به نام خدا

مرکز دانلود رایگان مهندسی مطالوری و مواد

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Shape-memory Alloys Handbook

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WILEY
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Foreword

Shape-memory alloys (SMAs), often also qualified as “smart materials”, were discovered over 60 years ago (Au–Cd in the 1930s and NiTi alloys in the early 1960s). The first applications were for mechanical purposes. In particular, these materials “remember” their original un-deformed shape. When they are preformed at a given temperature, they recover their original shape if they are heated above this temperature. These materials are solid-state alternatives to conventional actuators, such as hydraulic, pneumatic and motor-based systems. Shape-memory alloys have applications in industrial fields including medicine and aerospace. There is another type of SMA, called a ferromagnetic shape-memory alloy (FSMA), which changes shape when subjected to strong magnetic fields. These materials are of particular interest, as their magnetic response tends to be faster and more efficient than temperature-induced responses.

In this book, Christian Lexcellent gives a detailed analysis, both physical and mechanical, of the properties of these fascinating materials. The author, who belongs to the French school of mechanics of materials, has devoted a large part of his scientific career to working on these materials and has supervised about 20 PhD students who have investigated various aspects of these alloys. Christian Lexcellent is a well-known scientist and has published many technical papers dealing with various aspects of these materials.

It is real pleasure to introduce this comprehensive book on SMAs. In his book, Christian Lexcellent has found the right balance between physical metallurgy (Chapter 2), the various mechanical and thermodynamic facets of these materials (Chapters 3, 4, 5, 6 and 7), their applications (Chapter 8) and magnetic SMAs (Chapter 9). The main chapters are characterized by the fact that all the aspects (theory and thermodynamics of phase transformation, phenomenological models, models based on internal variables) are approached. A broad overview of the literature, in addition to the authors own work, is presented.
This book covers the most important fundamental and practical aspects of SMA in a clear and logical manner, and provides a sound basis that should make it as attractive to English-speaking students, practicing engineers and researchers.

André PINEAU
Professor École des Mines ParisTech
January 2013
In this age of “immediacy”, in which it is often the case that people have lost the memory of their history, there are some materials which have, beyond a doubt, kept theirs.

In this context, I came to discover the wondrous world of shape-memory alloys (SMAs) in the late 1980s, while working on a project financed under a CIFRE grant with the company Aug Decoupage in Besanon.

Our task was to create, characterize and model small elements made of copper-based SMAs, such as springs. In the end, the contract was never signed, because the company was alarmed by what it called the “exotic” or mysterious behavior of these alloys.

Therefore, Claude Oytana and I went to study under Grard Gunin in the Materials Laboratory at INSA Lyon. Thus, the first academic terms regarding these metallic alloys saw the light of day (one-way shape-memory effect, pseudo-elasticity, double-way shape memory effect, training, etc.).

Armed with this priceless knowledge, Pierre Vacher (now at the IUT Annecy) and I endured the trials and tribulations of early “hiccups” in the context of his thesis. For instance, what thermal treatment should be carried out on Cu-Zn-Al alloys under traction in order to obtain a hysteresis loop corresponding to a pseudo-elastic behavior of the alloy?

We soon came into contact with Marcel Berveiller and Etienne Patoor at the LPMM in Metz, who were more knowledgeable on the subject than we were. This contact gave rise to enriching exchanges and amicable debates which are still going on even today.

“The discovery” of the concept of training these alloys, in our small world, was an important part of what has been an epic journey.
Certain researchers have discovered mysterious treatments to make the four leaves of a clover open at ambient temperature when removed from a refrigerator. Water memory, the treasured theory of Jacques Benveniste, was compared to the shape memory of these alloys. When it was realized that a simple appropriate thermomechanical treatment was all that was required in order to train these materials, research in the field regained in rigor what it had lost in poetry.

Thus, the domain is strewn with theses: Pierre Vacher, 1991; Ccile Rogueda, 1993; Gilles Bourbon, 1994; Byong Chong Goo, Sylvain Leclercq, 1995; Hellal Benzaoui, Bertrand Gabry, Sylvain Moyne, 1998; Alexandre Vivet, 1999; Jol Abadie, James Rejzner, 2000; Christophe Bouvet, 2001; Benot Vieille, 2003; Nicolas Creton*, 2004; Pierrick Malecot, 2005; Jean-Yves Gauthier*, Frdric Thiebaud, 2007; Karine Taillard, 2008; Zoltan Palanki, Elie Gibeau, 2009; these are 19 theses about SMAs, of which two (marked *) are devoted to magnetic shape-memory alloys.

Virginie Taillebot has recently completed the coverage of the area in 2012, presenting her works on the fracture mechanics of SMAs.

We have been joined in this exalting adventure by partners such as Christian Licht, Bodgan Raniecki, Lamine Boubakar, Sylvain Calloch, Rachid Laydi for thermomechanical modeling, Jean Bernardini, Deszo Beke, Patrick Delobelle for knowledge of the materials, Nicolas Chaillet and Arnaud Hubert for the command and control of these alloys, and finally Manuel Collet and Emmanuel Foltte for the dynamic and damping responses of SMAs. This book is an attempt to reconstruct what these doctoral candidates and my colleagues have taught me about “the world of shape-memory alloys”.

Without the technical assistance of Joël Abadie and Scott Cogan at FEMTO-ST, it would have been difficult, or even impossible, to put this book together. Thanks to my status as Professor Emeritus, I have benefited from the facilities at the Department of Applied Mechanics, for which I am very thankful.
Chapter 1

Some General Points about SMAs

1.1. Introduction

What are these alloys that we call “shape-memory alloys”?

To begin with, they are metallic alloys with two, three or even four components, with very special compositions.

There are two main families of SMAs:
– “copper-based” materials – Cu-Al (Zn, Ni, Be, etc.);
– nickel-titanium-X materials (where X is an element present in small proportions) – NiTi (Fe, Cu, Co, etc.).

These materials are called “memory” materials, meaning that they have the property of “remembering” thermomechanical treatments to which they have been subjected (traction, torsion, flexion, etc.).

Specifically, the geometric shape that they had, at high and low temperatures, constitute two states which they “remember”. This memory is developed by way of training – i.e. often by the repetition of the same thermodynamic loading: this is in terms of stress or strain imposed and/or in terms of temperature.

The physical key to “shape memory” lies in a phase transformation between a parent phase called austenite (A) and a produced phase called martensite (M). For SMAs, this phase transformation is described as thermoelastic. It involves a change of crystalline lattice between the phase A, also known as the “high temperature” phase,
and a phase M, also known as the “low temperature” phase. This change is called a “martensitic transformation”. The austenite is transformed into “martensite variants” (a term which will be explained later on).

As shown by the photographs taken by Chu and James [CHU 93] of “copper-based SMAs”, the microstructure may prove very complex, which makes it difficult to analyze them (Figures 1.1 to 1.4).

**Figure 1.1.** Optical micrograph of a microstructure of a Cu-Al-Ni alloy: a “complex lattice”; horizontal extent 0.75 mm: reproduced with kind permission from C. Chu and R.D. James [BHA 03]

### 1.2. Why are SMAs of interest for industry?

SMAs belong to the category of so-called “adaptive” materials. Not only are they useful as structural elements, appreciable for their mechanical properties such as toughness; they are also capable of fulfilling functions such as that of a sensor or an actuator.

They are very widely used in domains with high financial added value – for example:

- the biomedical industry: used for implants, prostheses or stents, which are “latticed” tubes that are inserted into a conduit – e.g. a bronchus;
- aeronautics: filtering out of harmful frequencies, noise reduction (Boeing);
- aerospace: deployment of antennas;
- watch-making: insertion of an SMA spring into the mechanism of a watch;
- the nuclear industry: for pipes.
Some General Points about SMAs

Figure 1.2. Optical micrograph of a microstructure of a Cu-Al-Ni alloy: a “corner”-type microstructure; horizontal extent 0.75 mm: reproduced with kind permission from C. Chu and R.D. James [BHA 03]

Figure 1.3. Optical micrograph of a microstructure of a Cu-Al-Ni alloy: “cross-twinning”; horizontal extent 0.75 mm: reproduced with kind permission from C. Chu and R.D. James [BHA 03]
However, the cost of the alloy has hitherto been a serious hindrance for potential applications in the automobile industry, because of the tight budget in terms of mechanical parts in this sector.

Indeed, this cost is very heavily dependent on the delivery state, i.e. on the metallurgic treatment, shaping and geometry of the manufactured parts.

For instance, according to information provided by Nimsis-Technologies:

– a polycrystalline Cu-Al-Be alloy, in the raw spun state, costs around $390 per kilogram. If it is trained, the cost of a spring made of the same alloy may run to dozens of dollars;

– a round nickel-titanium wire 1, 2 or 3 mm in diameter sells for between $190 and $450 per kilogram; thin bands between $1300 and $1950, and a stent around $13.

At present, in France, there are three companies which supply SMAs:

– “Mmomtal technologies”. Bought on 6 July 2011 by Stryker, one of the world leaders in the domain of orthopedics and medical devices, Mmomtal is a specialist in the production of implants and prostheses made of nitinol, and generally everything from the choice of alloy to the design of the parts. This entails possible training
of the components, including the different stages of transformation (wire-drawing, metal-shaving, and shaping of the parts);

– “NiTiFrance”. This company has been in existence since 1998. It is a branch of the biomedical group Lpine. It has a market presence in the United States as “Nitinol Devices and Components” and specializes primarily in osteosynthesis staples.

Mmontal produces its alloys using the “hot crucible” technique, which is excellent for obtaining homogeneity in the resulting composition, but causes the problem of excessive oxygen absorption. NiTiFrance uses a “cold copper crucible”, which increases the ductility of the alloy (by 15 to 30% between the two solutions) by decreasing the percentage of oxygen absorbed. Remember that titanium is highly oxyphilic, and that oxygen tends to position itself in the interstitial site in crystalline lattices, which causes an increase in the fragility of the material.

As regards the activity of Nimésis-Technologies, it covers the main sectors of applications for SMAs, satisfying the demand for sensors and actuators.

Founded a century ago in Besanon, the company “MICRO-MEGA” is an uncontested leader in endodontics. In October 2009, it was bought by a German industrial dentistry corporation. It has developed a profitable niche market in NiTi “nerve lag” for root-canal work. It is the pseudo-elasticity of the alloy which is exploited here (see Chapter 2).

One of the drawbacks to these alloys is that they have a relatively slow dynamic of use, due to the prolonged period of heat transfer. However, the use of thin films can greatly improve the situation. An operational frequency of 100 Hz has been obtained by exploiting the austenite to R phase transformation for certain NiTi based alloys [TOM 06].

With massive SMAs, even a slow dynamic does not prevent their use in development of actuators.

The specific uses of SMAs, relating to their particular properties associated with phase transformation, will be discussed in detail in Chapter 2, entitled “The world of SMAs”.

1.3. Crystallographic theory of martensitic transformation

Let us first examine the crystallographic aspect of martensitic transformation. At a low temperature, the phase M (hereafter called \( M_T \) – self-accommodating martensite) obtained from A by simple cooling of the alloy and therefore isotropic redistribution
of the variants, may, under external stresses, produce major deformations associated with the reorientation of the martensite variants. This associated behavior is qualified as “pseudo-plastic” (Figure 1.5).

“Shape memory” constitutes a particular manifestation of crystalline phase transformation, known as “martensitic phase transformation”. This is a solid-to-solid phase transformation where the parameters of the crystalline lattice change suddenly (e.g. \( A \rightarrow M \) when cooled) at a specific temperature of the alloy in question. Although the change is abrupt and the distortion of the lattice is very significant, there is no diffusion and no alteration in the relative positions of the atoms during the transformation. This transformation is said to be “displacive”, of the first order (sudden change in the crystalline parameters) (see Figure 1.6).

If the alloy is heated, it undergoes thermal expansion until the reverse transformation (\( M \rightarrow A \)) occurs at another critical temperature. The difference between the two critical temperatures (\( A \rightarrow M \)) and (\( M \rightarrow A \)) shows that the behavior of SMAs is hysteretic. The conventional SMAs exhibit a small amount of hysteresis.
Some General Points about SMAs

Figure 1.7 illustrates the so-called “pseudo-elastic” traction curve representing a phase transformation under stress.

![Figure 1.7. The pseudo-elastic stress/strain curve](image)

One observable characteristic of martensitic transformation is the microstructure that it causes. In a typical transformation, the austenite, which is often “cubic” has a greater degree of symmetry than the produced phase. This is shown diagrammatically in two-dimensions in Figure 1.6, where the austenite is a square (a) and the martensite a rectangle (b and c). Consequently, we have multiple martensite variants – in this case two: (b and c). The number $\nu$ of variants obtained depends on the change in symmetry during the transformation.

More specifically:

$$\nu = \frac{\text{number of rotations in } P_a}{\text{number of rotations in } P_m}$$  \[1.1\]

where $P_a (P_m)$ is the symmetry group of A(M).

Indeed, there is no reason why the austenite crystal should transform into only one martensite variant. However, the microstructure must be consistent and may be presented in the architecture shown in Figure 1.6 (d), which is corroborated by transmission electron microscope (TEM) observations of a nickel-aluminum alloy (see the images of microstructures in Figures 1.1 to 1.4 [BHA 03]).

This need of the crystals to form mixtures of variants, while the whole must remain consistent, gives rise to complex structures which we refer to as the microstructure of the martensite.
1.4. Content of this book

1.4.1. State of the art in the domain and main publications

The first widely-recognized work in French on the topic was a basic introduction to SMAs, by Patoo and Berveiller [PAT 90]. Their second book was more significant in terms of the mechanical behavior of these alloys [PAT 94].

The question of the microstructure of martensite: “why it forms and how it gives rise to the shape-memory effect” constitutes the premise of the book with the same name by Bhattacharya [BHA 03]. The first founding theorems in this theory can be attributed to Ball and James [BAL 87], [BAL 92]. The chapter on martensitic transformation (Chapter 3) will make use of their proposals about the mathematical description of the microstructure.

Wayman’s book [WAY 64] is largely used as an introduction to crystallography of martensitic transformation (CMT).

With regard to the book by Khachaturyan [KHA 83] and the review by Roytburd [ROY 78], they predate the discipline of CMT (by linear or nonlinear construction) and deal with linear geometric theory.

The monograph published by Abeyaratne and Knowles [ABE 04] consists of an introduction to the dynamics of phase transformations.

The reader will find fairly general information about SMAs and their use in Shape Memory Alloys, the book written by Japanese scientists such as Shimizu, Tadaki, Homma, Miyazaki, Otsuka, Suzuki and Sekiguchi, translated into English [FUN 87].

Structural calculations about SMAs can be found in a special edition of the Revue des éléments finis (Finite Element Journal) [REF 98].

Finally, Smith [SMI 05] extended his study to intelligent systems such as ferroelectrics, ferromagnetics and of course, SMAs.

Note that these materials are not intrinsically intelligent; rather it is the usage that is made of them that can be intelligent (or not)! Also, the title Journal of Intelligent Materials and Structures may be considered to be ambiguous.

1.4.2. Content of this book

This chapter is an attempt to place shape-memory alloys in the context of physics and the mechanics of materials and to set out the key physical concepts of martensitic transformation and reorientation of martensite plates.
Chapter 2 contains a few elements on the basic metallurgy of SMAs, written by Michel Morin (MATEIS (Materials, Engineering and Science) lab at INSA in Lyon). Particular attention is paid to phase diagrams and *ad hoc* thermal treatments, drawing the distinction between copper-based SMAs and NiTi materials and their derivatives. The chapter closes with a description of the functional properties of SMAs (simple memory effect, pseudo-elasticity, recovering stress and training).

Chapter 3 borrows heavily from Kaushik Bhattacharya’s book, *Microstructure of martensite: why it forms and how it gives rise to the shape-memory effect* [BHA 03]. Following an overview of continuum mechanics, the kinematic (or Hadamard) compatibility conditions are examined, as well as the twinning equation between two martensite variants and special microstructures.

Chapter 4 defines the thermodynamic framework used for the modeling of the materials, referred to as generalized standards [HAL 75].

Chapter 5 touches on the earliest applications of the crystallographic theory of martensite on SMA monocrystals.

Chapter 6 also borrows from Chapter 5 (*Model development for shape memory alloys*) of Ralph Smith’s book *Smart Material Systems: Model Development* [SMI 05].

It consists of the description of the “all-or-nothing” Preisach models, Falk’s investigations into the deformation potential, the statistical approaches of Seelecke and Muller and Smith’s extensions of these.

Chapter 7 introduces three macroscopic models with internal variables: namely, those advanced by Raniecki and Lexcellent, referred to as the $R_L$ models; the Metz-Nancy approaches, which are more concerned with the microstructure [CHE 11]; and finally the more mathematical models put forward by Kelly and Bhattacharya [KEL 12]. An elastohysteresis model was also described [FAV 88].

In Chapter 8, “material strength”-type calculations are performed on beams in flexion or torsion and a number of distilled exercises.

Chapter 9 will examine the behavior of magnetic shape-memory alloys.

In Chapter 10, some elements of the fracture mechanics of SMAs will be set out.

A general conclusion will focus on the numerous problems which still need to be resolved in this domain of functional materials.

Although there is a common thread running throughout the book, the author has been careful to make sure that each chapter can be read independently of the others. For instance, a reader interested in metallurgy can focus on Chapter 2 and on Chapter 9 about magnetic shape-memory alloys.
Chapter 2

The World of Shape-memory Alloys

2.1. Introduction and general points

The term martensite was first put forward in honor of Adolf Martens, a German metallurgist who was the first to observe this microstructure in quenched steel. Regarding SMAs, Chang and Read [CHA 51] were the first to detect a phase transformation in a Au-Cd alloy by metallographic observations and measurements of electrical resistance. Thus, pseudo-elasticity was born.

Two decades later, the shape-memory effect was observed on a bent bar of that same alloy. In 1963, Buelher et al. [BUE 63] discovered the same properties on an equiatomic NiTi alloy. In the wake of this discovery, in 1969, the world witnessed the first industrial application with the simple memory effect used on a sleeve of hydraulic lines in a fighter plane. This created a particular interest in these new materials.

Yet the process of gaining true knowledge of the material and its thermomechanical behavior was slow, and would cause difficulties in practical perennial use in the 1970s–1980s. In fact, scientific research into the topic truly began in the 1980s associated with the first experimental investigations and the earliest attempts at modeling. The first mechanical tests were, naturally, uniaxial (traction/compression) as were the models. As in the study of any solid material, multiaxial tests – proportional or otherwise – such as traction-torsion-internal pressure tests, were performed, which necessitated the development of more complex models [BOU 02, GAL 98, ORG 98a].

Finally, in the 2000s, SMAs came to include the category of “smart materials”, but it is more accurate to speak of functional materials or adaptive materials.
12 Shape-memory Alloys Handbook

To begin with, we ask a simple question: what is the advantage of SMAs over conventional materials?

Normal metallic alloys exhibit a restricted domain of elasticity. For this reason, an elastic limit of 0.2% deformation has been defined for simple traction tests.

SMAs are able to accommodate extremely significant reversible deformations, of around 6–7% with certain NiTi alloys [TOB 98]. However, it is rare for any SMA to have the property of memory from the moment of its elaboration. In order to create this effect, a heat treatment must be performed.

Having set out these general points, let us now outline a number of elements regarding the metallurgy of these alloys.

2.2. Basic metallurgy of SMAs, by Michel Morin

“An overview of the basic metallurgy of commonly-used SMAs” has been written by Michel Morin (of the Materials and Engineering Sciences MATEIS lab at INSA Lyon).

There are various alloys which exhibit a shape-memory effect, e.g. Au-Cd, In-Tl, Au-Cu, Fe-Pd, Fe-Pt, etc., but very few of these alloys are used industrially, mainly because of the cost of them or their disadvantageous properties – for instance in the case of Fe-Mn-Si, which exhibits a very high phase transformation temperature and hysteresis.

Finally, only two categories of alloys are commonly used for applications: the category of copper-based materials includes Cu-Zn, Cu-Al, Cu-Sn, Cu-Zn-Al, Cu-Al-Ni, Cu-Al-Be and Cu-Al-Mn; and the NiTi category, either in the form of a binary alloy or with the addition of Cu, Fe or more exotic elements such as Pd or Hf. In this chapter, we shall give an overview of these different alloys and describe their main properties.

2.2.1. Copper-based shape-memory alloys

The centered cubic intermetallic phase $\beta$ of binary alloys Cu-Zn and Cu-Al exhibits a martensitic transformation, but the transformation temperatures that can be obtained by varying the composition are extremely low (practically lower than $-50^\circ$C for Cu-Zn) or too high (over 100°C for Cu-Al). The addition of a third element (Al for Cu-Zn, Ni or Be for Cu-Al) enables us to obtain martensitic transformations, the temperatures for which can be adjusted by the composition, over a wide range. Figures 2.1 and 2.2 show the phase diagrams for the binary alloys Cu-Al and Cu-Zn.
Figure 2.1. Phase diagram for binary Cu-Al

Figure 2.2. Phase diagram for binary Cu-Zn
As can be seen in these diagrams, the $\beta$ phase is only stable above temperatures of around 500°C. Given that for these alloys, the shape-memory effect can only take place below 200°C, it is necessary to perform quenching from the domain of stability of the $\beta$ phase. Quenching will enable us to obtain an alloy with a $\beta$ phase that is metastable at the transformation temperature. The goal of this process is somewhat different from the martensitic quenching of steels. In the case of steels, quenching from the $\gamma$ domain enables us to obtain the $\gamma$ phase at the temperature of martensitic transformation, but it also serves to prevent carbon diffusion in the form of cementite. As carbon diffuses very quickly in the matrix, for steels, we have to perform rapid quenching. In the case of copper-based shape-memory alloys (and the same is true for NiTi-based alloys), it is enough that the quenching process be sufficiently quick to prevent diffusion reactions. In certain cases, even air-quenching may suffice (e.g. in the case of Cu-Zn-Al (8% weight) alloys).

2.2.2. Cu-Zn-Al

Figure 2.3 shows vertical cross-sections with 0, 2, 4 and 6% weight aluminum of the ternary diagram for Cu-Zn-Al. In this figure, the martensitic transformation temperature is also shown as a function of the composition of the alloys.

Figure 2.3 shows that in the case of Cu-Zn (0% aluminum), the highest possible martensitic transformation temperature (around 0°C) corresponds to a concentration of 38.5% per weight of zinc. This concentration corresponds to the boundary of the domain of stability of the $\beta$ phase at 900°C. It is very difficult to obtain a sample at this concentration in a metastable $\beta$ phase at ambient temperature, because the homogenization temperature must be very precise, and the quenching very extensive in order to avoid diffusion reactions and obtain the metastable $\beta$ phase at ambient temperature. The other diagrams show that adding aluminum leads to a shift of the domain of stability of the $\beta$ phase in relation to the transformation temperature curve. At 6% per weight aluminum, the alloys which transform at ambient temperature have a zinc concentration of approximately 22% per weight. At this concentration, the $\beta$ phase is stable across an extensive range of temperatures (between 690 and 950°C approx.). Therefore, it is very easy to homogenize the samples. In addition, the quenching of the $\beta$ phase does not need to be very severe.

The shaping of the shape-memory alloys also poses a problem, because the $\beta$ phase is a phase which is not very malleable at all, which can only be molded or shaped at high temperatures (between 600 and 700°C). In order to shape parts made of Cu-Zn-Al, therefore, we use alloys with a 4% per weight aluminum content. At this concentration, and for a transformation temperature near to ambient temperature (around 28% zinc and 4% aluminum), the $\beta$ phase is stable between 720 and 950°C. If we take a sample of this composition to 550°C, in the $\alpha + \beta$ domain, the $\beta$ phase will decompose as per the reaction:

$$ \beta \Rightarrow \alpha + \beta $$
We thereby obtain a bi-phase alloy containing approximately 50% $\alpha$ phase and 50% $\beta$ phase (in accordance with the mixtures law on the diagram). In contrast to the $\beta$ phase, the $\alpha$ phase is a highly malleable cubic phase with centered faces. The remaining $\beta$ phase has changed composition (it has been enriched with zinc) and can no longer be transformed into martensite. This treatment enables us to shape the alloy at ambient temperature (metal-shaping, wire-drawing, etc.). After shaping, it is enough to re-homogenize the parts at around 800°C (in the $\beta$ domain) and then quench them in order to obtain the $\beta$ phase once more. After quenching, we obtain an alloy which is “poorly ordered” and which contains many vacancies. It is
therefore necessary to reheat it (30 minutes at 100°C, usually) in order to eliminate the oversaturation of vacancies and obtain a stable order of the \( \beta \) phase. The whole cycle of these thermomechanical treatments is summarized in Figure 2.4.

The alloys typically used have a concentration between 3 and 8% per weight of aluminum. In this range of concentration, martensite of type 9R is formed. The transformation of this 9R martensite is thermoelastic with slight hysteresis and slight spread, which is compatible with the good properties of memory effect and superelasticity. For higher aluminum concentrations, we obtain a 2H martensite, with burst-type transformation (i.e. non-thermoelastic) and a greater hysteresis.

Cu-Zn-Al alloys exhibit excellent properties of shape memory and pseudo-elasticity. It is possible to adjust the transformation temperatures within a very extensive range, between 0°C and over 150°C. It is relatively easy to shape these alloys. Yet the main problem with them means that they are not widely used for industrial applications and that they are not stable above or around 130°C. Beyond this temperature, the \( \beta \) phase, which is not at thermodynamic equilibrium, has a tendency to decompose, which leads firstly to a decrease in the transformation temperatures and then very quickly to the disappearance of the shape-memory effect properties. Hence, these alloys can only be used for applications where the temperature will never go above a hundred degrees centigrade.

2.2.3. Cu-Al-Ni

As we saw above, the \( \beta \) phase of the Cu-Al diagram also exhibits thermoelastic martensitic transformation. Figure 2.5 shows the equilibrium diagram for Cu-Al (solid
line) and the curve of the phase transformation start (“martensite start”, denoted “Ms” – dotted line). We can see in this diagram that it is possible to obtain a martensite start temperature at ambient temperature, but the corresponding alloy (with around 14% Al) is very brittle. In practical terms, we can only use alloys with lower aluminum concentrations, with a martensite start temperature of around 200°C. The addition of nickel causes a shift in the domain of stability of the $\beta$ phase in relation to the transformation temperature curve without noticeably changing the rest of the diagram.

![Equilibrium diagram for Cu-Al and Cu-Al-Ni with 4% nickel](percentage per weight)

Figure 2.5. *Equilibrium diagram for Cu-Al and Cu-Al-Ni with 4% nickel (percentage per weight)*

The dotted curve in Figure 2.5 shows the position of the $\beta$ domain for Cu-Al alloys with 4% of nickel. At this concentration of nickel, an alloy with 13.2% aluminum (and 4% nickel) is in the domain where the $\beta$ phase is most stable (eutectoid composition) with a martensite start temperature of around 150°C. We can increase the aluminum content in order to decrease the Ms temperature to around 50°C, with 14% Al. Beyond this 14% concentration of Al, the martensite formed becomes 2H (instead of 9R, as is the case with Cu-Zn-Al that is too rich in Al), and the alloys become brittle. Hence, in practical terms, for applications, usable Cu-Al-Ni alloys cannot have Ms temperatures lower than 50°C.

On the other hand, these alloys have a good resistance to high temperatures, up to around 200°C. Hence, they are well adapted for applications where the shape-memory element has to withstand high temperatures, but with a domain of function always above 50°C.
Cu-Al-Ni elements can only be shaped at high temperatures (around 600°C), because the $\beta$ phase is not sufficiently plastic at temperatures lower than this.

2.2.4. Cu-Al-Be

The addition of beryllium in a small proportion modifies the equilibrium diagram for Cu-Al: the temperature of the eutectoid plateau is reduced, and above all the curve of the transformation temperatures is brought down. The martensite formed is 9R. Unlike the effect of nickel, beryllium in a low concentration does not affect the composition or the temperature of the TTT (time-temperature-transformation) diagram. Figure 2.6 shows part of the phase diagram for Cu-Al-Be (vertical cross-section at 0.47%wt beryllium). Figures 2.7 show the influence of the beryllium and aluminum content on the Ms temperature.

For industrial use, Cu-Al-Be presents the cumulated advantages of Cu-Zn-Al and Cu-Al-Ni: the possibility to adjust the transformation temperatures between a very low temperature and 200°C by altering the concentrations of the elements in the alloys, and excellent heat resistance, up to 200°C. However, similarly as for Cu-Al-Ni, the samples can only be shaped at high temperatures, around 600°C. Another disadvantage of this alloy is the presence of beryllium, as beryllium oxides are very dangerous in terms of health. Even so, the beryllium is present only in very small amounts and in an alloy-bound form. The only precaution that needs to be taken with this alloy is not to overheat the samples, mainly during the manufacturing process.
For further information, the interested reader can refer to the regulations on the use of Cu-Be, which is a structural hardening alloy, commonly used in industry.

![Figure 2.7. Influence of the beryllium and aluminum content on the martensite start temperature of the Cu-Al-Be alloy](image)

### 2.2.5. The phenomena of aging, stabilization and fatigue

The properties of copper-based SMAs are very interesting, but they may be limited by a number of phenomena, about which we must have knowledge if we wish to use these alloys: these phenomena are aging, martensite stabilization and fatigue.

As regards aging, we have seen that the martensitic transformation responsible for the memory effect takes place from the $\beta$ phase. As this $\beta$ phase is not stable at ambient temperature, it is obtained by quenching. If, with this quenching, the alloy is heated to a temperature that facilitates the diffusion of the atoms, the metastable $\beta$ phase will decompose and tend toward thermodynamic equilibrium. This decomposition leads to a number of phenomena which are damaging for the martensitic transformation: an alteration of the composition of the resulting $\beta$ phase, and the formation of precipitates which will interfere with and then prevent the martensitic transformation. These processes exist for the three copper-based alloys described above, but their behavior is different:

- with Cu-Zn-Al, the $\beta$ phase decomposes in accordance with the equilibrium diagram into a bi-phase mixture of $\alpha$ and $\beta$ phases. The resulting $\beta$ phase becomes progressively richer in zinc, which leads to a decrease in the Ms temperature. However, because this increase in zinc is not homogeneous, we also observe a staggering of the transformation. The precipitates of the $\alpha$ phase counteracts the shifting of the interfaces during the martensitic transformation, causing an increase in hysteresis. Very soon, the martensitic transformation disappears completely. For this alloy, these phenomena of diffusion begin to manifest themselves at around 130°C, which is highly problematic for many applications;
– with Cu-Al-Ni and Cu-Al-Be, the presence of a peri-eutectoid transformation leads to the decomposition of the \( \beta \) phase into a mixture of \( \beta + \alpha + \gamma_2 \) (see the diagram in Figure 2.6), which causes an alteration in the composition of the \( \beta \) phase and the Ms temperature. However, these two alloys are far more stable than Cu-Zn-Al, meaning they can be used up to temperatures of over 200°C.

The stabilization of the martensitic phase is observed for alloys whose austenite start (As) temperature is higher than ambient temperature. After being kept at ambient temperature (or above, but still in the martensitic phase) for a prolonged period of time, we observe a degradation of the memory effect. Figure 2.8 illustrates this degradation, which manifests itself as an increase in the \( A_s \) and \( A_f \) (austenite finish) temperatures of the first inverse martensitic transformation, with an incomplete inverse martensitic transformation in certain cases (that is, there remains stabilized martensite at a high temperature). Only the temperatures of the first inverse martensitic transformation are altered (curves 1 and 1’ in Figure 2.8). After this first round of heating, the sample returns to “normal” transformation temperatures (curves 2, 3, 2’ and 3’).

![Figure 2.8](image-url)

**Figure 2.8. Schematic representation of the stabilization of copper-based alloys.** 1) First inverse martensitic transformation (increase in temperature) after prolonged maintenance in the martensitic phase at ambient temperature; 2) and 3) The subsequent martensitic transformations are “normal”; 1’), 2’ and 3’) Example of stabilization with incomplete martensitic transformation

Martensite stabilization may result from two different physical phenomena:

– the trapping of the interfaces between the martensite variants by vacancies;

– a structural change in the martensitic phase, probably due to a reordering of the atoms.

In order to reduce this phenomenon of stabilization, therefore, we need to decrease the concentration of vacancies (given that reordering is a diffusional process governed by these vacancies). By reheating after quenching (or staggered quenching), we are able to eliminate nearly all quenching vacancies.
2.2.6. Methods for copper-based SMA elaboration

The different stages of the elaboration of a copper-based shape-memory alloy include the choice of raw materials, smelting, shaping and betatization treatments and reheating:

− raw materials: in order to avoid a decrease in the properties of the alloys, primarily due to interactions between the movement of the variants and impurities, the purity of the different components needs to be very high – greater than 99.99%;

− smelting: the different elements of the alloy in a sufficient quantity are melted; however, before proceeding with the casting, it is crucial to very precisely monitor its composition. As we saw above, the martensitic transformation temperatures are very highly dependent upon the composition of the alloys. For instance, for Cu-Zn-Al, an 0.5%wt increase in the zinc content causes a 30°C drop in the Ms temperature and 0.5% more aluminum decreases this temperature by 80°C. Thus, the proportion of the different elements in the alloy is extremely critical. The conventional analytical methods for this type of operations (spark spectrometry) are not accurate enough. In practical terms, a sample is taken just before casting; this sample is subjected to thermal betatization treatment and reheated, and then its transformation temperatures are measured (e.g. by resistivity measurement). If these temperatures do not correspond to those being sought for the planned application, the composition of the bath of molten metal is corrected by the addition of metal just before casting;

− shaping: the procedures for shaping depend on the alloy which has been made. As we saw above, Cu-Zn-Al can be shaped at ambient temperature if the alloy is in the bi-phase state \((\alpha + \beta)\) (Figure 2.3). In the case of Cu-Al-Be and Cu-Al-Ni, shaping can only be done at a high temperature of over 600°C;

− “betatization” treatments: the martensitic transformation responsible for the shape-memory properties occurs from the beta phase. As this phase is not thermodynamically stable at ambient temperature, it is therefore necessary to raise the alloys to the temperature of the beta domain and then quench them in order to stabilize them in that state. The quenching is followed by a reheating in order to eliminate the quenching vacancies and stabilize the state of order of the alloy (Figure 2.4).

2.2.7. Ti-Ni-based alloys

All alloys in this category are made from the equiatomic alloy Ti-Ni. The diagram for Ti-Ni, shown in Figure 2.9, exhibits an intermetallic \(\beta\) around the equiatomic composition. It is this \(\beta\) phase, a cubic B2-ordered (Cs-Cl-type) phase, which is transformed into martensite. The martensitic phase obtained after transformation exhibits a compact crystallographic structure which varies depending on the transformation temperature and the composition (between a 2H and a 9R structure).
2.2.8. **Ti-Ni alloy**

The maximum $M_s$ transformation temperature that can be obtained with this alloy is around 70°C. Figure 2.10 shows that a slight increase in the Ni content of the alloy causes a decrease in this temperature. Below 50% nickel, the $M_s$ temperature is independent of the composition and remains at its maximum value. This is very easy to understand in view of the equilibrium diagram (Figure 2.9) which shows that for these sub-stoichiometric concentrations, the alloys are in the bi-phase domain $Ti_2Ni + \beta$, with a concentration of the $\beta$ phase which remains nearly equiatomic.

![Equilibrium diagram of Ti-Ni](image)

**Figure 2.9.** *Equilibrium diagram of Ti-Ni*

In the case of over-stoichiometric concentrations, it is necessary to perform quenching from the $\beta$ domain. After this quenching treatment, prolonged maintenance at 600°C leads to a precipitation of $TiNi_3$ or $Ti_2Ni_3$, which decreases the nickel content of the $\beta$ phase and increases the transformation temperatures (see Figure 2.9).

In certain conditions, an intermediary phase can be formed upon cooling before the martensitic transformation. This “pre-martensitic” phase has been called the R phase (trigonal structure). It is indeed a martensitic transformation which exhibits a (very slight) hysteresis and a small memory effect. This transformation begins to compete with the martensitic transformation. If it occurs first, when the substance is cooled, we observe the following successive transformations: $\beta \Rightarrow R \Rightarrow M$. Conversely, if the martensitic transformation occurs first, we do not observe the R phase. It is very uncommon, when the substance is heated, to observe the reverse transformation $M \Rightarrow R \Rightarrow \beta$. The factors which favor the existence of the R phase are:
The substitution of a few percent of nickel by iron or aluminum;

– the formation of precipitates $Ti_3Ni_4$ by aging of Ti-Ni with a high nickel content;

– reheating after cold deformation.

The R phase is used for a number of applications which require low hysteresis, but the memory effect obtained with the $A \rightarrow R$ transformation produces a small deformation, of around 1%.

![Figure 2.10. $M_s$ temperature depending on the Ni concentration. The different symbols correspond to experimental measurements, and the line to a thermodynamic calculation [TAN 97]](image)

### 2.2.9. Ti-Ni-X alloys

Numerous elements have been tested to increase the transformation temperatures of Ti-Ni (see Figure 2.11). Unfortunately, nearly all the elements tested actually decrease the transformation temperatures. The only elements which increase these temperatures are gold, hafnium, platinum and palladium, but even then, only with high concentrations of them (except in the case of gold). The price of these elements is prohibitive for their extensive use.

At present, the most commonly used element in an alloy with Ti-Ni is copper, substituting for some of the nickel. The effect of copper is to decrease the hysteresis and the spread of the martensitic transformation without having too great an effect on the values of the transformation temperatures. In addition, copper inhibits the
formation of the R phase. It is this alloy which is most often used in applications, except in surgery and medicine for reasons of problems of biocompatibility.

![Graph of alloy elements on martensite start temperature](image)

**Figure 2.11. Effect of alloy elements on the martensite start temperature $M_s$ on the Ti-Ni system**

### 2.2.10. Elaboration

The elaboration of Ti-Ni-based alloys is a fairly complex process, because the titanium is highly oxyphilic. Oxygen has a very damaging effect on the martensitic transformation (see Chapter 1). For fusion, therefore, we have to carry out the process
(similarly as for titanium) in vacuum fusion ovens, which considerably increases the price of the alloys. The other techniques used are for different concentrations in powder form, pack rolling or vapor phase deposit. All these techniques can be used to produce good alloys, with the greatest difficulty in all cases being in preventing oxygen penetrating the material.

2.2.11. Shaping

After casting, the ingot is forged, rolled or indeed extruded at high temperature (between 850 and 950°C). Forging and rolling are carried out at around 800°C. At this temperature, the metal is still malleable, and surface oxidation is relatively slight. Then, the alloy is shaped at cold temperatures, before being subjected to a final heat treatment in order to obtain good mechanical and shape-memory properties. During the manufacturing process, a layer of oxide forms on the surface – mainly TiO₂. Depending on the thickness of this oxidized layer, we distinguish various surface states: shiny black if the oxide layer is thick (around 400 nm); brownish gray if the thickness is around 100 nm; white-ish gray if the surface has been acid-scoured, which gives a less smooth surface; or shiny with the appearance of stainless steel if the metal has been polished.

2.2.12. Final heat treatments

After shaping (wire-drawing, stretching or rolling), Ti-Ni alloys present no memory effect. In order to endow them with it, we need to subject them to a heat treatment with decreases the amount of defects (mainly dislocations), thereby enabling the martensitic transformation to occur in a satisfactory manner. However, the matrix needs to retain sufficient mechanical strength so as not to undergo plastic deformation. This strength is obtained by preserving a sufficient amount of defects. The temperature and duration of the heat treatment are therefore fairly critical, and depend on the type of application envisaged. For applications in which the alloy will be subject to major stress, with only small a deformation with memory effect or super-elasticity, we would choose a treatment of a few minutes at 400°C. In order to favor the amplitude of the memory effect or super-elastic effect, to the detriment of the force exerted by the SMA piece, the treatment could be performed at 500°C for durations exceeding ten minutes. Ti-Ni alloys can be supplied in two main states: pre-treated or raw, with no heat treatment. This latter state is particularly advantageous if the user wishes to shape it for a particular purpose before use.
2.2.13. Table comparing the physical and mechanical properties

<table>
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<td>950-1020</td>
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<td>7100-7200</td>
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<td>Tensile resistance</td>
<td>MPa</td>
<td>800-1000</td>
<td>800-900</td>
<td>1000</td>
<td>900-1000</td>
</tr>
<tr>
<td>Fracture elongation (in martensite)</td>
<td>%</td>
<td>30-50</td>
<td>15</td>
<td>8-10</td>
<td>15</td>
</tr>
<tr>
<td>Yield fatigue resistance</td>
<td>MPa</td>
<td>350</td>
<td>270</td>
<td>350</td>
<td></td>
</tr>
<tr>
<td>Grain size</td>
<td>µm</td>
<td>20-100</td>
<td>50-300</td>
<td>30-300</td>
<td>100-500</td>
</tr>
<tr>
<td>Transformation domain</td>
<td>°C</td>
<td>-100 to 100</td>
<td>-100 to 100</td>
<td>-100 to 170</td>
<td>200 to 150</td>
</tr>
<tr>
<td>Hysteresis (As-Mf)</td>
<td>°C</td>
<td>20-40</td>
<td>10-20</td>
<td>20-25</td>
<td>20-25</td>
</tr>
<tr>
<td>Spread (AI-As)</td>
<td>°C</td>
<td>30</td>
<td>10-20</td>
<td>20-30</td>
<td>15-20</td>
</tr>
<tr>
<td>Maximum strain:</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>- one way shape memory effect</td>
<td>%</td>
<td>8</td>
<td>3-5</td>
<td>3-6</td>
<td>3-5</td>
</tr>
<tr>
<td>- two way shape memory effect</td>
<td>%</td>
<td>5</td>
<td>2</td>
<td>3</td>
<td>2</td>
</tr>
<tr>
<td>Cycle (N) = 10²</td>
<td>%</td>
<td>5</td>
<td>1</td>
<td>1.2</td>
<td></td>
</tr>
<tr>
<td>Cycle (N) = 10⁵</td>
<td>%</td>
<td>2</td>
<td>0.8</td>
<td>0.8</td>
<td></td>
</tr>
<tr>
<td>Cycle (N) = 10⁷</td>
<td>%</td>
<td>2.5</td>
<td>0.5</td>
<td>0.5</td>
<td></td>
</tr>
<tr>
<td>Maximum temperature use (1 hour)</td>
<td>°C</td>
<td>400</td>
<td>160</td>
<td>300</td>
<td>400</td>
</tr>
<tr>
<td>Supercritical maximum strain:</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>- polycrystal</td>
<td>%</td>
<td>4</td>
<td>2</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>- monocystal</td>
<td>%</td>
<td>10</td>
<td>10</td>
<td>10</td>
<td>10</td>
</tr>
<tr>
<td>Damping</td>
<td>SDC-%</td>
<td>15</td>
<td>30</td>
<td>10</td>
<td></td>
</tr>
<tr>
<td>Corrosion resistance</td>
<td></td>
<td>Excellent</td>
<td>Average</td>
<td>Good</td>
<td>Average</td>
</tr>
<tr>
<td>Biocompatibility</td>
<td></td>
<td>Good</td>
<td>Bad</td>
<td>Bad</td>
<td></td>
</tr>
</tbody>
</table>

2.2.14. Biocompatibility of SMAs

As the table indicates, there is no guarantee of biocompatibility for copper-based SMAs, and particularly for Cu-Al-Be, as previously stressed. It appears to be better for NiTi. The problem with this alloy lies in the fact that the Ni ions, which are particularly toxic, must not separate from the nickel-titanium. However, corrosion studies have shown that a NiTi element dipped in fetal bovine serum (FBS) at 37°C decreased the thickness of its protective oxidized layer and increased its porosity and lost Ni ions [HAN 10b]. The same authors [HAN 10a] deposited a coating of “diamond-like carbon” (DLC) on NiTi. The effects of the albumen protein serum at 37°C were analyzed. The results obtained show that depositing carbon on NiTi increases its corrosion resistance.
2.3. Measurements of phase transformation temperatures

There are two classic techniques:

– differential scanning calorimetry (DSC). This enables us to measure the four temperatures characteristic of phase transformation:

- $M_0^s$: appearance of the first martensite platelet in the austenite during cooling;
- $M_0^f$: appearance of the last martensite platelet during cooling, i.e. when the austenite has disappeared completely;
- $A_0^s$: disappearance of the first martensite platelet during heating (for energy reasons this is the platelet which appeared last);
- $A_0^f$: disappearance of the last martensite platelet during heating (the platelet which appeared first).

Furthermore, the amounts of heat given off during the direct transformation $A \rightarrow M$ and absorbed during the reverse transformation $M \rightarrow A$ can be measured (see Figure 2.12);

– measurements of electrical resistance can be used, as the resistivity of austenite is different from that of martensite. Thus, the measurement of the electrical resistance becomes an indicator of the advancement of the phase transformation.

The curve in Figure 2.13 shows that the response (volume fraction of martensite depending on the temperature) is hysteretic.

Finally, DSC measurements or electrical resistance measurements can be used to validate the heat treatment performed to “force $\beta$ phase formation”.

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Figure 2.12. Measurement of the characteristic temperatures of phase transformation by DSC.
2.4. Self-accommodating martensite and stress-induced martensite

Details about the martensitic transformation will be given in Chapter 3.

However, there is a distinction to be made between the martensite obtained by simply cooling the alloy, when no particular direction is favored during the phase transformation, and the martensite induced under stress, when the direction of the stress favors the appearance of certain variants over others.

This distinction between thermally-induced martensite $M_T$ and stress-induced martensite $M_\sigma$ was drawn by Brinson et al. [BRI 93].

Figure 2.14 gives a schematic representation of the difference between the two martensite microstructures.
Figure 2.15, for the case of a CuAlNiMn polycrystal, presents images of self-accommodating martensite on the one hand and “oriented” martensite on the other [LEC 96]. We can clearly distinguish the martensite platelets in both cases.

As we shall see, this dichotomy is very useful, in terms of a macroscopic simulation, particularly in the case of anisothermal loading.

2.5. Fatigue resistance

2.5.1. Causes of degradation of the properties

SMAs are very susceptible to fatigue. Indeed, in addition to undergoing the phenomena encountered on conventional crystalline materials (increase in the density of dislocations, formation of dislocation lattices, presence of grain joints in polycrystalline materials which are an additional cause of crack initiation, etc.) they possess additional characteristic mechanisms relating to phase-change.

These mechanisms are grouped into one mode of thermal fatigue and three modes of mechanical fatigue.

Thermal fatigue results from thermal cycling between the domains of stability of the two phases (austenite and martensite).

As regards mechanical fatigue, it is defined depending on the domain of temperature:

- at $T \leq M_f$ during the reorientation of the martensite variants;
- at $M_s \leq T \leq A_f$ during martensite formation under stress;
- at $T \geq A_f$ classic fatigue in the austenitic phase.
In most applications, the different mechanisms intervene in a coupled manner and the phenomenon becomes a highly complex one. In order to study it, we need to take account of multiple parameters such as the loading temperature, the phase transformation temperatures, the stresses or strains imposed.

We distinguish two types of fatigue [EGG 04]:

– functional fatigue corresponds to the loss of the thermomechanical properties during cycling;
– structural fatigue relates to the lifetime of the material before fracture.

2.5.2. Fatigue of a Cu-Al-Be monocrystal

We observe a progressive change in the mechanical properties over the course of the cycles. In the case of a monocrystal, the transformation start stress decreases, but the stress throughout the course of the transformation, instead of remaining constant, increases. This can be attributed, depending on the testing temperature, to the creation of defects when the austenite/martensite interface shifts or to phenomena of diffusion such as the reordering that occurs with different kinetics in the austenite or martensite (see Figure 2.16).

Figure 2.16. Traction cycling of a monocrystalline Cu-Al-Be alloy [SIR 06]

2.5.3. Results

Figure 2.17 presents the lifetimes obtained [SIR 06]:

– for a monocrystal and a polycrystal of Cu-Al-Be subjected to flexural stress, with repeatedly-imposed strains. Polishing leads to a slight improvement in fatigue resistance;
– for a NiTi polycrystal subjected to rotative flexion by Miyazaki et al. [MIY 99].
The monocrystalline alloy Cu-Al-Be exhibits a longer lifetime, with greater strains than NiTi. However, we can see a great dispersion of the results (see Figure 2.17). Samples aged for five years clearly show a decrease in their fatigue lifetime. This tendency disappears when the tests are carried out in a nitrogenous environment.

Just like with conventional materials, the surface state at the crack initiation point plays an important role. As shown in Figure 2.17, careful polishing greatly improves the lifetime.

During “pseudo-elastic fatigue”, we observe a decrease in the stress corresponding to the start of the stress-induced martensitic transformation, and also a decrease in the super-elastic strain (see Figure 2.21).

If we look at the pseudo-elastic fatigue of a NiTi polycrystal, the evolution of the hysteresis loop is impressive over the first fifty cycles (Figure 2.18) as is the energy dissipated per cycle which constitutes the stress/strain area of the loop (Figure 2.19).

The decrease in dissipated energy $W$ is fast in the early cycles, and a stabilization occurs when a high number of $N$ is reached (in this case around 50), none of which

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**Figure 2.17. Fatigue lifetime of different shape-memory alloys (the arrows indicate that the samples did not fracture) [SIR 06]**

---
can use the relation between the number of cycles before fracture $N_f$ and the value of $W$ corresponding to the stabilized cycle suggested by Moumni et al. [MOU 05]:

$$N_f = \left( \frac{W}{\delta} \right)^{\frac{1}{\mu}}$$  \hspace{1cm} [2.1]$$

where $\delta$ and $\mu$ are constants.

**Figure 2.18.** Pseudo-elastic cyclic behavior of a NiTi alloy between $\varepsilon = 0$ and $\sigma = 800$ MPa and $\dot{\varepsilon} = 10^{-3} s^{-1}$ [MOR 11]

**Figure 2.19.** Evolution of the energy dissipated with the number of cycles (corresponding to the curve shown above) [MOR 11]
Thus, there is a need to know how the microstructure can be optimized in order to achieve good fatigue resistance. The term “functional fatigue” indicates that the memory effects such as the work associated with the movement of an actuator for the simple effect and the dissipated energy in cyclical pseudo-elasticity (Figures 2.18 and 2.19) give rise to applications in damping. Particular attention must be paid to the localization in strain during the formation of stress-induced martensite [EGG 04].

The classical mechanical fatigue induces an accumulation of defects in the material, and the formation and opening of cracks. The resistance to mechanical fatigue is highly dependent on the grain size, which is very significant for copper-based SMAs (see Figure 2.20).

In the course of pseudo-elastic fatigue of “copper-based” alloys, we also observe a decrease in the stress corresponding to the start of the stress-induced martensitic transformation, and a decrease in super-elastic strain (see Figure 2.21).

In the case of “shape-memory” fatigue, or thermomechanical fatigue, we observe a change in the phase transformation temperatures, a reduction in the amplitude of the memory effect and the strain of the alloy when the number of cycles increases.
Figure 2.21. Effect of mechanical cycling on the shape of the super-elastic cycles of a sample of Cu-Zn-Al [ROG 91]

It is about shape-memory fatigue that most research has been done, particularly with cycles of shape-memory effect assisted by a stress. In this type of experience, the sample, subjected to a constant stress, is cycled thermally between a temperature lower than $M_f$ and a temperature greater than $A_f$. Over the course of cooling, the austenitic sample is transformed into martensite, and the stress applied orients the martensite variants. This results in the deformation of the sample in the direction of the stress. When heated, the sample regains its initial shape, by virtue of the shape-memory effect. The number of cycles before fracture depends primarily on the stress applied and on the size of the grains.

During the course of thermal cycling, we observe a shift (of up to around 10°C) in the phase transformation temperatures: during cooling, the $M_s$ and $M_f$ temperatures increase, while during heating, $A_s$ and $A_f$ decrease. This leads to a decrease in hysteresis.

Figure 2.22 presents deformations of a sample of Cu-Zn-Al subjected to a static stress of 25 MPa and to thermal cycles between 16 and 70°C. The bottom curve represents the deformation of the sample when it is in the high-temperature phase (the austenitic phase) and the top curve corresponds to the martensitic phase. These two curves are almost parallel, which means that the shape-memory effect assisted by the stress (represented by the difference between the two curves) hardly varies at all. In Figure 2.22 with the logarithmic scale of the horizontal axis which has been used, the two curves are nearly straight lines. Thus, we have a logarithmic variation in the deformation of the sample as a function of the number of cycles. This variation is fairly significant (around 1%), even for the low value of stress imposed. Therefore, we need to take account of this deformation for applications which require a large number of cycles of memory effect.
Figure 2.22. Variation of the deformation of a sample of Cu-Zn-Al subjected to cycles of memory effect fatigue under static stress [BIG 95]

Figure 2.23 represents the Whler curves obtained after fatigue tests with double memory effect assisted by a stress, on two types of samples of Cu-Zn-Al: wires with large grains and tapes with fine grains [BIG 95]. As previously mentioned, it is obvious that the grain size is of great importance for the fatigue resistance of copper-based SMAs.

In summary, the study of fatigue in SMAs, which is far from being as advanced as for conventional materials, will be key for the perennial use of actuators and sensors.

2.6. Functional properties of SMAs

Martensitic transformation and the process of reorientation of the martensite variants lend SMAs specific functional properties.

2.6.1. The pseudo-elastic effect

Consider an alloy in the austenitic state, in the natural non-deformed state, i.e. at $T \geq A_f^0$. The stress-strain curve (Figure 2.24) can be decomposed as follows:
beginning of loading by elastic strain of the austenite;

– an $A \rightarrow M_{\sigma}$ phase transformation for $\sigma = \sigma_{c}^{AM}$ up to $\sigma_{f}^{AM}$. Even for NiTi alloys, the phase transformation is rarely complete. Often, plastification of the sample intervenes at the end of loading;

– if the phase transformation is total, when the stress is relieved, the martensite exhibits elastic behavior;

– then the reverse transformation $M_{\sigma} \rightarrow A$;

– and finally an elastic behavior on the part of the austenite until the stress becomes null.

The physical phenomenon of pseudo-elasticity is clearly the direct and reverse phase transformation under the influence of a stress.

The behavior tends to be hysteretic because the direct and reverse paths are not the same.

With regard to monocrystalline alloys, the detection of the transformation threshold stress for polycrystals is more random, as shown in Figure 2.24. Application: significant thermoelastic strains (up to several per cent) can be recovered.

Among the main medical applications, one might cite:

– an arch for dental braces: a NiTi wire exerts a small but near-constant force (see the $M_{\sigma} \Rightarrow A$ plateau) on badly-aligned teeth;

– a pseudo-elastic nerve lag developed by the company MICRO-MEGA.

The endodonic instrument (Figure 2.26) is used to carry out treatment at the level of the root canals of teeth (devitalization). The shape of the roots is often complex (Figures 2.27 and 2.28) with many curvatures, and the tool used must be able to match this shape as closely as possible in the interest of the best possible treatment.
Super-elastic nickel-titanium alloys are ideal materials for this application [SER 95]. Many systems of instruments made of NiTi exist [HUL 05]. These instruments may have different geometric characteristics, in terms of the shape of the cross-section, the step, the conicality, etc. [HUL 05]. Yet no matter what the instrument, if it fractures during the preparation of the root canal, the treatment may fail [PAR 06]. Certain authors associate this fracture with fatigue caused by the repetition of bending stresses in the curvaceous canals. Other authors emphasize the torsion, relating to the problem of the instrument’s getting stuck, as the principal cause of this fracture.

Figure 2.25. Pseudo-elastic stents

Figure 2.26. An endodontic dental instrument, “one shape R” (see MICRO-MEGA’s Website)

Other applications include:

– arms for glasses;
– pseudo-elastic stents: Figures 2.25 and 2.29.

2.6.2. One-way shape-memory effect

Consider an SMA in the stress-free state in the austenitic state (at $T_0 > A_0^f$).

First stage: cooling to $T_1 < T^f_0$: $A \rightarrow M_T$ ($M_T$ thermal martensite).

Second stage: with $T_1$ kept constant, we apply a stress $\sigma$: $M_T \rightarrow M_\sigma$ (reorientation of martensite plates).
Third stage: at $T_1$, the stress on the sample is relieved entirely. We obtain a point B of the operation ($T = T_1$, $\varepsilon = \varepsilon_R$: a few %).
We need only heat the material from $T_1$ to $T_0$ in order to recover the initial state: point A ($\varepsilon = 0$, $(T_1 - T_0)$ is approximately 30–60°C, which is small. This constitutes an excellent situation of actuation.

Applications: the main applications lie in cut-off switches and sensors:
- smoke detector;
- “smart” fryer [PAT 90];
- thermomechanical actuator;
- connection of two pipes.

Pseudo-elasticity and the one-way shape-memory effect are shown in Figure 2.31, in a ternary diagram $\{\sigma, \varepsilon, T\}$.

Figure 2.30. *Schematic representation of the one-way shape-memory effect*

Figure 2.31. *Pseudo-elasticity and one-way shape-memory effect in a SMA*
2.6.3. Recovery stress

In reference to the single memory effect, the procedure is strictly the same up to point B ($\sigma = 0$, $T = T_1$ and $\varepsilon = \varepsilon_R$). Then, the material is heated, while the deformation $\varepsilon_R$ is kept constant. This is a “countered phase return” between two antagonistic processes. Heating naturally tends to transform $M_\sigma$ into $A$, but maintaining a constant deformation prevents the intrinsic deformation associated with $M_\sigma$ from reducing, causing a high degree of stress called “recovery stress” (see Figure 2.32).

Figure 2.32. Measurement of the recovery stress for a NiTi alloy

One application made of this in the past has been the design of an adaptive beam.

Created in the Department of Applied Mechanics – DMA/FEMTO-ST in Besanon by Perreux and Lexcellent [PER 99], a double beam with a hinge, the cross-section of which is shown in Figure 2.33, presents a quadratic bending moment, variable depending on the state of strain of the NiTi wire (effective strain when the wire is in the oriented martensitic state $M_\sigma$ and null in the austenitic state).

Figure 2.33. Cross-section of the beam

For instance, simple heating enables us to reduce the natural bending of the beam by $2/3$ (see Figure 2.34).
2.6.4. Double shape-memory effect: training

If we subject an SMA to a specific thermomechanical treatment, called “training treatment”, it can memorize two geometric shapes: one in its austenitic phase and one in its martensitic phase, under simply thermal loading. As training is often tantamount to repeating, such treatments often constitute cyclic loading – e.g. thermal cycles under constant stress. The shape memorized in the martensitic phase “results from the preferred formation”, in the absence of any applied macroscopic stress, of variants oriented by the internal stress field generated in the material by the training process [PAT 87].

This can be represented schematically in the approach adopted by Frmond [FRE 98], [FRE 02] in a model with two martensite variants $M_1$ of volume fraction $z_1$ and $M_2$ of volume fraction $z_2$. Training an SMA is tantamount to “cutting a corner off the triangle”!

For the raw material, the domain of existence of martensite covers the entirety of the triangle $C_r$ (Figure 2.35).

**Figure 2.35. Triangle representing a raw material [FRE 02]**
For the trained material, the domain of existence of trained martensite is located in the triangle $C_{re}$ (Figure 2.36). This means that any and every point in the triangle $C_1$ can be reached, a priori, by the raw material. With the trained material, only the triangle $C_{re}$ remains accessible.

**Figure 2.36. Triangle representative of a trained material [FRE 02]**

### 2.7. Use of NiTi for secondary batteries

A flexible wire for a lithium battery has been made, using a thermal-sulfurized NiTi alloy as a cathode. Sulfides have a multi-layer structure consisting of Ni-S$_{1.97}$, Ni-S and Ti$_{8.2}$-S$_{11}$ [CHO 08] (Figure 2.37). The mechanical properties (pseudo-elasticity, etc.) of NiTi are apparently unchanged by sulfurization at 80 kPa. The discharge capacity of sulfurized NiTi applied to the Li battery has been measured as over 400 mAh/g-Ni-S$_{1.97}$, after the fifth cycle. The initial capacity of a battery wire 1 mm in diameter and 100 mm in length is 0.66 mAh/cell.

**Figure 2.37. A schematic process applied in order to manufacture a battery wire**

### 2.8. Use of SMAs in the domain of civil engineering

This section will summarize the works in this field of J.F. Destrebecq, X. Ballandraud and their doctoral candidate H. Tran at the IFMA in Clermont-Ferrand.

As mentioned above, frequently used for specific applications in mechanics, in the aerospace industry or in the medical domain, shape-memory alloys do not have much of a presence in the domain of civil engineering.
The delay in their adoption in this domain can partly be explained by the high cost of SMAs in relation to that of conventional construction materials, but also by the lack of knowledge of the mechanisms involved in their coupling with traditional construction materials such as masonry or concrete.

The first significant attempts to use SMAs in the domain of civil engineering were in the mid-1990s.

To begin with, the interest was in using SMAs’ properties of superelasticity and damping with a view to limiting the forces caused by dynamic effects in construction. These works led to the invention of damping devices based on nickel-titanium-type alloys with firm applications for the seismic protection of historic buildings, or more recently for controlling the vibrations in guyed bridges.

More recently, interest has also turned to the memory effect to create states of pre-stress in concrete components in order to improve their mechanical behavior.

From the point of view of its constitution, concrete presents a compact assembly of rigid and strong grains bound by a cement matrix. Although its compressive strength is very high when subjected to uniaxial or multiaxial compression, its mechanical performances are mediocre when it is subjected to a traction force. Regarding the peculiarities of its behavior, we can mention the existence of high degrees of withdrawal and creep deformations, and great susceptibility to damage, leading to brittle fracture under traction, or slightly ductile behavior under compression.

Traditional technological solutions involve reinforcing the concrete with steel bars in the stressed areas (reinforced concrete), or with extended cables to create states of compression that are able to compensate the traction forces likely to occur during the lifetime of the construction (pre-stressed concrete).

These arrangements are intended to guarantee the strength of the structural components and enhance their rigidity, while limiting the risk of cracking. In this context, various paths are beginning to be explored which would see shape-memory alloys used in conjunction with concrete components. At present, the works in question remain in the field of research alone; generally speaking they attempt to take advantage of the memory effect to create states of uni- or multiaxial pre-stress, in order to improve the behavior or strength of the concrete components.

Thus, we can cite:

– the creation of a one-dimensional state of pre-stress in bent concrete components using shape-memory alloy reinforcements;

– the creation of effects of two-dimensional confinement in concrete columns so as to improve their final performance in terms of strength and ductility;
– the use of SMA reinforcements to create self-repairing structures capable of reducing excessive cracking.

Finally, certain works are attempting to use SMAs in the form of short fibers included in the concrete during its manufacture, so that the activation of the memory effect in these “bimaterials” will create a state of three-dimensional internal stress capable of setting back the process of damage by cracking in the stressed areas.

By way of an example, in the following we present a few results obtained for the first two cases mentioned above. The first relates to the creation of pre-stressed states in concrete beams equipped with nickel-titanium wires (Figure 2.38). A key point relates to the procedure used to create a pre-stress force. Nickel-titanium wires are first stretched in the martensitic state, at ambient temperature, before being firmly fixed on the beams. The application of a thermal cycle then activates the memory effect, the result of which is that the wires are subjected to traction but their shortening is prevented by their fixture to the beam. This traction force plays the role of a pre-stress force which subjects the beam to compound bending loading.

![SMA wires (pre-strained at martensitic state)](image)

![Concrete beam](image)

![Strain gauge](image)

a) Initial state

![SMA wires (austenitic state)](image)

![Concrete beam](image)

b) After thermal activation of memory effect

**Figure 2.38. Principle behind the creation of a bending pre-stress using SMA wires [TRA 12a]**

An example of the result obtained after thermal activation of the memory and return to ambient temperature is presented in Figure 2.39. This result relates to three beams equipped with four, eight and twelve nickel-titanium wires 1 mm in diameter. The wires are previously stretched in the martensitic state, so that after the stress is relieved they exhibit residual pre-deformation between 0.16 and 1.02%. The obtained pre-stress effect is demonstrated by the curvature of the beams, deduced from the longitudinal deformations measured using extensometric gages placed on their upper and lower surfaces. We observe that the effect of pre-stress increases in a near-linear manner with the pre-deformation of the wires, as long as this does not go above 0.6%. Beyond this value, partial martensite production under stress occurs during
cooling. Consequently, the value of the predeformation no longer has any impact on the curvature obtained, which reaches an upper limit for each type of beam.

![Graph showing curvature induced in a concrete beam by pre-stress using SMA wires](image)

**Figure 2.39.** *Curvature induced in a concrete beam (520 × 48 × 60 mm³) by pre-stress using SMA wires SMA (Ni50.8-Ti49.2 at.%, Ms = −10°C, Mf = −25°C, As = 23°C, Af = 28°C, diameter 1 mm) depending on the pre-deformation applied before thermal activation of the memory effect [TRA 11]*

This result highlights the influence of the transformation temperatures on the effective pre-stress force. An inapt choice may lead to an instant loss by partial martensite production when cooled. Various losses of the same nature may also occur if the component is exposed to an excessive drop in temperature during its existence (as may be the case, in particular, with outdoor work). Thus we can see that the choice of transformation temperatures is crucial in terms of limiting losses and ensuring the permanence of the pre-stress created by the memory effect.

The second case relates to the use of SMA reinforcements to create states of active confinement in concrete cylinders (Figure 2.40). The SMA wire, previously stretched in the martensitic state at ambient temperature, is rolled with a constant interval on the lateral face of the cylinder before being firmly fixed at its two extremities. Thermal activation of the memory effect causes the application of stress to the wire, whose geometry is anchored by that of the concrete substrate. Because of its curvature, the wire exerts radial pressure on the cylinder, which is therefore subject to a confinement effect. The two-dimensional stress state thus created in the concrete contributes to the retardation of the process of damage, which improves the behavior of the cylinder when subjected to an axial compressive stress.

An example of the result obtained is presented in Figure 2.41. Two cylinders are confined, using a nickel-titanium wire previously stretched in the martensitic state,
with pre-deformations equal to 0.5% and 1.0% (active confinement). A third cylinder is confined by a wire rolled in the austenitic state (passive confinement). The last cylinder is made of non-confined concrete. The measurement of the axial and radial deformations shows that the rigidity, strength and ductility of the cylinders are greatly improved by the presence of the SMA wire. Conversely, the mode and intensity of the confinement appear to have only a slight influence on the behaviors observed.

![Extensometric gauge](image)

**Figure 2.40.** Example of a cylinder representing a concrete column, equipped with an SMA wire with the aim of causing an active confinement effect [DES 10]

![Graph](image)

**Figure 2.41.** Results of compression tests performed on concrete cylinders (tests stopped at 2% radial deformation). Demonstration of the improvement of the mechanical performances of the concrete actively confined by an SMA wire [TRA 12b]
This result illustrates the complex behavior of the wire rolled around the cylinder. The curvature imposed on the wire during rolling greatly modifies its state of deformation. Consequently the behavior of the rolled wire is very different from that observed for a straight sample of the same wire tested alone, as shown in Figure 2.42. This difference can be explained by the additional strain imposed on the wire in its martensitic state when being rolled, and by the asymmetry between traction and compression in the behavior of the SMA wire used. This result illustrates the complex interaction between the SMA wire and the concrete substrate during the phase of rolling and the phase of thermal activation of the memory effect. Therefore, the process of stress creation in traditional components using SMA reinforcements needs to be subject to a detailed analysis, using an appropriate thermomechanical model for the SMA reinforcement used.

![Figure 2.42](image)

**Figure 2.42.** Curvature influence on the average traction stress obtained by thermal activation of the memory effect in an SMA wire (Ni50.8-Ti49.2 at%, \(M_s = -10^\circ C\), \(M_f = -25^\circ C\), \(A_s = 23^\circ C\), \(A_f = 28^\circ C\)). Comparison between a straight wire and a wire rolled around a concrete cylinder 74 mm in diameter, as a function of the pre-deformation applied [DES 10]

The increasing number of studies published over the past few years demonstrates the interest aroused on an international level by the exceptional properties of SMAs in the domain of civil engineering. Thus, in addition to the studies relating to the damping effects or to the creation of pre-stress in concrete components, attempts have also been made to use the memory effect to create variable stress states in structural elements, with the aim of designing active structures capable of adapting their strength capacities to variable use conditions. In view of the size of the constructions and the amounts of materials involved, the impact on the cost is crucial in terms of validating the use of these new materials in civil engineering. There can be no doubt: the prospect of eventually having moderately-costed SMAs will be a crucial factor for the diffusion of these innovative technologies in the sector of civil engineering.
Chapter 3

Martensitic Transformation

NOTE.– This chapter may be partly considered as an attempt to summarize the book by Kaushik Bhattacharya [BHA 03] Microstructure of martensite: why it forms and how it gives rise to the shape memory effect.

3.1. Overview of continuum mechanics

We shall begin by briefly outlining a few basic elements of linear algebra in relation to a certain orthonormal basis and a number of kinematic concepts in continuum mechanics.

3.1.1. Main notations for vectors

A bold-type lowercase letter, e.g. a, will be used hereafter to denote a column vector of real components $a_i$, $i = 1, 2, 3$, in the form:

$$a = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$$

with a particular vector: $0$, which is the null vector.

We use the following notation:

– $a^T$: the transpose of $a$;

– $a \cdot b$: the scalar product of $a$ times $b$: $a \cdot b = a^T b = a_1 b_1 + a_2 b_2 + a_3 b_3$;
- $|a|$: the length of $a$: $|a| = (a \cdot a)^{\frac{1}{2}} = (a_1^2 + a_2^2 + a_3^2)^{\frac{1}{2}}$;
- $\hat{a}$: the unitary vector of components $a_i$, $i = 1, 2, 3$: $|\hat{a}| = 1$;
- $a \times b$: the vector product of $a$ times $b$: $a \times b = \begin{pmatrix} a_2 b_3 - a_3 b_2 \\ -a_1 b_3 + b_1 a_3 \\ a_1 b_2 - a_2 b_1 \end{pmatrix}$

We have:

$$a \times (b \times c) = (a \cdot c) b - (a \cdot b) c$$

$$\det (a, b, c): \text{ the determinant of } (a, b, c): \det (a, b, c) = a (b \times c)$$

### 3.2. Main notations for matrices

A bold-type uppercase letter, e.g. $A$, will be used to denote a real matrix with components $a_{ij}$, $i, j = 1, 2, 3$, in the form:

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$$

There are particular matrices which are, respectively, $\mathbf{O}$ – the null matrix, and $\mathbf{I}$ or $\mathbf{1}$ – the unit matrix.

We use the following notation:
- $\det (A)$: the determinant of $A$;
- $\text{tr}(A)$: the trace of $A$;
- $A^T$: the transpose of $A$;
- $A^{-1}$: the inverse of $A$ if $\det (A) \neq 0$;
- $A^{-T}$: the transpose of $A^{-1}$, and we have $A^{-T} = \frac{1}{\det(A)} \text{cof}(A)$;
- $\text{cof}(A)$: the matrix of cofactors of $A$ (defined by the above equality);
- $a \otimes b$: the dyadic product $a$ times $b$: $a \otimes b = ab^T$. We have:

$$(a \otimes b) c = (b \cdot c) a$$
3.3. Additional notations and reminders

3.3.1. Unit matrices

A matrix $A$ is a unit matrix if:

$$AA^T = I$$

Hence, necessarily:

$$\det (A) = 1 \text{ or } \det (A) = -1$$

In the first case, we say that $A$ is a rotation. In the second case, it is an inversion (the reverse of a rotation). In all cases, the compounded effect of two rotations or of two inversions is a rotation, and we have:

$$Ax \cdot Ay = x \cdot y \forall x, y$$

In particular, every rotation $A$ retains the same length, meaning that:

$$|Ax| = |x| \forall x$$

The reciprocal is also true – i.e. any matrix $A$ which retains the same length is necessarily a rotation.

3.3.2. Rotation matrix

Consider $\hat{u}$ a unitary vector and $P_{\hat{u}}$ and $Q_{\hat{u}}$ the associated matrices defined by:

$$P_{\hat{u}} = \begin{pmatrix} u_1^2 & u_1u_2 & u_1u_3 \\ u_1u_2 & u_2^2 & u_2u_3 \\ u_1u_3 & u_2u_3 & u_3^2 \end{pmatrix} \quad \text{and} \quad Q_{\hat{u}} = \begin{pmatrix} 0 & -u_3 & u_2 \\ u_3 & 0 & -u_1 \\ -u_2 & u_1 & 0 \end{pmatrix}.$$  

In other words, for any $x$:

$$P_{\hat{u}}x = (\hat{u} \odot \hat{u}) x = (\hat{u} \cdot x) \hat{u} \quad \text{and} \quad Q_{\hat{u}}x = \hat{u} \times x$$

We can see that $P_{\hat{u}}$ and $Q_{\hat{u}}$ are orthogonal:

$$P_{\hat{u}}Q_{\hat{u}} = Q_{\hat{u}}P_{\hat{u}} = O$$

$P_{\hat{u}}$ projects onto the axis directed by $\hat{u}$ and $Q_{\hat{u}}$ projects onto the associated orthogonal plane.

Let us set that:

$$R(\hat{u}, \theta) = P_{\hat{u}} + \cos \theta (I - P_{\hat{u}}) + \sin \theta Q_{\hat{u}}$$
It is easy to verify that $R(u, \theta)$ is a rotation. In addition:

$$
\begin{align*}
R(u, \delta \theta) &= R(\delta u, \theta) \\
R(u, \delta \theta) - (R(u, \delta \theta))^T &= 2\delta \sin(\theta) Q_u \\
\forall \delta &\in \{-1, 1\}
\end{align*}
$$

Conversely, we show (see Appendix 1 at the end of the book) that for any rotation $R$, there is at least one couple $(u_R, \theta_R)$, such that:

$$
R = R(u_R, \delta_R \theta_R) \text{ for a certain } \delta_R \in \{-1, 1\}
$$

where $u_R$ denotes a unitary vector, such that:

$$
R u_R = u_R
$$

and $\theta_R$ the angle defined in $[0, \pi]$ by:

$$
\theta_R = \arccos(\kappa_R) \text{ where } \kappa_R = \frac{1}{2} (\text{tr}(R) - 1)
$$

We say that $R$ is the rotation of $\delta_R \theta_R$ about the axis directed by $u_R$.

The parameter $\delta_R$ is closely linked to the direction of orientation of the angle $\theta_R$. Its value is unique for $\theta_R \in [0, \pi]$, where we have:

$$
\delta_R (Q_u)_{ij} (R - R^T)_{ij} \geq 0 \forall i, j = 1, 2, 3
$$

Unlike a situation where $\theta_R = 0$ or $\theta_R = \pi$, the value of $\delta_R$ may just as well be 1 as $-1$, because:

$$
R(u_R, \theta_R) = R(u_R, -\theta_R) \forall \theta_R \in [0, \pi]
$$

For example, consider: $R = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$

We verify that $R$ is a rotation because $RR^T = I$ and $\det(R) = 1$.

Thus, $R = R(u_R, \delta_R \theta_R)$ with the following values:

$$
\begin{align*}
\theta_R &= \arccos\left(-\frac{1}{2}\right) = \frac{2\pi}{3} \iff \kappa_R = -\frac{1}{2} \\
\frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} &\Rightarrow R u_R = u_R, \ |u_R| = 1 \\
\delta_R &= 1 \text{ or } \delta_R = -1
\end{align*}
$$
Martensitic Transformation

and:

\[ Q = \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & -1 & 1 \\ 1 & 0 & -1 \\ -1 & 1 & 0 \end{pmatrix} \]

Using [3.1] and choosing \((i, j) = (1, 3)\), for instance, we get:

\[
\delta_R \begin{pmatrix} Q \mathbf{u} \end{pmatrix}_{13} \begin{pmatrix} \mathbf{R} - \mathbf{R}^T \end{pmatrix}_{13} \times \begin{pmatrix} >0 \end{pmatrix} \Rightarrow \delta_R > 0 \Rightarrow \delta_R = 1
\]

Hence:

\[
\mathbf{R} = \mathbf{R} (\mathbf{u}_R, \theta_R)
\]

Another example:

\[
\mathbf{R} = \begin{pmatrix} 0.36 & 0.48 & -0.8 \\ -0.8 & 0.60 & 0 \\ 0.48 & 0.64 & 0.60 \end{pmatrix}
\]

We verify that \(\mathbf{R}\) is also a rotation. \(\text{because } \mathbf{R} \mathbf{R}^T = \mathbf{I} \text{ and } \det (\mathbf{R}) = 1\).

Thus, we also have \(\mathbf{R} = \mathbf{R} (\mathbf{u}_R, \delta_R \theta_R)\) where:

\[
\begin{align*}
\theta_R &= \arccos (0.28) \approx 73.74^\circ \iff \kappa_R = 0.28 \\
\mathbf{u}_R &= \frac{1}{3} \begin{pmatrix} -1 \\ 2 \\ 2 \end{pmatrix} \Rightarrow \mathbf{R} \mathbf{u}_R = \mathbf{u}_R, |\mathbf{u}_R| = 1 \\
\delta_R &= 1 \text{ or } \delta_R = -1
\end{align*}
\]

and \(Q \mathbf{u} = \frac{1}{3} \begin{pmatrix} 0 & -2 & 2 \\ 2 & 0 & 1 \\ -2 & -1 & 0 \end{pmatrix}\)

With:

\[
\delta_R \begin{pmatrix} Q \mathbf{u} \end{pmatrix}_{13} \begin{pmatrix} \mathbf{R} - \mathbf{R}^T \end{pmatrix}_{13} \times \begin{pmatrix} >0 \end{pmatrix} \Rightarrow \delta_R < 0 \Rightarrow \delta_R = -1
\]

so:

\[
\mathbf{R} = \mathbf{R} (\mathbf{u}_R, -\theta_R)
\]
3.3.3. Symmetric matrices

A matrix $S$ is symmetric if $S^T = S$. Such a matrix has three real eigenvalues $(\lambda_1, \lambda_2, \lambda_3)$ and three associated eigenvectors $(\hat{e}_1, \hat{e}_2, \hat{e}_3)$ which form a direct orthonormal trihedron, so $i, j = 1, 2, 3$, we have:

$$S\hat{e}_i = \lambda_i \hat{e}_i,$$

where $\hat{e}_i \cdot \hat{e}_j = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$ and $\det(\hat{e}_1, \hat{e}_2, \hat{e}_3) = 1$

Let $R_S$ be the matrix whose $j$th column vector is equal to the eigenvector $\hat{e}_j$. Therefore, $R_S$ is a rotation and we have:

$$S = R_SD_SR_T,$$

$$D_S = \begin{pmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{pmatrix},$$

Thus, every vector $x$ decomposes in a unique manner in the form:

$$x = x_1\hat{e}_1 + x_2\hat{e}_2 + x_3\hat{e}_3$$

where $x_i = x_i \hat{e}_i, i = 1, 2, 3$

and we have:

$$\begin{cases} Sx = x_1\lambda_1\hat{e}_1 + x_2\lambda_2\hat{e}_2 + x_3\lambda_3\hat{e}_3 \\ Sx \cdot x = \lambda_1 x_1^2 + \lambda_2 x_2^2 + \lambda_3 x_3^2 \end{cases}$$

3.3.4. Positive definite symmetric matrices

A symmetric matrix $S$ is positive definite if $Sx \cdot x > 0$ for any vector $x$ which is not identically null.

Hence, a symmetric matrix $S$ is positive definite if and only if all its eigenvalues $\lambda_i$ are positive. Thus, we can associate it with the following matrix:

$$D_S^\frac{1}{2} = \begin{pmatrix} \mu_1 & 0 & 0 \\ 0 & \mu_2 & 0 \\ 0 & 0 & \mu_3 \end{pmatrix},$$

where $\mu_i = \sqrt{\lambda_i}$

Thus:

$$S = R_SD_S^\frac{1}{2}D_S^\frac{1}{2}R^T_S = \left(R_SD_S^\frac{1}{2}R^T_S\right)\left(R_SD_S^\frac{1}{2}R^T_S\right) = U_S^2,$$

for $U_S = R_SD_S^\frac{1}{2}R^T_S$

The matrix $U_S$ is also symmetric positive definite and this decomposition is unique.
Proof of the unicity. Indeed, let $M$ be another matrix satisfying the criteria, i.e. $S = M^2$. Its eigenvalues are necessarily $(\mu_1, \mu_2, \mu_3)$. Hence, there is a rotation matrix $R_M$, such that:

$$M = R_M D_M R_M^T = R_M D_S^2 R_M^T$$

From this, we can deduce that:

$$U_S^2 = M^2 \Leftrightarrow R_M D_S R_M^T = R_M D_S R_M^T \Leftrightarrow A D_S = D_S A \text{ where } A = R_M^T R_M$$

Thus for $1 \leq i, j \leq 3$, $a_{ij} \mu_i^2 = \mu_j^2 a_{ij}$. If $\mu_i \neq \mu_j$, then $a_{ij} = 0$. In any case, however, we have: $a_{ij} \mu_i = \mu_j a_{ij}$ and therefore $AD_S^2 = D_S^2 A$, which does indeed give us $M = U_S$.

For any positive definite symmetric matrix $S$, we define the matrix $S^{\frac{1}{2}}$, called the root of $S$, by:

$$S^{\frac{1}{2}} = U_S$$

Obviously, $S^{\frac{1}{2}}$ is also symmetric positive definite.

We note:

$$S^{-\frac{1}{2}} = \left(S^{\frac{1}{2}}\right)^{-1}$$

3.3.5. Polar decomposition

Consider an invertible matrix $F$, such that: $\det (F) > 0$ and $S = F^T F$. In this case, $F$ decomposes in a unique manner in the form:

$$F = R S^{\frac{1}{2}}$$

where:

$$R = F S^{-\frac{1}{2}}$$

is a rotation matrix

**PROOF.**—The symmetric matrix $S$ is positive definite, i.e.:

$$\forall x \neq 0 : S x . x = F x . F x = |F x|^2 > 0 \text{ because } F \text{ is invertible.}$$
Therefore, \( \mathbf{S} \) can only have one root \( \mathbf{S}^\frac{1}{2} = \mathbf{R}_S \mathbf{D}_S^\frac{1}{2} \mathbf{R}_S^T \). Given that the matrix \( \mathbf{S}^\frac{1}{2} \) is invertible because \( \mathbf{F} \) is, \( \mathbf{R} = \mathbf{F} \mathbf{S}^{-\frac{1}{2}} \) satisfies the criterion, meaning that \( \mathbf{R} \) is a rotation because:

\[
\mathbf{R} \mathbf{R}^T = \mathbf{F} \mathbf{S}^{-\frac{1}{2}} \left( \mathbf{F} \mathbf{S}^{-\frac{1}{2}} \right)^T = \mathbf{F} \mathbf{S}^{-\frac{1}{2}} \mathbf{S}^{-\frac{1}{2}} \mathbf{F}^T = \mathbf{F} \left( \mathbf{F}^T \mathbf{F} \right)^{-1} \mathbf{F}^T = \mathbf{I}
\]

where \( \det(\mathbf{R}) = \frac{\det(\mathbf{F})}{\det(\mathbf{S}^\frac{1}{2})} > 0 \).

The example is illustrated in Figure 3.1. Consider:

\[
\mathbf{F} = \begin{pmatrix}
2^{-\frac{1}{2}} & -2^{\frac{1}{2}} & 0 \\
2^{-\frac{1}{2}} & 2^{\frac{1}{2}} & 0 \\
0 & 0 & 1
\end{pmatrix}
\]

![Figure 3.1. Example of a homogenous deformation [BHA 03]](image)

The matrix \( \mathbf{S} = \mathbf{F}^T \mathbf{F} \) has the eigenvalues \( (\lambda_1 = 1, \lambda_2 = 1, \lambda_2 = 4) \), associated with the direct orthonormal trihedron \( \hat{\mathbf{e}}_1 = \begin{pmatrix}0 \\ 0 \\ 1\end{pmatrix}, \hat{\mathbf{e}}_2 = \begin{pmatrix}1 \\ 0 \\ 0\end{pmatrix}, \hat{\mathbf{e}}_3 = \begin{pmatrix}0 \\ 1 \\ 0\end{pmatrix} \). Hence:

\[
\mathbf{D}_S^\frac{1}{2} = \begin{pmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 2
\end{pmatrix}
\quad \text{and} \quad
\mathbf{R}_S = \begin{pmatrix}
0 & 1 & 0 \\
0 & 0 & 1 \\
1 & 0 & 0
\end{pmatrix}
\]

From this we deduce \( \mathbf{F} = \mathbf{R} \mathbf{S}^\frac{1}{2}, \) with:

\[
\mathbf{S}^\frac{1}{2} = \mathbf{R}_S \mathbf{D}_S^\frac{1}{2} \mathbf{R}_S^T = \begin{pmatrix}
1 & 0 & 0 \\
0 & 2 & 1 \\
0 & 0 & 1
\end{pmatrix}
\]

\[
\mathbf{R} = \mathbf{F} \mathbf{S}^{-\frac{1}{2}} = \begin{pmatrix}
2^{-\frac{1}{2}} & -2^{-\frac{1}{2}} & 0 \\
2^{-\frac{1}{2}} & 2^{-\frac{1}{2}} & 0 \\
0 & 0 & 1
\end{pmatrix} = \mathbf{R}(\hat{\mathbf{e}}_1, \frac{1}{4} \pi)
\]

\( \mathbf{R} \) thus constitutes a rotation of angle \( \frac{\pi}{4} \) around the axis \( \hat{\mathbf{e}}_1 \).
3.4. Kinematic description

Consider two sub-domains $\Omega_0$ and $\Omega$ of $\mathbb{R}^3$ taken to a direct orthonormal trihedron (see Figure 3.2).

![Figure 3.2. Transport from the domain $\Omega_0$ to the domain $\Omega$: point, vector, surface, volume [BHA 03]](image)

This is a moving body which successively occupies $\Omega_0$ at rest and $\Omega$ at a given time $t$ definitively fixed. Suppose that there is a derivable biunivocal correspondence $f$ between $\Omega$ and $\Omega_0$, such that:

$$\Omega = f(\Omega_0)$$

By definition, the initial position $x$ of a material particle of $\Omega_0$ is currently in $\Omega$ at the point:

$$y = f(x)$$

or indeed, in terms of components:

$$y_i = f_i(x), i = 1, 2, 3$$

The displacement vector at point $x$ is defined by:

$$u = y - x$$

3.4.1. Strain gradient

Let us express the differentials of $f_i$ in the form:

$$df_i = \frac{\partial f_i}{\partial x_1} dx_1 + \frac{\partial f_i}{\partial x_2} dx_2 + \frac{\partial f_i}{\partial x_3} dx_3 = \nabla f_i, dx, i = 1, 2, 3$$

This may be converted into matrix form:

$$dy = F dx$$
where:

\[ \mathbf{F} = \nabla \mathbf{f} = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \frac{\partial f_1}{\partial x_3} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \frac{\partial f_2}{\partial x_3} \\ \frac{\partial f_3}{\partial x_1} & \frac{\partial f_3}{\partial x_2} & \frac{\partial f_3}{\partial x_3} \end{pmatrix} \]

The matrix \( \mathbf{F} \), whose components have no physical dimensions, is the gradient tensor of the transformation.

Thus:

\[ \mathbf{F} = \mathbf{I} + \nabla \mathbf{u} \]

\( \mathbf{F} \) is said to be homogeneous if and only if \( \mathbf{F} \) is a constant matrix, independent of \( \mathbf{x} \).

### 3.4.2. Dilatation and strain tensors

In all cases, we shall always assume that:

\[ \det (\mathbf{F}) > 0 \]

and we set:

\[ \mathbf{C} = \mathbf{F}^T \mathbf{F} \]

Hence, \( \mathbf{C} \) is a positive definite symmetric matrix and we have the decomposition of \( \mathbf{F} \) in the form:

\[ \mathbf{F} = \mathbf{R} \mathbf{C}^{\frac{1}{2}} \]

where \( \mathbf{R} = \mathbf{F} \mathbf{C}^{-\frac{1}{2}} \) is a rotation.

Thus, the length of \( d \mathbf{y} \) has the following value:

\[ |d\mathbf{y}| = |\mathbf{F}d\mathbf{x}| = |\mathbf{R} \mathbf{C}^{\frac{1}{2}}d\mathbf{x}| = |\mathbf{C}^{\frac{1}{2}}d\mathbf{x}| = \left( \lambda_1 |dx_1|^2 + \lambda_2 |dx_2|^2 + \lambda_3 |dx_3|^2 \right)^{\frac{1}{2}} \]

where \( \lambda_1, \lambda_2 \) and \( \lambda_3 \) denote the positive eigenvalues of \( \mathbf{C} \).

The tensor \( \mathbf{C} \) is called the dilatation tensor. Its expression as a function of \( \mathbf{u} \) is quite simply:

\[ \mathbf{C} = (\mathbf{I} + \nabla \mathbf{u})^T (\mathbf{I} + \nabla \mathbf{u}) = \mathbf{I} + \nabla \mathbf{u} + (\nabla \mathbf{u})^T + (\nabla \mathbf{u})^T \nabla \mathbf{u} \]

We can see that it is expressed in a nonlinear fashion in relation to the components of the gradient of the displacement vector \( \mathbf{u} \).
The Lagrangian strain tensor is defined by:

\[ \mathbf{E} = \frac{1}{2} (\mathbf{C} - 1) = \frac{1}{2} \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T + (\nabla \mathbf{u})^T \nabla \mathbf{u} \right) \]

If the continuum moves as a rigid body, i.e. if:

\[ |d\mathbf{y}| = |d\mathbf{x}| \]

then the symmetric matrix \( \mathbf{C}^{\frac{1}{2}} \) is orthogonal, which implies that:

\[ \mathbf{C} = \mathbf{C}^{\frac{1}{2}} \left( \mathbf{C}^{\frac{1}{2}} \right)^T = \mathbf{I} \]

We therefore have the following necessary and sufficient condition for a body to move without deformation:

\[ \mathbf{E} = 0 \]

With small strains, we often ignore the quadratic terms and write:

\[ \epsilon = \frac{1}{2} \left( \nabla \mathbf{u} + (\nabla \mathbf{u})^T \right) \]

**EXAMPLE.** – (see Figure 3.1) We shall place ourselves in the context of the homogeneous case (where \( \mathbf{F} \) is constant):

\[ \mathbf{F} = \begin{pmatrix} 2^{-\frac{1}{2}} & -2^{-\frac{1}{2}} & 0 \\ -2^{-\frac{1}{2}} & 2^{-\frac{1}{2}} & 0 \\ 0 & 0 & 1 \end{pmatrix} \]

We have:

\[ \mathbf{C} = \mathbf{F}^T \mathbf{F} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 1 \end{pmatrix} \Rightarrow \mathbf{E} = \frac{1}{2} (\mathbf{C} - \mathbf{I}) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \frac{3}{2} & 0 \\ 0 & 0 & 0 \end{pmatrix} \]

Thus, in the direction \( \mathbf{\hat{e}} = \begin{pmatrix} 2^{-\frac{1}{2}} \\ -2^{-\frac{1}{2}} \\ 0 \end{pmatrix} \) for instance, we find a deformation equal to

\[ e = \mathbf{E} \cdot \mathbf{\hat{e}} = \frac{3}{4}. \]
3.4.3. Transformation of an element of volume or surface (see Figure 3.2)

Consider an elementary parallelogram \( s_{\Omega_0} \) in \( \Omega_0 \), with infinitesimal sides \( dx_1, dx_2 \) and surface \( ds_{\Omega_0} \), i.e.:

\[
d s_{\Omega_0} = |dx_1 \times dx_2|
\]

The image of \( s_{\Omega_0} \) by \( f \) is a parallelogram \( s_\Omega \) in \( \Omega \), with surface:

\[
d s_\Omega = |Fd x_1 \times Fd x_2|
\]

The elementary volume \( d\Omega_0 \) of the parallelepiped constructed on a trihedron of infinitesimal particle vectors \((dx_1, dx_2, dx_3)\) is equal to the determinant of \((dx_1, dx_2, dx_3)\):

\[
d\Omega_0 = \det (dx_1, dx_2, dx_3)
\]

The image by \( f \) of this parallelepiped is the parallelepiped constructed on the trihedron \((Fdx_1, Fdx_2, Fdx_3)\), whose volume is given by:

\[
d\Omega = \det (Fdx_1, Fdx_2, Fdx_3) = \det (F) d\Omega_0
\]

Consider the unitary vectors \( \hat{n}_{\Omega_0} \) and \( \hat{n}_\Omega \) defined by:

\[
\hat{n}_{\Omega_0} = \frac{dx_1 \times dx_2}{|dx_1 \times dx_2|} \quad \text{and} \quad \hat{n}_\Omega = \frac{Fdx_1 \times Fdx_2}{|Fdx_1 \times Fdx_2|}
\]

They are orthogonal respectively to \( s_{\Omega_0} \) and to \( s_\Omega \).

Using the volume formula, we write:

\[
d s_\Omega \hat{n}_\Omega \cdot Fdx_3 = ds_{\Omega_0} \det (F) \hat{n}_{\Omega_0} \cdot dx_3 \\
\Rightarrow ds_{\Omega_0} \hat{n}_{\Omega_0} \cdot Fdx_3 = ds_{\Omega_0} \det (F) F^{-T} \hat{n}_{\Omega} \cdot Fdx_3 = ds_{\Omega_0} \text{cof} (F) \hat{n}_{\Omega_0} \cdot Fdx_3
\]

This last equality occurs for every infinitesimal vector \( dx_3 \), from which we deduce:

\[
d s_\Omega \hat{n}_\Omega = ds_{\Omega_0} \text{cof} (F) \hat{n}_{\Omega_0}
\]

In particular:

\[
d s_\Omega = ds_{\Omega_0} |\text{cof} (F) \hat{n}_{\Omega_0}|
\]
3.5. Kinematic compatibility

We shall now focus on a crucial problem of shifting at the plane interface $\Gamma$ between two sub-parts $\Omega_1$ and $\Omega_2$ of the sample $\Omega$ (see Figure 3.3):

$$y(x) = \begin{cases} F_1 x + c_1 & \text{in } \Omega_1 \\ F_2 x + c_2 & \text{in } \Omega_2 \end{cases}.$$

Consider $\hat{n}$ to be a unitary vector normal to the plane surface $\Gamma$. Continuity means that:

$$x \in \Gamma: (F_1 - F_2)x = c_2 - c_1 \Rightarrow \begin{cases} c_2 - c_1 \in \text{image} (F_1 - F_2) \\ \dim (\ker (F_1 - F_2)) = 2 \end{cases}$$

If we suppose that:

$$\forall x \ (c_2 - c_1 \in \text{image} (F_1 - F_2), \dim (\ker (F_1 - F_2)) = 2)$$

then:

$$x = P_{\hat{n}}x + (I - P_{\hat{n}})x \Rightarrow F_1 x = F_1 P_{\hat{n}}x + F_1 (I - P_{\hat{n}})x, \ i = 1, 2$$

$$\Rightarrow (F_1 - F_2)x = (F_1 - F_2)P_{\hat{n}}x + (F_1 - F_2)(I - P_{\hat{n}})x$$

i.e.:

$$F_1 - F_2 = (F_1 - F_2)P_{\hat{n}}\hat{n} + c_2 - c_1 = (F_1 - F_2)\hat{n}\hat{n}^T + c_2 - c_1$$

$$F_1 - F_2 = a\otimes\hat{n} + c_2 - c_1$$
Example: consider 

\[
Q = \begin{bmatrix}
\cos \theta & -\sin \theta & 0 \\
\sin \theta & \cos \theta & 0 \\
0 & 0 & 1
\end{bmatrix}
\]

\[
U_1 = \begin{bmatrix}
\beta & 0 & 0 \\
0 & \alpha & 0 \\
0 & 0 & \alpha
\end{bmatrix}
\]

\[
U_2 = \begin{bmatrix}
\alpha & 0 & 0 \\
0 & 0 & \beta \\
0 & 0 & \alpha
\end{bmatrix}
\]

\[F_1 = QU_1, \quad F_2 = U_2\]

where:

\[
F_1 - F_2 = QU_1 - U_2 = \begin{pmatrix}
\beta \cos \theta - \alpha & -\alpha \sin \theta & 0 \\
\beta \sin \theta & \alpha \cos \theta - \beta & 0 \\
0 & 0 & 0
\end{pmatrix}
\]

Verification of the conditions:

\[c_2 - c_1 \in \text{image } (F_1 - F_2) \Rightarrow 0 \in \text{image } (F_1 - F_2)\]

and:

\[\dim (\ker (F_1 - F_2)) = 2 \Leftrightarrow 3\alpha \beta - (\alpha^2 + \beta^2) \cos \theta = 0\]

We find:

\[F_1 - F_2 = a \otimes \hat{n}\]

where:

\[
a = (F_1 - F_2) \hat{n} = \begin{pmatrix}
\beta \cos \theta - \alpha & -\alpha \sin \theta & 0 \\
\beta \sin \theta & \alpha \cos \theta - \beta & 0 \\
0 & 0 & 0
\end{pmatrix} \begin{pmatrix}
n_1 \\
n_2 \\
n_3
\end{pmatrix} = \begin{pmatrix}
(\beta \cos \theta - \alpha) n_1 - \alpha \sin \theta n_2 \\
(\alpha \cos \theta - \beta) n_2 + \beta \sin \theta n_1 \\
0
\end{pmatrix}
\]

### 3.6. Continuous theory of crystalline solids

In this section, we shall develop the continuous theory of crystalline solids. We begin with an overview of crystalline lattices and their symmetry. We draw the link between the lattice and the continuum using the Cauchy–Born rule.
3.6.1. Bravais lattices

A Bravais lattice \( L(e_i, 0) \) is an infinite array of points in a three-dimensional space generated by the translation operation of a single point \( O \) by three lattice vectors \( e_1, e_2, e_3 \), i.e.:

\[
L(e_i, 0) = \{ x = \nu^1 e_1 + \nu^2 e_2 + \nu^3 e_3 | \nu^1, \nu^2, \nu^3 \text{ are integers} \}
\]  \[3.3\]

The vectors \( e_1, e_2, e_3 \) define a unit cell. It is conventional to denote a direction in the lattice by \([u,v,w]\), where \( u, v \) and \( w \) are numbers.

The direction \( d \) is given by the vector:

\[
d = u e_1 + v e_2 + w e_3
\]  \[3.4\]

An equivalent class of directions is denoted \(<uvw>\). By a simple cubic lattice with lattice vectors parallel to the vertices:

\(<100> = \{[100], [010], [001], [100], [010], [001] \} \] \[3.5\]

In Figure 3.4 we see some examples of Bravais lattices.
We describe a plane in a lattice with its normal (hkl). To this effect, we introduce the reciprocal vectors by \( \{ e^1, e^2, e^3 \} \) such that:

\[
e_i e_j = \begin{cases} 
0 & \text{if } i \neq j \\
1 & \text{if } i = j 
\end{cases}
\]  

[3.6]

Thus, the plane \((hkl)\) is the plane whose normal is:

\[
\hat{n} = he^1 + ke^2 + le^3
\]  

[3.7]

3.6.2. Deformation of lattices and symmetry

Consider two Bravais lattices \( L(e_i, 0) \) and \( L(f_i, 0) \) generated by \( \{ e_i \} \) and \( \{ f_i \} \) respectively. Therefore, there is a matrix \( F \) (with \( \det F \neq 0 \)) such that

\[
f_i = Fe_i
\]  

[3.8]

Thus, we consider the lattice \( L(e_i, 0) \) to be the transformed lattice \( L(f_i, 0) \) by \( F \). In continuous theory, we limit ourselves to those deformations which preserve the orientation, i.e. those such that \( \det F > 0 \). In more explicit terms, \( e_1(\varepsilon_2 \wedge \varepsilon_3) > 0 \).

There are deformations which transform a Bravais lattice into itself. This is a consequence of the symmetry of the lattice. Two arrays of lattice vectors \( e_1, e_2, e_3 \) and \( f_1, f_2, f_3 \) with the same orientation generate the same Bravais lattice \( L(e_i, 0) = L(f_i, 0) \) if and only if:

\[
f_i = \mu_i e_j
\]  

[3.9]

For \( 3 \times 3 \) matrices of integers such that:

\[
\det \left[ \mu_i \right] = 1
\]  

[3.10]
In the decomposed form:

\[ f_i = \mu_i^1 e_1 + \mu_i^2 e_2 + \mu_i^3 e_3 \]

For example, in Figure 3.5, we see:

\[ f_1 = e_1, f_2 = e_1 + e_2, f_3 = e_3 \]

Thus:

\[ \begin{bmatrix} \mu_i^j \\ \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \]

We can say that a matrix \( H \) transforms a lattice into itself if and only if:

\[ H e_i = \mu_i^j e_j \]  

[3.11]

where \( \mu_i^j \) satisfies the conditions [3.10].

Thus, the set of operations that transforms a lattice into itself is given by:

\[ G(e_i) = \left\{ H : H e_i = \mu_i^j \text{ for values of } \mu_i^j \text{ that satisfy equation } [3.10] \right\} \]  

[3.12]

\( G(e_i) \) is a group and is called the symmetry group of the lattice.

More specifically, the punctual group of the matrix \( P(e_i) \) is a set of rotations which transforms the lattice into itself:

\[ P(e_i) = \left\{ R / R \text{ is a rotation and } R e_i = \mu_i^j e_j \text{ satisfy equation } [3.10] \right\} \]  

[3.13]

There are seven punctual groups of symmetry in Bravais lattices, a list of which may be found, for instance, on page 35 of Bhattachary’s book [BHA 03].

### 3.6.3. Link between lattices and the continuous medium: Cauchy–Born hypothesis

We have just discussed lattices. Our aim is to obtain the continuous medium theory. The Cauchy–Born hypothesis is explicitized in Figure 3.6.

This hypothesis states that the direction vectors of the crystalline lattice deform such that:

\[ e_i(x) = F(x)e_i^0(x) \]  

[3.14]

In other words, the direction vectors of the lattice behave like infinitesimal linear elements in the continuum. We refer to a homogenous reference configuration, so \( e_i^0 \) is independent of \( x \).
3.6.4. Energy density in crystalline solids

Returning now to Bravais lattices \( L(e_1, 0) \), we assume that the Helmholtz free energy, specific to the lattice is written thus:

\[
\hat{\varphi}(F e_1^0, \theta) = \varphi(F, \theta) \quad \text{[3.15]}
\]

Its properties are as follows:

1) material indifference:

\[
\varphi(QF, \theta) = \varphi(F, \theta) \text{ no matter what the rotation } Q \quad \text{[3.16]}
\]

2) material symmetry:

\[
\varphi(FH, \theta) = \varphi(F, \theta) \text{ no matter what } H \in G(e_1) \quad \text{[3.17]}
\]

Demonstration:

\[
\begin{align*}
\varphi(F, \theta) &= \hat{\varphi}(F(x)e_1^0, \theta) = \hat{\varphi}(e_1, \theta) = \hat{\varphi}(\mu_1^1 e_j, \theta) \\
&= \hat{\varphi}(\mu_2^0 e_j^0, \theta) = \hat{\varphi}(FHe_1^0, \theta) = \varphi(FH, \theta)
\end{align*} \quad \text{[3.18]}
\]

For material symmetry, we can write:

\[
\varphi(FR, \theta) = \varphi(F, \theta) \text{ for any rotation } R \in P(e_1^0) \quad \text{[3.19]}
\]

If we combine the symmetry with the material indifference, we obtain:

\[
\varphi(R^TFR, \theta) = \varphi(F, \theta) \text{ for any rotation } R \in P(e_1^0) \quad \text{[3.20]}
\]
3.7. Martensitic transformation

3.7.1. Introduction

Our objective is to develop a continuous theory for materials subject to a so-called “martensitic phase transformation”. In particular, we are seeking to understand the nature of the microstructure which is observed in these materials. For the moment, we shall focus on monocrystalline samples in their austenitic state (the highest-temperature phase). We shall describe a number of crystallographic states of the material. The total energy of the material, in $\Omega$, subject to the transformation gradient $F = \nabla y$, at temperature $\theta$, is given by:

$$\int_{\Omega} \varphi(F = \nabla y, \theta) \, dV \quad [3.21]$$

We assume that the energy depends on the distortion of the lattice. We postulate that the material will be in a state which “minimizes its total energy”. Specifically, we shall find that this energy has multiple minima called “multi-well structures”.

3.7.2. Martensitic transformation: Bain matrix or transformation matrix

Let us examine a simple crystallographic transformation between cubic austenite and quadric martensite. Such is the case of the magnetic shape-memory alloy $\text{Ni}_2\text{MnGa}$ studied by J.Y. Gauthier et al. [GAU 07a][GAU 11] or $1n = 23at\%Th$ [GUT 50].

Consider the direction vectors of the austenitic lattice $e_{a1}^a, e_{a2}^a, e_{a3}^a$ and those of the martensitic lattice $e_{m1}^m, e_{m2}^m, e_{m3}^m$ (Figure 3.7).

In the description of the transformation of the austenitic lattice into a martensitic lattice, we can find the matrix $U_1$ such that:

$$e_{m_i}^m = U_1 e_{a_i}^a \forall i = 1, 2, 3 \quad [3.22]$$

$U_1$ is called a Bain matrix; it is a positive definite $3 \times 3$ matrix. The vectors of the two lattices are written in $R_0$ (orthonormal framework associated with the cubic cell of austenite):

$$e_{a1}^a = \frac{1}{2} \begin{bmatrix} 0 \\ a_0 \\ a_0 \end{bmatrix}, \quad e_{a2}^a = \frac{1}{2} \begin{bmatrix} 0 \\ -a_0 \\ +a_0 \end{bmatrix}, \quad e_{a3}^a = \frac{1}{2} \begin{bmatrix} 0 \\ -a_0 \\ -(-a_0) \end{bmatrix} \quad [3.23]$$

$$e_{m1}^m = \frac{1}{2} \begin{bmatrix} 0 \\ a \\ a \end{bmatrix}, \quad e_{m2}^m = \frac{1}{2} \begin{bmatrix} 0 \\ -a \\ -a \end{bmatrix}, \quad e_{m3}^m = \frac{1}{2} \begin{bmatrix} c \\ 0 \\ a \end{bmatrix} \quad [3.24]$$
In $R_0$, it is easy to verify that the transformation matrix is given by:

$$U_1 = \begin{bmatrix} \beta & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \alpha \end{bmatrix}$$

[3.25]

where $\alpha = a/a_0$, $\beta = c/a_0$.

For instance, for $Ni_2MnGa$: $a_0 = 5.82 \text{ Å}$ and $a = 5.95 \text{ Å}$, $c = 5.60 \text{ Å}$; we get $\alpha = 1.0188$ and $\beta = 0.9589$ [HEC 01]; and for $InTh$: $a_0 = 4.7445 \text{ Å}$ and $a = 4.619 \text{ Å}$, $c = 4.8451 \text{ Å}$, which gives us $\alpha = 0.9889$ and $\beta = 1.02012$ [GUT 50].

For this crystalline transformation, there are three martensite variants named:

$$U_1 = \begin{bmatrix} \beta & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \alpha \end{bmatrix}, \quad U_2 = \begin{bmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & \alpha \end{bmatrix}, \quad U_3 = \begin{bmatrix} \alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \beta \end{bmatrix}$$

[3.26]
As this is the simplest crystallographic transformation, we shall use it as the pervading example in this chapter.

The cubic-to-orthorhombic transformation (Figure 3.8) is characterized by the following Bain matrix:

\[
U_1 = \begin{bmatrix}
\frac{a+\gamma}{2} & 0 & \frac{a-\gamma}{2} \\
0 & \beta & 0 \\
\frac{a-\gamma}{2} & 0 & \frac{a+\gamma}{2}
\end{bmatrix}
\] [3.27]

where \( \alpha = \sqrt{2}a/a_0 \), \( \beta = b/a_0 \) and \( \gamma = \sqrt{2}c/a_0 \).

Figure 3.8. Cubic-to-orthorhombic martensitic transformation [BHA 03]

This is the case with Cu−14.2wt%Al−4.3%Ni with \( \nu = 6 \{ U_1, \ldots, U_6 \} \).

As regards NiTi, Hane and Shield [HAN 99b] showed that the transformation was type I cubic-to-monoclinic with \( \nu = 12 \) and:

\[
U_1 = \begin{bmatrix}
\gamma & \epsilon & \epsilon \\
\epsilon & \alpha & \delta \\
\epsilon & \delta & \alpha
\end{bmatrix}
\] [3.28]

where:

\[
\gamma = \frac{a(\sqrt{2}a + c\sin\beta)}{a_0\sqrt{2a^2 + c^2 + 2\sqrt{2ac}\sin\beta}},
\] [3.29]

\[
\epsilon = \frac{ac\cos\beta}{\sqrt{2a_0\sqrt{2a^2 + c^2 + 2\sqrt{2ac}\sin\beta}}},
\]

\[
\alpha = \frac{1}{2\sqrt{2a_0}} \left( \frac{c(c + \sqrt{2a_0}\sin\beta)}{\sqrt{2a^2 + c^2 + 2\sqrt{2ac}\sin\beta}} + b \right),
\] [3.30]

\[
\delta = \frac{1}{2\sqrt{2a_0}} \left( \frac{c(c + \sqrt{2a_0}\sin\beta)}{\sqrt{2a^2 + c^2 + 2\sqrt{2ac}\sin\beta}} - b \right),
\]
where, for \( Ni = 49.75\% Ti \): \( a_0 = 3.015\ A^\circ, \ a = 2.889\ A^\circ, \ b = 4.12\ A^\circ, \ c = 4.622\ A^\circ, \ \beta = 96.8^\circ\)

This gives \( \alpha = 1.0243, \gamma = 0.9563, \epsilon = -0.04266, \delta = 0.05803 \) [OTS 71].

![Figure 3.9. Type I cubic-to-monoclinic transformation in nickel-titanium (only the position of the titanium atoms is shown) [BHA 03]](image)

As regards the copper-based alloys Cu-Al-Ni, Cu-Al-Zn, Cu-Ga-Zn, etc., there are Type II cubic-to-monoclinic transformations (Figure 3.9) where \( \nu = 12 \) and:

\[
\mathbf{U}_1 = \begin{bmatrix} \alpha & \delta & 0 \\ \delta & \beta & 0 \\ 0 & 0 & \gamma \end{bmatrix}
\]  

\[\text{[3.31]}\]

3.7.2.1. Summary

We can find the Bain matrices of the different martensite variants \( \mathbf{U}_1, \mathbf{U}_2, \ldots, \mathbf{U}_\nu \) in the form \( \mathbf{R}^T \mathbf{U}_i \mathbf{R} \) where \( \mathbf{R} \) is a rotation belonging to the symmetry group of \( A: \mathbf{P}_a \) (\( \mathbf{R}^T \mathbf{R} = \mathbf{R}^T \mathbf{R} = 1 \)). It is important to highlight that for any material, the number of variants \( \nu \) and the transformation matrix \( \mathbf{U}_1 \) are determined using crystalline parameters of the austenite and martensite, determined experimentally by X-ray measurements.

In order to go further with the knowledge of the microstructure, let us first look at the equation governing the interface between two martensite variants.

3.8. Equation governing the interface between two martensite variants \( M_i/M_j \) or the “twinning equation”

Let us examine an interface between two martensite variants (Figure 3.10: variant \( M_i \) in \( \Omega_1 \) and variant \( M_j \) in \( \Omega_2 \)). We are looking for a movement such that:

\[
\mathbf{F} = \nabla \mathbf{y} : \left\{ \begin{array}{l} \mathbf{Q}_1 \mathbf{U}_i \ \text{in} \ \Omega_1 \\ \mathbf{Q}_2 \mathbf{U}_j \ \text{in} \ \Omega_2 \end{array} \right\} \text{for two rotations} \ \mathbf{Q}_1 \ \text{and} \ \mathbf{Q}_2 
\]

\[\text{[3.32]}\]
The compatibility equation must satisfy:

\[ \mathbf{Q}_1 \mathbf{U}_i - \mathbf{Q}_2 \mathbf{U}_j = \mathbf{b} \otimes \mathbf{n} \quad [3.33] \]

where \( \mathbf{n} \) is the unitary normal to the interface and \( \mathbf{b} \) is a vector.

By multiplying the above equation by \( \mathbf{Q}_2^T \) and positing \( \mathbf{Q} = \mathbf{Q}_2^T \mathbf{Q}_1 \) and \( \mathbf{a} = \mathbf{Q}_2^T \mathbf{b} \), we get:

\[ \mathbf{QU}_i - \mathbf{U}_j = \mathbf{a} \otimes \mathbf{n} \quad [3.34] \]

We call this equation: the “twinning equation” between two martensites \( i \) and \( j \).

If we are looking for the solution to this “twinning equation”, the procedure is as follows (demonstrated by Ball and James in 1987 and 1992 [BAL 87], [BAL 92]):

1) we calculate the matrix \( \mathbf{C} \):

\[ \mathbf{C} = (\mathbf{U}_i \mathbf{U}_j^{-1})^T (\mathbf{U}_i \mathbf{U}_j^{-1}) \]

2) if \( \mathbf{C} = \mathbf{I} \) (identity matrix), equation \([A4.1]\) has no solution;

3) if \( \mathbf{C} \neq \mathbf{I} \), we calculate the eigenvalues of the matrix \( \mathbf{C} \). Automatically, \( \lambda_i > 0 \), and we shall classify them such that \( \lambda_1 \leq \lambda_2 \leq \lambda_3 \);

4) equation \([A4.1]\) has a solution if and only if the eigenvalues satisfy:

\[ \lambda_1 \leq 1, \quad \lambda_2 = 1, \quad \lambda_3 \geq 1 \quad [3.35] \]

5) if the condition \([3.35]\) is satisfied, then there are precisely two solutions, given by:

\[ \mathbf{a} = \rho \left( \sqrt{\frac{\lambda_1(1-\lambda_3)}{\lambda_3-\lambda_1}} \mathbf{e}_1 + \sqrt{\frac{\lambda_1(1-\lambda_2)}{\lambda_3-\lambda_1}} \mathbf{e}_3 \right) \quad [3.36] \]

\[ \mathbf{n} = \frac{\sqrt[\rho \sqrt{\lambda_3 - \lambda_1} - \sqrt{\lambda_1}]}{-\sqrt{1 - \lambda_1} \mathbf{U}_2^T \mathbf{e}_1 + \kappa \sqrt{\lambda_3 - 1} \mathbf{U}_2^T \mathbf{e}_3} \quad [3.37] \]
where $\kappa = \pm 1$, $\rho \neq 0$ chosen such that $\|\hat{\mathbf{n}}\| = 1$ and $\hat{\mathbf{e}}_i$ are the unitary eigenvectors associated with the eigenvalues $\lambda_i$ ($i = 1, 2, 3$).

Choosing $\kappa = 1$ yields one solution, while $\kappa = -1$ gives the other solution. For both solutions, we obtain $\mathbf{Q}$ by substituting $\mathbf{a}$ and $\hat{\mathbf{n}}$ into the expression (3.34).

In Appendix 2, we give some elements of a demonstration of the procedure used for the twinning equation as regards the eigenvalues $\lambda_i$ and the obtention of the vectors $\mathbf{a}$ and $\hat{\mathbf{n}}$.

### 3.8.1. Cubic $\rightarrow$ quadratic transformation

Let us apply this procedure to the cubic $\rightarrow$ quadratic transformation. To begin the calculation, we choose the variants 1 and 2.

Let $\mathbf{R}$ be a matrix of $180^\circ$ rotation around the $\hat{\mathbf{e}}$ axis defined by:

$$\hat{\mathbf{e}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$$

[3.38]

It is easy to verify that $\mathbf{R}^T \mathbf{U}_1 \mathbf{R} = \mathbf{U}_2$, and we get:

1. $\mathbf{a} = \frac{\sqrt{2}(\beta^2 - \alpha^2)}{\beta^2 + \alpha^2} \begin{pmatrix} -\beta \\ \alpha \\ 0 \end{pmatrix}$, $\hat{\mathbf{n}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$

[3.39]

2. $\mathbf{a} = \frac{\sqrt{2}(\beta^2 - \alpha^2)}{\beta^2 + \alpha^2} \begin{pmatrix} -\beta \\ -\alpha \\ 0 \end{pmatrix}$, $\hat{\mathbf{n}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$

[3.40]

Similarly, if we examine variants 1 and 3, we obtain the solution with $180^\circ$ rotation about the axis:

$$\hat{\mathbf{e}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

[3.41]

An explicit calculation of $\mathbf{a}$, $\hat{\mathbf{n}}$ and $\mathbf{Q}$ satisfying the twinning equation is given in Appendix 3 (at the end of the book).
3.8.2. Cubic $\rightarrow$ orthorhombic transformation

We shall begin with variants 1 and 2. Consider a 180° rotation about the axis:

$$\hat{e} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$ \[3.42\]

It is easy to verify that $R^T U_1 R = U_2$, and once again, we obtain:

1. $a = \frac{\gamma^2 - \alpha^2}{\gamma^2 + \alpha^2} (\alpha - \gamma) \\
   \hat{n} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$ \[3.43\]

2. $a = \frac{\gamma^2 - \alpha^2}{\gamma^2 + \alpha^2} (\alpha + \gamma) \\
   \hat{n} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$ \[3.44\]

The calculations for the cubic $\rightarrow$ monoclinic transformation are considerably more complicated, but are in the same vein, and the results are detailed in [BHA 03].

3.9. Origin of the microstructure

In section 3.8, we saw that twinned martensites were obtained by minimization of the strain energy. Yet it is unusual to find $M_i/M_j$ interfaces isolated in the material. The observations show that the microstructures are complex with many interfaces (Figures 1.1 to 1.4).

In fact, the microstructures are very fine and the size of the domains extremely small. A question therefore arises: why does a classic image of martensite constitute a complex lattice with a very fine scale? In fact, why does martensite form a microstructure?

The “crystallographical theory of martensite” (CTM) school of thought, including Ball, James, Kohn, Bhattacharya, etc., interprets “the existence of a very fine microstructure as a consequence of the multi-well structure” of the energy density.

Let us consider a monocrystal, subject to boundary conditions of mechanical loading. In energetic terms, it is preferable that the boundary condition should correspond to an energy well, so the material can easily accommodate this. In addition, if the boundary condition imposed does not correspond to any one of the wells, but rather to a combination of different wells, the material can “normally” accommodate it. However, the combination of energy wells cannot be arbitrary, because the conditions of compatibility at the $M_i/M_j$ interfaces must be respected. We shall see that “forming very fine structures” increases the materials’ capacity to satisfy the conditions of compatibility at the interfaces.
We shall demonstrate this with a well-known example which constitutes the calculation of the variations initiated by Bolza and Young [YOU 80]. It is a one-dimensional example. Unfortunately, in this case, the need to respect consistency is not a severe constraint. Nevertheless, it will serve as a good educational example for two-dimensional or three-dimensional cases.

### 3.9.1. Simplified one-dimensional case

Consider a bar with unit length whose axial displacement is $y(x)$. In this case, the gradient $f$ is scalar:

$$f = \frac{dy}{dx}$$

We assume that the energy density is:

$$\varphi(f) = (f^2 - 1)^2$$

As Figure 3.11 shows, there are two “variants” characterized by the wells $f = 1$ and $f = -1$.

![Figure 3.11. Energy density in the one-dimensional case [BHA 03]](image)

The total energy is:

$$\xi(f) = \int_{0}^{1} (\varphi(f(x)) + (y(x))^2) dx = \int_{0}^{1} ((f(x) - 1)^2 + (y(x))^2) dx$$

We seek to minimize this total energy whatever the continuous displacements $y(x)$. We shall show that this leads to a fine microstructure between variants $f = 1$ and $f = -1$. Note that the lowest energy value is, obviously, equal to zero. This means that the terms below the integral sign must be equal to zero. In other words, we have to find a movement $y$ which satisfies:

$$\frac{dy}{dx} = f(x) = \pm 1 \text{ and } y(x) = 0$$

which is, of course, impossible.
A numerical solution is possible. For any integer $n$, let $y^n$ represent the movement with $n$, just as shown in Figure 3.12:

$$y^n(x) = \begin{cases} x & 0 < x < \frac{1}{2n} \\ \frac{1}{n} - x & \frac{1}{2n} < x < \frac{2}{2n} \end{cases}$$

It is easy to calculate the deformation energy:

$$\xi(y^n) = n \int_0^{1/2n} x^2 \, dx + n \int_{1/2n}^{2/2n} \left( \frac{1}{n} - x \right)^2 \, dx = \frac{1}{12} n^2$$

Clearly:

$$\lim_{n \to \infty} \xi(y^n) = 0$$

In prosaic terms, this is equivalent to dividing an interval into $n$ segments.

### 3.9.2. Simplified two-dimensional case

We work on a square with length of side $L$:

$$\{(x_1, x_2), 0 < x_1 < L, 0 < x_2 < L\}$$
The following movement \( x \) is written \( y(x_1, x_2 - x) \). The displacement gradient is now a vector:

\[
f = \left\{ \frac{\partial y}{\partial x_1}, \frac{\partial y}{\partial x_2} \right\} = \{ f_1, f_2 \}
\]

Consider the energy density \( \varphi(f) = \varphi(f_1, f_2) \):

\[
\varphi(f) = (f_1^2 - 1)^2 + f_2^2
\]

We impose \( y = 0 \) at the edge, and try to find \( y \) which minimizes the total energy.

The procedure is identical to the one-dimension case demonstrated above, and we obtain:

\[
\xi(y^n) = \frac{L^2}{n}
\]

### 3.9.3. Three-dimensional case

The three-dimensional case will not be discussed in detail here because it is too complex. We associate “minimizing series” with increasingly fine microstructures and the relaxed energy density, in addition to the critical size of the microstructure. Some information will be given in section 3.10.

### 3.10. Special microstructures

#### 3.10.1. Austenite-martensite interface

We shall draw on two ideas. The first is that the microstructure can be represented more and more finely, by a usually converging sequence of displacements (see the measurements taken by Bolza and Young). The second idea is that energy minimization forces the strains associated with these sequences to assume values which situate the energy in wells of potential.

As regards the austenite-martensite interface, also known as the “habitat plane”, the microstructure is interesting and is historically important. In most SMAs, the interface between the austenite and martensite is not a simple interface. We have the austenite \( A \) on one side and a couple of martensite variants \( (M_i/M_j) \) on the other. A question arises: why do SMAs choose to form such a habitat plane (or such a microstructure)?

The issue investigated by Weschler et al. [WES 53] and Bowles and MacKenzie [BOW 54] led each of these author groups independently to put forward the phenomenological theory of martensite, which we shall now outline briefly.
3.10.2. Phenomenological theory of martensite

A structural transformation is considered to be martensitic if it fulfills a number of criteria:

– the passage from the crystalline structure of the parent phase to the produced phase occurs by way of a homogeneous deformation of the lattice. This mechanism corresponds to a cooperative displacement of all the atoms;

– the transformation takes place without diffusion (the displacements of all the atoms are smaller than an interatomic distance).

In summary, martensitic transformation is defined as “a transformation dominated by a shearing component obtained by distension of the lattice, without diffusion and occurring by germination and growth of a new phase which is totally or partially consistent with the parent phase” (Elisabeth Gautier, lecture at IPSI, 2001) [GAU 01].

The observations of the microstructures of transformation can be used to establish different characteristics: relations of orientation between the crystalline structure of the parent phase and that of the produced phase, plane of side-by-side mutual accommodation of the two phases (which we shall call the “invariant plane – an internal structure of martensite platelets” which we have called “martensite variants”).

Let us examine, in the simple case of $\text{Ni}_2\text{Mn-Ga}$ (or $\text{In} - \text{Tl}$), the crystallographic transformation of austenite.

In its “high-temperature” austenitic phase, the Ni-Mn-Ga alloy has an $L2_1$ structure, called a Heusler structure, discovered by Heusler, Starck and Haupt in 1903: in fact it is an assembly of eight centered cubic lattices, with a particular distribution of the three atoms making up the alloy (Figure 3.13).

![Figure 3.13. Superlattice of austenite in Ni2-Mn-Ga](www.iran-mavad.com)
This lattice has a parameter $a_0$, whose value is essentially the same, irrespective of the chemical composition of the particular alloy: we shall take it as being equal to 5.82 Å.

By phase transformation, austenite undergoes a distortion and then gives rise to martensite, a phase which is stable at “low temperature”. We shall now see how it is possible to deduce the martensitic structure on the basis of the austenitic structure.

In the lattice shown in Figure 3.14, it is possible to show another, quadratic lattice, possessing the parameters of the lattices $a_0$ and $a_0/\sqrt{2}$.

**Figure 3.14. Quadratic lattice within the cubic lattice of austenite**

Given these two lattices, let us now look at how to define the martensitic transformation from a crystallographic point of view.

During this transformation, the austenitic phase is deformed: there is a movement of the atoms making up the material, to the point where the structure is no longer that which best represents the atomic distribution. The martensite rather has a quadratic-type structure deduced from the former (modifying the values of the lattice parameters: $a$ becomes $c$ and $a_0/\sqrt{2}$ becomes $a/\sqrt{2}$ (Figure 3.15)).

**Figure 3.15. Passage from the austenite lattice to the martensite lattice**
As can be seen in Figure 3.15, the martensite lattice is rotated by 45° in relation to the austenite lattice and is contained within it; it is indeed quadratic, with lattice parameters \( c \) and \( b = a/\sqrt{2} \). Wescbler, Liebermann and Read developed a geometrical phenomenological model in order to describe these transformations [WES 53]. The deformation, on the invariant plane \( F \), is a combination of a deformation with an invariant lattice \( S \) followed by a Bain deformation \( U \) and a rotation \( Q \) of a lattice, enabling the invariant plane to be returned to its original position. We obtain:

\[
F = QUS
\]

Shearing of the invariant lattice occurs by twinning or slip.

The Bain deformation \( U \) has already been calculated on the basis of the lattice parameters of the austenite and martensite.

For all these approaches, the displacement vector can be written:

\[
b = \eta s + \xi m
\]

where \( \eta \) is the angular distortion caused by shearing on the plane \((m, s)\) and \( \xi \) is the subsequent linear dilatation, normal to the habitat plane.

\[\text{Figure 3.16. Austenite-to-martensite transformation}\]

Figure 3.16 explicitizes the geometric construction. In finite transformation, \( F \) can be written as:

\[
F = 1 + \nabla b
\]

and the transformation strain tensor:

\[
E_T = \frac{1}{2}(F^T F - I)
\]

In the small perturbation theory, \( \varepsilon_t = (\nabla b)^t \), the symmetric part of gradient \( b \) quite simply.
3.10.3. Crystallographic theory of martensite

Let us place ourselves in the simplest situation, where a plane interface separates
the austenite from the i-th martensite variant (Figure 3.17):

\[
F = \begin{cases} 
1 & \text{in } \Omega_1 \\
QU_i & \text{in } \Omega_2 \text{ for any rotation } Q 
\end{cases}
\]  \hspace{1cm} [3.45]

So that the displacement is continuous, the conditions of compatibility must be satisfied – i.e.:

\[
QU_i - 1 = b \otimes \hat{m} \hspace{1cm} [3.46]
\]

Figure 3.17. An exact austenite/martensite interface

The procedure is absolutely identical to the twinning equation between two
martensite variants (see equation \([A4.1]\)).

Calculate \(C\):

\[
C = (QU_i)^T (QU_i) = U_i Q^T Q U_i = U_i^2 \hspace{1cm} [3.47]
\]

\(C\) must have three eigenvalues \(\lambda_i\) such that:

\[
\lambda_1 \leq 1, \quad \lambda_2 = 1, \quad \lambda_3 \geq 1
\]

The large majority of materials do not satisfy these conditions. In his book, K.
Bhattacharya cites only two materials which do: Ti-29%Ta obtained by Bywater and
Christian [BYW 72] and a Ti-Ni-Cu by Miyazaki and Ishida [MIY 94].

Note that this is only true for very special compositions of the alloy. Certain
Cu-Zn-Al or Cu-Al-Be alloys have values of \(\lambda_2\) which are around the value of 1
[LEX 04] for cubic-to-monoclinic phase transformations, as previously highlighted
by Hane [HAN 99a], but taking an elementary \(6M_1\) lattice different to the monoclinic
\(18M\) lattice. In this context, let us note the crystallographic investigations of
Balandraud and Zanzotto[BAL 07], in search of a simple \(\text{A}/M_i\) interface.
In general, we have the austenite on the one hand, and a couple $M_i/M_j$ of martensite variants, on the other.

This microstructure represented in Figure 3.18 leads us to verify two very distinct equations:

– the compatibility equation between the two variants $I$ and $J$:

$$QU_1 - U_j = a \otimes \hat{n}$$  \[3.48\]

which we have already discussed;

– the compatibility equation between the austenite $A$ and the couple of martensite variants $M_i/M_j$ in proportion $(1-\lambda)$ and $\lambda$ respectively:

$$Q\left(\lambda QU_j - (1-\lambda)U_i\right) = 1 + b \otimes m$$  \[3.49\]

![Figure 3.18. a) A typical interface between the austenite and martensite; b) a sequence of deformations which characterize the austenite/martensite interface](image)

Let us hypothesize that the twinning equation of the variants $i$ and $j$ has a solution. Once again, Ball and James [BAL 87], [BAL 92] give the procedure in order to obtain the solution to the equation of the austenite/martensite interface.

1) Calculate:

$$\delta = a. U_i(U_i^2 - 1)^{-1}\hat{n}$$  \[3.50\]

and:

$$\eta = tr(U_i^2) - det(U_i^2) - 2\times \frac{|a|^2}{\delta}$$  \[3.51\]

The equation of the austenite/martensite interface has a solution if and only if:

$$\delta \leq -2 \text{ and } \eta \geq 0$$  \[3.52\]
2) In order to find the solutions, calculate:

\[ \lambda = \frac{1}{2} (1 - \sqrt{1 + \frac{2}{\delta}}) \]  

[3.53]

3) Calculate:

\[ C = (U_1 + \lambda a \otimes \hat{n})(U_1 + \lambda \hat{n} \otimes a) \]  

[3.54]

Find the eigenvalues \( \lambda_1 \leq \lambda_2 \leq \lambda_3 \) and the eigenvectors \( \hat{e}_1, \hat{e}_2, \hat{e}_3 \) of \( C \). Automatically, \( \lambda_2 = 1 \) and:

\[ b = \rho \left( \frac{\lambda_3 - \lambda_1}{\lambda_3 - \lambda_1} \hat{e}_1 + \frac{\lambda_3}{\lambda_3 - \lambda_1} \hat{e}_3 \right) \]  

[3.55]

\[ \hat{m} = \frac{\lambda_3 - \sqrt{\lambda_1}}{\rho \sqrt{\lambda_3 - \lambda_1}} (-\sqrt{1 - \lambda_1} U_1^T \hat{e}_1 + \kappa \sqrt{\lambda_3 - 1} U_1^T \hat{e}_3) \]  

[3.56]

with \( \rho \) chosen in order to obtain \( |\hat{m}| = 1 \) and \( \kappa = \pm 1 \).

Two solutions for \( \kappa = 1 \): \((b^+, \hat{m}^+); \kappa = -1 \): \((b^-, \hat{m}^-)\).

4) If \( \delta > -2 \), repeat calculation 3), replacing \( \lambda \) with \((1 - \lambda)\). Note that \( C \) is quadratic in \( \lambda \); the condition of \( \lambda_2 = 1 \) gives us a root for this quadratic equation:

\[ \lambda = \frac{1}{2} (1 \pm \sqrt{1 + \frac{2}{\delta}}) \]  

[3.57]

An attempt to explain this calculatory procedure will be made in Appendix 4 (at the end of the book).

For the cubic austenite \( \rightarrow \) quadratic martensite transformation.

Look again at the Bain matrices \( U_1 \) and the vectors \( a \) and \( \hat{n} \) obtained by solving the twinning equation. The equation of the \( A/(M_i, M_j) \) interface has a solution if and only if:

\[ \alpha < 1 < \beta \text{ and } \frac{1}{\alpha^2} + \frac{1}{\beta^2} \leq 2 \]  

[3.58]

or:

\[ \beta < 1 < \alpha \text{ and } \alpha^2 + \beta^2 \leq 2 \]  

[3.59]

From this we deduce:

\[ \lambda = \frac{1}{2} \left( 1 - \sqrt{1 + \frac{2(\alpha^2 - 1)(\beta^2 - 1)(\alpha^2 + \beta^2)}{(\beta^2 - \alpha^2)^2}} \right) \]  

[3.60]
The two solutions with $\lambda$ and $(1-\lambda)$ are given by:

$$b^\pm = \rho \frac{1 - \alpha^2}{1 + \beta^2} \left[ \pm \frac{\delta + \tau}{\beta} + \pm \frac{\delta - \tau}{2} \right] \quad \tilde{m}^\pm = \frac{1}{\rho} \left[ \pm \frac{\delta + \tau}{\beta} + \pm \frac{\delta - \tau}{2} \right]$$

[3.61]

where:

$$\delta = \sqrt{\frac{\alpha^2 + \beta^2 - 2}{1 - \alpha^2}}, \quad \tau = \sqrt{\frac{2\alpha^2\beta^2 - \alpha^2 - \beta^2}{1 - \alpha^2}}$$

[3.62]

$\varphi$ is chosen such that $||\tilde{m}^\pm|| = 1$.

The numerical applications for In –23% at.Th give:

$$\lambda = 0.3382$$

$$b \left[ 0.01503, 0.00034, 0.01553 \right]$$

$$\tilde{m} \left[ 0.7033, 0.0161, 0.7108 \right]$$

of around 1° of difference with the predictions made by Basinski and Christian [BAS 54a][BAS 54b].

More complex structures may exist, such as “wedges” (see Figure 3.19). The principle is the same but the calculations are more complicated and there are precise conditions regarding the value of the lattice parameters. For instance, for quadratic martensite, the parameter $\alpha$ is linked to $\beta$ by the following relation:

$$\alpha^2 = \frac{(1 - \beta^2)^2 + 4\delta^2(1 + \beta^2)}{(1 - \beta^2)^2 + 8\beta^4}$$

Figure 3.19. Schematic representation of a “wedge”-type microstructure

The calculation for In –23%Tl gives us:

– for $\beta = 1.0221$, $\alpha$ calculated = 0.9893 as opposed to $\alpha$ measured = 0.9889.
The calculation for $Ni_2Mn - Ga$ gives us:
– for $\beta = 0.9589$, $\alpha$ calculated = 1.0216 as opposed to $\alpha$ measured = 1.0188.

This means that wedge-type microstructures may potentially exist for these two alloys.

A counter-example is discussed by Balandraud and Zanzotto [BAL 07].

Contrary to the prediction of the crystallographic theory of martensite, a “wedge” of martensite, which ought not to exist in reference to the values of the crystallographic parameters, is observed in a Cu-Zn-Al (Figure 3.20). Certainly, we observe a stress gradient effect which is not taken into account by the CTM. Balandraud and Zanzotto resolve the problem by attempting to close the angle of “non-compatibility” between the two variants (Figure 3.21) and introduce a criterion of “near compatibility” related to the value of this angle [BAL 10].

**Figure 3.20. Presence of a wedge of martensite in a Cu-Zn-Al alloy [SAB 79]**

**Figure 3.21. Angle of “non-compatibility” between two martensite variants**

3.11. From the scale of the crystalline lattice to the mesoscopic and then the macroscopic scale

The continuity, even if only in the monocrystal, of so-called “special” microstructures, comes up against boundary conditions imposed on the edges (whether in terms of displacement, stress vector or mixed conditions), and this causes
problems of homogenization – an area in which France’s academics in particular have garnered recognition on an international scale. There is another hurdle to be overcome: the issue of the transition from the monocrystal to the polycrystal.

The situation is not always clear-cut. On the one hand, there is the very seductive mathematical theory of martensitic transformation (Ball, James, Bhattacharya, Kohn, etc.) and on the other, there is (what I would call “reality”) the macroscopic behavior of the polycrystal.

Let us give an overview of the basic ideas regarding scale-change, developed by Christian Licht [LIC 98].

3.11.1. Approach at the level of the crystalline lattice

As already detailed, there are in existence crystallographic lattices which are stable at different temperatures. At high temperature, there is a single lattice: that formed by the parent phase, or austenite. At low temperature, there are several lattices. A lattice is determined to the nearest rotation: the classes of equivalence, by way of rotations, are called variants. Thus, if the austenitic phase is cubic centered and the martensite quadratic, there are three martensite variants. For the sake of an easier understanding, we shall only illustrate three phases called $A, M_1, M_2$ (austenite + two martensite variants) (see Figure 3.22).

The energy of these crystalline lattices is of the type:

$$
\begin{align*}
\varphi(e_i^\alpha, \theta) & \leq \varphi(e_i, \theta) & \theta > \theta_0 \\
\varphi(e_i^\alpha, \theta) & = \varphi(e_i^m, \theta) & \theta = \theta_0 \\
\varphi(e_i^m, \theta) & \leq \varphi(e_i, \theta) & \theta < \theta_0
\end{align*}
$$

[3.63]

for any vector in the lattice $e_i$.

The free energy $\varphi$ is obviously non-convex.
3.11.2. **Microscopic approach**

By the Cauchy–Born rule, we associate a continuum with the crystalline medium.

– The linear application $F$ which leads from the austenitic crystalline lattice to the martensitic crystalline lattice becomes $\nabla y(x)$, the transformation gradient which transforms the point $x$ from the abstract continuous medium into a point $y(x)$.

– The continuous medium is supposed to be thermoelastic with an energy $\varphi(\nabla y(x), \theta(x))$ which inherits energetic properties from the previous crystalline model.

In order to solve the problem, R.V. Kohn [KOH 91] worked on the basis of the linearized deformation hypothesis (sometimes called the small strain hypothesis). This means that the strain tensor $\varepsilon(u)$ is equal to the symmetrized gradient of displacement $u$. The energy (though the nonlinear energy) of the system is written:

$$\varphi = \text{Min}_{i} \varphi_i(\varepsilon(u))$$

$i = 0$: austenite; $i = 1, 2, ..., \nu$: martensite variants;

where:

$$\varphi_i(\varepsilon(u)) = \alpha(\varepsilon(u) - a_i) : (\varepsilon(u) - a_i)/2 + \varphi_0^i$$

[3.64]

where:

– $\alpha$: elastic constant tensor (the same no matter what the phase state);

– $a_i(\theta)$: deformation in the stress-free state;

– $\varphi_0^i(\theta)$: level of energy at the well $\varepsilon_i$.

The dependency of $\varphi_i$ on the temperature $\theta$ is crucial – it is this which renders both the austenite and martensite stable.

3.11.3. **Mesoscopic approach**

The calculation of part of a monocrystal, occupying the domain $\Omega$ and subjected to a displacement on its boundary $\partial \Omega$, leads to the formulation (P).

Mathematicians have shown that the problem (P) usually has no solution, but that:

– the minimizing series $\tilde{u}(x)$ of (P) usually accept limits for convergences. We shall denote this as $\tilde{u}(x)$;

– the $\tilde{u}(x)$ minimizes another total energy $\int_{\Omega} Q\varphi(\varepsilon(u(x)))dx$;

where $Q\varphi$ is the quasi-convex function of $\varphi$. 
One mechanical interpretation may be as follows: \( \hat{u}(x) \) (constituting an average limit) describes, at the mesoscopic scale, the equilibrium of the crystalline element, whose behavior is then described by an apparent energy, the quasi-convex \( Q\phi \) of the real energy \( \phi \) which described it at the microscopic scale.

An example is to be found in the work of Kohn [KOH 91], who calculates “the relaxation of a double-well energy” of the form:

\[
\phi(\varepsilon(u)) = Min(\phi_1(\varepsilon(u)), \phi_2(\varepsilon(u)))
\]

where:

\[
\phi_1(\varepsilon(u)) = \alpha(\varepsilon(u) - a_1); (\varepsilon(u) - a_1)/2 + \phi_1^0
\]

A useful expression of the quasi-convex is given by:

\[
Q\phi(\xi) = Min_{0 \leq z \leq 1} \left( \frac{1}{2} \alpha(\xi - za_1) - (1 - z)a_2 \right); (\xi - za_1 - (1 - z)a_2) + z\phi_1^0 + (1 - z)\phi_2^0 + \frac{z(1 - z)}{2}h
\]

\( z \) the volumetric fraction of phase 1 and \( (1-z) \) the volumetric fraction of phase 2.

Note that the term \( z(1-z) \) is indeed worthy of the appellation of term of interaction between the two phases:

- it exists only if there is incompatibility between the two wells \( a_1 \) and \( a_2 \), which corresponds to \( h \neq 0 \);
- it is minimal at \( z = 0 \) and at \( z = 1 \);
- the value of \( h \) is fixed by \( a_1 \) and \( a_2 \).

\( Q\phi \) can be written in the form:

\[
Q\phi(\xi) = Min_{z \in [0, 1]} QZ\phi(\xi)
\]

where \( QZ\phi(\xi) \) is a function of \( z \) and \( \xi \). It is this expression that we get when we propose a model dependent on \( \xi \) (i.e. \( \varepsilon \)) and \( z \).

In addition, reversibility necessitates the counteraction of the thermodynamic force \( \Theta = -\frac{\partial QZ\phi(\xi)}{\partial z} \), and therefore that \( z \) does the minimum on the interval \( (0, 1) \) of \( QZ\phi(\xi) \), which means that the variable \( z \) can be eliminated.

Finally, the coefficient \( h \) is either positive or null (equation [3.12], in [KOH 91]). The consequence of this is that \( QZ(\xi) \) is not necessarily convex at \( z \). \( h \) is perfectly defined as a function of the wells \( a_i \) and the energy levels \( \phi_i^0 \).
The result of this will be a mesoscopic energy $Q_\phi$ which is quasi-convex, not necessarily convex. It will only be convex if $h = 0$, which requires that $(a_1 - a_2)$ be written in the form of a dyadic product (see the Hadamard compatibility equations).

In certain macroscopic approaches such as those of Muller [MUL 89], [MUL 91] or Raniecki et al. [RAN 92], we find some similarities with the term of interaction in $A\zeta(1-\zeta)$.

### 3.11.4. Macroscopic approach

The polycrystal is considered to be an aggregate of monocrystals of energy $Q_\phi$ in a homogenized whole. The orientations of the grains depend on the spatial variable. The same is true of $Q_\phi$ (because the $a_i$ are dependent on $x$). An illustration of the problems encountered is to be found in Figure 3.23.

![Figure 3.23. A polycrystal with its incompatibilities between the grains to be accommodated](image)

### 3.12. Linear geometric theory

This simplified theory is used when the strains are small. For an analysis under “large strains”, the phase transition leads to a “multi-well energy” and the material’s physical behavior is extremely nonlinear. If there are several consecutive transformations, we have to multiply the rigid rotation matrices, as demonstrated by polar decomposition.
The linearized theory simplifies the calculations relating to microstructure, and for instance transforms polar decomposition, which is multiplicative, into an additive decomposition.

### 3.12.1. Linearized kinematics

Let \( x \mapsto y(x) \) with the transformation gradient \( F/F(x) = \nabla y(x) \). We define the vectorial displacement \( u(x) \) by:

\[
    u(x) = y(x) - x
\]  \[3.65\]

If we define the matrix \( H(x) = \nabla u(x) \), we obtain:

\[
    H(x) = F(x) - 1
\]  \[3.66\]

Take the Lagrangian strain tensor in finite transformation:

\[
    E = \frac{1}{2} (F^T F - 1) = \frac{1}{2} (H + H^T + H^T H)
\]  \[3.67\]

We are under small strain conditions if \( H \) is small in comparison to 1, which means that \( u_{i,j} \) is infinitely small of order 1 and \( u_{k,i} u_{k,i} \) is infinitely small of order 2 and we introduce the small strain tensor \( \varepsilon \) by ignoring \( H^T H \) in the face of \( H \):

\[
    \varepsilon = \frac{1}{2} (H + H^T)
\]  \[3.68\]

Note that only by calculating the value of the components \( u_{i,j} \) of \( H \) will we be able to vindicate or invalidate this choice of measurement of deformation. By way of a counter-example, with \( F \) chosen as before (equation [3.2]):

\[
    F = \begin{bmatrix}
        \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 \\
        \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\
        0 & 0 & 1
    \end{bmatrix}
\]

This being the case:

\[
    H = F - 1 = \begin{bmatrix}
        \frac{1}{\sqrt{2}} - 1 & -\frac{1}{\sqrt{2}} & 0 \\
        \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} - 1 & 0 \\
        0 & 0 & 0
    \end{bmatrix}
\]

and the “small strain” hypothesis would not be relevant at all.
For the polar decomposition $F = QU$, we shall show, by use of an example, that in the small strain situation:

$$U \approx 1 + \varepsilon \text{ and } Q \approx 1 + \Omega$$

where:

$$\Omega = \frac{1}{2}(H - H^T)$$

$\Omega$ is called the infinitesimal rotation matrix.

Thus, the multiplicative polar decomposition is approximated by an additive decomposition:

$$H = \varepsilon + \Omega$$

EXAMPLE.— Consider the transformation $x \implies y(x)$:

$$\begin{pmatrix}
  y_1 &=& x_1 \cos \theta - \lambda x_2 \sin \theta + \delta \\
  y_2 &=& x_1 \sin \theta - \lambda x_2 \cos \theta \\
  y_3 &=& x_3
\end{pmatrix}$$

Thus:

$$F(x) = \begin{pmatrix}
  \cos \theta - \lambda \cos \theta & 0 \\
  \sin \theta & \lambda \cos \theta \\
  0 & 0 & 1
\end{pmatrix} = \begin{pmatrix}
  \cos \theta - \cos \theta & 0 \\
  \sin \theta & \cos \theta \\
  0 & 0 & 1
\end{pmatrix} \begin{pmatrix}
  1 & 0 & 0 \\
  0 & \lambda & 0 \\
  0 & 0 & 1
\end{pmatrix} = QU$$

$Q$ performs a rotation of axis $x_3$ and angle $\theta$.

$H$ is small in comparison to $1$ if and only if $(\lambda - 1)$ and $\theta$ are small. We get:

$$\varepsilon = \begin{pmatrix}
  0 & 0 & 0 \\
  0 & \lambda - 1 & 0 \\
  0 & 0 & 0
\end{pmatrix}, \quad \Omega = \begin{pmatrix}
  1 - \theta & 0 \\
  \theta & 1 & 0 \\
  0 & 0 & 1
\end{pmatrix}$$

where $\theta$ is in radians.
The axial deformation \( \varepsilon_{\hat{e}\hat{e}} = \hat{e} \cdot \varepsilon \hat{e} \) for \( \hat{e} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \):

\[
\varepsilon_{\hat{e}\hat{e}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \begin{pmatrix} 0 & 0 & 0 \\ 0 & \lambda - 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} = \frac{1}{2} (\lambda - 1)
\]

is small, with \( \lambda - 1 \) also being small.

3.12.2. Linear geometric theory for phase transformation

Consider the total energy of the specimen subject to a displacement \( u \) at temperature \( \theta \) given by:

\[
\int_{\Omega} \varphi(\nabla u, \theta) dV
\]

[3.72]

As an input, the specimen takes a state which minimizes the total energy.

We assume:

– material indifference; this energy density \( \phi \) is invariant for any infinitesimal rotation of the lattice:

\[
\phi(H + W, \theta) = \phi(H, \theta) \ \forall \theta
\]

\[
\Rightarrow \phi(H, \theta) = \psi(\varepsilon, \theta)
\]

– material symmetry:

\[
\psi(R^T \varepsilon R, \theta) = \psi(\varepsilon, \theta) \ \forall R \in P
\]

The transformation from austenite to martensite can be described as a homogeneous deformation of tensor \( \varepsilon_1 \), with the definition:

\[
\varepsilon_1 = U_1 - 1
\]

For instance, for a cubic \( \rightarrow \) quadratic transformation:

\[
\varepsilon_1 = \begin{bmatrix}
\varepsilon_\beta &=& \beta - 1 & 0 & 0 \\
0 & \varepsilon_\alpha &=& \alpha - 1 & 0 \\
0 & 0 & \varepsilon_\alpha &=& \alpha - 1
\end{bmatrix}
\]

[3.73]
and $\varepsilon_2 = \begin{bmatrix} \varepsilon_\alpha & 0 & 0 \\ 0 & \varepsilon_\beta & 0 \\ 0 & 0 & \varepsilon_\alpha \end{bmatrix}$, $\varepsilon_3 = \begin{bmatrix} \varepsilon_\alpha & 0 & 0 \\ 0 & \varepsilon_\alpha & 0 \\ 0 & 0 & \varepsilon_\beta \end{bmatrix}$.

We can define:

$$\begin{cases} 
\psi(0, \theta) \forall \varepsilon, \theta > \theta_0 & \text{austenitic state} \\
\psi(0, \theta) = \psi(\varepsilon_1, \theta) \quad \psi(\varepsilon_N, \theta) \leq \psi(\varepsilon, \theta) \forall \varepsilon, \theta = \theta_0 & \text{austenite/martensite boundary} \\
\psi(\varepsilon_1, \theta) = \psi(\varepsilon_N, \theta) \leq \psi(\varepsilon, \theta) \text{ for any } \varepsilon, \theta < \theta_0 
\end{cases}$$

### 3.12.3. Some microstructures and comparison

#### 3.12.3.1. Twinning

Consider a displacement gradient involving two variants $I$ and $J$ in the two sub-domains:

$$\begin{align*}
\nabla u &= \varepsilon_1 + \omega_1 \text{ in } \Omega_1 \\
\nabla u &= \varepsilon_2 + \omega_2 \text{ in } \Omega_2
\end{align*}$$

for a number of antisymmetric matrices $\omega_1, \omega_2$ which will perform rotations.

The compatibility conditions require that:

$$\varepsilon_1 - \varepsilon_J = \frac{1}{2} (a \otimes \hat{n} + \hat{n} \otimes a)$$

Procedure to find the vectors $a \neq 0$ and $\hat{n}$ such that:

$$\varepsilon_I - \varepsilon_J = \frac{1}{2} (a \otimes \hat{n} + \hat{n} \otimes a)$$

1) calculate $\varepsilon = \varepsilon_I - \varepsilon_J$;

2) if $\varepsilon = 0$, there is no solution;

3) if $\varepsilon \neq 0$, calculate the eigenvalues of $\varepsilon$ and order such that $\epsilon_1 \leq \epsilon_2 \leq \epsilon_3$;

4) equation [3.75] has a solution if and only if the eigenvalues satisfy:

$$\epsilon_1 \leq 0 \epsilon_2 = 0 \epsilon_3 \geq 0$$
5) if the condition in equation [3.75] is satisfied, then we have exactly two solutions which are given by

\[ a = \sqrt{3}(\varepsilon_3 - \varepsilon_1)(\kappa \sqrt{-\varepsilon_1 \mathbf{e}_1} + \sqrt{\varepsilon_3} \mathbf{e}_3) - twinning \]

where \( \kappa = \pm 1 \) and \( \mathbf{e}_i \) are the eigenvectors of \( \varepsilon \) corresponding to the eigenvalues \( \varepsilon_i, i = 1, 2, 3; \kappa = 1 \) delivers one solution and \( \kappa = -1 \) the other.

Cubic \( \rightarrow \) quadratic transformation

Take \( I = 1 \) and \( J = 2 \). We can easily verify that we switch from variant 1 to variant 2 by a 180° rotation about the axis:

\[
\frac{1}{\sqrt{2}} \begin{bmatrix}
1 \\
1 \\
0
\end{bmatrix}
\]

We can find two possible forms of twinning between variants 1 and 2:

1) \( a = \sqrt{2}(\beta - \alpha) \begin{bmatrix}
-1 \\
1 \\
0
\end{bmatrix}, \quad \mathbf{n} = \frac{1}{\sqrt{2}} \begin{bmatrix}
1 \\
1 \\
0
\end{bmatrix} \)

2) \( a = \sqrt{2}(\beta - \alpha) \begin{bmatrix}
1 \\
1 \\
0
\end{bmatrix}, \quad \mathbf{n} = \frac{1}{\sqrt{2}} \begin{bmatrix}
-1 \\
1 \\
0
\end{bmatrix} \)

The same calculations can be performed for the cubic \( \rightarrow \) orthorhombic transformation.

3.12.3.1.1. Austenite/martensite interface

Let us consider an interface between the austenite and a simple martensite variant called \( I \).

The condition of compatibility requires that:

\[ \varepsilon_i - 0 = \frac{1}{2}(a \otimes \mathbf{n} + \mathbf{n} \otimes a) \]

In this case, one of the eigenvalues of \( \varepsilon_i \) must be zero. Remember that this is a non-generic condition which very few materials satisfy.

Hence, we shall attempt to make an interface between \( A \) and a couple \((M_i, M_j)\) of martensite variants.
Suppose that the infinitesimal rotation of the austenite is equal to zero.

Without sacrificing generality, we need to solve the following system:

1) \( \varepsilon_I - \varepsilon_J = \frac{1}{2}(a \otimes \hat{n} + \hat{n} \otimes a) \)

2) \( \lambda \varepsilon_J + (1 - \lambda) \varepsilon_I = \frac{1}{2}(b \otimes \hat{m} + \hat{m} \otimes b) \)

In more explicit terms, we examine the cubic \( \rightarrow \) quadratic transformation, where \( I = 1 \) and \( J = 2 \).

We know the two solutions \( (a_1, \hat{n}_1) \) and \( (a_2, \hat{n}_2) \).

Consider the matrix:

\[
\begin{bmatrix}
\lambda \varepsilon_\alpha + (1 - \lambda) \varepsilon_\beta & 0 & 0 \\
0 & \lambda \varepsilon_\beta + (1 - \lambda) \varepsilon_\alpha & 0 \\
0 & 0 & \varepsilon_\alpha
\end{bmatrix}
\]

one of the eigenvalues of which must be null.

There is the trivial scenario \( \varepsilon_\alpha = 0 \), which gives us an \( A/M_I \) interface that is uninteresting.

Thus, we have to choose \( \lambda \) such that:

\( \lambda \varepsilon_\alpha + (1 - \lambda) \varepsilon_\beta = 0 \) or \( \lambda \varepsilon_\beta + (1 - \lambda) \varepsilon_\alpha = 0 \)

Thus:

\( \lambda = \lambda^* \) or \( \lambda = 1 - \lambda^* \) or \( \lambda^* = \frac{\varepsilon_\beta}{\varepsilon_\beta - \varepsilon_\alpha} \)

In any case, we have \( 0 < \lambda < 1 \), which requires:

\( \varepsilon_\beta > 0 > \varepsilon_\alpha \) ou \( \varepsilon_\beta < 0 < \varepsilon_\alpha \)

Assuming one of the conditions and choosing \( \lambda = \lambda^* \):

\[
\lambda \varepsilon_J + (1 - \lambda) \varepsilon_I = \begin{bmatrix}
0 & 0 & 0 \\
0 & \varepsilon_\alpha + \varepsilon_\beta & 0 \\
0 & 0 & \varepsilon_\alpha
\end{bmatrix} = \frac{1}{2}(b \otimes \hat{m} + \hat{m} \otimes b)
\]
For variants 1 and 2, we find, by identification:

\[
\lambda = \frac{\epsilon_\beta}{\epsilon_\beta - \epsilon_\alpha} \ b = \rho \epsilon_\alpha \ (0, \kappa \delta, 1) \ \hat{m} = \frac{1}{\rho} \ (0, -\kappa \delta, 1)
\]

\[
\lambda = 1 - \frac{\epsilon_\beta}{\epsilon_\beta - \epsilon_\alpha} \ b = \rho \epsilon_\alpha \ (\kappa \delta, 0, 1) \ \hat{m} = \frac{1}{\rho} \ (-\kappa \delta, 0, 1)
\]

where \( \delta = \sqrt{-\epsilon_\alpha + \beta/\epsilon_\alpha}, \kappa = \pm 1 \) and \( \rho \) is chosen such that \(|\hat{m}|=1\).

**EXAMPLE.**– Ni\(_{2}\)-Mn-Ga [HEC 01]

*Numerical application*

\[\alpha = 1.0188; \beta = 0.8589\]

\[\epsilon_\alpha = 0.0188; \epsilon_\beta = -0.0411; \epsilon_\alpha - \epsilon_\beta = 0.0599; l = 0.3186; \delta = 1.0891, \rho = 1.4786\]

### 3.13. Chapter conclusion

Readers wishing to gain deeper knowledge about microstructure can consult the work of K. Bhattacharya.

There, the reader will find additional information about the memory effect and recoverable deformations and about thin films and polycrystals.
Chapter 4

Thermodynamic Framework for the Modeling of Solid Materials

4.1. Introduction

This chapter opens the door to thermomechanical modeling of SMA monocrystals, dealt with in Chapter 5, then that of polycrystals, which are the subject of Chapter 7, and finally that of magnetic SMAs (Chapter 9).

It stems from the desire to define a constitutive framework for the modeling of solid materials. The modeling of conventional (and magnetic) shape-memory alloys will be done within the framework thus defined.

Modeling is the art of producing an abstract representation (a mathematical model) of a natural phenomenon (a physical problem) [DUV 84]. Physics is classically regulated by two types of laws:

– conservation laws: these are universal and exact laws, which are valid irrespectively of the medium’s behavior;

– constitutive laws: these seek to describe the response of the medium to given thermomechanical loading (or, for instance, thermo-magneto-mechanical loading for magnetic SMAs). They are approximated laws, determined by the identification of coefficients (e.g. the measurement of the Young’s modulus associated with a uniaxial traction test for a linear elastic solid).

These laws only partially express reality, and lead to uncertainties.

In the case of complex materials and loads, we often need to adapt the model in order to make it correspond as closely as possible to the physical reality. This is the
model-adjustment phase. However, this comes at a price: in terms of the computation time for the structures, but also in terms of readability, the more sophisticated a model becomes.

### 4.2. Conservation laws

These are the:
- mass balance;
- momentum balance;
- first and second principles of thermodynamics;
- diffusion;
- etc.

#### 4.2.1. Concept of a material system

Consider $\omega_0$ to be any “fairly small” subdomain of the domain $\Omega_0$.

At all times, we can match the subdomain $\omega_t$ of $\Omega_t$ such that:

$$\forall \left\{ \begin{array}{l} x \in \omega_0 \\ t > 0 \end{array} \right. y = f(x, t) \in \omega_t$$  \[4.1\]

$$x \left( \begin{array}{c} x_1 \\ x_2 \\ x_3 \end{array} \right)$$  \[4.2\]

$x_i, i = 1, 2, 3, t$ the Lagrange variables:

$$y \left( \begin{array}{c} y_1 \\ y_2 \\ y_3 \end{array} \right)$$  \[4.3\]

$y_i, i = 1, 2, 3, t$ the Euler variables.

The Lagrange variables describe the trajectory over time of a particle located at a point $x$ at time $t_0 = 0$: the conventional origin in time graphs.

The Euler variables, for their part, hold the velocity field to be known at every point in space-time:

$$V = V(y, t)$$  \[4.4\]
4.2.2. Concept of a particulate derivative

Consider $G$ an application which, for the coordinate pair $(y, t)$, matches $G(y, t)$, which can also be written as $G(f(x, t), t)$ or $G(y(t), t)$.

The time derivative is written:

$$
\frac{dG}{dt} = \frac{\partial G}{\partial t} + \sum_{i=1}^{3} \frac{\partial G}{\partial y_i} \frac{dy_i}{dt} = \frac{\partial G}{\partial t} + \nabla_y G \cdot V
$$

This derivative, known as a particulate derivative, represents the unitary variation of $G$ in relation to time as we follow the trajectory of the particulate animated with velocity $V$: we denote it $DG_{Dt}$.

The derivative $\frac{\partial}{\partial t}$ measures the extent of variation at a given point in space.

The result can, naturally, be extended to the vector functions:

$$
\frac{dU}{dt} = \frac{\partial U}{\partial t} + \nabla_y U \cdot V
$$

where:

$$
\nabla_y U = \begin{pmatrix}
U_{1,1} & U_{1,2} & U_{1,3} \\
U_{2,1} & U_{2,2} & U_{2,3} \\
U_{3,1} & U_{3,2} & U_{3,3}
\end{pmatrix}
$$

Derivative of the integral of a scalar function on a domain $\omega_t$, time-dependent:

$$
\frac{d}{dt} \int_{\omega_t} G(y(t), t) \, d\omega_t = \frac{d}{dt} \int_{\omega_0} G(y(t), t) \, d\omega_0 = \int_{\omega_0} \left( \frac{dG}{dt} J + G \frac{dJ}{dt} \right) \, d\omega_0
$$

where:

$$
\frac{dJ}{dt} = (\text{div} V) J
$$

where $J$ constitutes the Jacobian of the transformation.

This gives us:

$$
\frac{d}{dt} \int_{\omega_t} G(y(t), t) \, d\omega_t = \int_{\omega_t} \left( \frac{dG}{dt} + G \text{div} V \right) \, d\omega_t
$$

By introducing the equation:

$$
\text{div}(GV) = V \cdot \text{grad} G + G \text{div} V
$$
we obtain:

\[
\frac{d}{dt} \int_{\omega_t} G(y(t), t)d\omega_t = \int_{\omega_t} \left( \frac{\partial G}{\partial t} + \text{div}(GV) \right)d\omega_t = \int_{\omega_t} \frac{\partial G}{\partial t}d\omega_t + \int_{\partial\omega_t} G(y(t), t)V\cdot\nu dS_t
\]

This derivation can be interpreted as being the sum of a term representing the eigenvariation of \(G\) in relation to time and a flux on the boundary \(\partial\omega_t\) (\(\nu\) the unitary normal on the boundary).

4.2.3. Mass balance

\textit{Lagrange variables}

Consider \(d\omega_0 \rightarrow d\omega_t\); thus \(\rho_0 d\omega_0 = \rho d\omega_t\) where \(d\omega_t = J d\omega_0\)

\(J\) is the Jacobian of the transformation, which gives us:

\[
\rho J = \rho_0 \tag{4.13}
\]

\textit{Euler variables}

Consider \(\rho(y, t)\) the density at point \(y\) at \(t\):

\[
m(t) = \int_{\omega_t} \rho(y, t)d\omega_t
\]

The principle of mass conservation imposes:

\[
\frac{dm(t)}{dt} = 0
\]

meaning that:

\[
\frac{\partial \rho}{\partial t} + \text{div}(\rho V) = 0 \tag{4.14}
\]

or:

\[
\frac{d\rho}{dt} + \rho \text{div} V = 0 \tag{4.15}
\]
This means that an incompressible solid is such that:

\[
div V = 0
\]  

[4.16]

### 4.2.4. Motion balance equation

The fundamental law of dynamics indicates that for a material system \( \omega_t \), if we use the notation \( V(y, t) \) for the velocity field, the time derivative of the momentum torsor is equal to the torsor of external applied forces. This is expressed by:

\[
\frac{d}{dt} \int_{\omega_T} \rho V d\omega_t = \int_{\partial \omega_T} \Sigma \nu dS_t + \int_{\omega_T} \rho f d\omega_t
\]

This gives us:

\[
\int \rho \frac{dV}{dt} d\omega_t = \int_{\omega_T} (div \Sigma + \rho \Sigma) d\omega_t
\]

and finally:

\[
div \Sigma + \rho \Sigma = \rho \gamma
\]

[4.17]

with the acceleration \( \gamma = \frac{dV}{dt} \).

This is the Cauchy equation or dynamic equilibrium equation.
The second equation:

\[
\frac{d}{dt} \int_{\omega_t} \bar{M} \wedge \rho \mathbf{V} dV_t = \int_{\partial \omega_t} \bar{P} \wedge \Sigma \cdot \mathbf{v} dS_t + \int_{\omega_t} \bar{M} \wedge \rho \mathbf{f} d\omega_t \tag{4.18}
\]

can be used to obtain the symmetry of the stress tensor \((\Sigma_{ij} = \Sigma_{ji})\).

### 4.2.5. Energy balance: first law of thermodynamics

For any material system, the time-derivative of the total energy is equal to the power of the external forces increased by the heat input.

To begin with, there is a scalar \(e\), the internal energy per unit mass, such that the total energy is the sum of this internal energy and the mass kinetic energy.

Thus:

\[
\frac{d}{dt} \left[ \int_{\omega_t} \rho e d\omega_t + \frac{\rho V^2}{2} d\omega_t \right] = \int_{\omega_t} W d\omega_t - \int_{\partial \omega_t} \mathbf{q} \cdot \mathbf{V} dS_t + \int_{\omega_t} \rho \mathbf{f} \cdot \mathbf{V} d\omega_t \\
+ \int_{\partial \omega_t} \Sigma \cdot \mathbf{v} dS_t
\]

where \(W\) is an internal heat source and \(\mathbf{q}\) is the heat-flow vector; classically, with the divergence theorem:

\[
\int_{\partial \omega_t} \mathbf{q} \cdot \mathbf{V} dS_t = \int_{\omega_t} \text{div} \mathbf{q} d\omega_t \tag{4.19}
\]

and:

\[
\int_{\partial \omega_t} \Sigma \cdot \mathbf{v} dS_t = \int_{\omega_t} \text{div} (\Sigma \cdot \mathbf{v}) d\omega_t \tag{4.20}
\]

where:

\[
\text{div} (\Sigma \cdot \mathbf{v}) = \Sigma : \dot{\mathbf{E}} + \mathbf{V} \cdot \text{div} \Sigma
\]

and \(\dot{\mathbf{E}}\) is the Eulerian tensor of the strain velocities such that:

\[
\dot{E}_{ij} = \frac{1}{2} \left( \frac{\partial V_i}{\partial y_j} + \frac{\partial V_j}{\partial y_i} \right) \tag{4.22}
\]

Finally, we get:

\[
\rho \frac{de}{dt} = \Sigma : \dot{\mathbf{E}} + W - \text{div} \mathbf{q} \tag{4.23}
\]
4.2.6. Variation of entropy: second law of thermodynamics

There is a function $s$, per unit mass, called entropy, such that, for any material system, the variation in entropy is greater than the integral of the ratio of the heat input divided by the absolute temperature:

$$\frac{d}{dt} \int_{\omega_t} \rho s d\omega_t \geq \int_{\omega_t} \frac{W}{T} d\omega_t - \int_{\omega_t} \frac{q}{T} \nu dS_t$$ \[4.24\]

Alternatively, using the divergence theorem:

$$\int_{\omega_t} \frac{dS}{dt} d\omega_t \geq \int_{\omega_t} \left( \frac{W}{T} - \text{div} \left( \frac{q}{T} \right) \right) d\omega_t$$ \[4.25\]

Given that this is true for all values of $\omega_t$, we have:

$$\rho \frac{ds}{dt} \geq \frac{W}{T} - \text{div} \left( \frac{q}{T} \right)$$ \[4.26\]

Summary:

$$\frac{d\rho}{dt} + \rho \text{div} V = 0 \ (I)$$ \[4.27\]

$$\text{div} \Sigma + \rho f = \rho \gamma \ (II)$$ \[4.28\]

$$\rho \frac{de}{dt} = \Sigma : \dot{E} + W - \text{div} q \ (III)$$ \[4.29\]

$$\rho \frac{ds}{dt} \geq \frac{W}{T} - \text{div} \left( \frac{q}{T} \right) \ (IV)$$ \[4.30\]

4.3. Constitutive laws

Let $y = f(x, t)$

Let $\mathbf{F} = \nabla_x y$

respectively represent the motion law, the geometric transformation gradient and the temperature.

We generally accept the existence of laws called “constitutive laws” linking the stresses, the internal energy, the heat flux and the entropy in the state of transformation.
gradients and temperature at a given time:
\[
\Sigma(t) = \sum_{\tau \leq t} (F(\tau), T(\tau)) \tag{4.31}
\]
\[
e(t) = \sum_{\tau \leq t} E(\tau) (F(\tau), T(\tau)) \tag{4.32}
\]
\[
q(t) = \sum_{\tau \leq t} Q(\tau) (F(\tau), T(\tau)) \tag{4.33}
\]
\[
s(t) = \sum_{\tau \leq t} S(\tau) (F(\tau), T(\tau)) \tag{4.34}
\]

4.3.1. Clausius-Duhem inequality

A question arises: is it possible to choose any values for the functionals \(\Sigma, e, q, s\)?

Suppose we take the rate law \(V\) and the history of the transformation gradients \(F(\tau)\) and temperatures \(T(t)\).

As \(V\) is a known entity, equation [4.27] can be used to discover \(\rho\).

Equation [4.28] is satisfied by choosing the value of \(f\).

Equation [4.29] is satisfied by adopting \(W\).

Equation [4.30] therefore gives us an inequality which must be verified for all the constitutive laws of equation [4.29]. We find the value of \(W\) and then substitute it into equation [4.30], so that:
\[
\rho T \frac{ds}{dt} \geq \rho \frac{de}{dt} - \sum \frac{\dot{E}}{t} + \text{div} q - T \text{div} \left( \frac{q}{T} \right) \tag{4.35}
\]

Noting that \(\text{div} \left( \frac{q}{T} \right) = \frac{1}{T} \text{div} q + q \frac{\text{grad} T}{T}\), we obtain:
\[
\Phi = \rho T \frac{ds}{dt} - \frac{de}{dt} + \sum \frac{\dot{E}}{t} - q \frac{\text{grad} T}{T} \geq 0 \tag{4.36}
\]
which is called the Clausius-Duhem inequality. If we introduce the specific free energy \(\psi\) defined by:
\[
\psi = e - Ts \tag{4.37}
\]
This leads to \(T \frac{ds}{dt} = \frac{de}{dt} = -(\frac{d\psi}{dt} + s \frac{dT}{dt})\):
\[
\rho \frac{de}{dt} = \sum \frac{\dot{E}}{t} + W - \text{div} q \tag{4.38}
\]
We gather the terms together in two types of dissipation, namely:

- the intrinsic dissipation:
\[
\Phi_i = \sum \frac{d\dot{E}}{dt} - \frac{d\psi}{dt} - s \frac{dT}{dt} \tag{4.39}
\]
– the thermal dissipation:

\[
\Phi_{th} = -q \frac{\nabla T}{T} \tag{4.40}
\]

Classically, we make the hypothesis of uncoupling between the two sorts of dissipation (which is absolutely not obligatory), meaning that each of the dissipations separately must verify the inequality:

\[
\left\{ -q \nabla T \geq 0 \\
\Sigma : \frac{dE}{dt} - (\frac{d\psi}{dt} + s \frac{dT}{dt}) \geq 0 \right\} \tag{4.41}
\]

**INTERPRETATION.**

– The first inequality implies that the “heat flux” vector \( q \) must form an obtuse angle with the vector \( \nabla T \). This is satisfied for isotropic materials, which are governed by Fourier’s law:

\[
q = -k \nabla T \tag{4.42}
\]

If the material is not isotropic:

\[
q = -K \nabla T \tag{4.43}
\]

where \( K \) constitutes the \((3 \times 3)\) matrix of calorific diffusivity which must be positive definite.

– The second inequality can be interpreted using the local state method. The local state method postulates that the thermomechanical state of a material medium at a given point and at a given time is entirely defined by the known value, at that time, of a certain number of variables which depend only on the point in question (and on the physical problem at hand). These variables, called state variables, are the observable variables and the internal variables:

– observable variables: the temperature \( T \), the strain tensor \( E \);

– internal variables: for dissipative phenomena, the state at any given moment also depends on the previous history, represented by values at each moment of other variables, called internal variables.

The plasticity and viscoplasticity require the introduction of deformation variables such as the plastic deformation \( E^{pl} \) with:

\[
E = E^{el} + E^{pl} \tag{4.44}
\]

where, in the small deformation hypothesis, \( E^{el} \) is the elastic tensor and \( E^{pl} \) is the plastic or viscoplastic strain tensor.
In order to describe the phase transformation, we need to introduce a deformation associated with the transformation called $E^{tr}$, with:

$$E = E^{el} + E^{tr}$$ \[4.45\]

One or more internal variables will be necessary, e.g. $z$ the volume fraction of martensite in the austenite ($z \in [0, 1]$).

However, there is no objective method to choose the nature of the internal variables which are best adapted for such-and-such a phenomenon: it is the necessity to describe the physics which prevails.

Thus, for phase transformation:

$$\psi = \psi(E^{el} = E - E^{tr}, z, T)$$ \[4.46\]

which shows that:

$$\frac{\partial \psi}{\partial E^{el}} = \frac{\partial \psi}{\partial E} - \frac{\partial \psi}{\partial E^{tr}}$$ \[4.47\]

We use the Clausius-Duhem inequality with:

$$\frac{d\psi}{dt} = \frac{\partial \psi}{\partial E^{el}} \frac{dE^{el}}{dt} + \frac{\partial \psi}{\partial T} \frac{dT}{dt} + \frac{\partial \psi}{\partial z} \frac{dz}{dt}$$ \[4.48\]

$$\left[ - \frac{\partial \psi}{\partial E^{el}} \right] \frac{dE^{el}}{dt} + \Sigma \left( \frac{dE^{tr}}{dt} - \rho(s + \frac{\partial \psi}{\partial T}) \frac{dT}{dt} - \rho \frac{\partial \psi}{\partial z} \frac{dz}{dt} \right)$$ \[4.49\]

A classic hypothesis can be used to independently eliminate certain terms from the inequality. We obtain:

$$\Sigma = \frac{\partial \psi}{\partial E^{el}} - \frac{\partial \psi}{\partial E} - \frac{\partial \psi}{\partial E^{tr}}, s = \frac{\partial \psi}{\partial T}$$ \[4.50\]

If we introduce the variables of “thermodynamic forces” associated with the internal variables, e.g. here:

$$\Pi^f = -\rho \frac{\partial \psi}{\partial z}$$ \[4.51\]

the Clausius-Duhem inequality is reduced to:

$$dD = \Pi^f dz$$ \[4.52\]
We shall see that knowing the specific free energy function $\psi$ and two pseudo-potentials of dissipation $\phi_1$ and $\phi_2$, dependent upon the strain rates of phase transformation and of the kinetics of direct transformation $\text{A} \Rightarrow \text{M}$ and reverse transformation $\text{M} \Rightarrow \text{A}$, is entirely sufficient to determine the pseudo-elastic behavior of the SMA (see the works of J.J. Moreau on convex analysis [MOR 70]).

If for a monocrystal, we choose the fractions of the $n$ martensite variants as internal variables $z_i \ i = 1... n$, then:

$$dD = \sum_{i=1}^{i=n} \Pi_i^f dz_i$$ \ [4.53]

where:

$$\Pi_i^f = -\rho \frac{\partial \psi}{\partial z_i}$$ \ [4.54]
Chapter 5

Use of the “CTM” to Model SMAs

5.1. Introduction

On the basis of the crystallographic theory of martensite (CTM), a number of problems can be viewed in a new light, and sometimes solved.

Obviously, in Chapter 3, the microstructure is described in the absence of external stresses, but these external stresses are the driving forces for the reorientation of martensite plates or the (A → M) (austenite to martensite) phase-change.

Three cases will be solved here:
– the process of reorientation of the martensite variants in a monocrystal;
– the pseudo-elastic behavior of a monocrystal;
– the prediction of the threshold surfaces for the beginning of the phase-change for monocrystals and polycrystals.

For the purposes of these applications, we need to introduce a classic “micro-macro” model. It is a thermodynamic model with \((n + 1)\) internal variables: \(z_0\) is the volume fraction of austenite and \(z_1...z_n\) are the volume fractions of the \(n\) martensite variants.

5.2. Process of reorientation of the martensite variants in a monocrystal

In the existing body of literature, convergent constitutive models (see [BUI 91, LEX 96, PAT 98, SUN 93]) have been developed, in order to integrate the
phase-change induced under stress (austenite $\Rightarrow$ martensite) and the reorientation of the martensite plates in monocrystals in SMAs. The volume fractions of the different martensite variants are chosen as internal variables, in order to describe the evolution of the microstructure. In the context of thermodynamics of irreversible processes (TIP) and a micromechanical behavior homogenization method, the Gibbs free energy is established on the scale of the monocrystal. As happens with plasticity, criteria of phase-change or reorientation and kinetics of transformation are put forward.

In addition, biaxial traction tests on a Cu-Al-Ni monocrystal, causing a transition from one martensite variant to another, were carried out by Chu in his doctoral thesis [CHU 93]. An exploitation of the main experimental results obtained, based on the concept of minimization of energy on a local scale, enabled Abeyaratne et al. [ABE 96] to analyze the kinetics of transition between two martensite variants under biaxial stress.

In this chapter, it is our intention to evaluate the predictive capabilities of the model used as a reference point for the experimental results.

In the first section, we shall briefly outline the foundations of the model. The next section will be given over to describing the testing conditions and the results of the experiment. Finally, in the third section, we shall compare and contrast the experimental results and the model’s predictions.

\[ \text{Figure 5.1. Interface between austenite and two variants } i \text{ and } j \text{ of twinned martensite} \]
5.2.1. Internal variable model of the thermomechanical behavior of an SMA monocystal

As highlighted above, the formulation of the Gibbs free energy, on the macroscopic scale, is long-established and classic. It is the choice of the expression of the interaction energy $\phi_{\text{it}}$ induced by the field of internal stresses which differentiates one “micro-macro” model from another. In addition, an analysis of the overall behavior associated with the movements of the interfaces between the martensite variants can be found in Buisson et al. [BUI 91].

$$\rho G(\Sigma, T, z_0, z_1, \ldots, z_n) = u^a_0 - T s^a_0 - z \Pi^f_0(T) + C_v \left[ (T - T_0) - T \ln \frac{T}{T_0} \right]$$

where in this case:

$$\phi_{\text{it}} = Az_0(1 - z_0) + \frac{1}{2} \sum_{k=0}^{n} \sum_{l=1}^{n} H_{kl} z_k z_l$$

where $l$ is different to $k$ and:

$$z = \sum_{k=1}^{n} z_k = 1 - z_0$$

In these relations, $A$ expresses the interaction between the austenite and the martensite variants, and $H_{kl}$ the interactions between the variants $k$ and $l$ of martensite; $z_0$ is the volume fraction of austenite, $z_k$ the volume fraction of the variant $k$ of martensite ($k = 1, \ldots, n$) and $z$ is the total fraction of martensite; $\rho, C_v, M$ are, respectively, the density, the specific heat and the (fourth-order) compliance tensor, for which identical values are chosen for all phases. $\Pi^f_0(T) = \Delta u - T \Delta s$ where $\Delta u = u^a_0 - u^m_0$, $\Delta s = s^a_0 - s^m_0$ where $u^a_0$, $u^m_0$, $s^a_0$ and $s^m_0$ respectively represent the internal energy and the specific entropy of the austenite and the martensite at the reference temperature $T_0$.

From equation [5.1], we get the total macroscopic deformation $E$:

$$E = -\rho \frac{\partial G}{\partial \Sigma} = \Sigma: \mathbf{E}^{\text{el}} + \sum_{k=0}^{n} z_k \mathbf{E}^k = \mathbf{E}^{\text{el}} + \mathbf{E}^{\text{tr}}$$

where $\mathbf{E}^{\text{tr}}_0 = 0$: the austenite representing the untransformed reference state.

Let $\Pi_k$ be the thermodynamic force associated with the creation (or elimination) of the variant $k$.

By definition:

$$\Pi_k = -\rho \frac{\partial G}{\partial z_k} = \Sigma: \mathbf{E}^{\text{tr}}_k + \Pi^f_0(T) - \frac{\partial \phi_{\text{it}}}{\partial z_k}$$
The Clausius-Duhem inequality is written in the conventional form of the intrinsic dissipation increment $dD$ (see Chapter 4):

$$dD = \sum_{k=0}^{n} \Pi_k dz_k$$  \[5.6\]

Let us now look at the process of reorientation. Suppose that the material initially comprising only the variant $i$ is transformed into the variant $j$. In order to make this assumption, we need to make sure that the variants $i$ and $j$ are compatible, i.e. that they satisfy Hadamard’s formula (compatibility equation at the interface between $i$ and $j$).

In this case, ($i \rightarrow j$) the Clausius-Duhem inequality is reduced to:

$$dD = \Pi_j dz_j + \Pi_i dz_i = \Pi_{ij} dz_j$$  \[5.7\]

where $dz_i = -dz_j$, expressing the fact that $dD$ is not an exact total differential. We have:

$$\Pi_{ij} = \Pi_j - \Pi_i = \Sigma: (E_{ij}^{tr} - E_{ji}^{tr}) - \left( \frac{\partial \phi_{ik}}{\partial z_j} - \frac{\partial \phi_{id}}{\partial z_i} \right)$$  \[5.8\]

where:

$$E_{ij}^{tr} = \frac{1}{2} \Sigma: (U_{ij}^2 - U_{ji}^2) - H_{ji}(1 - 2z_j)$$  \[5.9\]

where:

$$E_k^{tr} = \frac{1}{2} (U_k^2 - 1)$$  \[5.10\]

where $k = (1...n)$.

In these relations, $U_i$ denotes the Bain strain tensors, which depend on the lattice parameters of the austenite and martensite, and therefore on the type of phase-change induced (cubic $\Rightarrow$ trigonal, tetragonal, orthorhombic, monoclinic, etc. – see Chapter 3). $\Pi_{ij}$ represents the thermodynamic force associated with the reorientation of variant $i$ into variant $j$.

We accept that the critical force for the reorientation of variant $i$ into variant $j$ is given by:

$$\Pi_{ij}(z_j = 0) = \frac{1}{2} \Sigma: (U_j^2 - U_i^2) - H_{ji} = \Pi_{cr}^+$$  \[5.11\]

and the reverse transformation $j \rightarrow i$ by:

$$\Pi_{ij}(z_j = 1) = \frac{1}{2} \Sigma: (U_j^2 - U_i^2) - H_{ij} = -\Pi_{cr}^-$$  \[5.12\]

where evidently $H_{ij} = H_{ji}$. 

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In addition, the evolution equation for the reorientation can be written for $i \Rightarrow j$:

$$d\Pi_{ij} = \lambda_1 dz_j (dz_j \geq 0)$$  \[5.13\]

and for $j \Rightarrow i$:

$$d\Pi_{ji} = \lambda_2 dz_j (dz_j \leq 0)$$  \[5.14\]

5.2.2. Experimental procedure and results obtained

The testing machine created by [CHU 93] is a (“dead-load”) biaxial traction machine on which uniform traction forces are applied at the boundary of a square plate of a monocrystalline SMA. The alloy examined by Chu is a Cu–14.0-Al-3.9-Ni (\% wt) and the dimensions of the plate are 22.4 mm side and 0.54 mm thickness. Extreme care was taken when creating the machine so that the traction forces would remain static even if the sample were to spontaneously undergo extensive shearing due to the reorientation of the martensite plates.

The tests were performed at a fixed temperature, lower than $A_0$ (the “austenite start” temperature, i.e. the temperature at which austenite begins to appear, at the stress-free state) so that the sample would remain entirely martensitic throughout all the stages of mechanical loading. The martensite $\gamma_1$ of which the monocrystal is formed is orthorhombic, and may therefore be composed of six variants $U_i$ ($i = 1, \ldots, 6$).

In all the tests carried out by Chu[CHU 93] and analyzed by Abeyaratne et al. [ABE 96], the orientation particular to the martensitic lattice, in reference to the geometric framework of the plate, was chosen such that at most two of the martensite variants, $i$ and $j$, would be present. In general, the normal to the plate is [001] and the normals to the sides of the samples are [110] and [T1] in the framework associated with the austenite ($i_1$, $i_2$, $i_3$). If $x_1$ is the direction of application of $\sigma_1$, we have $\theta_1 = (i_1, x_1) = \pi/4$.

During the application of the strain, the volume fraction of variant $j$, which increases at the expense of the other variant $i$, was measured. When at all times $t$, the Piola-Kirchhoff stresses $\sigma_1(t)$ and $\sigma_2(t)$ were positive, the program of stress application was as follows: $\sigma_1(t)+\sigma_2(t)$ was kept constant and $\sigma_1(t)−\sigma_2(t)$ varied in a “sawtoothed” wave pattern with period $T$.

Because the transformation of one variant into another occurs rapidly, it is reasonable to define “specific stresses for reorientation” for the direct and inverse reorientations by two pairs of $(\sigma_1(t), \sigma_2(t))$ for $z_i = z_j = 0.5$: direct $(\sigma_1 = 4.3$MPa, $\sigma_2 = 6.4$MPa) and inverse $(\sigma_1 = 6.05$MPa, $\sigma_2 = 4.65$MPa) (see Figure 5.2).
Tests with different programs of stress application (e.g. with $\sigma_1$ kept constant and $\sigma_2$ varying periodically) were carried out, and the specific stresses determined. Note from Figure 5.2 that the position of the points in the plane, $(\sigma_1, \sigma_2)$ corresponding to these specific stresses, can be represented by two parallel lines whose slope is equal to 1.

The effect of the orientation was also analyzed. Another sample was tested with the normal to the plate being [001] and $\theta_2 = \theta_1, \phi_1 = \pi/8$. Figure 5.3 shows that the amplitude of the hysteresis is highly sensitive to the crystallographic orientation of the sample in relation to the axes of loading.

5.2.3. Modeling of the experiments

Such modeling was performed for this monocrystalline Cu-Al-Ni alloy by Blanc and Lexcellent ([BLA 03]).

In general, any solid-solid phase transformation is described by $\mathbf{F} = \mathbf{R}\mathbf{U}$ where $\mathbf{R}$ is a rotation matrix and $\mathbf{U} = (\mathbf{F}\mathbf{F}^T)^{1/2}$ characterizes the Bain strain of the lattice during the phase transformation. Because of the symmetries of the phases present,
there are six distinct variants $U_1...U_6$ for the CC $\rightarrow$ orthorhombic transformation. These variants may be linked by the rotations $Q$ which render invariant the austenitic lattice $U_1 = Q^i U_j Q$. In the cubic austenitic base, with the parameters $\alpha, \beta, \gamma$ dependent upon the lattice parameters $a_0$ of the austenite and $a, b, c$ on the orthorhombic martensitic lattice, these variants are written:

$$
\begin{align*}
U_1 &= \begin{pmatrix}
\frac{\alpha + \gamma}{2} & \frac{\alpha - \gamma}{2} & 0 \\
\frac{\alpha - \gamma}{2} & \frac{\alpha + \gamma}{2} & 0 \\
0 & 0 & \beta
\end{pmatrix}, \\
U_2 &= \begin{pmatrix}
\frac{\alpha + \gamma}{2} & \frac{\gamma - \alpha}{2} & 0 \\
\frac{\gamma - \alpha}{2} & \frac{\alpha + \gamma}{2} & 0 \\
0 & 0 & \beta
\end{pmatrix}, \\
U_3 &= \begin{pmatrix}
\frac{\alpha + \gamma}{2} & \frac{\alpha - \gamma}{2} & 0 \\
\frac{\alpha - \gamma}{2} & \beta & 0 \\
0 & 0 & \frac{\alpha + \gamma}{2}
\end{pmatrix}, \\
U_4 &= \begin{pmatrix}
\frac{\alpha + \gamma}{2} & \frac{\gamma - \alpha}{2} & 0 \\
\frac{\gamma - \alpha}{2} & \beta & 0 \\
0 & 0 & \frac{\alpha + \gamma}{2}
\end{pmatrix}, \\
U_5 &= \begin{pmatrix}
\frac{\beta}{2} & 0 & 0 \\
0 & \frac{\alpha + \gamma}{2} & \frac{\alpha - \gamma}{2} \\
0 & \frac{\alpha - \gamma}{2} & \frac{\alpha + \gamma}{2}
\end{pmatrix}, \\
U_6 &= \begin{pmatrix}
\beta & 0 & 0 \\
0 & \frac{\alpha + \gamma}{2} & \frac{\gamma - \alpha}{2} \\
0 & \frac{\gamma - \alpha}{2} & \frac{\alpha + \gamma}{2}
\end{pmatrix}
\end{align*}
$$

[5.15]

where $\alpha = 1.0619$, $\beta = 0.9178$, $\gamma = 1.023$ obtained for Cu-14.2–Al-4.3-Ni (Wt) [OTS 75], i.e. for a composition very similar to that of the alloy under discussion here.

Figure 5.3. Hysteresis loop for two different orientations [ABE 96]
In the initial state, the material is composed entirely of variant 2 \((i = 2)\) [ABE 96], [CHU 93].

Under mechanical stress, variant 2 may give way to variant \(j\) if the compatibility equation between 2 and \(j\) is satisfied; in other words if:

\[
RU_j - U_i = a \otimes n
\]

where \(i = 2\) and \(j = [1,3,4,5,6]\), where \(n\) is the unitary external normal to the interface between variants \(i\) and \(j\) and \(a\) is the shearing at the interface. The calculations show that 2 is compatible with the other five variants. The variant which will appear is that which maximizes \(\Pi_{2j}\), and reorientation will begin when \(\max \Pi_{2j}\) attains the value \(\Pi^\text{cr}_{2j}\), which is a constant in the material. This, and \(\Pi_{21}\), is determined on the basis of the characteristic points (start of transformation 1 \(\rightarrow\) 2 and 2 \(\rightarrow\) 1) on the experimental curves (Figure 5.3).

The external mechanical strains are applied in accordance with \(\hat{x}_1(\sigma_1)\) and \(\hat{x}_2(\sigma_2)\).

From this, we deduce:

\[
\Sigma = \sigma_1 \hat{x}_1 \otimes \hat{x}_1 + \sigma_2 \hat{x}_2 \otimes \hat{x}_2
\]

The thermodynamic forces can be calculated using the formula in equation [5.9]:

\[
\Pi_{21} = \frac{1}{2} (\sigma_1 - \sigma_2)(\alpha^2 - \gamma^2) \sin 2\theta - H_{21}
\]

\[
\Pi_{2j}(j = 3, 4) = \frac{1}{4} [-(\alpha^2 - 2\beta^2 + \gamma^2)(\sigma_2 \cos^2 \theta + \sigma_1 \sin^2 \theta) + 2(\sigma_1 - \sigma_2)(\alpha^2 - \gamma^2) \sin 2\theta] - H_{22}
\]

\[
\Pi_{2j}(j = 5, 6) = \frac{1}{4} [-(\alpha^2 - 2\beta^2 + \gamma^2)(\sigma_1 \cos^2 \theta + \sigma_2 \sin^2 \theta) + 2(\sigma_1 - \sigma_2)(\alpha^2 - \gamma^2) \sin 2\theta] - H_{2j}
\]

where \(H_{2j}\) is identical for any \(j\) (excluding 2).

The calculations show that \(\Pi_{21}\) is far greater than \(\Pi_{2j}, j = [1,3,4,5,6]\) for \(\theta_1 = \pi/8\) (see Figure 5.5) or \(\theta_2 = \pi/4\), with the reversion occurring obviously from 1 to 2 (see Figures 5.4 and 5.5). This confirms the experimental observations [ABE 96], [CHU 93] made on the basis of Figure 5.3.
Figure 5.4. Thermodynamic forces, reorientation of martensite 2 into other variants $\theta = \pi / 4$

Figure 5.5. Thermodynamic forces, reorientation of martensite 2 into other variants $\theta = \pi / 8$
In addition, the term $H_{21}$ can be measured on the experimental curves ($H_{21} = 0.017$ MPa). In all cases, we observe a linear dependence of $z_1 (2 \rightarrow 1)$ or of $z_2 (1 \rightarrow 2)$ with $(\sigma_1 - \sigma_2)$.

In the space $(\sigma_1, \sigma_2)$, the critical stresses of reorientation can be traced with $z_1 = z_2 = 0.5$ (Figure 5.2):

$$(1 \Rightarrow 2) \Pi_{21}(z_1 = 0.5) = \text{Const.} \Rightarrow \sigma_2 = \sigma_1 + C_{21} \quad [5.21]$$

$$ (2 \Rightarrow 1) \Pi_{12}(z_2 = 0.5) = \text{Const.} \Rightarrow \sigma_1 = \sigma_2 + C_{12} \quad [5.22]$$

Finally, the hysteresis loops representing the evolution of $z_1$ with $(\sigma_1 - \sigma_2)$ can be modeled for $\theta_1$ and $\theta_2$ (Figure 5.3). In order to render the simulation less schematic, kinetics that more closely represent the physics of reorientation will be introduced later on.

5.2.4. Conclusion

We have now begun to exploit the potentials of a model with $(n + 1)$ specific internal variables of the mechanical behavior of an SMA monocrystal. Thus, the process of reorientation of one martensite variant into another has been analyzed and the experimental results simulated. Another step, which is more difficult, for the same alloy, is modeling the phase transformation from austenite into martensite. Indeed, the martensite created is constituted by a couple $(i, j)$ of variants interfacing with the parent phase.

The compatibility needs to be examined on two levels – that of the $ij$ interface and that of the austenite with the couple $(i, j)$. Pseudoelastic traction tensile tests on three monocrystals with different orientations, again on the same alloy, were carried out by Shield [2].

Our simulation will be compared with the very different one presented in [STU 02].

5.3. Process of creation of martensite variants in a monocrystal: pseudoelastic behavior

5.3.1. Modeling the pseudoelastic behavior of the monocrystal

The model employed is the micromechanical approach developed in section 5.2.1 with austenite of volume fraction $z_0$ and the $n$ martensite variants of volume fraction $z_n$. Remember that the thermodynamic force $\Pi_k$ associated with the variant $k$ is written:

$$\Pi_k = -\rho \frac{\partial G}{\partial z_k} = \Sigma : E_t^k + \Pi_0(T) - \frac{\partial \phi_{it}}{\partial z_k} \quad [5.23]$$
with the intrinsic dissipation:
\[ dD = \sum_{k=0}^{n} \Pi_k dz_k \] [5.24]

and the stress tensor:
\[ \mathbf{E} = -\rho \frac{\partial G}{\partial \Sigma} = \Sigma + \sum_{k=0}^{n} z_k \mathbf{E}_{tr} = \mathbf{E}^{el} + \mathbf{E}^{tr} \] [5.25]

As explained in the previous chapter, only the transformation from the cubic parent phase \( \beta_1 \) into the orthorhombic phase \( \gamma_1 \) is taken into account; it is assumed that the other phase transformations do not take place. The initially monophase austenitic material is transformed under mechanical loading into a “twinned” martensite which consists of a very fine lattice of two martensite variants \( i \) and \( j \) against the austenite (Figure 5.1).

The crystallographic data show that the twinning equation between two martensite variants \( i \) and \( j \) is satisfied, as is that between the austenite \( A \) and the couple \( (M_i, M_j) \)
and with \( \lambda \) the volumetric ratio of variant \( i \) and \( (1 - \lambda) \) the volumetric ratio of variant \( j \).

We can write:
\[ z_i = \lambda z_m , z_j = (1 - \lambda) z_m \] [5.26]

Note that \( z_m = z_i + z_j \ldots z_m \) is the total fraction of martensite. Consider the thermodynamic force \( \Pi_{A/M} \) to be:
\[ \Pi_{A/M} = \lambda \Pi_i + (1 - \lambda) \Pi_j = \Sigma: \mathbf{E}_{tr} + \Pi_0(T) = \left[ \lambda \frac{\partial \phi_{it}}{\partial z_i} - (1 - \lambda) \frac{\partial \phi_{it}}{\partial z_j} \right] \] [5.27]

where, in line with the small strain theory:
\[ \mathbf{E}_{tr} = \frac{1}{2} (\mathbf{b} \otimes \mathbf{m} + \mathbf{m} \otimes \mathbf{b}) \] [5.28]
for the phase transformation, we assume that:
\[ \phi_{it} = A z_m (1 - z_m) \] [5.29]

Thus:
\[ \Pi_{A/M} = \Sigma: \mathbf{E}_{tr} + \Pi_0(T) - A(1 - 2z_m) \] [5.30]
If $\Pi_{cr}$ is the critical force of initiation of $A \rightarrow (Mi, Mf)$ then:

$$\Pi_{A/M}(z_m = 0) = \sum^{AM}_m \mathbf{F}^{tr}_{lm} + \Pi_{f}^{ij}(T) - A(T) = \Pi_{cr}^{+} \geq 0$$ \[5.31\]

Coupled with a complete phase transformation, the reverse transformation is expressed by:

$$\Pi_{M/A}(z_m = 1) = \sum^{MA}_m \mathbf{F}^{tr}_{lm} + \Pi_{f}^{ij}(T) + A(T) = \Pi_{cr}^{-} \leq 0$$ \[5.32\]

5.3.2. Traction curves

Simple traction tests have been performed by Shield [SHI 95] on three samples of monocrystalline Cu 13.95 (\% Wt) – Al 3.93 (\% Wt) – Ni with their crystallographic orientations measured (Figure 5.6). The results associated with the simple traction applied at $T_o = 313$ K are thus analyzed.

![Figure 5.6. Traction in Cu-Al-Ni monocrystals for three different orientations [SHI 95]](image)

The transformation in question is cubic-orthorhombic (see section 5.1) with six Bain matrices ($U_1, \ldots, U_6$). The lattice parameters used were measured by Otsuka and Shimizu [OTS 75] on Cu 14.2 (\% Wt) – Al 4.3 (\% Wt)–Ni (which constitutes a slightly different composition of the alloy to that used in Shield’s samples).

The couples $(i, j)$ obtained by calculation under traction and under compression are listed in Table 5.1. A characteristic angle between the direction of traction (or compression) and the $A/M$ interface was chosen. The comparison between the angles measured by Shield and the calculated values validated the CTM approach employed by Blanc and Lexcellent [BLA 04].
Use of the “CTM” to Model SMAs

Table 5.1. Comparison between the “twin” solutions by simulation under traction and compression [BLA 04] with those measured by Shield [SHI 95]

<table>
<thead>
<tr>
<th>Specimen</th>
<th>J</th>
<th>Type</th>
<th>Measured angle (a)</th>
<th>Predicted angle (b)</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Traction</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>E1</td>
<td>3</td>
<td>I</td>
<td>0.3008</td>
<td>46.8</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>I</td>
<td>0.3008</td>
<td>46.8</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>II</td>
<td>0.3008</td>
<td>46.8</td>
</tr>
<tr>
<td></td>
<td>3</td>
<td>II</td>
<td>0.3008</td>
<td>46.8</td>
</tr>
<tr>
<td>E2</td>
<td>6</td>
<td>II</td>
<td>0.3008</td>
<td>21.4</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>II</td>
<td>0.6992</td>
<td>21.4</td>
</tr>
<tr>
<td>E3</td>
<td>6</td>
<td>II</td>
<td>0.3008</td>
<td>9.8</td>
</tr>
<tr>
<td></td>
<td>6</td>
<td>II</td>
<td>0.6992</td>
<td>9.8</td>
</tr>
</tbody>
</table>

| **Compression** |    |      |                   |                   |
| E1           | 5 | II   | 0.3008            | 50.59             |
|              | 6 | II   | 0.3008            | 50.59             |
| E2           | 4 | II   | 0.3008            | 82.68             |
|              | 5 | II   | 0.6992            | 82.68             |
| E3           | 4 | II   | 0.3008            | 67.14             |
|              | 5 | II   | 0.3008            | 62.207            |
|              | 5 | II   | 0.6992            | 67.15             |
|              | 5 | II   | 0.3008            | 46.51             |

For these uniaxial tests, our model is able to calculate the deformation associated with the complete phase transformation and the stress thresholds for transformation \( \sigma^{AM} \) and \( \sigma^{MA} \). The Young’s moduli are given by Shield.

In our model, if we make the hypothesis that \( \Pi_{\sigma} = \Pi_{\sigma} = 0 \), the measurements of the \( \sigma^{AM}(T_0) \) for the three samples enable us to obtain the following parameters:

\[
\Pi_0^f(T_0) = -4.523 \text{ MJ/m}^3, \quad A(T_0) = 0.089 \text{ MJ/m}^3
\]

In Figure 5.7, we show our results [BLA 04] and those obtained by Stupkiewicz and Petryk [STU 02].

Stupkiewicz and Petryk constructed a micromechanical model more sophisticated than our one, with particular attention paid to the different elastic anisotropy between the two phases and the redistribution of the associated internal stresses.

The difference between traction and compression in terms of the level of stress is less pronounced than in our investigation.
5.4. Prediction of the surfaces for the austenite → martensite phase transformation

5.4.1. Case of a monocrystal

On a monocrystalline plate of Cu-Zn-Al, biaxial traction tests were performed by Vivet and Lexcellent [VIV 01]. The optical system comprises a microscope and a CCD camera with a data acquisition system. The surface of the start of the phase transformation is detected experimentally and predicted theoretically. Thus, as can be seen in Figure 5.8, the surface is divided into a series of sectors. Each sector represents an activated variant. On the boundary between two sectors, the two variants corresponding to the two sectors may be activated. As Figure 5.8 shows, the boundary curve resembles a deformed Tresca curve. Its geometric shape is entirely dependent upon the crystallographic orientation of the plate.

Thus, for any imposed direction of the stress vector, the martensite variant activated is that which gives the greatest deformation of transformation in the direction of the stress, because the associated stress of phase transformation is lesser (in reference to equation [5.33]).

For radial loading, a cubic crystal of austenite is subjected only to a normal strain $\Sigma_{nn}$ in the direction $\hat{n}$ (from the geometric framework $R$ of the sample).
The phase transformation start criterion is regulated by:

$$\Sigma_{nn}(\text{threshold}) = \frac{K(T)}{\max_i(\varepsilon_{tr}^i)_{nn}}$$  \[5.33\]

where obviously:

$$(\varepsilon_{tr}^i)_{nn} = n_i \varepsilon_{tr}^i n$$  \[5.34\]

and:

$$\varepsilon_{tr} = R^T \varepsilon_{tr} R$$  \[5.35\]

$R$ is the rotation matrix defined by the Euler angles $\Phi, \Theta, \psi$ which are used to describe the orientation of a grain ($\Phi, \Theta, \psi$ varying from 0 to $2\pi$):

$$R = \begin{pmatrix}
\cos \Phi \cos \Theta - \sin \Phi \sin \Theta \cos \psi & \sin \Phi \cos \Theta + \sin \Phi \cos \Theta \cos \psi & \sin \Phi \sin \psi \\
-\sin \Phi \cos \Theta - \sin \Phi \cos \Theta \cos \psi & -\sin \Phi \cos \Theta + \sin \Phi \cos \Theta \cos \psi & \cos \Phi \sin \psi \\
-\sin \Theta \sin \Psi & -\cos \Theta \sin \Psi & \cos \Psi
\end{pmatrix}$$  \[5.36\]

It is reasonably simple to calculate the surface of the start of the phase transformation. Under a condition of radial loading, the intensity of this loading is increased until one possible variant out of the twelve satisfies the criterion defined in equation [5.33], and so on for another direction of strain application (see Figure 5.8).
Very recently, Laverhne-Taillard et al. [LAV 11] have used a rather similar procedure to predict the threshold surfaces of NiTi monocrystals (cubic to monoclinic phase transformation II), subjected to biaxial strains.

5.4.2. Case of a polycrystal

The procedure used to calculate the threshold surfaces of the polycrystal is purely phenomenological, and is adapted from a publication by Huang [HUA 99]:

– a polycrystal is considered to be an aggregate of \( n \) grains (\( n \) is chosen as 100) defined by their crystallographic orientation. Here, an isotropic texture which is represented by a random distribution of crystallographic orientations, in the Euler angles space, is chosen. Evidently, the number \( m \) of possible variants \( U_1 \) is equal to 12 (for a cubic \( \rightarrow \) monoclinic transformation). The interactions between the grains are not taken into account, which is a strong hypothesis but is acceptable in order to obtain the surface representing the appearance of the martensite plates;

– for a given direction of mechanical strain represented by \( \Sigma_0 \), for each grain \( k \) and of the \( m \) possible variants, that which represents the greatest factor \( K \) (see equation [5.33]) is selected. Remember that this variant is the one which represents the greatest deformation of transformation, along the direction of the applied stress, which is equivalent to the smallest transformation stress. A set of \( n \) factors \( K_{k}^{\text{max}} \) is thus determined;

– a new set of \( K_{k}^{\text{max}} \) may be determined for uniaxial traction, called \( K_{\text{traction},k}^{\text{max}} \);

– a ratio \( \lambda_0 \) and the tensor of the stress threshold for transformation \( \Sigma_{\text{tr}} \) may be obtained:

\[
\lambda_0 = \frac{\sum_{k=1..n} K_{k}^{\text{max}}}{\sum_{k=1..n} K_{\text{traction},k}^{\text{max}}} ; \Sigma_{\text{tr}} = \frac{1}{\lambda_0} \Sigma_0 \quad [5.37]
\]

– a new direction of loading is applied and the new tensor of the stress thresholds is obtained, and so on.

This is a simple process of homogenization and the results obtained are indeed representative of the measurements carried out on a Cu-Al-Zn polycrystal (see Figure 5.9) and a Cu-Al-Be (see Figure 5.10).

Another technique based on a self-consistent approach gives isodeformation surfaces for isotropic or textured Cu-Zn-Al polycrystals (Aleong et al. [ALE 02]) (Figure 5.11).
**Figure 5.9.** Criterion surface for phase transformation simulated in the space \((\Sigma_1, \Sigma_2)\): Austenite \(\Rightarrow\) non-twinned martensite [LEX 02, LEX 04]

**Figure 5.10.** Criterion surface for phase transformation simulated in the space \((\Sigma_1, \Sigma_2)\): Austenite \(\Rightarrow\) non-twinned martensite [LEX 04]
Figure 5.11. Isodeformation surface. Left: isotropic texture; right: stretched texture [ALE 02]

Figure 5.12. Criterion surface for phase transformation simulated in the space $\left(\Sigma_1, \Sigma_2\right)$: Austenite $\rightarrow$ twinned martensite [LEX 04]
As usual, the polycrystals are represented by aggregates of $n$ grains ($n = 1000$ in this particular case). The self-consistent method offers a direct solution to the overall problem. This is done by adding the effects of each grain individually.

In order to do so, each grain is considered to be encapsulated in an equivalent medium, which has the property of all the embedded grains. In addition, the grains are considered to be spherical in order to simplify the calculation. By this method, a problem with $n$ inclusions is transformed into $n$ problems with one inclusion each. As before, all interaction between neighboring grains is ignored. Finally, there is no difficulty in taking account of any initial texture [ALE 02]. We shall now close this chapter with a calculation of the elastic domain for a Cu-Al-Ni alloy with an interface between the austenite and a couple of martensite variants ($M_i$, $M_j$) (Figure 5.12).
Chapter 6

Phenomenological and Statistical Approaches for SMAs

6.1. Introduction

As previously mentioned, SMAs are characterized by solid-to-solid displacive transformations between austenite and the martensite variants or between these variants themselves, in response to mechanical loading, thermal loading, electromagnetic loading (the case of magnetic SMAs will be dealt with specifically in Chapter 9) or possibly even ultrasonic loading.

This lends these materials the capacity to retain or recover deformations of up to 10%; this property makes them unique actuators and potential sensors in adaptive systems.

The inherent thermomechanical (magnetic) couplings and their hysteretic responses associated with phase transformation thus pose significant challenges in terms of the modeling which needs to be carried out in order to fully exploit the transduction capacities of these alloys.

NOTE.— The work of Ralph C. Smith (Smart Material systems: Model Development – SIAM – Frontiers in Applied Mathematics, Chapter 5, 2005 [SMI 05]) has been essential with regard the writing of this chapter. SIAM has kindly given us permission to use Figures 5.13, 5.14, 5.17 and 5.18 (respectively 6.7, 6.9, 6.8 and 6.12 in our chapter) from their publication Smart Material Systems: Model Development with “Copyright© 2005 Society for Industrial and Applied Mathematics. Reprinted with permission. All rights reserved” for these figures.
The macroscopic models are based on the concept of REV (representative elementary volume), which is linked to the local state method (detailed in Chapter 4). This constitutive framework includes a wide range of models, stemming from the thermodynamics of irreversible processes, in addition to the phenomenological Preisach models.

Let us begin by examining Preisach models.

6.2. Preisach models

As will be explained later on, Preisach models have the advantage of a “mature” mathematical structure; also, it is unsurprising that many researchers have used them for applications on SMAs. A non-exhaustive list might include the works of Gorbet, Wang and Morris [GOR 98], Huo, Ktena et al. [HUO 89], Lagoudas and Bhattacharya [LAG 97] and Webb, Kurdila and Lagoudas [WEB 00].

The idea of using the Preisach representations for the hysteretic stress/strain curves originates with Everett and Whitton [EVE 52], but the main developments were made for SMAs by Ortin [ORT 91][ORT 92]. He chose the Mayergoyz formulation [MAY 86] of the Preisach model [PRE 35] and adapted it to the problem of phase transformation induced under stress. The control parameter (intensive variable) is the traction stress \( \Sigma \) and the output variable (extensive variable) is the resulting deformation \( E(t) \). The elementary hysteresis operator \( \gamma_{\alpha\beta} \) is defined in Figure 6.1.

\[ E(t) = \int_{\alpha \geq \beta} \mu(\alpha, \beta) [\gamma_{\alpha\beta} \Sigma(t)] d\alpha d\beta \]  

[6.1]
This equation represents the Preisach model for hysteresis. The function \( \mu(\alpha, \beta) \) represents the population of elementary operators with the commutable values \( \alpha \) and \( \beta \).

In reference to Figure 6.1, it should be noted that \( [\gamma_{\alpha \beta}\Sigma(t)] \) can only take a value of 0 or 1; thus, equation [6.1] is reduced to:

\[
E(t) = \int_{S^+(t)} \mu(\alpha, \beta)d\alpha d\beta
\]

where \( S^+(t) \) is the region (in the triangular support \( \alpha \geq \beta \)) containing all the points \( (\alpha, \beta) \) of the elementary operators in state +1 at time \( t \), and only at these points.

\[\text{Figure 6.2. Left: determination of } E_\alpha \text{and } E_{\alpha \beta} \text{for the first-order inverse transformation. Right: triangular support of the integration associated with } F(\alpha, \beta) \text{ [ORT 92]}\]

The population \( \mu(\alpha, \beta) \) of the elementary operators can be evaluated with a limited set of experimental data. In order to validate this proposal, let us consider the path constituted by a branch of increasing mechanical loading up to a value \( \Sigma(t) \), followed by a release of this loading. Figure 6.2 illustrates this path and how to determine the deformations \( E_\alpha \) and \( E_{\alpha \beta} \) which, in terms of a Preisach model, are written:

\[
E_\alpha = \int_{a \geq b \geq 0} \mu(a, b)dadb
\]

\[
E_{\alpha \beta} = \int_{a \geq b \geq 0} \mu(a, b)dadb - \int_{a \geq b \geq \beta} \mu(a, b)dadb
\]
From these two values, we can construct the function:

\[ F(\alpha, \beta) = E_\alpha - E_{\alpha\beta} \]  \[6.5\]

which, according to equations [6.3] and [6.4], gives us:

\[ F(\alpha, \beta) = \int_\alpha^\beta \mu(a, b) db = \int_\beta^\alpha da \int_\beta^a \mu(a, b) db \]  \[6.6\]

It is easy to show that:

\[ \mu(\alpha, \beta) = -\frac{\partial^2 F(\alpha, \beta)}{\partial \alpha \partial \beta} \]  \[6.7\]

Thus, the population \( \mu(\alpha, \beta) \) of elementary operators can be computed on the basis of \( F(\alpha, \beta) \) which, in turn, can be obtained by a collection of first-order “reversible” paths.

This Preisach approach yields a good description of the internal loops in the pseudo-elastic external loop, and is able to fully take account of the memory points (the points where the mechanical deformation is reversed). (See Figures 6.3 to 6.6)

Figure 6.3. Diagrammatic representation of the ascending branch A and its corresponding line \( S^+ \) defining the domain of integration \( \mu(\alpha, \beta) \) [ORT 92]

Although the physics of the martensitic transformation is not taken into account, this model is very useful for commanding or controlling SMA-based adaptive systems (partial loading or partial unloading, etc.).

6.3. First-order phase transitions and Falk’s model

6.3.1. Falk's model

The earliest models in the context of thermodynamics of irreversible processes (TIP) were put forward by Falk between 1980 and 1983 [FAL 80, FAL 83].
This theory is based on the Landau-Devonshire theory for ferroelectric and ferromagnetic compounds.

The discussion is based, primarily, on the construction of different Helmholtz free energies $\psi(\varepsilon, T)$, where $\varepsilon$ represents the uniaxial shear stress with an equilibrium value $\varepsilon = 0$ for austenite and $\varepsilon = \varepsilon_T$ for martensite, in the non-stressed state.

The Gibbs free energy is naturally defined by:

$$G(\varepsilon, T) = \psi(\varepsilon, T) - \sigma \varepsilon$$

[6.8]
Falk introduced $\psi$ as an even-power polynomial of $\varepsilon$, in the form:

$$\psi(\varepsilon, T) = \psi_0(T) + \alpha_1(T - T_0)\varepsilon^2 - \alpha_2\varepsilon^4 + \alpha_3\varepsilon^6$$  \[6.9\]

Here, $\alpha_1, \alpha_2, \alpha_3$ are positive constants and $T_0$ the Curie temperature.

A classic representation of $\psi_0(T)$ is:

$$\psi_0(T) = -Ts$$  \[6.10\]

where:

$$s = c\rho ln\left(\frac{T}{T_R}\right) + \eta$$  \[6.11\]

denotes the specific entropy, $\eta$ is a constant, $\rho$ the density, $T_R$ a reference temperature and $c$ the specific heat.

Secondly, the necessary equilibrium condition is expressed by:

$$\frac{\partial G}{\partial \varepsilon} = 0 \iff \sigma = \frac{\partial \psi}{\partial \varepsilon}$$  \[6.12\]

This naturally leads us to the constitutive law:

$$\sigma = \sigma(\varepsilon, T) = 2\alpha_1(T - T_0)\varepsilon - 4\alpha_2\varepsilon^3 + 6\alpha_3\varepsilon^5$$  \[6.13\]
In order to incorporate the non-local effects such as the interfacial energies, Falk added a squared strain gradient term of \(x\), at the initial free energy \(\psi\):

\[
\tilde{\psi}(\varepsilon, \varepsilon_x, T) = \psi(\varepsilon, T) + \frac{\gamma}{2} (\varepsilon_x)^2 \tag{[6.14]}
\]

where:

\[
\varepsilon_x = \frac{\partial \varepsilon}{\partial x} \tag{[6.15]}
\]

We shall illustrate this reasoning by introducing a partial differential equation quantifying the longitudinal movement of an SMA bar, of length \(l\) and cross-section \(A\) which is subjected to a linear density of force \(f(t, x)\). Note that \(u\) and \(\varepsilon\) are linked by:

\[
\varepsilon(t, x) = \frac{\partial u}{\partial x}(t, x) = u_x \tag{[6.16]}
\]

The total energy of the system at time \(t\) is given by:

\[
U(t) = A \int_0^l \rho \left[ \psi(\varepsilon(t, x), T) \frac{\gamma}{2} (\varepsilon_x)^2 - \rho u(t, x) f(t, x) \right] dx \tag{[6.17]}
\]

and the kinetic energy is written:

\[
K(t) = A \int_0^l \frac{\rho}{2} u_x^2(t, x) dx \tag{[6.18]}
\]

The application of Hamilton’s principle with the Lagrange operator \(L = U - K\) yields the partial differential equation:

\[
\rho u_{tt} - \frac{\partial}{\partial x} \left( \frac{\partial \psi(\varepsilon, T)}{\partial \varepsilon} \right) + \gamma u_{xxxx} = \rho f(t, x) \tag{[6.19]}
\]

or in partial differentials of \(u(t, x)\):

\[
\rho u_{tt} - (2\alpha_1(T - T_0) - 12\alpha_2(u_x)^2 + 30\alpha_3(u_x)^4)u_{xx} + \gamma u_{xxxx} = \rho f(t, x) \tag{[6.20]}
\]
6.3.2. Extension of Falk’s model

In order to refine the system, we can take higher-order polynomials, using the same procedure.

For instance, Massad and Smith [MAS 03] chose:

$$\psi(\varepsilon, T) = \psi_0(T) + \alpha_1(T - T_0)\varepsilon^2 - \alpha_2 \varepsilon^4 + \sum_{j=3}^{m} \alpha_j \varepsilon^{2j}$$  \[6.21\]

where $m = 4$ and 5.

As an extension, we can also choose quadratic polynomials, by domains of existence, for the expression of the free energy $\psi(\varepsilon, T)$, i.e.:

- for $\varepsilon \leq -\varepsilon_M(T)$:
  $$\psi(\varepsilon, T) = \frac{E_M}{2} (\varepsilon + \varepsilon_T)^2$$  \[6.22\]

- for $-\varepsilon_M(T) < \varepsilon \leq -\varepsilon_A(T)$:
  $$\psi(\varepsilon, T) = -\frac{E_0(T)}{2} (\varepsilon + \varepsilon_0(T))^2 + \psi_0(T)$$  \[6.23\]

- for $|\varepsilon| < \varepsilon_A(T)$:
  $$\psi(\varepsilon, T) = \frac{E_A}{2} \varepsilon^2 + \Delta \beta(T)$$  \[6.24\]

- for $\varepsilon_A(T) < \varepsilon \leq \varepsilon_M(T)$:
  $$\psi(\varepsilon, T) = -\frac{E_0(T)}{2} (\varepsilon - \varepsilon_0(T))^2 + \psi_0(T)$$  \[6.25\]

- for $\varepsilon \geq \varepsilon_M(T)$:
  $$\psi(\varepsilon, T) = \frac{E_M}{2} (\varepsilon - \varepsilon_T)^2$$  \[6.26\]

where $E_A$ and $E_M$ are the Young’s moduli for the austenite and martensite.

As shown in Figure 6.7, the free energy $\psi(\varepsilon, T)$, thus defined “by parts”, is non-convex overall. The points of inflection $\pm \varepsilon_M(T)$ and $\pm \varepsilon_A(T)$ delimit the transition from the convex regions (which represent stable phases) to concave regions (which represent unstable phases). The maxima of the concave parabolas are located at points $(\pm \varepsilon_0(T), \psi_0(T))$, and $E_0(T)$ is chosen to ensure the continuity $C^1$. 

The austenitic minimum is situated at the height \( \Delta \beta(T) \), where:

\[
\Delta \beta(T) = \beta_A(T) - \beta_M(T)
\]

[6.27]

where:

\[
\beta_\alpha(T) = C_\alpha(T - T_R) + u_\alpha - TS_\alpha
\]

[6.28]

represents the chemical part of the energy and \( \alpha = A, M^+, M^- \).

Here, \( C_\alpha, \rho_\alpha, u_\alpha, T_R \) represent the specific heat, the density, the intrinsic free energy of each phase, and the temperature in the reference state. These data are used to calculated the energies. In addition:

\[
S_\alpha = C_\alpha \rho_\alpha \ln \left( \frac{T}{T_R} \right) + \eta_\alpha
\]

[6.29]

constitute the specific entropies and \( \eta_\alpha \) entropic constants dependent upon the state of phase.

Note that the term \( TS_\alpha \) is none other than the average term \( \psi_0(T) = -TS \) employed by Falk in his polynomial distribution (equation [6.21]).

In summary, this is the free energy of three phases \( A, M^+, M^- \); often used in the existing literature, particularly by Seelecke [SEE 02], Seelecke and Heintze [SEE 11a], Seelecke and Kastner [SEE 11b] and Seelecke and Muller [SEE 04]. (See Figure 6.8)

### 6.3.3. Description of hysteresis loops

Depending on the testing temperature chosen and the intensity of the mechanical loading, the behavior of the material will differ.
The behavior of an SMA in temperature intervals delimited by transition temperatures $T_0 < T_C < T_1 < T_2$ can be summarized as follows:

- for $T < T_0$: the material is purely in the martensitic state and exhibits a ferroelastic behavior such as a simple memory effect, i.e. the reorientation of $M^+$ into $M^-$ (or vice versa);

- for $T_0 < T < T_1$: the austenitic phase nucleates at $T = T_0$ and is metastable for $T_0 < T < T_C$ and absolutely stable at $T_C < T < T_1$. Thus, the Curie temperature $T_C$ delimits the zone of transition from absolute stability of martensite to absolute stability of austenite;

- for $T_1 < T < T_2$: the austenite is only present at the stress-free state, but martensite variants may be induced with sufficient stresses. The behavior of the material is pseudo-elastic;

- for $T \geq T_2$: the material has a purely elastic (or elastoplastic) behavior of the austenite.

For temperatures varying within the intervals thus defined, the Helmholtz free energy and the $\sigma - \epsilon$ relation dictated by the condition $\sigma = \frac{\partial \psi}{\partial \epsilon}$ resulting from the minimization of $G(\epsilon, T) = \psi(\epsilon, T) - \sigma \epsilon$ are given in Figure 6.9.

Because the model takes no account of either the thermal effects or the inhomogeneities of the materials, the phase transformations are instantaneous, so $A_0 = A_F = T_1$ and $M_0 = M_F = T_0$ correspond to the stress-free state.

This first approach correctly represents the behavior of an SMA monocrystal, on condition that the skewness between the traction and compression is not taken into account (i.e. we do not content ourselves with a free energy that is symmetrical in $\epsilon$).

### 6.3.4. Phase domains with moving boundaries

The theory of “phase domains with moving boundaries or walls” is the second unified theory associated with ferroelectrical materials. This theory was put forward...
Phenomenological and Statistical Approaches for SMAs


Figure 6.9. Helmholtz energy and stress-strain relations

6.3.4.1. Development of the model

The theory of phase domains with moving boundaries or walls is based on the quantification of the energy dissipated when the boundaries shift. In SMAs, the domains are made up of segregated martensite and also martensite variants, and the elimination or reorientation of the domains is quantified by the elastic energy.

The model comprises three components:

– anelastic strains $\varepsilon_{an}$;
– irreversible strains due to the shifting of the walls $\varepsilon_{irr}$;
– reversible strains due to the bending of the walls $\varepsilon_{rev}$.

Thus, surreptitiously, internal variables are introduced, in order to take account of the hardening of the $\sigma \leftrightarrow \varepsilon$ curves during the phase transformation or the reorientation of the martensite variants.
6.3.4.2. Equilibrium deformations

Equilibrium deformations $\varepsilon_{an}$ minimize the Gibbs free energy:

$$G(\sigma, \varepsilon, T) = \psi(\varepsilon, T) - \sigma \varepsilon$$ [6.30]

where $\sigma_e$ is the effective stress defined by:

$$\sigma_e = \sigma + \sigma_I$$ [6.31]

$\sigma$ applied stress, $\sigma_I$ interaction stress.

In order to introduce the general interactions, we consider the effective stress in the form:

$$\sigma_e = \sigma + \alpha \varepsilon$$ [6.32]

where $\alpha$ is a constant.

The necessary equilibrium condition $\frac{dG}{d\varepsilon} = 0$ yields the following relation:

$$\sigma_e = \sigma(\varepsilon_{an}, T) = 2\alpha_1(T - T_0)\varepsilon_{an} - 4\alpha_2\varepsilon_{an}^3 + \sum_{j=3}^{m} 2j\alpha_j\varepsilon_{an}^{2j-1}$$ [6.33]

which, implicitly, quantifies the behavior of $\varepsilon_{an} : \varepsilon_{an} = \varepsilon_{an}(\sigma_e, T)$.

6.3.4.3. Irreversible deformations

The second component is the irreversible deformation which accompanies the shifting of the walls. Using the expression of the elastic energy:

$$U = \int \sigma_e(\varepsilon)d\varepsilon$$ [6.34]

in order to quantify the amount of work required for reorientation of the martensite variants and phase transformation, Massad and Smith [MAS 03] show that $\varepsilon_{ir}$ can be written in the form:

$$\varepsilon_{ir} = \varepsilon_{an} - \delta k_p \frac{d\varepsilon_{ir}}{d\sigma_e}$$ [6.35]

where $k_p$ is a constant of the material, $\delta = \text{sgn}(d\sigma)$ ensures that the energy required to break the anchoring sites is opposite to the change in stress. The calculations give:

$$\frac{d\varepsilon_{ir}}{d\sigma} = \frac{\varepsilon_{an}(\sigma_e) - \varepsilon_{ir}(\sigma)}{\delta k_p + \alpha(\varepsilon_{an}(\sigma_e) - \varepsilon_{ir}(\sigma))}$$ [6.36]
Here, $\delta = 1$ for all values $(\sigma, \varepsilon)$ which are located outside of the region bounded by the equilibrium curve $(\sigma, \varepsilon_{an})$, and $\delta = 0$ otherwise.

6.3.4.4. Reversible deformations

The reversible deformations are given by:

$$\varepsilon_{rev} = C(\varepsilon_{an} - \varepsilon_{irr})$$  \[6.37\]

where the constant $C$ quantifies the degree of reversibility and is necessarily situated in the interval $[0, 1]$.

6.3.4.5. Total deformations

The total macroscopic deformations are given by:

$$\varepsilon = \varepsilon_{irr} + \varepsilon_{rev} = (1 - C)\varepsilon_{irr} + \varepsilon_{an}$$  \[6.38\]

6.3.5. Properties of the model and validation

These can be found in [MAS 03].

6.3.5.1. Properties of the model

The $\sigma \leftrightarrow \varepsilon$ curves are given for four temperatures (a) $T = 273$ K, (b) $T = 283$ K, (c) $T = 291$ K and (d) $T = 298$ K in Figure 6.10.

The simulation parameters are:

$$T_0 = 273 \text{ K}, \quad k_p = 10 \text{ MJ/Km}^3, \quad \alpha = 7 \times 10^3 \text{ MPa}, \quad \alpha_1 = 0.638 \times 10^3 \text{ MPa/K}, \quad \alpha_2 = 4.908 \times 10^6 \text{ MPa}, \quad \alpha_3 = 6.108 \times 10^8 \text{ MPa} \quad \text{and} \quad C = 0.5.$$

6.3.5.2. Experimental validation

The model’s performances, in terms of characterizing the external and internal loops of the pseudo-elastic behavior of NiTi, are illustrated in Figure 6.11.

The data given by Bundara et al. correspond to traction tests on polycrystalline wires of Ni-55\%at.Ti [BUN 00]. In order to minimize the effects of aging and of training, stabilized hysteresis loops were measured after 22 cycles at 295 K. Following the external loop, the internal loops were generated by partial loading followed by cycles of complete unloading.

The Curie temperature of this material is $T_0 = 288$ K, and the least squares method can be used to adjust the value of the parameters:

$$k_p = 29.39 \text{ MJ/Km}^3, \quad C = 0.9, \quad \alpha = 698.8 \text{ MPa}, \quad \alpha_1 = 8.43 \times 10^3 \text{ MPa/K}, \quad \alpha_2 = 1.059 \times 10^8 \text{ MPa}, \quad \alpha_3 = 8/775 \times 10^{10} \text{ MPa}, \quad \alpha_4 = -3.224 \times 10^3 \text{ MPa} \quad \text{and} \quad \alpha_5 = 4.465 \times 10^{15} \text{ MPa} \quad \text{and} \quad \text{the model is indeed representative of the experiment.}$$
Further details about this example and the characterization of a monocrystal of NiTi can be found in the publication by Massad and Smith [MAS 03].

![Simulated behavior of the model and equilibrium deformations](image)

**Figure 6.10.** Simulated behavior of the model and equilibrium deformations
a) $T = 272$ K, b) $T = 283$ K, c) $T = 291$ K, d) $T = 298$ K [MAS 03]

### 6.4. Constitutive framework of the homogenized energy model

The peculiarity of this constitutive framework of the “homogenized energy model” lies in the theory of thermally activated processes, developed for SMAs by Muller, Achenbach and Seelecke between 1980 and 2004 [ACH 85, ACH 89]. At the heart of it, the theory is based on an equilibrium between the Gibbs energies and the thermal energies, applying Boltzmann principles for monocrystals. In the Paperfu and Seelecke publication of 1999 [PAP 99], the initial effects of the polycrystallinity are incorporated, in order to integrate the distribution of crystalline lattices and the effects of orientation of the stresses. Thus, this gives us a summary to analyze these distributions. Models incorporating relative stress- (which will later be defined as...
the thickness of hysteresis of the traction curves) and effective stress distributions were developed by Massad et al. [MAS 03] for thin SMA films and for massive materials.

![Simulation of the NiTi polycrystal](image)

Figure 6.11. Simulation of the NiTi polycrystal [BUN 00]

This produced a framework for modeling SMAs which describes their ferroelastic and pseudo-elastic behaviors, as well as other memory effects. In addition, this approach takes into account the internal loops, associated with partial phase transformations, and incorporates the dynamic behavior, the temperature change (integration of the heat equation) and thermal relaxation.

In order to obtain a sufficient degree of reliability which is necessary for transducers and models based on command control, a multiscale approach is employed.

The energy relations are developed at the mesoscopic scale in order to integrate the operative physical mechanisms. The effects of variation in the lattice parameters, of polycrystallinity and of variable stresses are incorporated, assuming that the parameters such as the relative and effective stresses are manifestations of the distribution of the microstructure rather than simple constants.

Thus, homogenization provides us with macroscopic models which are fairly simple and therefore easy to embed in computer coding.
6.4.1. One-dimensional mesoscopic model

To summarize the theory developed for uniaxial behavior, the material is formed of three phases \( A, M^+, M^- \) (the lattices of which are represented diagrammatically in Figure 6.8), with respective volume fractions of \( z_A, z_{M^+}, z_{M^-} \) with the following conservation equation:

\[
z_A + z_{M^+} + z_{M^-} = 1 \tag{6.39}
\]

6.4.1.1. Helmholtz and Gibbs free energies

The quadratic expressions “by parts” are repeated here:

- for \( \varepsilon \leq -\varepsilon_M(T) \):
  \[
  \psi(\varepsilon, T) = \frac{E_M}{2} (\varepsilon + \varepsilon_T)^2 \tag{6.40}
  \]

- for \( -\varepsilon_M(T) < \varepsilon < -\varepsilon_A(T) \):
  \[
  \psi(\varepsilon, T) = -\frac{E_0(T)}{2} (\varepsilon + \varepsilon_0(T))^2 + \psi_0(T) \tag{6.41}
  \]

- for \( |\varepsilon| < \varepsilon_A(T) \):
  \[
  \psi(\varepsilon, T) = \frac{E_A}{2} \varepsilon^2 + \Delta\beta(T) \tag{6.42}
  \]

- for \( \varepsilon_A(T) < \varepsilon \leq \varepsilon_M(T) \):
  \[
  \psi(\varepsilon, T) = -\frac{E_0(T)}{2} (\varepsilon - \varepsilon_0(T))^2 + \psi_0(T) \tag{6.43}
  \]

- for \( \varepsilon \geq \varepsilon_M(T) \):
  \[
  \psi(\varepsilon, T) = \frac{E_M}{2} (\varepsilon - \varepsilon_T)^2 \tag{6.44}
  \]

where \( E_A \) and \( E_M \) are the Young’s moduli for the austenite and martensite, with:

\[
G(\sigma, \varepsilon, T) = \psi(\varepsilon, T) - \sigma \varepsilon \tag{6.45}
\]

Figure 6.12 illustrates the pseudo-elastic behavior at a fixed temperature \( T \geq A_F^0 \). The material is austenitic at the stress-free state (\( \sigma = 0 \)). The stress increases up to a threshold value \( \sigma_{AM^+} \) when the stable equilibrium of the austenite ceases to be a local minimum and \( M^+ \) becomes the stable phase. When the stress decreases, a new threshold stress \( \sigma_{M^+A} \) is attained for the reversion of \( M^+ \) into \( A \).
6.4.1.2. Local stress-strain relation with negligible thermal activation

The $\sigma \Leftrightarrow \varepsilon$ relations satisfy the necessary conditions:

$$\frac{\partial G}{\partial \varepsilon} = 0, \quad \frac{\partial^2 G}{\partial \varepsilon^2} \geq 0 \quad [6.46]$$

associated with the minimization of $G$.

Because of the quadratic definition of $G$ in $\varepsilon$, the local $\sigma \Leftrightarrow \varepsilon$ relation is linear in the absence of thermal activation. It is written with $\sigma = \frac{\partial G}{\partial \varepsilon}$:

- for $\varepsilon \leq -\varepsilon_M(T)$:
  $$\sigma = E_M(\varepsilon + \varepsilon_T) \quad [6.47]$$

- for $-\varepsilon_M(T) < \varepsilon \leq -\varepsilon_A(T)$:
  $$\sigma = -E_0(T)(\varepsilon + \varepsilon_0) \quad [6.48]$$

- for $|\varepsilon| < \varepsilon_A(T)$:
  $$\sigma = E_A \varepsilon \quad [6.49]$$

- for $\varepsilon(T) < \varepsilon \leq \varepsilon_M(T)$:
  $$\sigma = -E_0(T)(\varepsilon - \varepsilon_0) \quad [6.50]$$
\[
\sigma = E_M (\epsilon - \epsilon_T) \quad [6.51]
\]

We can define the threshold stress for the transformation \(A \Rightarrow M^+\): \(\sigma_{AM^+}\) by:
\[
\sigma_{AM^+} = E_M (\epsilon_M(T) - \epsilon_T) \quad [6.52]
\]

where the threshold stress for the transformation \(\sigma_{AM^-}\) is given by:
\[
\sigma_{AM^-} = E_M (-\epsilon_M(T) + \epsilon_T) = -\sigma_{AM^+} \quad [6.53]
\]

In the case of symmetrical traction-compression behavior.

Similarly, for the reverse transformation \(M^+ \Rightarrow A\) or \(M^- \Rightarrow A\), the stress for total elimination of the martensite \(\sigma_{M\pm A}\) is written:
\[
\sigma_{M\pm A} = E_A (\pm \epsilon_A(T)) \quad [6.54]
\]

For the construction of macroscopic models, it may be useful to introduce the relative stress \(\sigma_R(T)\) defined by:
\[
\sigma_R(T) = \sigma_{AM^+} - \sigma_{M+A} \quad [6.55]
\]

The inverse relations \(\sigma \Rightarrow \epsilon\) are written thus, for instance, under traction \((A \Rightarrow M^+):\)
\[\epsilon \geq \epsilon_M(T):\]
\[
\epsilon = \frac{\sigma}{E_A} \quad [6.56]
\]

\[\sigma_{M+A} \leq \sigma \leq \sigma_{AM^+}:\]
\[
\epsilon = \frac{\sigma_{AM^+}}{E_A} + (\Delta \epsilon + \sigma_R(\frac{1}{E_M} - \frac{1}{E_A})) z \quad [6.57]
\]

\[\sigma_{M+A} < \sigma < \sigma_{AM^+}:\]
\[\sigma = \sigma_{M+A}:\]
\[
\epsilon = \frac{\sigma_{M+A}}{E_A} + (\Delta \epsilon) z \quad [6.58]
\]

\[\sigma_{M+A}:\]
\[
\sigma = \frac{\sigma}{E_A} \quad [6.59]
\]

where \(z\) is the volume fraction of the martensite \(M^+:\) \(z \in [0, 1]\) and \(\Delta \epsilon = \epsilon_M - \epsilon_A\).
6.4.1.3. Local stress-strain relation with thermal activation

In order to quantify the average local strains for operational regimes for which the thermal activation is significant, it is necessary to balance the Gibbs free energy $G$ with the thermal energy $kT$, using the Boltzmann equation:

$$
\mu(G) = C \exp \left( \frac{G}{kT} \right) \quad [6.60]
$$

In physical terms, high values of $kT$ mean that the material will reach a minimum of energy required before the threshold stresses are reached. This gives the pseudo-elastic curves a rounded form and decreases the transition values, as illustrated on the curve in Figure 6.12.

This phenomenon was detailed by Massad and Smith in 2003 [MAS 03] and Seelecke et al. in 2004 and 2011 [SEE 04, SEE 11b].

The probabilities $p_{A\pm}$ that $A$ will be transformed into $M \pm$ and $p_{\pm}$ that $M \pm$ will be transformed into $A$ or into the other variant are:

$$
p_{A\pm}(\sigma, T) = \frac{1}{\tau(T)} \int_{\chi_{A\pm}} e^{(-G(\sigma, \varepsilon, T)/kT)} d\varepsilon \quad [6.61]
$$

$$
p_{\pm}(\sigma, T) = \frac{1}{\tau(T)} \int_{\chi_{M\pm}} e^{(-G(\sigma, \varepsilon, T)/kT)} d\varepsilon \quad [6.62]
$$

where $\tau(T) = \tau_1 \sqrt{\frac{V}{kT}}$ denotes the relaxation time $\chi_A(T) = (\varepsilon_A(T), \varepsilon_A(T))$, $\chi_{M+} = (\varepsilon_M(T), \infty)$, $\chi_{M-} = (-\infty, -\varepsilon_M(T))$ represent the regions where $A, M^+, M^-$ are stable and $\pm \varepsilon_A, \pm \varepsilon_M$ represent the intervals concerning the transition strains $\pm \varepsilon_A, \pm \varepsilon_M$.

Note that in practice, we often employ the following relations:

$$
p_{A\pm}(\sigma, T) = \frac{1}{\tau(T)} \int_{\chi_{A\pm}} e^{(-G(\sigma, \pm \varepsilon_A(T)/kT)} d\varepsilon \quad [6.63]
$$

$$
p_{\pm}(\sigma, T) = \frac{1}{\tau(T)} \int_{\chi_{M\pm}} e^{(-G(\sigma, \pm \varepsilon_M(T)/kT)} d\varepsilon \quad [6.64]
$$
The expected deformations are written:

\[
<\varepsilon^-> = \int_{\chi^-} \varepsilon \mu(G(\sigma, \varepsilon, T)) d\varepsilon
\]

\[
<\varepsilon^+> = \int_{\chi^+} \varepsilon \mu(G(\sigma, \varepsilon, T)) d\varepsilon
\]

\[
<\varepsilon_A> = \int_{\chi_A} \varepsilon \mu(G(\sigma, \varepsilon, T)) d\varepsilon
\]

where \(\mu(G)\) is defined in [6.60].

The phase transformation kinetics are given by:

\[
\dot{z}^-(t) = p_A z_A(t) - p^- z^-(t)
\]

\[
\dot{z}^+(t) = p_A z_A(t) - p^+ z^+(t)
\]

\[
\dot{z}_A(t) = -p_A z_A(t) + p^- z^-(t) - p_A z_A(t) + p^+ z^+(t)
\]

with the conservation equation:

\[
\dot{z}^- + \dot{z}^+ + \dot{z}_A = 0
\]

and finally:

\[
\bar{\varepsilon} = <\varepsilon^- > z^- + <\varepsilon^+ > z^+ + <\varepsilon_A > z_A
\]

6.4.2. Thermal change

Massad and Smith [MAS 03] establish the heat equation in the following form:

\[
M \frac{\partial T}{\partial t}(t) = -\Omega [h_c + \chi/\zeta] [T - T_e(t)] + J(t) - \sum_\alpha h_\alpha z_\alpha
\]

where \(h_\alpha = G_\alpha + T S_\alpha\) and the average specific heat \(\bar{\tau} = \sum_\alpha c_\alpha z_\alpha\).

\(J(t)\) is defined for an intensity of electric current \(I(t)\), by a classic equation:

\[
J(t) = \bar{\rho}(t) \frac{\bar{I}^2(t)}{A}
\]
where:
- $\bar{\rho}(t) = \sum_\alpha \rho_\alpha z_\alpha$ is the average resistivity per unit length of the bar;
- $J(t)$ represents the heat generated by the Joule effect;
- $M$: the mass of the actuator;
- $\Omega$: a heat transfer coefficient;
- $\lambda$: the thermal conductivity;
- $l$: the length of the bar;
- $T_e(t)$: the variable temperature of the environment surrounding the bar;
- $A$: the area of the cross-section of the bar;

and finally:

$$\bar{c}(t) = \sum_\alpha c_\alpha z_\alpha(t) \tag{6.75}$$

### 6.4.3. Macroscopic model

The mesoscopic relations were developed under the auspices of the representative Elementary volume (REV) hypothesis.

In order to incorporate the effects of polycrystallinity, non-homogeneity of the material and also to take into account of the effect of grain boundaries, we consider that $\sigma_R(T) = \sigma_{AM+} - \sigma_{M+A}$ represents these different distributions. Owing to the fact that $\sigma_{AM+} \geq \sigma_{M+A}$, the density $\nu_1$ for $\sigma_R(T)$ is only defined for $\sigma_R(T) \geq 0$.

A log-normal law is chosen in order to facilitate embedding:

$$\nu_1(\sigma_R) = c_1 e^{-[\ln(\sigma_R/\sigma_{\text{bar}})^2/2]} \tag{6.76}$$

As before, we introduce the stress in the form $\sigma_e = \sigma + \sigma_I$; rather than choosing $\sigma_I = \alpha \varepsilon$, we consider that $\sigma_I$ and also $\sigma_e$ are statistically distributed with a density $\nu_2$.

In this particular case, two representations have been employed for the normal density:

$$\nu_2(\sigma_I) = c_2 e^{-\sigma_I^2/2\sigma^2} \tag{6.77}$$
or Laplace’s equation:

\[ \nu_2(\sigma_1) = c_2 e^{-|\sigma_1|/b} \]  \[6.78\]

The macroscopic deformation is defined by:

\[ [\varepsilon(\sigma, T)](t) = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \nu_1(\sigma_R) \nu_2(\sigma_I) \left[ \Xi(\sigma_e, T; \sigma_R, z) \right](t) d\sigma d\sigma_R \]  \[6.79\]

\( \nu_1 \) and \( \nu_2 \) satisfy the following conditions of positivity, symmetry and integrability:

- \( \nu_1(x) \) defined for \( x \geq 0 \);
- \( \nu_2(x) = \nu_2(-x) \);
- \( |\nu_1(x)| \leq c_1 e^{-a_1 x} \), \( |\nu_2(x)| \leq c_2 e^{-a_2 |x|} \);

for positive values of \( c_1, a_1, c_2, a_2 \).

6.4.4. Performance of the model and material characterization

6.4.4.1. Simulation of the model

The model’s capability to characterize the pseudo-elastic behavior, the shape memory effect and the internal loops are illustrated in Figures 6.13, 6.14, 6.15 and 6.16 in Massad and Smith [MAS 05].

![Figure 6.13. Pseudo-elastic curve monitoring the temperature and volume fraction of martensite [MAS 05]](image)

Figure 6.13 illustrates the \( \sigma \leftrightarrow \varepsilon \) behavior with the change in temperature delivered by the heat equation [6.73]. The simulation reflects the role played by the
enthalpic terms $\sum h_{\alpha} \dot{z}_{\alpha}$ in equation [6.74], which quantify the amounts of heat generated and absorbed during phase transformations. Some of this heat is transferred by convection as the residual heat changes $\sigma_{AM+}$ and $\sigma_{M+A}$.

The memory effect is illustrated in Figures 6.14 and for stresses imposed. In both cases, the temperature is controlled by convection, at the rate of 0.1 K/s. While the enthalpies do have an effect on the internal temperature, this effect is small in comparison to the changes due to convection. It is logically observed that the temperatures for phase transformation (under stress) $A_F^\sigma$, $A_S^\sigma$, $M_F^\sigma M_S^\sigma$ are different.

![Hysteresis loop monitoring the temperature and the volume fraction of martensite [MAS 05]](image1)

**Figure 6.14.** Hysteresis loop monitoring the temperature and the volume fraction of martensite [MAS 05]

![Stress dependency of the thermal hysteresis loop [MAS 05]](image2)

**Figure 6.15.** Stress dependency of the thermal hysteresis loop [MAS 05]

The simulation of the effects of warming by the Joule effect and convective cooling for a thin film 10 $\mu$m in thickness is given in Figure 6.16:
– warming by the Joule effect (see $J(t)$) is applied for 10 ms in order to increase the temperature by 50 K, and this causes a partial transformation $M \Rightarrow A$;

– then, convective cooling until $t = 0.05$ s causes a decrease in $z_A$ and an increase in $z_\gamma$, producing the first part of the internal loop;

– the resulting warming above $A_F$ completes the transformation into austenite.

In passing, the internal loop is closed. The external loop is obtained by a cooling/warming cycle.

![Figure 6.16. Simulation of warming by the Joule effect and forced convective cooling on a thin film in order to produce a hysteresis loop [MAS 05]](image)

Note that the dependency of $\dot{T}$ with $\dot{z}_\alpha$ corroborates the observation made by Ma et al. in 2000 [MA 00], that the response time of thin films is limited more by the rate of phase transformations than by the cooling time. This indicates the limited response speeds of transducers in the form of thin films.

6.4.4.2. Characterization of the materials

We shall now give two examples in order to demonstrate the robustness of the model.

– NiTiFe specimen

Consider a NiTiFe alloy of 500 $\mu$m in thickness made by Furakawa Techno-Materials as reported by Matsuzaki et al. in 2002 [MAT 02].

The data shown in Figure 6.17 correspond to the pseudo-elastic curve obtained at $\dot{\varepsilon} = 10^{-2}$ s$^{-1}$ of the associated internal loops.
Material parameters:

\[ A_S = 234 \, K, \quad A_F = 281 \, K, \quad M_S = 280 \, K, \quad M_F = 244 \, K; \]
\[ \rho = 6450 \, kg/m^3, \quad E_A = 37.2 \, GPa, \quad E_M = 25.5 \, GPa; \]
\[ \varepsilon_T = 0.0253, \quad \sigma_R = 70 \, MPa, \quad V = 6903 \, nm^3; \]
\[ \tau = 11.9 \, ms, \quad m^3, \quad E_A = 37.2 \, GPa, \quad E_M = 25.5 \, GPa; \]
\[ \varepsilon_T = 0.0253, \quad \sigma_R = 70 \, MPa, \quad V = 6903 \, nm^3; \]
\[ C_A = C_M = 2.9025 \, MJ/m^{-3} \, K^{-1}; \]
\[ b = 55 \, MPa, \quad c = 52 \, MPa, h_c = 10 \, W \, m^{-2}K^{-1}m^3, \quad E_A = 37.2 \, GPa, \]
\[ E_M = 25.5 \, GPa; \]
\[ \varepsilon_T = 0.0253, \quad \sigma_R = 70 \, MPa, \quad V = 6903 \, nm^3. \]

**Figure 6.17.** Pseudo-elastic curve with internal loops and simulation \[\text{[MAT 02], [MAS 05]}\]

The model reflects the experimental results relatively closely, in quantitative terms (see Figure 6.17).

– NiTi film

Consider a slender film 8 \( \mu \)m in thickness made in the UCLA “Active Material Laboratory” by Woolman *et al.* in 2003 [WOO 03].

The stress-strain curves at \( T = 353 \, K \) and \( T = 298 \, K \) are shown in Figure 6.18.
The simulations are reasonably representative of the pseudo-elastic behavior at 353 K and pseudo-plastic behavior (reorientation of the martensite variants) at 298 K.

6.4.4.3. Software

Matlab® m-files to embed their homogenized SMA model [SMI 05]

www.siam.org/books/fr32

6.5. Conclusion

Because of their intrinsic mathematic construction, the Preisach approaches are operational in command and in control of systems, and are therefore very widely used in automation engineering.

As regards the Falk analyses and their extensions, they are based on the derivation of the free energy \( \sigma = \frac{\partial F}{\partial \varepsilon} \) of a material with three possible phases \( A, M^+, M^- \).

The works of Seelecke and Muller introduce the thermal activation into the analysis (in reference to Boltzmann). All foregone research was integrated into a homogenized energy framework by Smith and his colleagues. Their model is entirely predictive, and gives a good representation of the curves discussed in the existing literature (pseudo-elasticity, internal loops, simple memory effect, etc.).
However, these models are, by construction, one-dimensional (1D). Their extension into multiaxial (three-dimension) space may prove somewhat complicated.

This is one of the reasons why Chapter 7 will discuss macroscopic models with internal variables that are able to take account of multiaxial loading, proportional or otherwise.
Chapter 7

Macroscopic Models with Internal Variables

7.1. Introduction

Most of these models are constructed under the auspices of thermodynamics of irreversible processes (TIP), applied to the standard materials made popular by Bernard Halphen and N’Guyen Quoc Son [HAL 74, HAL 75] (see Chapter 4).

The contribution of France’s academics to solid mechanics has been an important one: we can cite, in particular, the work of Zaki, Moumni and N’Guyen at ENSTA in Palaiseau; Calloch and Arbab Chirani at ENSTA and ENI in Brest; Patoor and Ben Zineb and their doctoral students for the axis LEM3 in Metz and LEMTA in Nancy; Favier and Orgas from L3S in Grenoble, Laverhne-Taillard from LMT in Cachan and finally Lexcellent and Boubakar and their doctoral students at the DMA-FEMTO in Besancon.

The main difference between these models is their description of the phenomenon of hysteresis. “Generalized standard materials”-type models use approaches similar to the theory of plasticity, and are therefore based on the definition of threshold functions for the $A \Rightarrow M$ transformations. Models with non-convex free energies describe hysteresis in the form of phenomena of instability. The hereditary approach considers rheological models based on springs and frictional dampers, putting forward a thermomechanical conception of hysteresis.

For the other phenomenological investigations, it is primarily the choice of the internal variables associated with the martensitic transformation which distinguishes these models from one another. As in Chapter 4, the behavior of the solid material is regulated by the choice of a specific free energy and a potential for dissipation or criterion functions for phase transformation (forward $A \Rightarrow M$ or reverse $M \Rightarrow A$).
Historically, the first “empirical” (so to speak) models were those advanced by Tanaka [TAN 82, TAN 86] which use the volume fraction of martensite \( z \) as an internal variable and the total strain \( E \) and temperature \( T \) as observable variables. With:

- \( \Sigma \) is the traction stress;
- \( E^{tr}, E^{th}, E^{el} \) the uniaxial traction deformations, respectively associated with phase transformation, thermal elongation and elastic contribution;
- note that \( E^{tr} = \gamma z \) and \( E^{th} = \alpha (T - T_0) \);
- \( E^* \) Young’s modulus.

They give a one-dimensional (1D) constitutive law:

\[
\Sigma = E^* (E - E^{tr} - E^{th}) = E^* (E - \gamma z - \alpha (T - T_0)) = E^* (E^{el}) \quad [7.1]
\]

with phase transformation kinetics in exponential laws.

For \( A \Rightarrow M \):

\[ z = 1 - \exp(a_1 < \Sigma - b_1 (T - M^0_S) >) \quad [7.2] \]

For \( M \Rightarrow A \):

\[ z = \exp(-a_2 < b_2 (T - A_0^0_S) - \Sigma >) \quad [7.3] \]

where \( < x > = x \) if \( x \geq 0 \) and 0 if \( x \leq 0 \) and \( a_1, a_2, b_1, b_2 \) constants.

This theory was extended in 1990 by Liang and Rogers, who gave a “sinusoidal form” to the phase transformation kinetics [LIA 90].

In 1993, Brinson [BRI 93] introduced a distinction between martensite of purely thermal origin \( M_T \) (created simply by cooling of austenite, i.e. the stress-free state) and a martensite obtained under the influence of an applied stress called \( M_S \). This enables us to simulate the response to mechanical loads or to varying external temperature, which may constitute the controlling variable in the system [BEN 97].

In 1992, Raniecki, Lexcellent and Tanaka [RAN 92] took the advances made by Tanaka et al. [TAN 82, TAN 86] and placed them in the context of thermodynamics of irreversible processes.

In this chapter, there is no question of giving a complete inventory of all the existing macroscopic models relating to SMAs – there are far too many of them in the literature. We shall content ourselves with highlighting a few of the salient points of some of these models.
However, we shall shift from a one-dimensional (1D) formulation, where all the variables are scalars, to a three-dimensional formulation where the strains and stresses become second-order tensors. For instance, $E \Rightarrow \mathbf{E}$ or $\Sigma \Rightarrow \mathbf{\Sigma}$, etc. This results from the desire to take account of the multiaxial mechanical loads such as traction/torsion on a tube.

7.2. $R_L$ model

This model was published by Raniecki et al. [RAN 92] and extended to the anisothermal case by Leclercq and Lexcellent [LEC 96].

We define the representative elementary volume (REV) by martensite platelets (whose overall volume fraction is $z$) disseminated in the austenitic parent phase (with overall volume fraction $(1-z)$).

The free energy of the two-phase mixture ($A + M$) can be defined by:

$$\psi(E, T, z) = (1 - z)\psi_A(E_A, T) + z\psi_M(E_M, T) + \psi_{int}(z, T)$$  \[7.4\]

where $\psi_A(\psi_M)$ represents the free energy of the austenite $A$ (or of the martensite $M$) and $\psi_{int}$ represent the interaction energy between the austenite and martensite. The choice of this expression proves both delicate and crucial in terms of modeling. We shall therefore come back to it later.

Let us examine the simplest choice: $\psi_{int}(z, T) = 0$, which will give us a reversible model referred to as $R$.

7.2.1. Reversible $R$ model

In this case, with $\psi_{int}(z, T) = 0$, the free energy becomes:

$$\psi(E, T, z) = (1 - z)\psi_A(E_A, T) + z\psi_M(E_M, T)$$  \[7.5\]

Let the free energy of the $\alpha$ phase:

$$\rho\psi^{\alpha}(E_\alpha, T) = u_0^{\alpha} - T s_0^{\alpha} + \frac{1}{2}(E_\alpha - E_\alpha^{tr} - E_\alpha^{th}) L (E_\alpha - E_\alpha^{tr} - E_\alpha^{th})$$

$$+ C_v \left( T - T_0 - T_n \ln \left( \frac{T}{T_0} \right) \right)$$  \[7.6\]

$\alpha = 1$ for austenite and $\alpha = 2$ for martensite.

In the expression of the free energy $\psi_\alpha(E_\alpha, T)$, the first term on the right represent the chemical contribution, the second the elastic energy and the third the thermal contribution.
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1st hypothesis
We assume the same values for the elastic constants $L$, density $\rho$, specific heat $C_v$ and thermal expansion coefficient $\alpha$ for both austenite and martensite. It is possible not to do so, but the expressions become more complicated, for a gain of only 5–8% in terms of precision, as per the analyses performed by Raniecki and Lexcellent [RAN 94].

Thus:

$$E_{\alpha}^{th} = E_{1}^{th} = E_{2}^{th} = E^{th} = \alpha(T - T_0)1$$

[7.7]

By definition:

$$\Sigma_\alpha = \rho \frac{\partial \psi_\alpha}{\partial E_\alpha} = L(E_\alpha - E_{\alpha}^{tr} - E_{\alpha}^{th}) = LE_{\alpha}^{el}$$

[7.8]

where:

- $E_\alpha$ represents the total deformation of the $\alpha$ phase;
- $E_{\alpha}^{tr}$ represents the transformation deformation associated with the $\alpha$ phase;
- $E_{\alpha}^{th}$ represents the thermal deformation of the $\alpha$ phase;
- $E_{\alpha}^{el}$ represents the elastic deformation of the $\alpha$ phase.

2nd hypothesis

$$E_{1}^{tr} = 0, E_{2}^{tr} = \kappa$$

We apply the mixture law to the total deformation:

$$E = (1 - z)E_1 + zE_2$$

[7.9]

where:

$$E_\alpha = (E_{\alpha}^{el} + E_{\alpha}^{tr} + E_{\alpha}^{th})$$

3rd hypothesis

The stress state is indifferent to the phase state – put differently:

$$\Sigma_\alpha = \Sigma_1 = \Sigma_2 = \Sigma \Rightarrow E_{\alpha}^{el} = E_{1}^{el} = E_{2}^{el} = E^{el}$$

[7.10]

and:

$$E = E^{el} + \kappa z + \alpha(T - T_0)1$$

[7.11]
The free energy of the biphase $(A + M)$ mixture is written:

$$\rho \psi(E, z, T) = u_0^1 - Ts_0^1 - z\Pi_0^f(T)$$

$$+ \frac{1}{2}(E - \kappa z - \alpha(T - T_0)1)\mathbf{L}(E - \kappa z - \alpha(T - T_0)1)$$

$$+ C_v(T - T_0 - T.Ln\left(\frac{T}{T_0}\right))$$

[7.12]

where:

$$\Sigma = \rho \frac{\partial \psi}{\partial E} = \mathbf{L}(E - \kappa z - \alpha(T - T_0)1); s = -\frac{\partial \psi}{\partial T}$$

[7.13]

where $s$ constitutes the specific entropy and $\Pi_0^f(T) = \Delta u - T\Delta s$, with $\Delta u = u_0^1 - u_0^2$; $\Delta s = s_0^1 - s_0^2$.

The increment of mechanical dissipation (in reference to Chapter 4) is written as:

$$dD = \Pi^f dz \geq 0$$

[7.14]

with:

$$\Pi^f(\Sigma, z, T) = -\frac{\partial \psi}{\partial z} = \Pi_0^f(T) + \frac{\kappa}{\rho} \Sigma$$

[7.15]

or:

$$\Pi^f(E, z, T) = -\frac{\partial \psi}{\partial z} = \Pi_0^f(T) + \frac{\kappa}{\rho} \mathbf{L}(E - \kappa z - \alpha(T - T_0)1)$$

[7.16]

A (thermodynamically) reversible model such as $R$ means that the dissipation is null, and consequently, during the forward or reverse phase transformation $\forall dz$; $z \in [0, 1]$:

$$\Pi^f(\Sigma, z, T) = 0; \Pi^f(E, z, T) = 0$$

[7.17]

1st application: uniaxial application of traction stress

In this case, we can reduce $\kappa$ to a scalar $\gamma$ and the threshold stress is written:

$$\Sigma_{am} = -\frac{\Pi_0^f(T)}{\gamma}$$

[7.18]
In the Clausius–Clapeyron diagram ($\Sigma, T$), we can deduce the slope of separation between the austenitic and martensitic domains:

$$\frac{d\Sigma_{am}}{dT} = \rho \frac{\Delta s}{\gamma} \quad [7.19]$$

As Figure 7.1 shows, the deformation at the start of phase transformation $E_{am}^m (z = 0)$ is governed by $E_{am}^m (z = 0) = \Sigma_{am}^m / E^* \gamma$ and at the end of transformation $E_{am}^m (z = 1) = \Sigma_{am}^m / E^* + \gamma$ and an intermediary deformation $E_{am}^m (z) = \Sigma_{am}^m / E^* + \gamma z$.

![Figure 7.1. Traction curve corresponding to the R model [RAN 92]](image)

This simple model is particularly well adapted to the description of monocrystals with little hysteresis such as Cu-Zn-Al [PAT 87]:

**7.2.2. R$_L$ model with a hysteresis loop [MUL 89]**

In this case, the free energy integrates the mixture law for the two phases in the $R$ model (equation [7.12]) and the interaction term $\psi_{int}(z, T)$:

$$\rho \psi(E, z, T) = a_1^0 - T s_1^0 - z \Pi_0^f (T)$$

$$+ \frac{1}{2} (E - \kappa z - \alpha (T - T_0)) \mathbf{L} (E - \kappa z - \alpha (T - T_0)) \mathbf{1} \quad [7.20]$$

$$+ C_v (T - T_0 - T \ln \left( \frac{T}{T_0} \right)) + \psi_{int}(z, T)$$

where:

$$\Sigma = \rho \frac{\partial \psi}{\partial E} = \mathbf{L} (E - \kappa z - \alpha (T - T_0)) \mathbf{1} ; \quad s = - \frac{\partial \psi}{\partial T} \quad [7.21]$$

which represents the same expression as equation [7.13] in the $R$ model.
As we shall go on to demonstrate, the choice of tensor $\kappa$ is very important in terms of the modeling of multiaxial experiments (taking into account the asymmetry between traction and compression, for example). The choice of $\psi_{int}(z, T)$ proves crucial as regards dissipation and hysteresis.

A logical reasoning would be to hold that there is no interaction when only one of the two phases is present (although to make this assumption is to somewhat overlook the fact that the martensitic phase, “in passing” into the parent phase, may have left traces!). We write:

$$\psi_{int}(z = 0) = \psi_{int}(z = 1) = 0$$

[7.22]

Hence, a natural choice was made first by Muller [MUL 89] and then by Muller and Xu [MUL 91] in their one-dimensional theory regarding the formation of hysteresis loops due to phase transformation:

$$\psi_{int}(z, T) = Az(1 - z)$$

[7.23]

Raniecki et al. [RAN 92] replaced the constant $A$ with $\psi_{it}(T) = u_0 - T s_0$.

This is reminiscent of the thinkings of Licht, published in “z(1-z), j’aime assez” (“z(1-z): I quite like that”) [LIC 98].

We can also identify the mathematical expression of $\psi_{int}(z, T)$ by determining parameters on the experimental hysteretic traction curves, for instance, as outlined by Boubakar in his qualification to supervise PhD candidates [BOU 02, BOU 07]. This can be done in the context of finite transformations [VIE 03].

In comparison to the R model, here dissipation exists and is written thus, in reference to Chapter 4:

$$dD = \Pi^f dz \geq 0$$

[7.24]

where:

$$\Pi^f(\Sigma, z, T) = \Pi_0^f(T) + \frac{\kappa: \Sigma}{\rho} - (1 - 2z)\psi_{it}(T)$$

[7.25]

The threshold stress tensor $\Sigma^{am}$ for the start of the forward ($A \Rightarrow M$) transformation is governed by:

$$\Pi^f(\Sigma^{am}, z = 0, T) = \Pi_0^f(T) + \frac{\kappa: \Sigma^{am}}{\rho} - \psi_{it}(T) = 0$$

[7.26]
and the threshold stress tensor $\mathbf{\Sigma}^{ma}$ for the start of the reverse ($M \Rightarrow A$) transformation is governed by:

$$
\Pi^f(\mathbf{\Sigma}^{ma}, z = 1, T) = \Pi_0^f(T) + \frac{\kappa}{\rho} \mathbf{\Sigma}^{ma} + \psi_{it}(T) = 0 \quad [7.27]
$$

The forward transformation $A \Rightarrow M$ takes place when $dz > 0 \Rightarrow \Pi^f \geq 0$, and the reverse transformation $M \Rightarrow A$ occurs when $dz < 0 \Rightarrow \Pi^f \leq 0$.

In order to specify the equations for the phase transformation kinetics, we hypothesize that there are two functions $\phi_\alpha(\Pi^f, z) (\alpha = 1, 2)$ such that an active process of parent phase decomposition ($dz > 0 \Rightarrow A \Rightarrow M$) can take place only if $\phi_1 = \text{const.} (d\phi_1 = 0)$. Similarly, an active process of martensite decomposition ($dz < 0 \Rightarrow M \Rightarrow A$) can only progress if $\phi_2 = \text{cont.} (d\phi_2 = 0)$:

$$
\phi_1 = \Pi^f - k_1(z), \phi_2 = -\Pi^f + k_2(z) \quad [7.28]
$$

So as to be in agreement with metallurgists such as Koistinen and Marburger [KOI 59] as regards the expression for the phase transformation kinetics, we choose:

$$
k_1(z) = 2\psi_{it}(M^0_s)z + \frac{s_0 - \Delta s - 2s_0z}{a_1} \ln(1-z) \quad [7.29]
$$

$$
k_2(z) = 2\psi_{it}(A^0_s)(1-z) + \frac{s_0 + \Delta s - 2s_0(1 - z)}{a_2} \ln(z) \quad [7.30]
$$

Thus, laborious series of calculations give us the phase transformation kinetics in both directions:

$$
d\phi_1 = 0 \Rightarrow dz^{a\rightarrow m} \quad [7.31]
$$

$$
d\phi_2 = 0 \Rightarrow dz^{m\rightarrow a} \quad [7.32]
$$

The hysteresis size is defined in one-dimension (e.g. simple traction) by:

$$
\Delta \mathbf{\Sigma} = \mathbf{\Sigma}^{am} - \mathbf{\Sigma}^{ma} \quad [7.33]
$$

Note that in this case, $\kappa: \mathbf{\Sigma} = \gamma \mathbf{\Sigma}$ where $\mathbf{\Sigma}$ is the traction stress and $\gamma$ is the complete transformation deformation, with $\mathbf{\Sigma}^{am}$ such that $\Pi^f(\mathbf{\Sigma}^{am}, z = 0, T) = 0$, therefore giving us:

$$
\mathbf{\Sigma}^{am} = \frac{\rho}{\gamma} (-\Pi_0^f(T) + \psi_{it}(T)) \quad [7.34]
$$

Similarly, $\mathbf{\Sigma}^{ma}$ such that $\Pi^f(\mathbf{\Sigma}^{ma}, z = 1, T) = 0$, which gives:

$$
\mathbf{\Sigma}^{ma} = \frac{\rho}{\gamma} (-\Pi_0^f(T) - \psi_{it}(T)) \quad [7.35]
$$
We get the hysteresis size:

$$\Delta \Sigma = \Sigma^{ma} - \Sigma^{ma} = \frac{\rho}{\gamma} 2\psi_{it}(T)$$ \[7.36\]

If we wish to analyze thermomechanical coupling, we need to introduce the heat equation. Note in particular that the phase transformations are highly exothermic for \( A \Rightarrow M \) (and endothermic for \( M \Rightarrow A \)).

7.2.2.1. Heat equation

Let it be known that to say we are performing an “isothermal test” is a convenient but incorrect use of the language. We can simply impose a constant temperature at the boundary of the sample, which constitutes a structure whose internal temperature we do not control. Studies on thermomechanical coupling, with infrared imagery and estimations of the energy stored in the material, can be found in Chrysochoos et al. [CHR 00, CHR 09].

This equation is crucial in order to establish the contribution to the “slow” dynamic response of an SMA (in comparison to piezoelectric materials).

As stated in Chapter 4, the first principle of thermodynamics applied to the “Representative Elementary Volume” is written as follows:

$$\rho \dot{e} = \Sigma : \dot{\mathbf{E}} + r - \text{div} \mathbf{q}$$ \[7.37\]

where \( e = (\psi + Ts) \) and:

$$\rho \dot{\psi}(\mathbf{E}, z, T) = u^0_1 - Ts^0_1 - z\Pi^f_0(T)$$

$$+ \frac{1}{2}(\mathbf{E} - \kappa z - \alpha(T - T_0))L(\mathbf{E} - \kappa z - \alpha(T - T_0)) \mathbf{1}$$ \[7.38\]

$$+ C_v(T - T_0 - T.Ln(T/T_0)) + \psi_{int}(z, T)$$

and:

$$\rho \dot{\psi} = \Sigma : \dot{\mathbf{E}} + r - \text{div} \mathbf{q} - \rho s \dot{T} - \rho s T$$

$$\dot{\rho} \dot{\psi} = \rho \frac{\partial \psi}{\partial \mathbf{E}} : \dot{\mathbf{E}} + \rho \frac{\partial \psi}{\partial z} \dot{z} + \rho \frac{\partial \psi}{\partial T} \dot{T}$$ \[7.39\]

$$\rho \dot{\psi} = \Sigma : \dot{\mathbf{E}} - \rho \Pi^f \dot{z} - \rho s \dot{T}$$

and also:

$$\rho s \dot{T} = -\rho T \frac{\partial^2 \psi}{\partial \mathbf{E} \partial T} : \dot{\mathbf{E}} - \rho T \frac{\partial^2 \psi}{\partial T^2} \dot{T} - \rho \frac{\partial^2 \psi}{\partial z \partial T} \dot{z}$$ \[7.40\]
Finally, we find:

$$\rho C_v \dot{T} - \kappa \Sigma \dot{z} - \rho (\Delta u - (1 - 2z)u_0) \dot{z} - r + \text{div} \mathbf{q} + 3\alpha TK_0 tr \dot{\mathbf{E}} = 0 \quad [7.41]$$

In practice, not all the terms are of the same importance, and often, the heat equation is reduced to:

$$\rho C_v \dot{T} - \kappa \Sigma \dot{z} - \rho(\Delta u) \dot{z} - r + \text{div} \mathbf{q} = 0 \quad [7.42]$$

Let us examine the case of a SMA wire with diameter \(d\) and length \(l\) [BEN 97]. Its exterior surface and its volume are, respectively, \(S_{amf} = \pi dl\) and \(V_{amf} = \frac{\pi d^2 l}{4}\).

For a wire with electrical resistance \(R\) heated by the Joule effect by the passage of an electrical current \(i\), the internal heat source \(r\) is written:

$$r = \frac{Ri^2}{V_{amf}} = \frac{16\rho_e \pi d^2 i^2}{\pi^2 d^4 i^2} \quad [7.43]$$

where:

$$\rho_e = z\rho_m + (1 - z)\rho_a \quad [7.44]$$

with \(\rho_a\), \(\rho_m\) and \(\rho_e\) respectively representing the resistivity of the austenite, the martensite and the biphase mixture.

Furthermore, the term \(\text{div} \mathbf{q}\) corresponds to the conductive and convective heat exchanges at the surface of the wire. For a thin wire (i.e. whose length-to-diameter ratio is greater than 50), in order to be able to discount the radial temperature gradients, to begin with, \(\text{div} \mathbf{q}\) represents the density of heat lost by convection on the lateral surface of the wire, so that:

$$\text{div} \mathbf{q} = \frac{h S_{amf}}{V_{amf}} = \frac{4h}{d^2} (T - T_a) \quad [7.45]$$

where \(h\) is the convection coefficient of the SMA and \(T_a\) the ambient temperature.

7.2.3. Extension to reversible phase transformation: austenite\(\Rightarrow\)R phase for NiTi [LEX 94]

This phase transformation between the austenite and a pre-martensite called the \(R\) phase as regards NiTi, is mechanically reversible, i.e. without hysteresis. As explained in Chapter 2, the existence of this transformation is dependent on the composition and the thermomechanical treatment of the alloy in question.
Although the amplitude of the deformation of the transformation $A \Rightarrow R$ never exceeds 0.7% (a little over 10% of that corresponding to the $A \Rightarrow M$ transformation for the same alloy), because the dissipation at each cycle is very small, the fatigue resistance is excellent. The use of this phase transition is absolutely operational for NiTi wires covered in an epoxide matrix, for instance; the whole forms an adaptive structure (see Chapter 9, exercise 3).

It is elementary to model simple traction.

Let the free energy be:

$$\rho \psi(E, z, T) = u_0^0 - T s_0^0 - z \Pi_f^0(T) + \frac{1}{2} E^*(E - \gamma z)^2$$

$$+ C_v(T - T_0 - T_Ln(T/T_0)) + \psi_{it}(1 - z)$$

[7.46]

[7.47]

where $E_A = E_R = E^*$ are the Young’s moduli of the austenite (taken to be equal to one another), and the stress:

$$\Sigma = \rho \frac{\partial \psi}{\partial E} = E^*(E - \gamma z)$$

[7.48]

and:

$$dD = \Pi^I dz = 0 \text{ for } [0, 1]$$

[7.49]

because there is no hysteresis.

This gives us:

$$\Pi^I(\Sigma, z, T) = - \frac{\partial \psi}{\partial z} = \Pi_f^0(T) + \frac{\gamma \Sigma}{\rho} + (1 - 2z) \psi_{it}(T) = 0 \forall z$$

[7.50]

and in particular:

$$\Pi^I(\Sigma = \Sigma^{ar}, z = 0, T) = - \frac{\partial \psi}{\partial z} = \Pi_f^0(T) + \frac{\gamma \Sigma^{ar}}{\rho} - \psi_{it}(T) = 0$$

[7.51]

$$\Pi^I(\Sigma = \Sigma^{ra}, z = 0, T) = - \frac{\partial \psi}{\partial z} = \Pi_f^0(T) + \frac{\gamma \Sigma^{ra}}{\rho} + \psi_{it}(T) = 0$$

[7.52]

We obtain the threshold stresses for the start of the forward transformation $\Sigma^{ar}$ and the reverse transformation $\Sigma^{ra}$:

$$\Sigma^{ar} = \frac{\rho}{\gamma} (-\Pi_f^0(T) + \psi_{it}(T))$$

[7.53]

$$\Sigma^{ar} = \frac{\rho}{\gamma} (-\Pi_f^0(T) - \psi_{it}(T))$$

[7.54]
where:
\[ \Sigma^{ar} - \Sigma^{ra} = 2\frac{\rho}{\gamma} \psi_{it} < 0 \]  [7.55]

which tells us that \( \psi_{it} < 0 \), by contrast to the classic \( A \Rightarrow M \) transformation.

The measurements of \( \Sigma^{ar} \) and \( \Sigma^{ra} \) at a given temperature \( T \) can be used to determine \( \Pi_0(T) \) and \( \psi_{it}(T) \).

It is elementary to model the traction curve (Figure 7.2) – that is:
– for the elastic austenitic domain, we plot a straight line from the origin \( \Sigma = 0 \) to \( \Sigma = \Sigma^{ar} \);
– we draw a second line between \( \Sigma^{ar} \) and \( \Sigma^{ra} \);
– beyond \( \Sigma^{ra} \), we draw a line parallel to the first with slope \( E^* \).

![Figure 7.2. Traction curves associated with the \( A \Rightarrow R \) transformation: a) experiment; b) simulation [LEX 94]](image)

While this method of modeling is easy, it introduces into the energy expression a term of interaction \( \psi_{it} z (1 - z) \) which is negative, which poses a problem in terms of the mixture of the two phases.

### 7.2.4. Multiaxial isothermal behavior

Shape-memory alloys used as actuators, for instance, are not simply wires subject to a traction stress. Examples of structural elements made of SMAs as well may be beams subject to flexion stress (see Chapter 8) which means we need to know the material’s response both under traction and compressive stress. The use of tubes, subjected to a twisting torque, requires us to be familiar with the SMAs’ behavior under shearing, and so on.

More generally speaking, for an increasingly broad range of applications, it is necessary to know the SMAs’ response to complex stresses.
Hitherto, models of thermomechanical behavior have been validated by way of uniaxial tests (using traction). Yet results on samples under traction and torsion (Rogueda et al. [ROG 96], Raniecki et al. [RAN 99], Taillard et al. [TAI 08], Grabe and Bruhns [GRA 09]) or under triaxial loading [GAL 98] (“carrot” of SMA subjected to lateral pressure and axial compression) show that their behavior is affected by a multiaxial stress state. Comparisons between the classic models and the experimental results under non-proportional loading demonstrate the need to enrich the databases in order to understand and model the mechanisms of formation and reorientation of martensite platelets ([LIM 99, MAR 96, SIT 95]).

The first task was to take account of the asymmetry between traction and compression. This asymmetry was measured on Cu-Zn-Al polycrystals by Vacher and Lexcellent in 1991 [VAC 91] and NiTi polycrystals by Orgas and Favier in 1998 [ORG 98a] (Figure 7.3).

Figure 7.3. Pseudo-elastic curve for NiTi under traction and compression: experiments performed by Orgas and Favier, simulation by Raniecki and Lexcellent [ORG 98a, RAN 98]

Indeed, in the domain of pseudo-elasticity ($T > A_f^0$), experimental observations show that:

a) the threshold stress for the start of transformation under traction $\Sigma_{am}^{T}$ has a smaller modulus than that measured under compression $\Sigma_{am}^{C}$;

b) the deformation for phase transformation associated with traction $\gamma_T$ is greater than that obtained under compression $\gamma_C$. However, the energies for traction and compression are equal – that is to say that:

$$\Sigma_{am}^{T} \gamma_T = \Sigma_{am}^{C} \gamma_C = C(T)$$  \hspace{1cm} [7.56]
c) as the threshold stresses $\Sigma_{am}^T$ and $\Sigma_{am}^C$ are linear functions of the temperature, it results that, is shown in Figure 7.4:

$$- \frac{d\Sigma_{am}^C}{dT} > \frac{d\Sigma_{am}^T}{dT}$$  \[7.57\]

\[\text{Figure 7.4. Clapeyron diagram showing traction and compression: schematic illustration}\]

\[d\) the hysteresis thickness obtained under compression is greater than that obtained under traction (Figure 7.3);

e) the behavior observed with pure shearing is symmetrical (see Figure 7.5).

\[\text{Figure 7.5. Hysteresis loop with pure shearing: Orgas and Favier’s experiment [ORG 98a]}\]

Figure 7.6 shows the theoretical modeling of the pseudo-elastic loop under tension/compression.
Now, the crux of the problem is to come up with an acceptable formula for $g^*(\Sigma)$ which is the equation governing the boundary of the elastic austenitic domain. The appropriate tools to do this are suggested by the plasticity.

Because the behavior of the two-phase medium is isotropic, and $\kappa$ is independent of the hydrostatic pressure, we suggest writing $g^*(\Sigma)$ in the form:

$$\rho g^*(\Sigma) = \gamma \Sigma g(y_\Sigma)$$  \[7.58\]

where $g(y_{\Sigma} = 0) = 1$.

If $S = \text{dev}(\Sigma)$ is the stress deviator, then:

$$\Sigma = \left(\frac{3}{2}SS\right)^\frac{1}{2}$$  \[7.59\]

corresponds to the equivalent Huber-von Mises stress.

$y_\Sigma$ is a function of $\Sigma$ and of the third invariant of the stress deviator tensor $J_3^S = \text{det}(S)$ and is chosen in dimensionless form:

$$y_\Sigma = \frac{27\text{det}(S)}{2\Sigma^3}$$  \[7.60\]

with $-1 \leq y_\Sigma \leq 1$. 

**Figure 7.6.** Theoretical illustration of the pseudo-elastic loop under traction/compression [RAN 98]
The value of $g(y_{\Sigma})$ may be freely chosen, with the proviso that it guarantees the convexity of the austenitic elastic domain.

Figure 7.6 illustrates the simulation by the $R_L$ model of the pseudo-elastic traction/compression curves.

With the introduction of the third invariant, it becomes possible to take account of the asymmetry between traction and compression, as done by Gillet et al. [GIL 96].

By derivation of $\rho g^*(\Sigma) = \gamma \Sigma g(y_{\Sigma})$ versus $\Sigma$, we obtain:

$$\kappa = \kappa + \kappa$$

where:

$$\kappa = \gamma \sqrt{\frac{3}{2}} g(y_{\Sigma}) N$$

$$\kappa = \gamma \sqrt{\frac{3}{2}} \frac{dg(y_{\Sigma})}{dy_{\Sigma}} (\sqrt{6} (N^2 - 1/3) - y_{\Sigma} N)$$

and $N = \sqrt{\frac{2}{3} S_{\Sigma}}$.

We obtain the equivalent transformation strain:

$$E^{tr} = \sqrt{\frac{2}{3}} E^{tr}; \quad E^{tr} = z \tau(y_{\Sigma})$$

where:

$$\tau(y_{\Sigma}) = \gamma \sqrt{(g(y_{\Sigma}))^2 + 9(1 - y_{\Sigma}^2) \left( \frac{dg(y_{\Sigma})}{dy_{\Sigma}} \right)^2}$$

This formulation was verified on a micromechanical model by Aleong et al. [ALE 02].

We have chosen two functions $g(y_{\Sigma})$:

– the first linear in $y_{\Sigma}$:

$$g(y_{\Sigma}) = 1 + ay_{\Sigma}$$

which guarantees the convexity of $g^*(\Sigma)$ if and only if $0 \leq a \leq 1/3$;

– the second in the form $\cos(\arccos)$, introduced by Bouvet et al. [BOU 02]:

$$g(y_{\Sigma}) = \cos(\frac{1}{3} \arccos(1 - a(1 - y_{\Sigma})))$$

which guarantees the convexity of $g^*(\Sigma)$ if and only if $0 \leq a \leq 1$. 
The phase transformation start surfaces can be obtained by:

\[ \rho g^*(\Sigma am(z = 0)) = b(T - M_0^s) \]  

[7.68]

The measurements show that the normality rule at the threshold phase transformation initiation surface \((A \Rightarrow M)\) regarding \(E^{IV}\) is verified in Figure 7.7.

![Figure 7.7. Curve of the boundary of the elastic austenitic domain obtained by way of biaxial mechanical tests performed on Cu-Al-Be [BOU 02]](image)

7.3. Anisothermal expansion [LEC 96] [LEX 06a]

The framework is strictly the same as the \(R_L\) model, except for the fact that instead of a single internal variable \(z\), we introduce two of them: the volume fraction of oriented martensite \(M_{\Sigma}^S\): \(z_{\Sigma}\) and the volume fraction of self-accommodating martensite \(M_T\): \(z_T\) as per the suggestion of Brinson et al. [BRI 93].

In the thermomechanical process, simple cooling of the austenite \(A\) gives rise to martensite \(M_T\), and simple heating causes the reverse transformation \(M_T \Rightarrow A\). An isothermal mechanical stress at \(T > M_0^s\) generates oriented martensite \(M_{\Sigma}\), and release of mechanical stress causes the reverse \(A \Rightarrow M_{\Sigma}\). The process of reorientation of the martensite variants, under stress, induces \(M_T \Rightarrow M_{\Sigma}\). Only the direct path \(M_{\Sigma} \Rightarrow M_T\) is not possible: this transformation has to pass through the intermediary austenitic phase \(A\). Any thermomechanical stress, particularly if it is non-proportional, will cause a martensitic transformation coupled with a reorientation of the martensite variants (Figure 7.8).
Figure 7.8. Possible phase transformation (T: temperature; Σ: stress)

The Helmholtz free energy of the “three-phase” system is written:

\[ \psi(E, T, z, z_T z_\Sigma) = (1 - z)\psi^{(1)} + z_T \psi^{(2)} + z_\Sigma \psi^{(3)} + \Delta \psi \]  \[7.69\]

with \( \alpha = 1 \) for austenite \( A \), \( \alpha = 2 \) for \( M_T \) and \( \alpha = 3 \) for \( M_\Sigma \), and:

\[ z = z_T + z_\Sigma \]  \[7.70\]

where \( z \) represents the overall volume fraction of martensite (and \( 1 - z \) that of austenite). \( z \) is divided into \( z_T \) – the volume fraction of self-accommodating martensite \( M_T \) – and \( z_\Sigma \) – the volume fraction of oriented martensite \( M_\Sigma \).

A “reasonable” expression of \( \Delta \psi \), which takes account both of the interaction between the austenite and martensite and that between the two martensite variants \( M_T \) and \( M_\Sigma \), is written:

\[ \Delta \psi = z(1 - z)\psi_{it} + z_T z_\Sigma \psi_{it}^{m} \]  \[7.71\]

where \( \psi_{it} \) and \( \psi_{it}^{m} \) are considered to be constant.

Consider:

\[ \rho \psi^{\alpha}(E_\alpha, T) = u_\alpha^0 - TS_\alpha^0 + \frac{1}{2}(E_\alpha - E_{\alpha}^{tr} - E_{\alpha}^{th})L(E_\alpha - E_{\alpha}^{tr} - E_{\alpha}^{th}) \]

\[ C_v(T - T_0 - T.Ln(T/T_0)) \]  \[7.72\]

with:

\[ \Sigma_\alpha = \rho \frac{\partial \psi^{\alpha}}{\partial E_\alpha} = L(E_\alpha - E_{\alpha}^{tr} - E_{\alpha}^{th}) = L E_\alpha^{el} \]  \[7.73\]

We shall extend what we wrote for the two-phase case \( (\alpha = 1, 2) \) to the three-phase case \( (\alpha = 1, 2, 3) \).
- 1st hypothesis:
  \[ E_{\alpha} = E_1^\text{th} = E_2^\text{th} = E_3^\text{th} = E_4^\text{th} = \alpha(T - T_0) \mathbf{1} \]  
  \[ \tag{7.74} \]

- 2nd hypothesis:
  \[ E_1^\text{tr} = E_2^\text{tr} = 0, \ E_3^\text{tr} = \kappa \]  
  \[ \tag{7.75} \]

- 3rd hypothesis:
  \[ E = (1 - z)E_1 + z_T E_2 + z_\Sigma E_3 \]  
  \[ \tag{7.76} \]

- 4th hypothesis: the stress state is indifferent to the phase state:
  \[ \Sigma = \Sigma_1 = \Sigma_2 = \Sigma_3 = \Sigma \Rightarrow E_\alpha = E_1 = E_2 = E_3 = E_4 = \Sigma \]  
  \[ \tag{7.77} \]

- and a 5th natural hypothesis because the two martensite variants are of the same crystallographic phase, i.e. \( u_2^0 = u_3^0 \) and \( s_2^0 = s_3^0 \), which gives us the expression of the free energy:
  \[ \rho \psi(E, z, T) = u_1^0 - T s_1^0 - z \Pi_0(T) \]
  \[ + \frac{1}{2} (E - \kappa z_\Sigma - \alpha(T - T_0) \mathbf{1}) L (E - \kappa z_\Sigma - \alpha(T - T_0) \mathbf{1}) \]
  \[ + C_v (T - T_0 - T_L n(\frac{T}{T_0})) + z(1 - z) \psi_{it} + z_T z_\Sigma \psi_{mt} \]  
  \[ \tag{7.79} \]

with:
  \[ \Sigma = \rho \frac{\partial \psi}{\partial E} = L(E - \kappa z_\Sigma - \alpha(T - T_0) \mathbf{1}); s = - \frac{\partial \psi}{\partial T} \]  
  \[ \tag{7.80} \]

and the thermodynamic forces associated with the internal variables:

\[ \Pi_0^\Sigma(T, z, z_T, T) = - \frac{\partial \psi}{\partial z_\Sigma} = \Pi_0^\Sigma(T) + \frac{\kappa}{\rho} (1 - 2z) \psi_{it}(T) - z_T \psi_{mt} \]  
\[ \Pi_0^z(T, z, z_\Sigma, T) = - \frac{\partial \psi}{\partial z_T} = \Pi_0^z(T) - (1 - 2z) \psi_{it}(T) - z_\Sigma \psi_{mt} \]  

In reference to Chapter 4, the dissipation of mechanical origin is written:

\[ dD = \Pi_0^\Sigma dz_\Sigma + \Pi_0^z dz_T \geq 0 \]  
\[ \tag{7.81} \]

In the particular case of reorientation, i.e. \( M_T \Rightarrow M_{\Sigma} \), we have:

\[ dz = 0 \implies dz_T = -dz_\Sigma \]  
\[ \tag{7.82} \]

and the mechanical dissipation term is then written:

\[ \Pi_0^{\Sigma, dz_\Sigma} \geq 0 \]  
\[ \tag{7.83} \]
where:
\[
\Pi_{T\Sigma}^\ell = \Pi_\Sigma^\ell - \Pi_T^\ell = \frac{\kappa}{\rho} \Sigma - (z_T - z_\Sigma) \psi_m^\ell
\]  \tag{7.84}

For any thermomechanical process in the field \((\Sigma, E, T)\), the Clausius-Duhem inequality must strictly be verified.

As before, we consider that for phase transformation processes, the start criterion will be the passage of the associated thermodynamic force through a value of 0. For instance, \(A \leftrightarrow M_\Sigma\) corresponds to \(\Pi_\Sigma^\ell = 0\) or \(A \leftrightarrow M_T\) corresponds to \(\Pi_T^\ell = 0\).

### 7.3.1. Kinetics of phase transformation or reorientation

As we have just seen, the explanation of the free energy enables us to determine the state equations and the thermodynamic forces associated with each internal variable. However, this information is not enough to describe a dissipative process. Consequently, there are no thermodynamic relations stemming from the free energy which can make explicit the kinetics of the volume fractions \(z_\Sigma\) and \(z_T\).

For any dissipative system, the missing equations can be obtained by introducing an additional thermodynamic function, namely a pseudo-potential of dissipation [MOR 70, HAL 74] or criterion functions like in elastoplasticity [LEC 96]. We assume the existence of five criterion functions \(\Phi_\Sigma^F, \Phi_\Sigma^R, \Phi_T^F, \Phi_T^R\) and \(\Phi_{T\Sigma}\) relating to the forward transformation: \(F:\ A \Rightarrow M_\Sigma,\ A \Rightarrow M_T\) and the reverse transformation \(R:\ M_\Sigma \Rightarrow A,\ M_T \Rightarrow A\) and to the reorientation of the martensite platelets \(M_T \Rightarrow M_\Sigma\).

In a formalism identical to that for plasticity, these functions \(\Phi\) are constant during the phase transformation associated with them; they are given by:

\[
\Phi_\Sigma^F = \Pi_\Sigma^\ell - k_\Sigma^F = Y_\Sigma^F \tag{7.85}
\]

\[
\Phi_\Sigma^R = -\Pi_\Sigma^\ell + k_\Sigma^R = Y_\Sigma^R \tag{7.86}
\]

\[
\Phi_T^F = \Pi_T^\ell - k_T^F = Y_T^F \tag{7.87}
\]

\[
\Phi_T^R = -\Pi_T^\ell + k_T^R = Y_T^R \tag{7.88}
\]

\[
\Phi_{T\Sigma} = \Pi_{T\Sigma}^\ell - k_{T\Sigma} = Y_{T\Sigma} \tag{7.89}
\]

\(Y_\alpha^F, Y_\alpha^R\) and \(Y_{T\Sigma}\) (\(\alpha = \Sigma\ or\ T\)) are non-negative constants, and \(k_\alpha^F, k_\alpha^R\) and \(k_{T\Sigma}\) [LEC 96] are functions which have the property of being null at the start of phase transformation (be it forward or reverse) or during reorientation.

The consistency equations \(d\Phi_\alpha^F = 0, \ d\Phi_\alpha^R = 0, \ d\Phi_{T\Sigma} = 0\) can be used to obtain the expressions of \(dz_\Sigma\) and \(dz_T\). The functions \(k_\alpha^F, k_\alpha^R\) and \(k_{T\Sigma}\) are chosen such that
we again find the classic kinetics used by metallurgists [KOI 59]:

\[
dz = (1 - z) \left[ \frac{\gamma aF}{\rho \Delta s} d\Sigma_{ef} - a^F b^F_s \left( e^{\exp(-b^F (T - M^0_s))} \right) dT \right]
\]
for \( A \Rightarrow M \) \[7.90\]

\[
dz_T = (1 - z_T) a^F T dz_T \text{ for } A \Rightarrow M_T \] \[7.91\]

\[
dz = (1 - z) \frac{\gamma a_T F}{\rho \Delta s} d\Sigma_{ef} \text{ for } M_T \Rightarrow M \Sigma \] \[7.92\]

with \( \Sigma_{ef} = \Sigma g(\gamma z) \) which is the effective stress.

Regarding the reverse phase transformation: \( M \Sigma \Rightarrow A, M_T \Rightarrow A \), a unique criterion function can be constructed in the plane of the stress deviator for any proportional or radial loading [LEX 06a]:

\[
\Phi^R_{\Sigma} = -\Sigma_{ef} + \Sigma^a_0 (z, z, T) \] \[7.93\]

\( \Sigma^a_0 \) being the threshold stress associated with the reverse transformation \( M \Sigma \Rightarrow A \).

The use of the maximum dissipation principle with the aim of obtaining the complementary laws (i.e. the kinetics) requires a convex elastic domain in order to ensure its unicity. However, in the case of the reverse transformation, this elastic domain is not convex, which suggests the construction of a “non-associated” constitutive “framework” using a function \( \chi(\Sigma, z, z, T) \) which verifies:

\[
\chi(\Sigma, z, z, T) < 0 \text{ when } \Phi^R_{\Sigma}(\Sigma, z, z, T) < 0 \\
\chi(\Sigma, z, z, T) = 0 \text{ when } \Phi^R_{\Sigma}(\Sigma, z, z, T) = 0 \] \[7.94\]

Such a function may be chosen thus:

\[
\chi(\Sigma, z, z, T) = -\Sigma \cdot \frac{E^r_{tr}}{E^{r}_{tr}} + \Sigma^a_0 (z, z, T) \] \[7.95\]

where \( E^r_{tr} = \gamma z \), and therefore:

\[
\frac{dE^r_{tr}}{dt} = \gamma \frac{dz}{dz_T} \frac{E^r_{tr}}{E^{r}_{tr}} \text{ i.e. } \kappa = \frac{\partial}{\partial \Sigma} \left( -\frac{\gamma}{\rho} \chi \right) \text{ and } E^r_{tr} = \kappa z \Sigma \] \[7.96\]

As before, \( dz \) derives from the consistency condition \( d\Phi_{\Sigma}^R = 0 \):

\[
dz = z \left[ \frac{\gamma a^F_{\Sigma}}{\rho \Delta s} d\Sigma_{ef} - a^F_{\Sigma} b^F_{\Sigma} \left( e^{\exp(-b^F (T - M^0_{\Sigma}))} \right) dT \right] \text{ for } M \Sigma \Rightarrow A \] \[7.97\]
The condition \( d\Phi_1^R = 0 \) gives us \( dz_T \):

\[
 dz_T = -a_T^R z_T dT 
\] \[7.98\]

The parameters are identified using traction curves (or compression curves) of the measurements of the anisothermal curves, in the stress-free state, and also the Clapeyron diagram \((\Sigma_{eff}, T)\) (Figure 7.9). This diagram is constructed on the basis of experimental observations: with small stresses, it is difficult to separate the stress-induced martensite \( M_{\Sigma} \) from purely thermally-induced martensite \( M_T \).

With the aim of getting around this problem in the space \((\Sigma_{eff}, T)\), a domain of self-accommodating martensite is defined at \( T < M_{f0} \) in addition to the two domains of austenite and oriented martensite.

For the practical identification of the parameters:

– the measurements of \( M_{s0} \) and \( A_{s0} \) give rise to two equations:

\[
 \Pi_T^f(\Sigma = 0, T = M_{s0}, z_T = 0, z_{\Sigma} = 0) = (\Delta u - u_0) - (\Delta s - s_0)M_{s0} = 0 \\
 f o r \ A \Rightarrow M_T 
\] \[7.99\]

\[
 \Pi_T^f(\Sigma = 0, T = A_{s0}, z_T = 1, z_{\Sigma} = 0) = (\Delta u + u_0) - (\Delta s + s_0)A_{s0} = 0 \\
 f o r \ M_T \Rightarrow A 
\] \[7.100\]

– regarding the pseudo-elastic behavior, the boundary values of initiation of the forward and reverse transformations are such that by integrating the fact that \( \Sigma: \kappa = \gamma \Sigma_{eff} \):

\[
 \Pi^f_{\Sigma}(\Sigma_{eff}, T, z_T = 0, z_{\Sigma} = 0) = \Pi^f_{\Sigma}(\Sigma_0, T = M_{s0}, z_T = 0, z_{\Sigma} = 0) \\
 f o r \ A \Rightarrow M_{\Sigma} 
\] \[7.101\]

Thus:

\[
 \Sigma_{eff} = \Sigma_0 - \rho \frac{(\Delta s - s_0)}{\gamma} (T - M_{s0}) = 0 
\] \[7.102\]

or by derivation:

\[
 \frac{d\Sigma_{eff}}{dT} = \rho \frac{(\Delta s - s_0)}{\gamma} = C_M 
\] \[7.103\]

\( C_M \) can be obtained on the basis of the measurement of the transformation start stresses for different isothermal traction curves \( \Sigma^{AM}_{\Sigma}(T) \) (Figure 7.9).
Similarly, for the reverse transformation $M_{\Sigma} \Rightarrow A$ we have:

$$
\Pi_{\Sigma}^{f}(\Sigma_{ef}, T, z_{T} = 0, z_{\Sigma} = 1 ) = \Pi_{\Sigma}^{f}(0, T = A_{0}^{s}, z_{T} = 0, z_{\Sigma} = 1 ) \tag{7.104}
$$

Thus:

$$
\Sigma_{ef} - \rho \frac{(\Delta s + s_{0})}{\gamma} (T - A_{0}^{s}) = 0 \tag{7.105}
$$

or by derivation:

$$
\frac{d\Sigma_{ef}}{dT} = \rho \frac{(\Delta s + s_{0})}{\gamma} = C_{A} \tag{7.106}
$$

$C_{A}$ is also determined experimentally (Figure 7.9).

With regard to the process of reorientation, the stress for initiation of this reorientation is governed by the following conditions:

$$
\Pi_{\Sigma T}^{f}(\Sigma_{ef}, T, z_{T} = 1, z_{\Sigma} = 0 ) = \Pi_{\Sigma T}^{f}(\Sigma_{0}, T = M_{0}^{s}, z_{T} = 1, z_{\Sigma} = 0 ) \tag{7.107}
$$

or by derivation:

$$
\Sigma_{ef} - \Sigma_{0} - \rho \frac{s_{0}^{m}}{\gamma} (T - M_{0}^{s}) = 0 \tag{7.108}
$$

thus:

$$
\frac{d\Sigma_{ef}}{dT} = -\rho \frac{s_{0}^{m}}{\gamma} = -C_{X} \tag{7.109}
$$
In addition, at every point at the start of reorientation, we have \(\Pi_{\Sigma}^{T} = 0\), so that:

\[
\Pi_{\Sigma}^{T}(\Sigma_0, T = M_0^s, \Sigma_T = 0) = \Sigma_0 - \frac{P}{\gamma}(u_{0}^{m} - M_0^s s_{0}^{m}) = 0 \quad [7.110]
\]

All these equations can be used to estimate the values of the six parameters of the model: \(\Delta u_0, \Delta s_0, u_0, s_0, u_0^{m}, s_0^{m}\), with \(\gamma\) being measured on one of the experimental curves.

7.3.1.1. Application of the \(R_L\) model

To date, no tools have been developed that are capable of truly modeling non-proportional loads. However, in Bouvet’s thesis, square and quarter-circle trajectories were carried out and made available to one and all (Figures 7.10 and 7.11).

![Figure 7.10. “Square” trajectory imposed under traction/internal pressure a); response in terms of strain b)](image)

![Figure 7.11. “Quarter-circle” trajectory imposed under bi-compression a); response in terms of strain b)](image)
7.3.2. Criticism of the $R_L$ approach

This approach, while it is very useful, does not really take account of the microstructure or of the changes in that microstructure during the course of thermomechanical loading. It assumes that the phase transformation is total, which is clearly not the case for polycrystals, because depending on their orientation in relation to the mechanical stress, some grains are not, or are scarcely, transformed!

Plainly speaking, there are phenomenological models inspired by plasticity such as the $R_L$ approach or the model developed by Aurrichio et al. [AUR 04, AUR 97].

Other models such as those of Panico and Brinson [PAN 07], Sadjadpour and Bhattacharya [SAD 07] and Chemisky et al. [CHE 11] introduce internal variables in order to incorporate certain microscopic data. To this end, Chemisky et al. [CHE 11] give an exhaustive review of these models including information about the microstructure.

Finally, there are other approaches such as the elasto-hysteresis models. These hereditary models “with discrete memory” put forward by Guelin et al. [GUE 76] will also be examined, at the end of this chapter. They are different in essence; indeed, it is not strains (elastic, transformation, etc.) which are added, but stresses (elastic, anelastic).

7.4. Internal variable model inspired by micromechanics

7.4.1. Introduction

We choose to describe the investigations by Chemisky et al. [CHE 11] followed by the approaches of Bhattacharya and his colleagues [KEL 08, KEL 12] and [SAD 07], which we compared with our own models, in a recent publication from Gibeau et al. [GIB 10].

7.4.2. Chemisky et al.’s model [CHE 11]

Their constitutive model includes martensitic transformation, martensite reorientation and accommodation of twinned martensite variants. This latter point is new in relation to $R_L$ and the choice of certain internal variables. It constitutes the extension of the works of Peultier et al. [PEU 06, PEU 08].

Conversely, the structure of the constitutive framework is the same as for $R_L$ – that of the generalized standard mediums described in Chapter 4.
7.4.2.1. Mechanisms of deformation considered

We shall examine the behavior of the REV, with – as usual – the size of this volume being statistically representative of the macroscopic behavior. When a thermomechanical stress is applied, five mechanisms cause macroscopic deformation:

– elastic deformation $E^{el}$;
– thermal expansion $E^{th}$;
– anelastic deformation due to the martensitic transformation $E^{tr}$;
– anelastic deformation due to the accommodation of twins between the martensite variants $E^{tw}$;
– plastic or visco-plastic deformation, which will not be discussed here.

If we assume that all the phases are isotropic and have the same thermoelastic constants, the elastic and thermal deformations are classic:

$$E^{el} = M \Sigma = L^{-1} \Sigma \quad [7.111]$$

$$E^{th} = \alpha (T - T_0) I \quad [7.112]$$

with:

$$E^{tr} = \frac{1}{V} \int_V \varepsilon^{tr}(r) dV = \frac{V_M}{V} \frac{1}{V_M} \int_{V_M} \varepsilon^{tr}(r) dV = z \kappa$$ \quad [7.113]

and:

$$E^{tw} = \frac{1}{V} \int_V \varepsilon^{tw}(r) dV = \frac{V_{FA}}{V} \frac{1}{V_{FA}} \int_{V_{FA}} \varepsilon^{tw}(r) dV = z_{FA} \kappa^{tw}$$ \quad [7.114]

where the "$\varepsilon$" values are considered to be deformations at the local scale.

This relation is obtained if we consider that the "twins" appear only in the volume occupied by the self-accommodating martensite $V_{FA}^A$, thus, the resulting local deformation $\varepsilon^{tw}(r)$ has a non-null value in this volume. $z_{FA}$ denotes the volume fraction of self-accommodating martensite $V_{FA}^A / V$. $z_T$ differs from $z_{FA}$, the volume fraction of martensite $M_T$ defined by Brinson [BRI 93] and used in $R_L$.

The total macroscopic deformation is written:

$$E = E^{el} + E^{th} + E^{tr} + E^{tw} \quad [7.115]$$

where:

$$E = M : \Sigma + \alpha (T - T_0) I + z \kappa + z_{FA} \kappa^{tw} \quad [7.116]$$
7.4.2.2. Internal variables and physical limitations

In this model, there are four internal variables, namely:
- the volume fraction of martensite \( z \);
- the martensite transformation deformation \( \kappa \);
- the volume fraction of self-accommodating martensite \( z_{FA} \);
- the accommodation of the “twins” \( \kappa_{tw} \).

The physical limitations are as follows:
- \( z \in [0, 1] \), obviously;
- the phase transformation takes place with no change in volume, as is assumed to be the case in most models existing in the literature;
- the existence of a maximum phase transformation modulus called \( E_{tr}^{max} \) which is greater than a \( E_{sat}^{tr} \) if the transformation saturates (i.e. is not complete);
- we naturally assume that \( E_{sat}^{tw} < E_{sat}^{tr} \).

A ratio between the two macroscopic deformations is defined by:
\[
\eta_e = 1 - \left( \frac{E^{tr}_{sat} z_{FA}}{E_{sat}^{tr}} \right) \tag{7.117}
\]
and:
\[
E_{max}^{tr} = E_{sat}^{tr} \left( 1 - \frac{z_{FA}}{z} \right) \eta_e \tag{7.118}
\]

This generalizes the formulation advanced by Peultier et al. [PEU 06], where \( E_{max}^{tr} \) was considered to be constant.

For the kinetics of the volume fraction of self-accommodating martensite \( z_{FA} \), we choose:
\[
\dot{z}_{FA} = \zeta_{FA} \dot{z} = \begin{cases} 
\frac{E_{sat}^{tr} - E_{sat}^{tr}_{eq} \dot{z}}{E_{sat}^{tr}_{eq}}, & \dot{z} > 0 \\
\frac{z_{FA} \dot{z}}{z}, & \dot{z} < 0
\end{cases} \tag{7.119}
\]
where \( E_{eq}^{tr} \) is the equivalent von Mises transformation strain. The symbol \( r \) corresponds to the point of inversion of the stress applications and the corresponding volume fractions.
7.4.2.3. Thermodynamic potential

Consider the Gibbs free energy $G$, typically defined by:

$$G = u^0_1 - T s^0_1 - z \Pi^0(T) - \Sigma: E + G_{\text{int}} + C_p \left( T - T_0 - T \ln \left( \frac{T}{T_0} \right) \right)$$ \[7.120\]

This formulation is in the same vein as the $R_L$ models, except that their interaction term $G_{\text{int}}$ is grounded in micromechanics. With $\sigma$ being the local stress, the elastic energy is written as:

$$G_{\text{int}} = \frac{1}{2V} \int_V \sigma(r): \varepsilon^{el}(r)dV $$ \[7.121\]

$G_{\text{int}}$ can be expressed as a function of the total deformation and of the other anelastic deformations:

$$G_{\text{int}} = \frac{1}{2V} \int_V \sigma(r): (\varepsilon(r) - \varepsilon^{th}(r) - \varepsilon^{tr}(r) - \varepsilon^{tw}(r))dV$$ \[7.122\]

or if we use the lemma put forward by Hill-Mandel [HIL 63], we can extract the macroscopic and thermal deformations of the integral:

$$G_{\text{int}} = \frac{1}{2} (\Sigma: E - \Sigma: E^{th}) - \frac{1}{2V} \int_V \sigma(r): (\varepsilon^{tr}(r) + \varepsilon^{tw}(r))dV$$ \[7.123\]

In order to consider the contribution of each mechanism in the internal energy, we write the local stress as the sum of an average contribution, i.e. the macroscopic stress and its local fluctuation around this value:

$$\sigma(r) = \Sigma + \delta \sigma(r)$$ \[7.124\]

This leads us to the following expression of $G_{\text{int}}$:

$$G_{\text{int}} = \frac{1}{2} \Sigma: (E - E^{th} - E^{tr} - E^{tw}) - \frac{1}{2V} \int_V \delta \sigma(r): \varepsilon^{tr}(r)dV$$

$$- \frac{1}{2V} \int_V \delta \sigma(r): \varepsilon^{tw}(r)dV$$ \[7.125\]

$$G_{\text{int}} = \frac{1}{2} \Sigma: M: \Sigma - \frac{1}{2V} \int_V \delta \sigma(r): \varepsilon^{tr}(r)dV$$

$$- \frac{1}{2V} \int_V \delta \sigma(r): \varepsilon^{tw}(r)dV$$ \[7.126\]

The fluctuation of the stress field must be linked to the intergranular and intragranular incompatibilities. We assume that $\delta \sigma$ must be decomposed into three on different scales:
– between each grain $\delta \sigma_1$;
– between each variant $\delta \sigma_2$;
– between each twin-pair in the variant $\delta \sigma_3$.

In addition, we assume that the fluctuation of $\delta \sigma_1$ increases proportionally with $\kappa$. Hence:

$$\frac{1}{2V} \int_V \delta \sigma_1(r) : \varepsilon^{tr}(r) dV = \frac{1}{2} \int_V H \kappa(r) : \kappa(r) dV = \frac{1}{2} z H \kappa : \kappa$$  \text{[7.127]}$$

The fluctuations between each variant $\delta \sigma_2$ were considered by Siredey et al. [SIR 99]. Using interfacial operators, the matrix $H^{mn}$ is defined in order to take the incompatibilities between each variant and the elastic energy in the grain $N$ thus written:

$$w^{N \text{int.}} = \frac{1}{2} \sum_{m,n} z_m H^{mn} z_n$$  \text{[7.128]}$$

and finally, they replace this term with a quadratic form of the energy in $z$ in the form:

$$\frac{1}{2V} \int_V \delta \sigma_2(r) : \varepsilon^{tr}(r) dV = \frac{1}{2} H z^2$$  \text{[7.129]}$$

In addition, the reasoning is the same for the accommodation of the “twins”:

$$\frac{1}{2V} \int_V \delta \sigma_3(r) : \varepsilon^{tw}(r) dV = \frac{1}{2} z_{FA} H_{tw} \kappa^{tw} : \kappa^{tw}$$  \text{[7.130]}$$

where:

$$- \mathbf{\Sigma} : \mathbf{E} = - \mathbf{\Sigma} : M \mathbf{\Sigma} - \mathbf{\Sigma} : \kappa z - \mathbf{\Sigma} : \kappa^{tw} z_{FA} - \mathbf{\Sigma} : \alpha(T - T_0) 1$$  \text{[7.131]}$$

We get the detailed expression of the Gibbs free energy $G$:

$$G = U^0_1 - T s^0_1 - z \Pi^0_0(T) - \frac{1}{2} \mathbf{\Sigma} : M \mathbf{\Sigma} - \frac{1}{2} \mathbf{\Sigma} : \kappa z - \mathbf{\Sigma} : \kappa^{tw} z_{FA} - \mathbf{\Sigma} : \alpha(T - T_0) 1$$  \text{[7.132]}$$

$$+ \frac{1}{2} z H E \kappa : \kappa + \frac{1}{2} H z^2 + \frac{1}{2} z_{FA} H_{tw} \kappa^{tw} : \kappa^{tw}$$

$$+ C_p(T - T_0 - T L n(T/T_0))$$

where $G = G(\mathbf{\Sigma}, T, \kappa, \kappa^{tw}, z)$. It should be noted that $z_{FA}$ does not have the status of an internal variable: its derivative is linked to the derivative of the volume fraction of martensite $z$ (see equation [7.119]):

$$E = - \frac{\partial G}{\partial \mathbf{\Sigma}} \quad s = - \frac{\partial G}{\partial T}$$  \text{[7.133]}$$
As indicated in Chapter 4, the Clausius-Duhem inequality is written in terms of free energy $G$, and we distinguish the intrinsic dissipation $\phi_1$ from the thermal dissipation:

$$\phi_1 = \Pi^f \dot{z} + \Pi_\kappa \dot{\kappa} + \Pi_{\kappa^{tw}} \kappa^{tw} [7.134]$$

$$\phi_2 = -q \frac{\text{grad}T}{T} [7.135]$$

with the definition of the three thermodynamic forces:

$$\Pi^f = -\frac{\partial G}{\partial z} = \Pi_0^f(T) + \Sigma : \kappa + \zeta_{FA} \Sigma : \kappa^{tw} - \frac{1}{2} H_{E \kappa} \kappa - H_z z [7.136]$$

$$\Pi_\kappa = -\frac{\partial G}{\partial \kappa} = (\text{dev} \Sigma) z - z H_\kappa [7.137]$$

$$\Pi_{\kappa^{tw}} = -\frac{\partial G}{\partial \kappa^{tw}} = (\text{dev} \Sigma) z_{FA} - H_{tw} \kappa^{tw} z_{FA} [7.138]$$

knowing that the phase transformation is deviatoric: $\text{tr} \kappa = \text{tr} \kappa^{tw} = 0$.

The accommodation of the “twins” is supposed to be reversible, i.e. without hysteresis in regard to transformation and reorientation.

Thus, we divide the intrinsic dissipation into two contributing factors (the third disappears):

$$\phi_{1z} = \Pi_{\kappa^{tw}}^e \dot{z} [7.139]$$

$$\phi_{1\kappa} = \Pi_{\kappa^{tw}}^e z \dot{\kappa} [7.140]$$

The authors choose $\Pi_0^f(T) = -B(T - T_0)$. For this reason, they introduce criterion functions that take account of the positivity of the dissipation:

$$\Pi_{\kappa^{tw}}^e = \Pi_{\kappa^{tw}}^{e_{max}} + (B_f - B)(T - T_0) \text{ if } \dot{z} > 0 [7.141]$$

$$\Pi_{\kappa^{tw}}^e = -\Pi_{\kappa^{tw}}^{e_{max}} + (B_f - B)(T - T_0) \text{ if } \dot{z} < 0 [7.142]$$

Furthermore, the stabilization of martensite observed by several authors ([LIU 00, PIA 93]) is linked to the transformation strain. This stabilization entails the modification of the Clausius–Clapeyron diagram including two critical temperatures for the reverse transformation, depending on whether the martensite is $M_\Sigma$ or $M_T$. A linear function of the equivalent martensite deformation is introduced in order to take account of the temperature dependency of the transformation, with the amplitude $\kappa_{eq}(\frac{1}{2} \kappa: \kappa)^\frac{1}{2} = |\kappa|$. Thus:

$$\phi_{1\text{stab}} = -H_s \kappa_{eq} \dot{z} [7.143]$$
We get:

$$\Pi_z = \Pi_{z}^{\text{max}} + (B_f - B).(T - T_0)H_z \kappa_{eq} \text{ if } \dot{z} > 0 \ A \Rightarrow M$$ [7.144]

$$\Pi_z = -\Pi_{z}^{\text{max}} + (B_f - B).(T - T_0)H_z \kappa_{eq} \text{ if } \dot{z} < 0 \ M \Rightarrow A$$ [7.145]

An isotropic criterion is chosen in order to describe the reorientation surface. When $\Pi_{\kappa}^{\text{max}}$ is constant, we get:

$$|\Pi_{\kappa}|_{\Sigma} = z\Pi_{\kappa}^c$$ [7.146]

where $|\cdot|_{\Sigma}$ corresponds to the equivalent von Mises stress. Consider $\Pi_{\kappa} = z\Pi_{\kappa}^c$; in this case:

$$|\Pi_{\kappa}^c|_{\Sigma} = \Pi_{\kappa}^{c\kappa}$$ [7.147]

As the dissipation associated with the accommodation of the “twins” is ignored, the associated thermodynamic forces are null, meaning that:

$$\Pi_{\kappa}^{tw} = z\Pi_{\kappa}^{c\kappa} = 0$$ [7.148]

It should not be forgotten that $z \in [0, 1]$ – a condition which may necessitate the introduction of the Lagrange multipliers; for instance:

$$\lambda_0 = 0 \ if \ z \geq 0 \ \lambda_0 > 0 \ otherwise$$ [7.149]

$$\lambda_1 = 0 \ if \ z \leq 1 \ \lambda_1 > 0 \ otherwise$$ [7.150]

The deformation $\kappa_{eq}$ must be limited by $\kappa_{max}$; we introduce $\lambda_2$ such that:

$$\lambda_2 = 0 \ if \ \kappa_{eq} \leq \kappa_{max} \ \lambda_2 > 0 \ otherwise$$ [7.151]

The thermodynamic forces are modified by adding the multipliers to the initial forces:

- Conjugate force of $z$:

$$F_Z = \Pi_z - \lambda_0 - \lambda_1 = -B(T - T_0) + \Sigma: \kappa + \zeta_{FA}\Sigma: \kappa^{tw}$$

$$-\frac{1}{2}H_{\epsilon}\kappa: \kappa - H_z z - \frac{1}{2}\zeta_{FA}H_{tw}\kappa^{tw}: \kappa^{tw} - \lambda_0 - \lambda_1$$ [7.152]

- Force conjugated to $\kappa$:

$$F_{\kappa} = \Pi_{\kappa}^c - \lambda_2 \kappa = (\text{dev} \Sigma) - H_{\epsilon}\kappa - \lambda_2 \kappa$$ [7.153]

- Force conjugated to $\kappa^{tw}$:

$$F_{\kappa}^{tw} = \Pi_{\kappa}^{c\kappa} = (\text{dev} \Sigma) - H_{tw}\kappa^{tw}$$ [7.154]
7.4.2.4. Description of the internal loops

With constant values of the threshold thermodynamic forces, if we seek to simulate an internal loop, the answer is that it does not exist (see Figure 7.12a)!

In the other cases, it is the experimental response that must be reproduced! Figure 7.12b corresponds to the approach advanced by Gillet et al. [GIL 98] and used by Peultier et al. [PEU 06], where the critical value for the internal loops is defined as being proportional to $z$.

Finally, Chemisky et al. [CHE 11] choose the scenario illustrated in Figure 7.12c.

Case (d) corresponds to the simulation run by Lexcellent and Tobushi [LEX 95] of experimental loops obtained for a NiTi alloy. The formulation uses the concept of memory points, first introduced by Wack et al. [WAC 83]. It is therefore necessary to introduce a variable $\gamma_z$ which defines the evolution of the phase transformation during the forward or reverse incomplete transformation:

$$\gamma_z = \left| \frac{z - z_{\text{mem}}}{z^{\text{obj}} - z_{\text{mem}}} \right|$$

where $z_{\text{mem}}$ is the typical fraction of martensite and $z^{\text{obj}}$ is the value obtained if the transformation reaches the saturation point:

$$F_{Z}^{cr} = (1 - \gamma_z)F_{Z}^{min} + \gamma_z F_{Z}^{max} + (1 - \gamma_z)F_{Z}^{mem}$$

$$+(B_f - B).(T - T_0) - H_s \kappa_{eq} A \Rightarrow M$$

$$F_{Z}^{cr} = (1 - \gamma_z)F_{Z}^{min} + \gamma_z F_{Z}^{max} - (1 - \gamma_z)F_{Z}^{mem}$$

$$+(B_r - B).(T - T_0) - H_s \kappa_{eq} M \Rightarrow A$$

$F_{Z}^{min}$ and $F_{Z}^{max}$ are material parameters which define the minimum and maximum critical forces and $F_{Z}^{mem}$ is memorized each time the applied load changes direction.

Empirically speaking, we define $F_{z}^{max}$ by:

$$F_{z}^{max} = B \frac{A_f - M_s}{2}$$

and the ratio between $F_{z}^{min}$ and $F_{z}^{max}$ by:

$$r_f = 1 - \frac{F_{z}^{min}}{F_{z}^{max}}$$

7.4.2.5. Asymmetry between traction and compression

For pseudo-elastic behavior, phase transformation surfaces have been defined on the basis of the Prager equation in order to take account of the asymmetry between
traction and compression ([PAT 95]). In this vein, many authors have proposed similar
criterion surfaces ([ORG 98a, QID 00, LEX 06a, CAL 06] and [LEX 06b]). In the
wake of the work of Peultier et al. [PEU 08], in order to integrate the asymmetry,
we propose an expression of $E_{\text{sat}}^{tr}$ in the space of transformation deformations, in the
form:

$$E_{\text{sat}}^{tr} = K \sqrt{1 + \frac{\beta J_3}{J_2^2}}$$

with:

$$J_2 = \frac{1}{2} \kappa \kappa; J_3 = \frac{1}{3} \kappa \kappa \kappa$$

This relation can be generalized to the power $1/n$:

$$E_{\text{sat}}^{tr} = K \left(1 + \frac{\beta J_3}{J_2^2}\right)^{\frac{1}{n}}$$

$K$ and $\beta$ can be identified using traction and compression tests, which enable us to
determine the saturation values $E_{\text{trac}}^{tr}$ and $E_{\text{comp}}^{tr}$:

$$K = E_{\text{trac}}^{tr} \left(1 + \frac{\beta}{\alpha}\right)^{-\frac{1}{n}}$$

$$\beta = \left(\frac{1 - \gamma}{1 + \gamma}\right) \alpha$$

where $\alpha$ is a constant value stemming from the definitions $J_2$ and $J_3$ ($\alpha \approx 2.6$) and $\gamma$
constitutes the ratio between traction and compression to the power $n$:

$$\gamma = \left(\frac{E_{\text{comp}}^{tr}}{E_{\text{trac}}^{tr}}\right)^n$$

$\beta$ is the asymmetry parameter. Note that if $\beta = 0$, i.e. if $E_{\text{trac}}^{tr} = E_{\text{comp}}^{tr}$, the
expression of $E_{\text{sat}}^{tr}$ gives the equivalent von Mises deformation.

The equations presented above are considered when the thermodynamic forces
$F_z, F_\kappa, F_{\kappa z}$ are activated. Otherwise, there are various different scenarios:

- $\dot{z} = 0, \dot{\kappa} = 0$ – neither reorientation nor transformation;
- $\dot{z} = 0, \dot{\kappa} \neq 0$ – reorientation;
- $\dot{z} \neq 0, \dot{\kappa} \neq 0$ reorientation and/or transformation;
- $\dot{z} \geq 0, \dot{\kappa} \neq 0$ forward transformation;
- $\dot{z} \leq 0, \dot{\kappa} \neq 0$ reverse transformation.
In addition:

\[ \dot{E}^{tr} = 0 \text{ equivalent to } z \dot{k} + \dot{k} = 0 \]  

[7.166]

Finally, the direction of \( \dot{k} \) follows the direction of \( F_k \) when reorientation occurs:

\[ \dot{k} = \hat{\lambda}_k \frac{F_k}{|F_k| \Sigma} \]  

[7.167]

When reorientation is not activated, then:

\[ \dot{k} = \hat{\lambda}_k \frac{\kappa}{|\kappa| E} \]  

[7.168]

In the next section, the model is used to describe the behavior of the REV when a homogenous stress state is applied.

7.4.2.6. Application to thermomechanical stresses

In this section, a unique set of parameters for classic NiTi alloys will be used.

| \( E \) (MPa) | \( \nu \) | \( E^{tr}_{irr} \) | \( E^{tr}_{irr}+E^{tr}_{comp} \) | \( E^{tr}_{comp} \) |
| 70,000 | 0.3 | 0.05 | 0.04 | 0.04 |
| \( B_Z \) (MPa°C\(^{-1}\)) | \( B_r \) (MPa°C\(^{-1}\)) | \( M_s \) (°C) | \( A_f \) (°C) | \( r_z \) |
| 0.25 | 0.3 | 20 | 60 | 0.6 |
| \( F_E \) (MPa) | \( H_Z \) (MPa) | \( H_m \) (MPa) | \( H_{irr} \) (MPa) | \( H_s \) (MPa) |
| 100 | 4 | 1,000 | 40,000 | 50 |

Figure 7.12. Internal loops for pseudo-elastic behavior: a) no internal loops; b) see [GIL 98]; c) proposed model; d) Lexcellent and Tobushi model [LEX 95]; e) nonlinear response
Simulations of the uniaxial tests:

- the possible internal loops for pseudo-elastic behavior are proposed in Figure 7.12;
- isothermal traction tests where the accommodation of the twins plays a part (Figure 7.13);

![Figure 7.13. Traction tests around the $M_s$ temperature. Impact of the mechanisms of accommodation of the “twins” [CHE 11]](image)

- pseudo-elastic behavior with internal loops (Figure 7.14);

![Figure 7.14. Behavior under traction/pseudo-elastic compression with internal loops [CHE 11].](image)

- for different levels of total strains imposed, there are anisothermal trajectories of stress (Figure 7.15). A similar simulation was offered by Gabry et al. [GAB 00] with $R_L$ anisothermal on thin films of NiTi;
Figure 7.15. Trajectory of anisothermal stresses at different levels of strain imposed [CHE 11]

– deformation/temperature loops at different levels of imposed stresses (Figure 7.16);

Figure 7.16. Anisothermal behavior under respective imposed stresses of 50, 100, 150, 200 and 300 MPa [CHE 11]

– recovering stress, which could be called “a forced return” (see Chapter 2 for the applications; Figure 7.17);
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Figure 7.17. Recovering stress: (left) pre-conditioning; (right) change in the recovering stress with changing temperature [CHE 11],

– strain/temperature loops at different levels of imposed stresses, with the associated Clausius–Clapeyron diagram (Figure 7.18).

Figure 7.18. (Left) Strain/Temperature loops; (right) Clausius–Clapeyron diagram according to [WU 03]

Multiaxial tests:

– surfaces of the start and end of phase transformation (see equation [7.162]) in the stress space (Figure 7.19); the form of these curves is identical to that determined by Bouvet et al. for Cu-Al-Be (Figure 7.7, [BOU 02]);

– surfaces of the start and end of reorientation (Figure 7.20); the start surface has already been identified on another NiTi alloy by Laverhne-Taillard et al. [LAV 08] by way of traction/torsion testing;

– in the square trajectory under shear strain/axial strain, it cannot be said that the effect of the temperature (which determines the initial state of the material: austenitic or martensitic, i.e. at the start of reorientation or phase transformation) is evident (Figure 7.21).
7.4.2.7. Criticism of Chemisky et al.’s model

This model offers an undeniable advantage for micromechanics with analysis of the intergranular and intragranular stresses between the variants, and also between “twinned pairs” of the same variant. This is to assume that all the variants are “twinned”, which is inconsistent with the findings of the CTM (Chapter 3) and of certain research by Balandraud and Zanzotto [BAL 07] and Lexcellent and
Blanc [LEX 04]. Perhaps it would be more advantageous to move away from the phenomenological theory of martensite (or WLR, for Wechsler, Lieberman and Read [WES 53, BOW 54]) used by the authors in their work, to the more modern CTM, founded by Ball and James [BAL 87, BAL 92]. However, the question of the evolution of the microstructure under stress in reorientation and/or transformation remains unanswered, and the associated observations will be invaluable in altering the models [BER 11].

![Figure 7.21](www.iran-mavad.com)

**Figure 7.21.** a) Square trajectory of load application in the stress space: shear strain versus axial strain; b) 0°C; c) 40°C; d) 80°C [CHE 11]

The model put forward by Kelly and Bhattacharya [KEL 12], which is more mathematical but which also integrates micromechanics into its construction, will complete this chapter.

**7.4.3. Kelly and Bhattacharya’s model [KEL 08, KEL 12]**

The starting point for this model is the observation that the mechanisms of initiation of the martensitic transformation are fundamentally different from those associated with saturation of the martensitic transformation, which occurs at the end of the loading.

To this effect, the authors of [KEL 12] carefully examine the pseudo-elastic curve (Figure 7.22) in order to introduce the finer points of their model:
The amplitude of the initial plateau, the intensity of the hardening, the saturation, etc., vary greatly depending on the material chosen or the control mechanism (using speed of displacement or force, for instance), but the curve (Figure 7.22) input is much more representative of NiTi-based SMAs than copper-based ones.

Figure 7.22. Schematic representation of a “NiTi-type” pseudo-elastic curve [KEL 12]

In order to understand the mechanisms at work, let us examine the behavior of a monocrystal at $T \geq A_f^0$. At this temperature, the austenite is a stable phase and the martensite metastable. The martensitic transformation $A \Rightarrow M_{\Sigma}$ takes place without hardening, and the reverse transformation $M_{\Sigma} \Rightarrow A$ does too, with a threshold stress slightly lesser than the initiation and a plateau (see Figure 7.23) [GOO 97]. If we take account of the anisotropies inherent to the monocrystal, it is not surprising that the pseudo-elastic response depends on the orientation (see Chapter 5: traction tests on a Cu-Al-Ni alloy).

The situation is considerably more complicated for a polycrystal. In the transformation strain, the microstructure is the response of the grains to a particular applied stress. Everything depends on the crystallographic orientation of each grain in the aggregate, giving rise to intergranular stresses.
In a polycrystal, phase transformation is a complex process. In the austenite, under mechanical loading, the stress in the polycrystal is largely uniform, except for an elastic anisotropy effect on the phase.

The grain in the best orientation in relation to the direction of loading will attempt to transform. It is impossible for the entire grain to completely transform, because of the stresses exerted by the surrounding grains, and transformation takes place in isolated regions, as observed by Brinson et al. [BRI 04] (Figure 7.24) and Daly et al. [DAL 08]. Finally, Sittner and Novak [SIT 00] noted that a model with uniform stress in the polycrystal, known as a Sachs-type model, accurately describes the initiation of the transformation, which corroborates our predictions concerning the surfaces of initiation of phase transformation [LEX 02].

In summary, the initiation of transformation is governed by well-oriented grains corresponding to the loading direction.

As the best-oriented grains begin to transform, the stress becomes extremely heterogeneous, which causes the transformation to advance rapidly (AB plateau on the curve shown in Figure 7.22). At the end of the plateau, the transformation is still nowhere near complete, and for it to continue, the stress must be increased, which results in hardening (BC curve). The transformation is entirely heterogeneous, as is the stress [BRI 04, DAL 08]. This means that variants other than those initially present appear, and this manifests itself by martensite reorientation.

As the transformation progresses, even the badly-oriented grains transform. However, their transformation deformation in the direction of loading is lesser, and we come to point C, which may be thought of as the saturation point. This is one of the reasons for which models with uniform deformation in the polycrystal (so-called Taylor models) [BHA 05] offer a good description of the macroscopic transformation strains. Thus, the saturation of the transformation is governed by “poorly”-oriented
grains. Figure 7.24 clearly shows initiation on the one hand and saturation on the other [BRI 04].

![Micrograph taken under polarized light by Brinson et al. on a polycrystalline NiTi alloy: a) initiation of phase transformation; b) saturation of phase transformation [BRI 04]](image_url)

One consequence of these observations lies in the fact that the initiation and saturation are governed by two different criteria (Sachs and Taylor) and that the straight-lined Clausius–Clapeyron diagram no longer holds true for a polycrystal.

With two different processes we associate two different kinematic quantities:

- the nominal martensite transformation strain $\kappa$ governs initiation;
- the effective transformation strain $E^{tr} = \kappa z$ governs saturation.

7.4.4. Internal variable model taking account of initiation, reorientation and saturation [KEL 12, SAD 07, KEL 08]

As already highlighted, this model exhibits similarities with those of Panico and Brinson [PAN 07] and Chemisky et al. [CHE 11].

7.4.4.1. Kinematics and limitations

The observable variables are the total strain $E$ and the temperature $T$. 
The internal variables are the volume fraction of martensite \( z \) and the nominal martensite transformation strain \( \kappa \).

The stress on the variable \( z \) is evident:

\[
z \in [0, 1]
\]

The existence of two domains of deformation – that of the nominal transformation strains \( G_i^* \) and that of effective transformation strains \( G_s^* \), where \( G_i^* \supset G_s^* \) (\( i \) as initiation; \( s \) as saturation) – imposes the following condition:

\[
\kappa \in G_i^* \text{ and } \mathbf{E}^{tr} = \kappa z \in G_s^*
\]

The domain \( G_i^* \) is defined as the domain of all the averages of the martensite variants in the grains:

\[
\kappa \in G_i^* = \left\{ \xi : \xi = \sum_{i,n} \mu_{i,n} Q_n^T \kappa_i Q_n \mu_{i,n} \geq 0, \sum \mu_{i,n} = 1 \right\}
\]

where \( \mu_{i,n} \) constitutes the volume fraction of the martensite variant \( i \) in the grain \( n \) and \( Q_n \) is the rotation matrix which describes the crystallographic orientation of the grain \( n \). Note that this domain considers all the possible arrangements of the martensite variants, regardless of the compatibility between these variants. However, let us not forget that \( G_i^* \) corresponds to the initiation of the transformation.

By contrast, \( G_s^* \) is limited to the microstructures which satisfy the compatibility conditions between the martensite variants and is limited by networks of “poorly-oriented” grains:

\[
\mathbf{E}^{tr} = \kappa z \in G_s^* = \left\{ \xi : \xi = \text{deformation of average transformation of a microstructure compatible with martensite} \right\}
\]

A schematic representation of the \( G_{i,s}^* \) domains can be given – see Figure 7.25.

In a one-dimensional regime, \( \kappa \) becomes a scalar and \( G_i \) and \( G_s \) are two overlapping intervals:

\[
G_{i,s}^* = [\kappa_{i,s}^c, \kappa_{i,s}^t], \quad \kappa_{i,s}^c \leq \kappa_{i,s}^s \leq \kappa_{i,s}^t
\]

This formulation integrates the asymmetry between traction and compression which has been demonstrated experimentally [ORG 98a, VAC 91].
Figure 7.25. Schematic representation of $G_{i,s}^*$

Figure 7.26 shows the area where the volume fraction of the martensite $z$ and the nominal transformation strain $\kappa$ are both limited.

Figure 7.26. The volume fraction of martensite $z$ and $\kappa$ are forced to remain within the gray area [KEL 08]

In a three-dimensional space, we consider transverse isotropic materials in direction $\hat{e}$, and postulate that the domains $G_{i,s}^*$ have the following geometric shape:

$$G_{i,s}^* = \left\{ \xi; tr\xi = 0 \text{ and } \frac{1}{2} |\xi|^2 + \frac{3}{2} b_{i,s} (det\xi)^{\frac{2}{3}} + \frac{1}{2} c_{i,s} (\hat{e}\xi\hat{e}) - g_{i,s} \leq 0 \right\}$$

[7.175]

This choice is consistent with the fact that phase transformation does not cause a change in volume: $tr\kappa = 0$. Obviously, $b_{i,s}$, $c_{i,s}$ and $g_{i,s}$ are material parameters. $g_i$ and $g_s$ determine the size of the surfaces of initiation and saturation, $b_i$ and $b_s$ the amount of asymmetry between traction and compression and $c_i$ and $c_s$ the degree of eccentricity in direction $\hat{e}$ (see examples in Figures 7.27 and 7.28).
We can show that the surface of initiation is the convex dual of that introduced into the stress space by Gibeau et al. [GIB 10].

### 7.4.4.2. Equations of the model

Cauchy equation, in a quasi-static regime:

\[
div \Sigma = 0
\]

[7.176]

Heat equation:

\[
\rho \frac{de}{dt} = \Sigma : \dot{E} + W - div q
\]

[7.177]
Local formulation of the second law of thermodynamics:

\[ \Sigma: \frac{dE}{dt} - \left( \frac{d\psi}{dt} + s \frac{dT}{dt} \right) - q \frac{\text{grad}T}{T} \geq 0 \]  \[ \text{[7.178]} \]

Helmholtz free energy

This thermodynamic potential is essentially the same as most internal variable models relating to SMAs. Here, the thermally-induced strain \( E_{\text{th}} \) is ignored:

\[ \psi(E, \kappa, z, T) = \frac{1}{2}(E - \kappa z) \cdot L(E - \kappa z) + z \omega(T) - C_v T L n \left( \frac{T}{T_0} \right) \]

\[ + z G_i(\kappa) + G_s(z \kappa) + G(z) \]  \[ \text{[7.179]} \]

where:

\[ \omega(T) = L_c \left( \frac{T - T_c}{T_c} \right) \]  \[ \text{[7.180]} \]

where \( L_c \) is the latent heat of transformation and \( T_c \) the thermodynamic temperature of transformation.

Further:

\[ G(z) = \begin{cases} 0 & \text{if } z \in [0, 1] \\ +\infty & \text{otherwise} \end{cases} \]  \[ \text{[7.181]} \]

\[ G_{i,s}(\xi) = \begin{cases} 0 & \text{if } \xi \in G_{i,s}^* \\ +\infty & \text{otherwise} \end{cases} \]  \[ \text{[7.182]} \]

As highlighted above, \( G_s \) may depend upon \( \Sigma \).

Driving forces and kinetics

In the generalized standard framework, we obtain the stress tensor and the entropy:

\[ \Sigma = \frac{\partial \psi}{\partial E} = L(E - \kappa z) \]  \[ \text{[7.183]} \]

\[ s = - \frac{\partial \psi}{\partial T} = - \frac{L_c}{T_c} + C_v \left( 1 + \text{Ln} \left( \frac{T}{T_0} \right) \right) \]  \[ \text{[7.184]} \]
We also obtain the thermodynamic forces associated with the two internal variables \( z \) and \( \kappa \). In writing the expression of these forces, it is useful to ensure that the functions \( G_i,s \) are regular. In these situations:

\[
\Pi^f_z = -\frac{\partial \psi}{\partial z} = \Sigma \kappa - \omega (T) G_i(\kappa) - \kappa: \left( \frac{\partial G_x}{\partial \xi} \right) z_{\kappa} - \left( \frac{\partial G}{\partial z} \right) z \quad [7.185]
\]

\[
\Pi^f_\kappa = -\frac{\partial \psi}{\partial \kappa} = z \Sigma - z \left( \frac{\partial G_x}{\partial \xi} \right) \kappa - z \left( \frac{\partial G}{\partial \xi} \right) z_{\kappa} \quad [7.186]
\]

We postulate that the kinetics of the internal variables are constitutive functions of the driving forces:

\[
\dot{\kappa} = \delta_{\kappa} \left( \Pi^f_\kappa \right) \quad [7.187]
\]

\[
\dot{z} = \delta_z (\Pi^f_z) \quad [7.188]
\]

Kelly and Bhattacharya [KEL 12, KEL 08] make the hypothesis that the martensite variants can reorient more easily than the process of phase transformation, and therefore the kinetics of \( \kappa \) is far faster than \( z \), and as we know, the slowest sets the pace!

Hence, we write two expressions for the kinetics of the volume fraction of martensite:

– an expression independent of the rate, with a threshold driving force \( \Pi^f_z \) for the initiation of the forward \( A \Rightarrow M \) transformation and a threshold driving force \( \Pi^f_{\kappa} \) for the initiation of the reverse transformation, \( M \Rightarrow A \):

\[
\dot{z} = 0 \text{ for } \Pi^f_z \in (\Pi^f_{\kappa}^- , \Pi^f_{\kappa}^+) \text{ and } \Pi^f_z \dot{z} \geq 0 \quad [7.189]
\]

This is represented by a dotted line in Figure 7.29;

– the slip limit. Here, we also need a driving force:

\[
\dot{z} = \begin{cases} 
\dot{z}^+ \left( 1 + \frac{1}{(\Pi^f_z - \Pi^f_{\kappa}^+)} \right)^{-\frac{1}{\eta}} & \text{for } \Pi^f_z \geq \Pi^f_{\kappa}^+ \text{ and } z \leq 1 \\
\dot{z}^- \left( 1 + \frac{1}{(\Pi^f_z - \Pi^f_{\kappa}^-)} \right)^{-\frac{1}{\eta}} & \text{for } \Pi^f_z \leq \Pi^f_{\kappa}^- \text{ and } z \geq 0 \\
0 & \text{otherwise}
\end{cases} \quad [7.190]
\]

This is shown with solid lines in Figure 7.29.
7.4.5. Certain constraints on simulation and modeling

7.4.5.1. Hard constraints

In the discussions mentioned above, the assumption has been that the functions $G$ are regular. In our case, the functions $G$ are not, which creates constraints. The domains $G_{i,s}$ are defined in the null-trace matrix subspace. Therefore, we need to project their derivatives into the appropriate subspaces. We have to rewrite the driving forces as follows:

$$-\Pi^I_{\xi} + 	ext{dev} \Sigma: \kappa - \omega(T) - G_i(\kappa) \in + \kappa: \partial G_s(z\kappa) + \partial G(z)$$  \[7.191\]

$$-\Pi^I_{\xi} + z.\text{dev} \Sigma \in \partial G_i(\kappa) + \partial G_s(z\kappa)$$  \[7.192\]

The kinetics for $\kappa$ becomes easier: $\kappa$ is the value which maximizes the projection on the applied stress out of all the values which satisfy the constraint:

$$\kappa(t) = \begin{cases} \arg \max_{\xi \in G_{i,s}} \omega \Sigma(t): \xi & \Sigma(t) \neq 0 \\ \kappa(t^-) & \text{for } \Sigma(t) = 0 \text{ and } z > 0 \\ 0 & \text{for } \Sigma(t) = 0 \text{ and } z = 0 \end{cases}$$  \[7.193\]

The kinetics of $z$ can be described as follows: as long as $z \in [0, 1]$ and $z\kappa$ is within $G_{i,s}$, then $\Pi^I_{\xi} = \Sigma: \kappa - \omega(T)$, and the evolution of $z$ is the same as in the normal case.

When the kinetics is independent of the rate (see equation [7.189]), we obtain:

$$\pm \Pi^I_{\xi} \pm \Sigma: \kappa - \omega(T) - G_i \in \kappa: \partial G_s(z\kappa) + \partial G(z)$$  \[7.194\]

We shall make use of this formulation for the analytical problems.
7.4.5.2. Flexible, adjustable constraints

As the “inflexible” constraints discussed above are hard to formulate mathematically, we shall replace them with high-degree polynomials, as done by Kelly [KEL 08] for his thesis:

\[
G_{i,s} = \left( \frac{\frac{4}{3} (\xi \cdot \xi)^{\frac{5}{3}} + b_{i,s} \det(\xi) + \frac{5}{3} c_{i,s} | \hat{\epsilon}_{i,s} \cdot \xi \hat{e}_{i,s} |^{3}}{y_{i,s}} \right)^{16}
\]  

[7.195]

We shall demonstrate the effectiveness of this approach in the next section.

We incorporate the kinetics by variational incremental principles, introducing the dissipation potentials as did Yang et al. [YAN 06]. Formally, we shall assume that it is possible to invert equation [7.188] and write \( \Pi^\nu = k_{m}^{-1}(\dot{\nu}) \). In addition, consider the dissipation potential defined by \( k_{m}^{-1}(v) = \partial \varphi^* / \partial v \). Hence, if we recall the definition of the driving force (equation [7.185]), we rewrite the kinetics in the form:

\[
- \frac{\partial \psi}{\partial z}(z) = \frac{\partial \varphi^*}{\partial \dot{z}}(\dot{z})
\]  

[7.196]

By discretizing this equation in relation to time, we get:

\[
\frac{\partial \psi}{\partial z}(z^N) + \frac{\partial \varphi^*}{\partial \dot{z}} \left( \frac{z^N - z^{N-1}}{\Delta t} \right) = 0
\]  

[7.197]

Note that this is the Euler-Lagrange equation associated with the variational problem:

\[
z^N = \text{arg min}_z \left\{ \psi(z) + \Delta t \varphi^* \left( \frac{z^N - z^{N-1}}{\Delta t} \right) \right\}
\]  

[7.198]

The function \( \varphi^* \) is known as the “dissipation potential” (see Figure 7.30). We include the evolution of the strain and of the transformation strain in this approach. From this, we conclude: consider given values of \( E_{N-1}^N, \kappa_{N-1}^N \) and \( z^{N-1} \), and the increment in loading with increasing potential \( L^N \):

\[
\begin{align*}
\{ E^N, \kappa^N, z^N \} &= \text{arg min}_{E,\kappa, z} \int_\Omega \left\{ \psi(E,\kappa,z) + \Delta t \varphi^* \left( \frac{z^N - z^{N-1}}{\Delta t} \right) \right\} dx + L^N
\end{align*}
\]  

[7.199]
This is a classic formulation for the dissipation potential $\varphi^*$:

1) for the rate-independent kinetics (equation [7.189]):

$$\varphi^*(\dot{z}) = \begin{cases} 
\Pi_{\text{f}+}^+ \dot{z} \geq 0 \\
\Pi_{\text{f}+}^- \dot{z} \leq 0 
\end{cases}$$

2) for the time-dependent kinetics ($p = 2$):

$$\varphi^*(\dot{z}) = \begin{cases} 
\Pi_{\text{f}+}^+ \dot{z} \geq 0 \\
\Pi_{\text{f}+}^- \dot{z} \leq 0 
\end{cases}$$

$\psi(E, \kappa, z, T) = \frac{1}{2} E^* (E - z\kappa)^2 + z\omega(T) - C_v T \ln \left( \frac{T}{T_0} \right) + z G_s(\kappa) + G_s(z) + G(z)$

where the functions $G_{i,s}$ are given by equations [7.174].

7.4.6. Certain ingredients of the model

7.4.6.1. One-dimensional case

We shall restrict ourselves, for the time being, to the one-dimensional case. Thus:

$$\psi(E, \kappa, z, T) = \frac{1}{2} E^* (E - z\kappa)^2 + z\omega(T) - C_v T \ln \left( \frac{T}{T_0} \right) + z G_s(\kappa) + G_s(z) + G(z)$$

where the functions $G_{i,s}$ are given by equations [7.174].
We assume that the kinetics of $\kappa$ is extremely quick, such that it minimizes the energy at each time. For stress-induced martensite, we shall use the kinetics given by case 1 (equation [7.189]):

\[
\dot{z} = 0 \text{ for } \Pi_{s}^{f} \in (\Pi_{s}^{f-}, \Pi_{s}^{f+}) \text{ and } \Pi_{s}^{f} \dot{z} \geq 0
\]

[7.204]

Consider an isothermal load at $T \geq A_{f}^{0}$, i.e. such that $\omega(T) > -\Pi_{s}^{f-} > 0$. As the material is austenitic, in the stress-free state, the initial state corresponds to $E = 0$ and $z = 0$. At the very beginning of loading, the behavior is elastic with $\Sigma(t) = E^{\star}E(t)$. The start of transformation occurs when $\Pi_{s}^{f} = \Pi_{s}^{f+}$. The nominal transformation strain $\kappa$ assumes its maximum value under traction $\kappa_{t}$ (or its maximum value under compression $\kappa_{c}$). Plainly put, under traction and at the start of phase transformation (point 1 in Figure 7.31), we can deduce the strain $E_{M,S}^{t}$ and the stress $\Sigma_{M,S}^{t}$ by:

\[
\Pi_{s}^{f+} = E^{\star}E_{M,S}^{f} \kappa_{t}^{t} - \omega = \Sigma_{M,S}^{f} \kappa_{t}^{t} - \omega
\]

[7.205]

where:

\[
E_{M,S}^{t} = \frac{\Pi_{s}^{f+} + \omega}{\kappa_{t}^{t}E^{\star}} , \quad \Sigma_{M,S}^{t} = \frac{\Pi_{s}^{f+} + \omega}{\kappa_{t}^{t}}
\]

[7.206]

As $z$ increases, the effective transformation $z\kappa$ increases and eventually saturates for the value of $z$ equal to:

\[
z^{t} = \frac{\kappa_{s}}{\kappa_{t}^{t}}
\]

[7.207]

This is indicated by point 2 in Figure 7.31, and we have:

\[
E_{M,P}^{t} = \frac{\Pi_{s}^{f+} + \omega}{\kappa_{t}^{t}E^{\star}} + \kappa_{s}^{t}, \quad \Sigma_{M,P}^{t} = \frac{\Pi_{s}^{f+} + \omega}{\kappa_{t}^{t}}
\]

[7.208]

As the transformation is saturated, both the stress and strain increase in a linear fashion until point 3.

The same reasoning can be applied when the load is relieved. The stress and driving force decrease until point 4, where $\Pi_{s}^{f} = \Pi_{s}^{f-}$. Here:

\[
E_{A,S}^{t} = \frac{\Pi_{s}^{f-} + \omega}{\kappa_{t}^{t}E^{\star}} + \kappa_{s}^{t}, \quad \Sigma_{A,S}^{t} = \frac{\Pi_{s}^{f-} + \omega}{\kappa_{t}^{t}}
\]

[7.209]

We pass from point 4 to point 5 with constant stress $\Sigma_{A,P}^{t}$ and constant driving force $\Pi_{s}^{f-}$:

\[
E_{A,P}^{t} = \frac{\Pi_{s}^{f-} + \omega}{\kappa_{t}^{t}E^{\star}} , \quad \Sigma_{A,P}^{t} = \frac{\Pi_{s}^{f-} + \omega}{\kappa_{t}^{t}}
\]

[7.210]
Finally, the material experiences elastic unloading until the original state is reached.

We can give the values of the transformation strain, the hysteresis size (under stress) and the average stress (with the superscript \( t \) for traction and \( c \) for compression), to say nothing of the fact that the asymmetry between traction and compression is well accounted for in the model, which was also true with the previous models.

\[
E_{\text{trans}}^{t,c} = \frac{1}{2}(E_{M_F}^{t,c} - E_{M_S}^{t,c} + E_{A_S}^{t,c} - E_{A_F}^{t,c}) = \kappa_s^{t,c}
\]

\[
\Sigma_{\text{hyst}}^{t,c} = \frac{1}{2}(\Sigma_{M_F}^{t,c} + \Sigma_{M_S}^{t,c} - \Sigma_{A_S}^{t,c} - \Sigma_{A_F}^{t,c}) = \frac{\Pi f^+ - \Pi f^-}{\kappa_s^{t,c}}
\]

\[
\Sigma^{t,c} = \frac{1}{4}(\Sigma_{M_F}^{t,c} + \Sigma_{M_S}^{t,c} + \Sigma_{A_S}^{t,c} + \Sigma_{A_F}^{t,c}) = \frac{1}{2} \Pi f^+ + \Pi f^- + 2\omega
\]

Figure 7.31. In a one-dimensional regime: stress-induced martensite: a) stress/strain curve; and b) the diagram \( z \) as a function of \( \kappa \) [KEL 12, KEL 08]

Note that the threshold stresses for forward and reverse transformation depend on the temperature by the intermediary of \( \omega(T) \), which is linearly dependent upon the temperature (see equation [7.180]). Hence, these stresses are linearly dependent on \( T \).

In addition, we can invert the above relations in order to obtain the temperatures for forward and reverse transformation, in the stress-free state:

\[
M^0_S = M^0_F = T_c - \frac{\Pi f^+}{L_c} \quad A^0_S = A^0_F = T_c + \frac{\Pi f^-}{L_c}
\]

We have seen that in the case of the rate-independent kinetics (equation [7.189]) \( \Sigma_{M_F}^{t,c} = \Sigma_{M_S}^{t,c} \), \( \Sigma_{A_S}^{t,c} = \Sigma_{A_F}^{t,c} \) and \( M^0_S = M^0_F, A^0_S = A^0_F \). If the material exhibits behavior dependent on the rate (equation [7.190]), then we have \( \Sigma_{M_S}^{t,c} < \Sigma_{M_F}^{t,c} \), the difference depending on the rate of loading.

We can also have \( \Sigma_{M_S}^{t,c} < \Sigma_{M_F}^{t,c} \) in anisothermal conditions. Remember than a mechanical test can only be performed at an imposed temperature, at the boundaries.
of the sample, and cannot be isothermal in the strict sense of the term. The fact that the $A \Rightarrow M$ phase transformation is exothermic accentuates the effect of thermomechanical coupling.

We can estimate the hardening, in the adiabatic situation, as done by Sadjadpour and Bhattacharya [SAD 07]. With $q = r = 0$, the temperature is determined by integrating the heat equation. If we consider that the effect of latent heat is predominant, equation [7.177] can be reduced to:

$$C_v \dot{T} = \frac{L_c}{T_c} \dot{z}$$  \[7.215\]

The integration of $t_1$ to $t_2$ yields:

$$\frac{T(t_2)}{T(t_1)} = \exp \left( \frac{L_c \left(z(t_2) - z(t_1)\right)}{C_v T_c} \right)$$  \[7.216\]

As the $M \Rightarrow A$ transformation progresses, the temperature increases. However, the driving force must retain its critical value $\Pi_f^+$, and thus:

$$\Sigma(t) - \frac{L_c}{T_c} (T(t) - T_c) = \Pi_f^+ \Rightarrow \Sigma(t) = \frac{\Pi_f^+}{\kappa_t} + \frac{L_c}{T_c} T_0 \exp \left( \frac{L_c z(t)}{C_v} \right) - 1\right)$$  \[7.217\]

The transformation saturates at $z = z^{t,c}$, the definition of which is given in equation [7.207], here:

$$\Sigma^{t.c} = \frac{\Pi_f^+}{\kappa_t} + \frac{L_c}{T_c} T_0 \exp \left( \frac{L_c z^{t,c}}{C_v} \right) - 1)$$  \[7.218\]

The hardening due to adiabatic conditions is given by:

$$\Sigma^{t,c}_{MF} = \Sigma^{t,c}_{MS} = \frac{L_c}{\kappa_s} \frac{T_0}{T_c} \exp \left( \frac{L_c z^{t,c}}{C_v} \right) - 1)$$  \[7.219\]

7.4.6.2. Two- or three-dimensional case

Consider a sample in the austenitic state, i.e. the initial state: $\Sigma = 0, \ z = 0, \ \kappa = 0$.

At time $t$, a proportional load $\Sigma(t) = s(t) \Sigma_0$ is applied, with $s(t)$ a scalar which begins at 0, increases monotonically until reaching a peak, and then decreases monotonically until it eventually returns to 0.

Note that the interconnection between $G_i$ and $G_s$ is more complex in a multi-dimensional case. This is illustrated schematically in Figure 7.32.
When \( z \) is very small, then \( \frac{G_s}{z} \) is very large, and the optimization of \( G_i \cap \frac{G_s}{z} \) is equal to that on \( G_i \) (see Figure 7.32a). We call this optimal value \( \kappa^0 \) and note that it is on the boundary of \( G_i \) and is independent of \( z \) if \( z \) is small enough. We define the largest value of \( z \) for which this condition is fulfilled (see Figure 7.32b):

\[
z_0 = \max \left\{ z \in [0, 1]: \max_{\xi \in G_i \cap \frac{G_s}{z}} \Sigma_0: \xi = \max_{\xi \in G_i \Sigma_0:} \Sigma_0: \xi \right\} \quad [7.220]
\]

As \( z \) increases beyond \( z_0 \), the issue is to determine the optimal value of \( \kappa: \kappa^{opt} \); this ideal value moves along the boundary of \( G_i \) as the value of \( z \) increases (see Figure 7.32c). However, if \( z \) becomes very large, the optimization on \( G_i \cap \frac{G_s}{z} \) becomes equal to that on \( \frac{G_s}{z} \) (see Figure 7.32e). We define \( z_1 \) as the smallest value of \( z \) for which it is true (see Figure 7.32c):
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\[ z_1 = \min \left\{ \max_{\xi \in G_i \cap G_s} \Sigma_0 : \xi = \max_{\xi \in G_i} \Sigma_0 : \xi \right\} \] [7.221]

\[ z_1 = \min \left\{ z \in [0, 1] : \max_{\xi \in G_i \cap G_s} \Sigma_0 : \xi = \max_{\xi \in G_s} \Sigma_0 : \xi \right\} \] [7.222]

The combination of these two equations gives us:

\[ \Pi^f = \max_{\xi \in G_i \cap G_s} s \Sigma_0 : \xi - \omega =: f(s, z) \] [7.223]

It is plain to see:
1) for any fixed value of \( z \), \( f \) increases monotonically with \( s \);
2) for any fixed value of \( s \), \( f \) decreases monotonically with \( z \);
3) for any fixed value of \( f \), \( f \) is constant for all values of \( z \in [0, z_0] \);
4) \( f < 0 \) when \( s \) is small enough.

This means that \( f \) can operate as a criterion function for the elastic austenitic domain in case 4. Figure 7.32f shows the level lines of the function \( f \) defined by equation [7.223].

Together, observations 1–3 imply that in the plane \( z - s \), the curve \( f \) is horizontal for \( z \leq z_0 \) and grows in a monotonic fashion beyond this range, as shown in Figure 7.32f.

7.4.6.3. Transformation criterion

As \( s \) begins with a value of zero, \( \kappa \) “jumps” to point \( \kappa^0 \) in \( G_i \), which is the maximum projection into \( \Sigma_0 \) (see Figure 7.32a). This is because \( z = 0 \) and \( G_s \) has no limit and \( G_i \cap G_s = G_i \). Because \( s \) is small, \( \Pi^f \) is negative and \( z \) is equal to 0. When \( s \) increases, the value of \( \kappa \) remains unchanged, but \( \Pi^f \) increases monotonically until it becomes positive and eventually attains the threshold value \( \Pi^f_+ \):

\[ s(t) = s_0 = \frac{\Pi^f_+ + \omega}{\Sigma_0 : \kappa^0} = \min_{\xi \in G_i} \frac{\Pi^f_+ + \omega}{\Sigma_0 : \xi} \] [7.224]

In the wake of the work done in Lexcellent et al. [LEX 02], we can define a criterion surface for phase transformation in the applied stress space, in the form:

\[ Y = \left\{ \Sigma : \text{dev} \Sigma = \min_{\xi \in G_i} \frac{\Pi^f_+ + \omega}{\Sigma : \xi} \text{ or } \Sigma = \sqrt{\Sigma : \Sigma} \hat{\Sigma} = \frac{\Sigma}{\Sigma} \right\} \] [7.225]

Note simply that \( Y \) is the convex dual function of \( G_i \).
7.4.6.4. Saturation of transformation

The transformation becomes saturated when $z = z_1$, and:

$$s(t) = s_1 = \frac{\Pi f^+ + \omega}{\Sigma_0: \kappa'} = \min_{\xi \in G} \frac{\Pi f^+ + \omega}{\Sigma_0: \xi}$$  \[7.226\]

If the stress continues to increase beyond $s_1 \Sigma_0$, there is no longer phase transformation, and the material responds elastically with the transformation strain fixed and the austenite retained (see Figure 7.32e).

7.4.6.5. Breaking the resolved stress criterion

It is common to make use of the resolved stress criterion, which stipulates that the product of the stress at the start of transformation by the component of the strain at saturation is a constant, independent of the loading direction. In the model put forward by Kelly and Bhattacharya [KEL 12], we can see that this product:

$$s_0 \cdot (z_1 \kappa'^1 : \Sigma_0) = (\Pi f + \omega) \frac{\max_{\xi \in G} \omega \Sigma_0: \xi}{\max_{\xi \in G} \Sigma_0: \xi}$$  \[7.227\]

generally depends on the direction of loading. The resolved stress criterion no longer works in their model [KEL 12], which would seem to be borne out by the experimental observations of Daly et al. [DAL 08].

7.4.6.6. Stress release

When the applied stress decreases, the material responds in an elastic fashion, until:

$$s(t) = s_2 = \frac{\Pi f^- + \omega}{\Sigma_0: \kappa'}$$  \[7.228\]

The reverse transformation begins at $s_2 \Sigma_0$, and continues until $z$ reaches $z_0$ at:

$$s(t) = s_3 = \frac{\Pi f^- + \omega}{\Sigma_0: \kappa'^0}$$  \[7.229\]

7.4.6.7. Parameters of the model

In the interests of consistency, unless otherwise specified, with the aim of replicating the asymmetry between traction and compression shown on the threshold surface in Lexcellent et al. [LEX 02], the initiation parameters are $b_i = -1.85$ and $g_i = 2.05 \times 10^{-4}$. There is no asymmetry for the saturation surface ($b_s = 0$). Because the saturation surface must be contained within the initiation surface (see Figure 7.25), $g_s$ is taken to be equal to $2.25 \times 10^{-5}$. The anisotropy is not taken into account in constructing these surfaces. The Young’s modulus $E^*$ is chosen as equal to 115MPa.

For the thermal parameters, we shall use the same ones as Sadjadpour and Bhattacharya [SAD 07]: the latent heat $L_c = 79$ MJ/m$^3$, $c_v = 5.4$ MJ/m$^3$ K,
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\( M_s^0 = 217.60 \text{ K} \) and \( A_s^0 = 266.79 \text{ K} \). They serve to select the parameters of the kinetics:

\[
\Pi^+_z = -\Pi^-_z = L_c \left( \frac{A_s^0 - M_s^0}{A_s^0 + M_s^0} \right) = 8 \times 10^6 \text{ J/m}^3
\]  

[7.230]

By exploiting the fact that the critical temperature \( T_c = \frac{A_s^0 + M_s^0}{2} \), the isothermal loads were taken to a temperature \( T = 333 \text{ K} \) so that \( \omega(T) \) is a round number:

\[
\omega(T) = L_c \left( \frac{T - T_c}{T_c} \right) = 1 \times 10^5 \text{ J/m}^3
\]  

[7.231]

The exponent \( p \) in the time-dependent kinetics (equation [7.190]) is chosen as equal to 2.

7.4.7. Traction and compression for an isotropic material

In this case, \( c_i = c_s = 0 \), with the time-independent kinetics (see equation [7.189]).

The uniaxial load corresponds to:

\[
\Sigma = s \text{ diag} \{0, 0, 1\}
\]  

[7.232]

and the transformation strain associated therewith (which is deviatoric):

\[
\kappa = \frac{\epsilon}{2} \text{ diag}(-1, -1, 2)
\]  

[7.233]

We conclude, in reference to equation [7.174], that the optimal value of \( \epsilon : \kappa_{t,c} \)
satisfies:

\[
g_i = \left( \frac{2}{3} (\kappa_{t,c})^2 \right)^{\frac{2}{3}} + \frac{3}{2} h_i \left( \frac{2}{27} (\kappa_{t,c})^3 \right) \Rightarrow \kappa_{t,c} = \pm \left( \frac{g_i}{\left( \frac{2}{3} \right)^{\frac{2}{3}} + \frac{2}{27} h_i} \right)^{\frac{3}{2}}
\]  

[7.234]

the transformation-start stresses and strains are written:

\[
E^{t}_{MS} = \frac{\Pi^+_t + \omega}{\kappa_{t,c} E^*}, \quad \Sigma^{t}_{MS} = \frac{\Pi^+_t + \omega}{\kappa_{t,c}}
\]  

[7.235]

The transformation becomes saturated when:

\[
z_{t,c} = \frac{\kappa_{t,c}}{\kappa_{t,c}^s} \quad \text{where} \quad \kappa_{t,c}^s = \pm \frac{2}{3} \left( \frac{g_s}{\left( \frac{2}{3} \right)^{\frac{2}{3}} + \frac{2}{27} h_s} \right)^{\frac{3}{2}}
\]  

[7.236]

and the associated stresses and strains are:

\[
E^{t}_{MP} = \frac{\Pi^+_t + \omega}{\kappa_{t,c}^s E^*} + \kappa_{t,c}^s, \quad \Sigma^{t}_{MP} = \frac{\Pi^+_t + \omega}{\kappa_{t,c}^s}
\]  

[7.237]

In this case, there is no reorientation of martensite or hardening.
7.4.8. Pure shearing of an isotropic material

The stress tensor is written:

\[
\Sigma = \begin{bmatrix}
0 & 0 & 0 \\
0 & 0 & \tau \\
0 & \tau & 0
\end{bmatrix}
\]  \[7.238\]

and the nominal transformation strain tensor (which is obviously symmetrical and deviatoric):

\[
\kappa = \begin{bmatrix}
-x - z & 0 & 0 \\
0 & z & y \\
0 & y & x
\end{bmatrix}
\]  \[7.239\]

The calculations performed by Kelly [KEL 08] give us:

\[
x = x_0 = \sqrt{P(b_i)} y_0
\]  \[7.240\]

\[
y = y_0 = \left(\frac{3g_i}{2(6P(b_i) + 2)^{1/2} + 6b_i \sqrt{P(b_i)(1 - P(b_i))}}\right)
\]  \[7.241\]

\[
z = z_0 = x_0
\]  \[7.242\]

where:

\[
P(b_i) = \frac{-3(24 + 2b_i^2) + (9(24 + 2b_i^2)^2 + 36b_i^2(24 - b_i^2))^{1/2}}{18(24 - b_i^2)}
\]  \[7.243\]

The driving force of the transformation is given by \(2\tau y_0 - \omega\). The transformation begins when:

\[
\tau = \tau_0 = \left(\frac{H_x^f + \omega}{2y_0}\right)
\]  \[7.244\]

It advances rapidly until \(z = z_0\), and becomes saturated at \(z = z_1\). The calculations are too complicated to give an explicit form to \(z_0\) and \(z_1\). However, it is possible to see that each of them may experience reorientation and hardening under shearing stress. Remember that the transformation becomes saturated when \(z\kappa\) reaches its optimal value in \(G_s\); \(\kappa\) will have the expression \[7.239\], with \(x_1, y_1, z_1\) with \(b_i\) replaced by \(b_s\) and \(g_i\) by \(g_s\). Note that the \(x_1/y_1\) ratio will be different to the \(x_0/y_0\) ratio (except in the non-generic case where \(P(b_i) = P(b_s)\)). From this, it follows that the transformation strain at saturation point will not be proportional to the transformation strain at initiation. In other words, even at \(T \geq A_0^f\), shearing may cause reorientation in addition to the phase transformation.
7.4.9. Examination of the parameters for a uniaxial extension combined with shearing

This prefigures the traction/torsion of a tube with imposed strain and austenitic in the stress-free state.

We focus on the material point where $E^N$ is given. Equation [7.199] becomes:

$$\{\kappa^N, z^N\} = \arg \min_{\kappa, z} \psi(E^N, \kappa, z) + \Delta t \varphi^* \left( \frac{z - z^{N-1}}{\Delta t} \right)$$  \[7.245\]

$$\Sigma^N = L(E^N - z^N \kappa^N)$$  \[7.246\]

We can also conduct imposed-stress tests. Then, $\Sigma^N$ is given and equation [7.199] becomes:

$$\{E^N, \kappa^N, z^N\} = \arg \min_{E, \kappa, z} \psi(E, \kappa, z) + \Delta t \varphi^* \left( \frac{z - z^{N-1}}{\Delta t} \right) - \Sigma^N : E$$  \[7.247\]

We shall use the set of parameters defined above.

7.4.9.1. Isotropic materials

We begin with the basic isotropic situation ($c_1 = c_s = 0$) with a biaxial and proportional load imposed by traction/shear strain:

$$E(t) = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & \gamma(t) \\ 0 & \gamma(t) & c(t) \end{pmatrix}$$  \[7.248\]

Note that the response under stress ($\tau - \sigma$) is non-proportional (see Figure 7.33a). This is in agreement with the observations made by Thamburaja and Anand [THA 01] and McNamey et al. [MCN 03]. The reason for this non-proportionality is the martensite reorientation, as shown in Figure 7.33b. This figure shows the components of shear and traction of the effective strain tensor $E^{tr} = \kappa z \in G_s^\kappa$ (illustrated by the solid-line curve). Figure 7.33b traces the surfaces $G_i$ and $G_s$, with the condition of a “hard constraint”, and we see that the trajectory calculated with the “soft constraint” is very similar to this, although slightly greater.
7.4.9.2. Anisotropic material

We consider uniaxial materials with \((e_i = e_a = e_3)\) and \(c_i, c_3 \neq 0\), with biaxial strain loading given by the matrix \([7.248]\). So as to separate anisotropy from asymmetry, we take \(b_i = b_a = 0\).

Figure 7.34 shows the results obtained for increasing anisotropy of the initiation surface \(G_i\) with \(c_i\) varying by equal increments between 0.3 and 1.5. When \(c_i = 0\), the initiation and saturation surfaces are homothetic; thus, there is no reorientation of martensite and the strains and stresses are proportional and close to the direction of the strain applied (the small difference stems from the elastic moduli).

When \(c_i\) is not equal to 0, the initiation surface is excentered. Thus, the nominal transformation strain deviates from the direction of loading. Indeed, the trajectory of effective strain goes in another direction, whereas the stress appears to keep the same direction. In addition, the initiation and saturation surfaces are no longer homothetic. Thus, when the effective transformation strains become great enough, we note the reorientation of the martensite and consequently non-proportional transformation strains and stresses (see Figure 7.34). With large values of \(c_i\), the curves \(\sigma_{eq} - \varepsilon_{eq}\) show a reduction in their gradient. However, this is not indicative of any instability.
Figure 7.34. Anisotropy of the initiation surface $G_i$, traction/shear strains imposed for values of the anisotropy parameter $c_i$ of 0.3 to 1.5: a) dotted lines: the trajectory $\gamma - \epsilon$ and trajectories of effective strains $\gamma_{eq} - \epsilon_{eq}$; b) $\tau - \sigma$; c) $\sigma_{eq} - \epsilon_{eq}$; d) $z - \epsilon_{eq}$ [KEL 08]

Figure 7.35 illustrates the situation when the saturation surface $G_s$ is anisotropic and the initiation surface $G_i$ is isotropic.

7.4.9.3. Proportional loads applied in different directions

Here, we shall examine the role of changing direction. We shall use the same basic parameters as before, with the exception of $c_s$, fixed at 1.5 in order to accentuate the reorientation of the martensite.

Figure 7.36 illustrates the material’s response for radial trajectories of the applied strains with different ratios. We can see the wide deviation between the direction of the strain applied and the initial direction of the transformation strain. The curves $\sigma_{eq} - \epsilon_{eq}$ also vary quite significantly. The volume fraction of martensite attained at the point of saturation depends heavily on the direction of loading (curve (d): $z - \epsilon_{eq}$).

Figure 7.37 shows the corresponding curves for loading under controlled strain. The observations are identical to those made above, except that the curve $\sigma_{eq} - \epsilon_{eq}$ exhibits no softening.
Figure 7.35. Anisotropy of the saturation surface $G_s$, traction/shear strains imposed for values of the anisotropy parameter $c_s$ between 0.3 and 1.5. a) Dotted lines: the trajectory $\gamma - \epsilon$, and the trajectories of effective strains $\gamma_M - \epsilon_M$; b) $\tau - \sigma$; c) $\Sigma_{eq} - E_{eq}$; d) $z - \epsilon_{eq}$ [KEL 08]

Figure 7.36. Variation of the direction of applied strain: a) the trajectory of effective strain with the trajectory of the applied strains (dotted lines); b) $\tau - \sigma$; c) $\sigma_{eq} - \epsilon_{eq}$; d) $z - \epsilon_{eq}$ [KEL 08]
7.4.9.4. **Non-proportional loading**

An interesting case is to be found in the experimental observations made by McNamey *et al.* [MCN 03], reproduced in Figure 7.38. These researchers looked at combined traction-and-torsion stress application to thin tubes, and observed a dual plateau when a uniaxial traction force is followed by torsion.

Thin NiTi tubes (.037 mm in thickness) are subjected to forces at slow rates (between $10^{-5}$ and $10^{-4}$ s$^{-1}$) in order to avoid the effects of quick loading.

The program followed consists of traction up to 6% followed by torsion of 2%. The stress is then relieved, first for torsion and then for traction.

This figure shows the results of the simulation which reproduces the dual plateau observed. The initiation and saturation surfaces are chosen so that there is a significant degree of asymmetry.

The authors of [KEL 12, KEL 08] explain why, when the tubes are subjected first to torsion and then to traction, the same dual plateaus are not observed.

---

**Figure 7.37.** Variation of the direction of applied stress: a) trajectory of effect strain; b) $\tau - \sigma$; c) $\sigma_{eq} - \varepsilon_{eq}$; d) $z - \varepsilon_{eq}$ [KEL 08]
7.4.10. Digital implantation

In order to exploit this model in an industrial context, we need to be able to build it into a finite element method computer code. A UMAT subroutine for ABAQUS has been developed for just this purpose.

Given $E^t$, the total strain field at time $t$, the fields $\kappa^t$ and $z^t$ are obtained by way of the procedure of implicit minimization at each timestep and every node.

\[
\begin{align*}
z^{t+1}, \kappa^{t+1} &= \arg \min_{g_{\kappa^{t+1}}} \{ z^{t+1} - \kappa^{t+1} \in G \} \\
&= \text{arg} \min \left\{ \frac{1}{2} (E^{t+1} - z^{t+1} \kappa^{t+1}) : L (E^{t+1} - z^{t+1} \kappa^{t+1}) \right\} + z^{t+1} \omega (T) + G_i (\kappa^{t+1}) + G_s (z^{t+1} \kappa^{t+1}) + \Delta t \phi^* \left( \frac{z^{t+1} - z^t}{\Delta t} \right) \}
\end{align*}
\]

[7.249]

Here, the functions $\phi^* (\dot{z})$ are the Legendre transforms of the dissipation potential associated with the kinetics, i.e. $\dot{z} = \frac{\partial \phi (\lambda)}{\partial \lambda}$ with the following potentials; $\phi^*$
depending on the rate with \( p = 2 \), with two formulations for the forward and reverse transformation:

\[
\varphi^+(\dot{z}) = \begin{cases} 
\pm \Pi^+_{zc} + \frac{\dot{z}}{2} \ln \left( \frac{\dot{z}^2}{Z_+^2 - Z_-^2} \right) + \frac{\dot{z}}{2} \left( \frac{Z_+^2}{Z_+^2 - Z_-^2} + \frac{1}{2} + \sqrt{\left( \frac{Z_+^2}{Z_+^2 - Z_-^2} \right)^2 + \left( \frac{Z_+^2}{Z_+^2 - Z_-^2} \right)^2} \right) \\
-\frac{\dot{z}}{2} \left( \frac{Z_+^2}{Z_+^2 - Z_-^2} \right)^2 + \left( \frac{Z_+^2}{Z_+^2 - Z_-^2} \right) \dot{z} \geq 0 
\end{cases}
\]

\[7.250\]

\[
\varphi^-(\dot{z}) = \begin{cases} 
-\dot{z} \Pi^-_{zc} - \frac{\dot{z}}{2} \ln \left( \frac{\dot{z}^2}{Z_+^2 - Z_-^2} \right) - \frac{\dot{z}}{2} \left( \frac{Z_+^2}{Z_+^2 - Z_-^2} + \frac{1}{2} + \sqrt{\left( \frac{Z_+^2}{Z_+^2 - Z_-^2} \right)^2 + \left( \frac{Z_+^2}{Z_+^2 - Z_-^2} \right)^2} \right) \\
\dot{z} \left( \frac{Z_+^2}{Z_+^2 - Z_-^2} \right)^2 + \left( \frac{Z_+^2}{Z_+^2 - Z_-^2} \right) \dot{z} \leq 0 
\end{cases}
\]

\[7.251\]

In addition, in order to simplify the calculations, we choose \( \Pi^+_{zc} = -\Pi^-_{zc} \).

---

Figure 7.39. Dual plateau obtained with non-proportional loading: a) the trajectory of effective strain with the trajectory of applied strains shown by dotted lines; b) \( \tau - \sigma \); c) \( \sigma_{eq} - \varepsilon_{eq} \); d) \( z - \varepsilon_{eq} \) [KEL 08]
With the goal of rendering the different stresses differentiable, we embed them in the computer code using the following standard penalties:

\[
G_i = \left( \frac{\frac{3}{2}(\kappa; \kappa)^{\frac{3}{2}} + b_i \det(\kappa) + \frac{3}{2} c_i \| \mathbf{\hat{e}}_i \cdot \kappa \mathbf{\hat{e}}_i \|^3}{g_i} \right)^N \tag{7.252}
\]

\[
G_s = \left( \frac{\frac{3}{2}(z \kappa; z \kappa)^{\frac{3}{2}} + b_s \det(z \kappa) + \frac{3}{2} c_s \| \mathbf{\hat{e}}_s \cdot z \kappa \mathbf{\hat{e}}_s \|^3}{g_s} \right)^N \tag{7.253}
\]

where \( N \) is large, positive and even - here, chosen as being equal to 16.

The result of the softening is visualized in Figure 7.40.

![Figure 7.40. The flexible constraint is calculated for a 10% imposed strain. The innermost dotted line is \( G_i^* \); the other is \( G_s^* \) at \( z = z_{sat} \), and the solid line is the polynomial with \( N=16 \) [KEL 08]](image)

Procedure for digital implantation:

1) give: \( E^{t+1} \);

2) minimize \( \psi(E, \kappa, z) \): obtain \( \kappa^{t+1}, z^{t+1} \);

3) calculate the stresses \( \Sigma^{t+1} = L \left( E^{t+1} - z^{t+1} \kappa^{t+1} \right) \);

4) calculate the “tangent modulus” matrix \( \partial \Sigma / \partial E \);

5) iteration.
7.4.10.1. *Criticism of Kelly and Bhattacharya's model*

As with the two models previously described, the difference between the Young's moduli of the austenite and the martensite, and other constants such as $C_v$, etc., are not taken into account by this model. As we have already pointed out, this may seriously complicate the approaches without thereby yielding any significant gain in terms of precision.

Like the others, this model does not integrate plasticity (or visco-plasticity), but this factor can be integrated without too many problems into the constitutive framework, as done by Sadjadpour and Bhattacharya [SAD 07] and Zaki and Moumni [ZAK 07].

This model is implanted into the finite element software package ABAQUS. The "small strain" approach can be extended to finite transformations.

7.5. Elastohysteresis model: formalism and digital implantation

7.5.1. *Experimentally-observed behaviors for shearing and traction/compression*

It is now accepted that traction tests alone are insufficient to give a full account of the three-dimensional behavior of SMAs (see Figure 7.3 in [ORG 98a]). The criterion of Huber-von Mises equivalent stress and strain does not apply to SMAs. In particular, the asymmetry between traction and compression can be taken into account in the simulation, similarly as with the previous three models.

Figure 7.41 shows the evolution of the threshold stresses for the start of $A \Rightarrow M$ phase transformation for traction, compression and shearing respectively with increasing temperature. The Clausius–Clapeyron relations are verified with $d\Sigma_{am}^{\text{t}}/dT = 6.11 \text{ MPa/K}$ and $d\Sigma_{am}^{\text{c}}/dT = 8.5 \text{ MPa/K}$ and $d\Sigma_{am}^{\text{s}}/dT = 10.26 \text{ MPa/K}$.

Figure 7.42 shows the position of the previous experimental points in the deviator plane, along with the transformation start surfaces as a function of the Lode angle (the azimuthal angle in the stress deviator plane).

7.5.2. *Elasto-hysteresis model*

7.5.2.1. *Formalism in finite transformations*

The constitutive equations are written using the Euler-Cauchy stress tensor $\Sigma$ and the Euler-Almansi strain tensor $E$. 

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In addition to the first invariant (which corresponds to the relative variation in volume), the other two invariants of $\mathbf{E}$ used by the elasto-hysteresis model are:

- a measure of the “intensity” $Q_e$ of the Almansi strain tensor $\text{dev}\mathbf{E}$:

$$Q_e = (2I_2)^{\frac{1}{2}}$$  \[7.254\]

with: $\text{dev}\mathbf{E} = \mathbf{E} - \frac{1}{3} \text{tr} (\mathbf{E}) \mathbf{1}$ and $I_2 = \frac{1}{2} E_{ij} E_{ij} - \frac{(\text{tr} (\mathbf{E}))^2}{3}$;

- the Lode angle $\phi_e$, such that:

$$\cos (3\phi_e) = 3\sqrt{6} \frac{I_3}{Q_e}$$  \[7.255\]

where: $I_3 = \frac{1}{3} E_{ij} E_{kj} E_{ik}$. 

---

**Figure 7.41.** Threshold stresses $\Sigma^{nm}$ for traction (Tra), compression (Com) and shearing (She) with changing temperature, for a polycrystalline NiTi [ORG 98a]

**Figure 7.42.** Transformation start surfaces in the stress deviator space for $T = 35, 50, 55, 60, 65$ and $70^\circ C$ [ORG 98a]
7.5.2.2. From the Duhem analysis to the elasto-hysteresis model

As suggested by Duhem [DUH 80] and Otsuka et al. [OTS 76], the stress tensor $\Sigma$ is obtained by adding a first, reversible stress tensor $\Sigma_{\text{rev}}$ and a second pure hysteresis (irreversible stress) $\Sigma_{\text{irr}}$ tensor [FAV 88] (Figure 7.43):

$$\Sigma = \Sigma_{\text{rev}} + \Sigma_{\text{hys}}$$  [7.256]

![Figure 7.43. Decomposition of the stress tensor into a reversible and hysteretic component](https://www.iran-mavad.com)

7.5.2.3. Calculation of the reversible stress

This calculation is performed using a hyper-elastic model which relies on a given value for an elastic energy density $E_{\text{rev}}$. For an isotropic material, it can be expressed as a function of the three invariants of the strain tensor, i.e. the variation of the volume $V$, a measure of the “intensity” $Q_e$ of the strain deviator and the Lode angle $\varphi_e$. The expression of $E_{\text{rev}}$ is constructed so as to track the evolution of the experimental results, by means of a set of control parameters, directly identifiable on the basis of a single shear test (see Figure 7.44).

$$E_{\text{rev}} = \omega_{\text{vol}} + \omega_{\text{dev}}$$  [7.257]

$$E_{\text{rev}} = \frac{K_{\text{rev}}}{2} \left[ n \left( V - Q_{\text{rev}} \right) + \nu_{\text{rev}} Q_{\text{rev}} + \mu_{\text{rev}} Q_{\text{rev}}^2 \right] + \frac{\nu_{\text{rev}}}{2} \left( Q_e \left( Q_{\text{rev}} + 2Q_{\text{rev}} \right) - (Q_e + Q_{\text{rev}}) \left( n^2 + (Q_e + Q_{\text{rev}})^{1/2} + Q_{\text{rev}} \left( \alpha_{\text{rev}}^2 + Q_{\text{rev}}^2 \right)^{1/2} \right) \right)$$

$$- \alpha_{\text{rev}} \left( \ln |Q_e + Q_{\text{rev}}| + (n^2 + (Q_e + Q_{\text{rev}})^{1/2} + Q_{\text{rev}} \left( \alpha_{\text{rev}}^2 + Q_{\text{rev}}^2 \right)^{1/2} \right) \right)$$

$$+ \frac{\mu_{\text{rev}}}{2} \left( Q_e \left( Q_e - 2 \left( \alpha_{\text{rev}}^2 + Q_{\text{rev}}^2 \right) \right) \right)$$

$$+ \alpha_{\text{rev}} \left( \ln |Q_e - Q_{\text{rev}} + (n^2 + (Q_e - Q_{\text{rev}})^{1/2} + Q_{\text{rev}} \left( \alpha_{\text{rev}}^2 + Q_{\text{rev}}^2 \right)^{1/2} \right) \right)$$

$$+ (Q_e - Q_{\text{rev}}) \left( \alpha_{\text{rev}}^2 + Q_{\text{rev}}^2 \right)^{1/2} + Q_{\text{rev}} \left( \alpha_{\text{rev}}^2 + Q_{\text{rev}}^2 \right)^{1/2} \right)$$  [7.258]
where:

\[ Q_{ec} = \frac{(\mu_{1rev}\alpha_{1rev})^2 - Q_{\Sigma rev}^2}{2\mu_{1rev}Q_{\Sigma rev}} \]  

\[ [7.259] \]

Figure 7.44. Example of hyper-elastic evolution for two levels of temperature: role of the control parameters [ORG 97]

Thus, the parameters of the model are: \( K_{rev} \), \( Q_{\Sigma rev} \), \( \mu_{1rev} \), \( \mu_{2rev} \), \( \mu_{3rev} \), \( \alpha_{1rev} \), \( \alpha_{3rev} \) and \( Q_{erev} \). These eight parameters control hyper-elastic evolution (see Figure 7.45a):

- \( K_{rev} \) for compressibility;
- \( Q_{\Sigma rev} \) for the level of the “plateau” regime;
- \( \mu_{1rev}, \mu_{2rev}, \mu_{3rev} \) for the slope of the three regimes: the response start, the plateau, the response for large strains;
- \( \alpha_{1rev} \) and \( \alpha_{2rev} \) respectively for the transitions between regimes 1 and 2 and between regimes 2 and 3;
- \( Q_{erev} \) for the strain at which the transition between regimes 2 and 3 takes place.

A single shear test is sufficient to identify the parameters, with the exception of the compressibility modulus \( K_{rev} \).

In order to take account of the asymmetry between traction and compression [ORG 98a, ORG 97], and more generally the dependency of the transformation stress on the trajectory of loading, the five parameters \( Q_{\Sigma}, \mu_{1}, \mu_{2}, \mu_{3} \) and \( Q_{e} \) may be functions of the Lode angle \( \varphi_{e} \) in the strain deviator plane (see Figure 7.45d).

\[ Q_{\Sigma} (\varphi) = Q_{\Sigma} f(\varphi), \mu_{i} (\varphi) = \mu_{i} f(\varphi), i = 1, 3, Q_{e} (\varphi) = Q_{e} f(\varphi) \]  

with \( f(\varphi) = \left( 1 + \gamma \cos (3\varphi) \right)^{-n} \). The coefficients \( \gamma \) and \( n \) may be different for each parameter \( Q_{\Sigma}, \mu_{1}, \mu_{2}, \mu_{3} \) and \( Q_{e} \).
Figure 7.45. Meaning of the constitutive parameters

In order to respect the independence of the transformation energy in relation to
the type of loading, the product $Q_2 Q_e$ is chosen as being independent of $\varphi_e$, which enables us to link the coefficients $\gamma$ and $n$ for $Q_2$ and $Q_e$; thus, only two coefficients remain to be freely identified.

7.5.2.4. Hysteresis stress: discrete memory

In essence, the contribution of hysteresis is always irreversible. It integrates
the coupled microstructural phenomena of dry friction and elastic energy storage. The
hysteresis stress $\Sigma_{\text{hys}}$ is taken to be purely deviatoric and is denoted as $S_{\text{hys}}$. The pure
hysteresis model constitutes a continuous extension of rheological models containing
elastic parts and plateaus [GUE 76] including the notion of “discrete memory”.

The tensorial constitutive equation is then written in the form:

$$\frac{\partial}{\partial t} \left[ \Delta R S^i_j \right] = 2\mu_{0\text{hys}} D^i_j + \beta \varphi \Delta R S^i_j with 2S_{\text{hys}j} = S^i_k g^{kj} + S^i_j g^{kj}[7.260]$$

In this equation, $\Delta R S_{\text{hys}}$ represents the variation of the stress deviator between
the current state “$t$” and a reference state “$R$” associated with the previous inversion. $\varphi$ is
the “intrinsic dissipation” proposed by Guelin [GUE 80]: it must always be positive
or null; this property enables us to determine the states of inversion. $\beta$ is a function of
the history of load application, so that:

- the behavior is noticeably linear with a shear modulus $\mu_{0\text{hys}}$ at the beginning of
load application and just after a state of inversion;
– the maximum intensity of hysteresis under shear stress/strain is $\tau_{0\text{hys}} = Q_0/\sqrt{2}$, as indicated in Figure 7.46.

$$\bar{\sigma} = \Delta_t^t S_s \Delta \frac{(Q_{\Delta \Sigma})^2}{2 \mu_{0\text{hys}}} \frac{w'}{w}$$
$$\beta = \frac{-2 \mu_{0\text{hys}}}{(w Q_0)^n (Q_{\Delta \Sigma})^{2-np}}$$

[7.261]

with:

$$Q_{\Delta \Sigma} = \sqrt{(\Delta_t^t S_s \Delta_t^t S_s)}$$
$$w' = w \cos (\alpha)$$

[7.262]

where $w$ is the Masing parameter, equal to 1 for the trajectory of the first load application and 2 for subsequent ones. $\alpha$ represents the angle between the tensors $\Delta_t^t S_s$ and $\Delta_R^R S_s$.

Figure 7.46. Pure hysteresis stress in the case of cyclical application of shear strain

Figure 7.45c shows the meaning of these three material parameters, which govern:

– $\mu_{0\text{hys}}$ the initial slope;
– $Q_0$ the level of saturation;
– $np$ the transition toward a state of saturation.

7.5.2.5. Temperature dependency

All the parameters of the model may depend on the temperature in line with a given evolutionary law, but usually three particular parameters are chosen to control the temperature dependency: the two parameters of the hyperelastic potential $Q_{\Sigma} (T)$ and...
and $Q_e(T)$ and the parameter of the hysteresis schema $Q_0(T)$. The evolution of these parameters with temperature is determined by isothermal traction tests at different temperatures, and on the basis of physical considerations.

For example, the evolution of $Q_e(T)$ shown in Figure 7.45b involves four parameters, $T_{0rev}$, $\frac{dQ_e}{dT}$, $Q_{\Sigma max}$, and $\alpha$. The parameter $\frac{dQ_e}{dT}$ satisfies the Clausius–Clapeyron relation.

7.5.2.6. Numerical model

The elasto-hysteresis model is implanted in a “home code” (see Herezh [RIO 95] [ORG 98b]) which can be used on its own or indeed connected to ABAQUS by way of a UMAT subroutine and a particular technique involving the passing of data through pipes. Readers can refer to [RIO 08] for details on the technique.

7.5.3. Illustrations

7.5.3.1. Modeling of homogenous tests

For the simulation of shearing cycles of different amplitudes, Figure 7.47 presents comparisons between the experimental results under shear on plates at a controlled testing temperature, drawn from [ORG 97], and the simulation carried out with the elasto-hysteresis model. Figures 7.47a and 7.47b relate to test temperatures leading respectively to a ferro-elastic-type behavior due to martensitic reorientations, and a super-elastic behavior, due to the mechanically-induced martensitic transformation, in the case of tests including loops and sub-loops. Figure 7.47c shows the experimental and simulated curves for superelastic behavior with shearing during a symmetrical cycle, for three temperatures.

Figure 7.47. Isothermal tests with loops and sub-loops a) ferroelastic materials b, c) superelastic materials

Another set of experimental data is used to analyze the model’s capacity to give an account of the evolution in the extent of hysteresis for shear tests including a series of small and large loops. One could refer to the work of Orgas [ORG 97] for one, and Liu et al. [LIU 06] for another, for further details about the experimental part.
With regard to non-proportional loading, e.g. under traction and compression/torsion, experimental data are provided by the works of C. Grabe and O.T. Bruhns [GRA 07, GRA 09]. The sample is presented in Figure 7.48. The material is a Ti-50.7 at.%Ni alloy exhibiting superelastic behavior at ambient temperature – ambient temperature is used for all the tests discussed here. Hereafter, we shall employ the notations introduced by Grabe. The experimental data available are the axial stresses $\sigma$, the axial strains $\varepsilon$, the scission stresses $\tau = \frac{3}{2} \tau$, the scission strains $\gamma = \frac{\gamma}{3}$. These values are calculated with the relations (7.263), on the basis on the measurements of elongation $\Delta l$ and the torsion angle $\Delta \varphi$ and the recorded values of the axial force $F$ and the moment $M_t$:

$$
\begin{align*}
\varepsilon &= \frac{\Delta l}{l}, \\
\gamma &= \frac{\Delta \varphi (d_0 + d_1)}{4l}, \\
\sigma &= \frac{F}{S}, \\
\tau &= \frac{16M_t}{\pi (d_0 + d_i)^2 (d_0 - d_i)}
\end{align*}
$$

[7.263]

$l$, $d_0$, $d_i$ and $S$ respectively represent the initial length, the initial exterior and interior diameters and the initial section of the sample. With these values being the initial values, and therefore constant, the stresses $\sigma$ and $\tau$ represent nominal stresses, rather than Cauchy stresses. Similarly, $\varepsilon$ and $\gamma$ represent nominal strains. Also at the level of comparisons with the experimental results, the same analytical formulae (equation [7.263]) are used to calculate the numerical values associated with the simulation.

The procedure of identification is based primarily on the results of a pure torsion experiment. In order to be able to suppose the test to be isothermal, we use the stress/strain curve obtained at the slowest rate of strain, $10^{-5}/s$, for identification. It should be noted, however, that the complex loading trajectories were carried out at $10^{-4}/s$, a strain rate with which phenomena of thermomechanical coupling may become significant. With simple loads, Grabe showed that the difference in response for these two strain rates was less than 5%. In what follows, we shall not take this coupling into account.

Figure 7.49 presents the response under shearing of the model identified, in comparison with the experimental results.
Figure 7.49. Identification of the parameters: pure torsion test → seven hyperelasticity parameters and three hysteresis parameters

Figures 7.50 and 7.51 respectively give the simulations of “square” and “butterfly” test trajectories with monitored deformation. The simulations of these complex tests performed by Grabe and Bruhns are particularly satisfactory.

Figure 7.50. “Square” imposed trajectory with strain under traction-compression-torsion: comparison between experimental results and the simulation
7.5.3.2. Simulation of anisothermal tests

This section describes the results of simulations obtained for NiTi wires subject to traction and torsion at different temperatures. The experimental data are drawn from the Roundrobin SMA Modelling\[sic\] benchmark [SIT 09]. The comparison between the potentialities of the different models – Metz-Nancy, Grenoble-Lorient, Pavie, College Station (Texas A&M), Leuwen and of course Besançon – has been performed on the basis of tests carried out in Prague, at an international symposium called ESOMAT 2009.

7.5.3.3. Simulation of non-homogeneous isothermal tests

This section relates to the case of holed plates, subject to tension stress in the plane, which causes non-homogeneous strain fields. The holes, which are 5, 6 and 7 mm in diameter, were made by electro-erosion in a plate 0.1 mm thick (see [CEL 12] and Figure 7.52 for further details).

The elastohysteresis parameters are identified on the basis of homogeneous tests involving traction, shearing and membrane bulging (equivalent to compression).
Figure 7.52. Geometry of the holed plate

Figure 7.53 shows the overall response of the holed plate subject to traction, with the nominal stress and nominal strain being $\sigma = F/s_0$ and $\varepsilon = \Delta L/L_0$. Based on the comparison with the experimental results, we can see that the simulation yields a similar overall behavior, a similar level of hysteresis as well, and the change in slope is accurately described. It should be noted, however, that the overall level of stress predicted by the simulation is a little lower than the experiment, and the response at the level of the second slope is smoother.

Figure 7.53. Non-homogeneous test: equivalent homogeneous behavior

Figure 7.54 presents the local responses. The experimental data are obtained by way of a system of measurement and analysis by image correlation. We observe the same order of appearance of localization bands; the distributions of the isovalues, for their part, are entirely similar.

7.6. Conclusion

Three models in the same vein have been abundantly described (superposition of the elastic and transformation strains, and choice of internal variables). These complement the investigations described in Chapters 5 and 6. Along the same
lines, the model advanced by Bouvet et al. [BOU 02] could have been described; it constitutes a variant of the previous three investigations. The hereditary models “with discrete memory” first put forward by Guelin et al. [GUE 76] have also been examined. These models are cut from a different cloth: it is not the strains (elastic strains, transformation strains) which are added here, but rather the stresses (elastic, anelastic stresses, etc.). As we have seen, these models are particularly effective for describing the hysteresis of the internal and external loops of shear curves, for instance [ORG 04].

Figure 7.54. Local behavior: main strain: experiment (above); simulation (below)
Chapter 8

Design of SMA Elements: Case Studies

8.1. Introduction

A simplified “strength of materials”-type method is used to perform calculations for bars or beams subject to bending stress, torsion, etc.

For instance, a simple spring works mainly under torsion. Therefore, we need to know the mechanical response of an SMA element subject to external mechanical loading, causing stress and strain gradients, as is the case under flexion or torsion.

In order to perform calculations for slender structures made of SMAs, such as beams, bars or plates, there is a simplified method equivalent to the strength-of-materials method for elastic bodies [GIL 96] or finite element method (FEM) calculations [BOU 98, VIE 01].

8.2. “Strength of materials”-type calculations for beams subject to flexion or torsion [REJ 99]

8.2.1. Beam with a rectangular cross-section, subject to pure flexion: theoretical study

A schematic curve of pseudo-elastic behavior of a NiTi alloy under isothermal traction can be described as follows (Figure 8.1).

This pseudo-elastic behavior without hardening can be qualified as “ideal”.

Consider a rectangular beam with a cross-section area $S$: height $2h$ (y axis), width $b$ (z axis), length $L = 2l$ (x axis) (Figure 8.2).
The only mechanical stress consists of a surface density of forces $\mathbf{T}(l, y, z)\mathbf{x} = \Sigma(l, y, z)\mathbf{x}$, of resulting torsor $-M\mathbf{z}$ at $x = l$ and another density of forces $\mathbf{T}(-l, y, z)(-\mathbf{x}) = \Sigma(-l, y, z)(-\mathbf{x})$, of resulting torsor $+M\mathbf{z}$ at $x = -l$.

Thus:

$$M = \int \int_{x=\text{const}} y \Sigma_{xx} dy dz \quad [8.1]$$

Elastic solution:

$$E_{xx} = \frac{y}{R} = Ky \quad [8.2]$$
$$\Sigma_{xx} = E^*E_{xx} = E^*Ky \quad [8.3]$$

where $R$ is the curvature radius of the neutral fiber (in fact of the neutral plane $y = 0$) $K (= 1/\rho)$, the curvature and $E^*$, the Young’s modulus (Figure 8.3).
Thus, for $0 \leq E = E_{xx} \leq E^{am}$, $0 \leq \Sigma = \Sigma_{xx} \leq \Sigma^{am}$, the momentum $M$ varies in a linear fashion with the curvature $K$ (Figure 8.4):

$$M = \frac{2}{3}bh^3E*K$$

[8.4]

with a phase transformation start value at both sides of the beam ($y = \pm h$):

$$M^{am}(z = 0) = \frac{2}{3}bh^2\Sigma^{am} = \frac{2}{3}bh^2E*K^{am}$$

[8.5]
Pseudo-elastic resolution of the bi-phase beam “A + M” (see Figure 8.5).

Figure 8.5. Stress gradient associated with pseudo-elastic loading

For $\Sigma = \Sigma^am$, $E^am \leq E \leq E^am + \gamma$.

If $2h_p$ constitutes the thickness of the austenitic core, then:

$$\Sigma = \begin{cases} \Sigma^am & \text{for } 0 \leq y \leq h_p \\ \Sigma^am & \text{for } h_p \leq y \leq h \end{cases}$$

[8.6]

This gives us:

$$M = 2b \left( \int_0^{h_p} \frac{\Sigma^am}{h_p} y^2 dy + \int_{h_p}^h \Sigma^am y dy \right)$$

[8.7]

$$M = bh^2 \Sigma^am \left( 1 - \frac{1}{3} \left( \frac{h_p}{h} \right)^2 \right) = \frac{3}{2} M^am (z = 0) \left( 1 - \frac{1}{3} \left( \frac{h_p}{h} \right)^2 \right)$$

[8.8]

$$M = M_L \left( 1 - \frac{1}{3} \left( \frac{h_p}{h} \right)^2 \right)$$

[8.9]

$h_p$ can be calculated as a function of $K$:

$$h_p = \frac{\Sigma^am}{E^am} \frac{1}{K}$$

[8.10]
Thus, there is a nonlinear relation between $M$ and $K$ (Figures 8.6 and 8.7):

$$M = \frac{3}{2} M^{am}(z = 0) \left(1 - \frac{1}{3h^2} \frac{\Sigma^{am}}{E} \right)^2 \frac{1}{K^2}$$  \quad [8.11]$$

with the limit momentum $M_L$:

$$M_L = \frac{3}{2} M^{am}(z = 0)$$  \quad [8.12]$$

Figure 8.6. Relation between the bending momentum $M$ and the radius of curvature $K = \frac{1}{R}$

The momentum at the end of transformation $M^{am}(z = 1)$ can be evaluated when $E = E^{am} + \gamma$ for $y = \pm h$:

$$M^{am}(z = 1) = \frac{3}{2} M^{am}(z = 0) \left(1 - \frac{1}{3} \left(\frac{E^{am}}{E^{am} + \gamma} \right)^2 \right)$$  \quad [8.13]$$

The stress release is more complex to define. While the stress-strain curve is unique when under loading, the same is not true for unloading. Indeed, the response curve is different for two samples containing different volume fractions of martensite.

The volume fraction of martensite $z$ (at the start of unloading and/or at the end of loading) is dependent on the distance $y$ to the neutral fiber:

$$\Sigma = E^* (E_{xx} - \gamma z)$$  \quad [8.14]$$
which gives us:

\[ z = \frac{1}{\gamma} (K_z y - \frac{\Sigma}{E}) \]  

[8.15]

where \( K_z \) corresponds to the value of \( K \) reached at the end of loading; the stress/strain relation is not independent of \( y \), so \( M = \int \int_{x=const} y \Sigma_{xx}(y) dy dz \) does not have a simple shape.

\[ M = \frac{3}{2} M_{ma}(z = 0) \left( 1 - \frac{1}{3h^2} \left( \frac{\Sigma_{ma}}{E} \right)^2 \frac{1}{K^2} \right) \]  

[8.16]

\[ M_{ma}(z = 1) = \frac{3}{2} M_{ma}(z = 0) \left( 1 - \frac{1}{3} \left( \frac{E_{ma}}{\Sigma_{ma} + \gamma} \right)^2 \right) \]  

[8.17]

\[ M_{ma}(z = 0) = \frac{2}{3} bh^2 \Sigma_{ma} \]  

[8.18]

\[ 0 \leq M \leq M_{ma}(z = 0) \]:

\[ M = \frac{2}{3} bh^3 E K \]  

[8.19]

\[ 0 \leq M_{ma}(z = 0) \leq M \leq M_{ma}(z = 1) \]:

\[ M = \frac{3}{2} M_{ma}(z = 0) \left( 1 - \frac{1}{3h^2} \left( \frac{\Sigma_{ma}}{E} \right)^2 \frac{1}{K^2} \right) \]  

[8.17]

\[ M_{ma}(z = 1) = \frac{3}{2} M_{ma}(z = 0) \left( 1 - \frac{1}{3} \left( \frac{E_{ma}}{\Sigma_{ma} + \gamma} \right)^2 \right) \]  

[8.19]
8.2.2. Experimental and theoretical validation [REJ 02]

The material chosen is a polycrystalline Cu-Zn-Al alloy (Cu: 70.17% Wt; Zn: 25.63% Wt; Al: 4.2% Wt). Following a “betatization” treatment, electrical resistance measurements yielded the following values: $M_s^0 = 17.8^\circ\text{C}; M_f^0 = 5.5^\circ\text{C}; A_s^0 = 16.7^\circ\text{C}; A_f^0 = 24.5^\circ\text{C}$.

Consider a rectangular beam with the following dimensions: $2l = 50 \text{ mm}, 2h = 12 \text{ mm}, b = 2 \text{ mm}$.

In order to perform pure bending testing, we had to put in place an adaptive experimental device (Figure 8.8) on a traction machine [REJ 02].

![Figure 8.8. Setup of adaptive flexion on a traction machine](image)

The experimental curves ($M \iff K$) obtained for three temperatures ($T_1 = 36^\circ\text{C}, T_2 = 46^\circ\text{C}$ and $T_3 = 56^\circ\text{C}$, greater than $A_f^0 = 24.5^\circ\text{C}$) are satisfactory. The phase transformation start momentum $M_{am}(z = 0)$ increases as $\Sigma_{am}$ increases (Figure 8.9).

In addition, visual observation carried out during the flexion reveals the appearance and disappearance of the martensite plates, within each grain, during the loading/unloading process (Figure 8.10). Figure 8.11 shows that the simulation of the experimental curves ($M \iff K$) is entirely correct.

A more sophisticated approach for flexion problems, with account taken, in particular, of the asymmetry between traction and compression, is also to be found in the works of Raniecki et al. [RAN 01].
8.2.3. Solving pure torsion problem: relation between the twisting torque \( C \) and the unitary angle of torsion \( \alpha \)

From the curve of ideal pseudo-elastic traction, the threshold shear transformation stresses \( \tau^{am} (\tau^{ma}) \) and the associated shear transformation strain are extrapolated on the basis of the equivalent von Mises stress and strain:

\[
\tau^{am} = \frac{\Sigma^{am}}{\sqrt{3}}, \quad \tau^{ma} = \frac{\Sigma^{ma}}{\sqrt{3}}, \quad \gamma_c = \sqrt{3}\gamma
\]

[8.20]

The procedure is identical to that used for flexion, so will not be discussed in detail.

Consider a circular beam with radius \( R \) and length \( l \) subject to two torques \( \pm Cz \) on its end surfaces \( (z = \pm l/2) \).

In the context of a kinematic approach, the shear strain is written:

\[
E_{Z\theta} = \frac{\alpha r}{2}
\]

[8.21]

where \( \alpha \) is the unitary angle of torsion.

The twisting torque \( C \) is conventionally defined by:

\[
C = \int \int_{z=\text{const}} r \Sigma_{z\theta} r dr d\theta
\]

[8.22]
Under loading:

– elastic torsion of the austenitic beam:

\[ 0 \leq E_{z\theta} \leq E_{c_{am}}, \quad 0 \leq \Sigma_{z\theta} \leq \tau_{am} (E_{c_{am}} = \frac{\tau_{am}}{2G}) \]

The torque \( C \) varies in a linear fashion with \( \alpha \):

\[ C = \frac{\pi R^4}{2} G \alpha \quad [8.23] \]

where \( G \) is the torsion shear modulus or Coulomb’s modulus with a value of transformation start torque \( C_{am}(z = 0) \) in \( r = R \), so that:

\[ C_{am}(z = 0) = \frac{\pi R^3}{2} \tau_{am} \quad [8.24] \]
– pseudo-elastic torsion of the biphased A + M beam:

\[
\Sigma_{z\theta} = \tau_{am} E_{c}^{am} \leq E_{z\theta} \leq E_{c}^{am} + \gamma_c
\]

**Figure 8.11.** Curve of the bending momentum \(M\) depending on the curvature \(K\): experiment and simulation

If \(2r_p\) is the thickness of the austenitic core of the cylinder, then:

\[
\Sigma_{z\theta} = \begin{cases} 
   \tau_{am} \frac{r_p}{r_p} & \text{for } 0 \leq r \leq r_p \\
   \tau_{am} & \text{for } r_p \leq r \leq R
\end{cases}
\]  
[8.25]

\[
C = 2\pi \left( \int_0^{r_p} \frac{\tau_{am}}{r_p} r^3 \, dr + \int_{r_p}^R \frac{r^3}{r_p} \, dr \right)
\]  
[8.26]

\[
C = \frac{2}{3} \pi R^3 \tau_{am} \left(1 - \frac{1}{4} \left(\frac{r_p}{R}\right)^3\right) = \frac{4}{3} C_{am}(z = 0) \left(1 - \frac{1}{4} \left(\frac{r_p}{R}\right)^3\right)
\]  
[8.27]

\(r_p\) can be calculated as a function of \(\alpha\):

\[
r_p = \frac{\tau_{am}}{G\alpha}
\]  
[8.28]

Now, there is a nonlinear relation between \(C\) and \(\alpha\):

\[
C \approx C_{am}(z = 0) \left(1 - \frac{1}{4R^3} \left(\frac{\tau_{am}}{G}\right)^3 \frac{1}{\alpha^3}\right)
\]  
[8.29]
The momentum at the end of phase transformation $C_{am}(z = 1)$ can be evaluated when $E_{z\theta} = E_{am} + \gamma_c$ for $r = R$:

$$C_{am}(z = 1) = \frac{4}{3} C_{am}(z = 0) \left( 1 - \frac{1}{4} \left( \frac{E_{am}}{E_{am} + \gamma_c} \right)^3 \right) \tag{8.30}$$

When the loading is released:

– for $0 \leq C \leq C_{ma}(z = 0)$, we have:

$$C = \frac{\pi R^3}{2} G \alpha \tag{8.31}$$

$$C_{ma}(z = 0) = \frac{\pi R^3}{2} \gamma_{ma} \tag{8.32}$$

– for $C_{ma}(z = 0) \leq C \leq C_{ma}(z = 1)$, we have:

$$C = C_{ma}(z = 0) \left( 1 - \frac{1}{4R^3} \left( \frac{\gamma_{ma}}{G} \right)^3 \frac{1}{\alpha^3} \right) \tag{8.33}$$

$$C_{ma}(z = 1) = \frac{4}{3} C_{ma}(z = 0) \left( 1 - \frac{1}{4} \left( \frac{E_{ma}}{E_{ma} + \gamma_c} \right)^3 \right) \tag{8.34}$$

### 8.3. Elements of calculations for SMA actuators

#### 8.3.1. Stress/position diagram: temperature parameterization

By transformation of energy which is often thermal, an actuator turns it into mechanical work.

Consider an SMA wire, in the martensitic state with an associated displacement $y_0$ under traction and subject to a constant force $F$.

The recoverable mechanical work is $F (y_0 - y_e)$ where $y_e$ constitutes the elastic elongation of the wire, in the austenitic state, subject to the force $F$.

In order for the wire to be able to return to its initial position when it is cooled, mechanical work $f_m \left( y_0 - y_e \right)$ needs to be injected into the wire (see Figure 8.12b).

If we suppose that for $y_0$, there is a buttress, then the cycle loops (see Figure 8.12b). The mechanical work provided by the wire, at each cycle, is equal to:

$$W = (F - f_m) \left( y_0 - \left( \frac{y_e + y_c}{2} \right) \right) \tag{8.35}$$
The maximum work provided by the actuator is obtained when $F$ and $y_0$ reach their maximum admissible values, i.e. $F_M$ and $y_M$:

$$W = (F_M - f_m) \left( y_M - \left( \frac{y_e + y_e'}{2} \right) \right)$$  \[8.36\]

Now, we add to the wire a recall element which provides a force $F$ between $f_m$ and $F_M$.

If:
- $F = f_m$, the work is available when the sample is heated (see Figure 8.13 and equation [8.36]);
- $F = F_M$, there is no work upon heating ($W = 0$) (see equation [8.36]); conversely, upon cooling, there is work available (see Figure 8.13b);
- $f_m < F < F_M$, work is available on heating and on cooling (Figure 8.13c).
Figure 8.13. Analysis of an actuator formed of an SMA wire with a recall element providing a constant force $F$ [GUE 96]

In reality, the actuator may not necessarily use all the available work; Figure 8.13d shows the point representative of functioning.

The recall force $F$ often produced by an elastic wire is no longer constant, and we obtain the diagram shown in Figure 8.14.

Figure 8.14. Diagram of the functioning of an SMA actuator with an elastic recall wire [GUE 96]
8.3.2. Work provided depending on the nature of the loading

We can define the efficiency of an actuator by its energy available per unit volume.

Let us examine some elementary loads.

8.3.2.1. Traction (or compression)

Consider a wire with length $L$ and section $S$, under the effect of $F_M$, we get:

$$\Sigma_M = \frac{F_M}{S}, \quad E_M = \frac{y_M}{L}, \quad E_e = \frac{y_e}{L}, \quad E_{TR} = E_M - E_e$$  \[8.37\]

and the maximum work provided when the sample is heated:

$$W_M = F_M (y_M - y_e) = \Sigma_M E_{TR} V$$ \[8.38\]

The efficiency $e$ is given by:

$$e = \frac{W_M}{V} = \Sigma_M E_{TR}$$ \[8.39\]

8.3.3. Torsion of a cylindrical wire

To begin with, we write:

$$W_M = \tau_M \gamma_{TR} \frac{V}{2}$$ \[8.40\]

where $\tau_M$ is the shear stress on the external fiber and $\gamma_{TR}$ is the transformation shear strain on the external fiber.

As we can show that $\Sigma_M E_{TR} = \tau_M \gamma_{TR}$, the efficiency of a wire under torsion is half that of a wire under traction.

8.3.4. Flexion of a beam

As in the previous case, we shall suppose that the equation of the deformation of the beam is the same in the elastic regime as during the transformation (which contradicts our previous calculations for flexion and torsion). This being the case, we can show on a rectangular beam anchored or under three-point flexion that (see Figure 8.15):

$$W_M = \Sigma_M E_{TR} \frac{V}{9}$$ \[8.41\]

and hence we get an efficiency value of $\frac{1}{9}$. 
8.3.5. Comparison of the different modes of loading

This is not entirely pertinent, because a mode is often associated with a type of actuation chosen and with stresses relating to usage. However, we can draw up a list of adjustable geometric parameters and efficiency factors (see Table 8.1).

<table>
<thead>
<tr>
<th>Mode of stress application</th>
<th>Efficiency factor</th>
<th>Adjustable geometric parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Traction, compression</td>
<td>1</td>
<td>Length L, diameter d</td>
</tr>
<tr>
<td>Torsion</td>
<td>1/2</td>
<td>L, d</td>
</tr>
<tr>
<td>Helix-shaped spring</td>
<td>1/2.8 to 1/2.3</td>
<td>Wire diameter d, rolling diameter D, number of spokes n and no spokes</td>
</tr>
<tr>
<td>Embedded flexion</td>
<td>1/9</td>
<td>L, b, h (Figure 8.15)</td>
</tr>
<tr>
<td>3-point flexion</td>
<td>1/9</td>
<td>L, b, h (Figure 8.15)</td>
</tr>
<tr>
<td>4-point flexion</td>
<td>1/9 to 1/3.3</td>
<td>L, l, b, h (Figure 8.15)</td>
</tr>
</tbody>
</table>

Table 8.1. Efficiency factors and adjustable parameters depending on the mode of loading [GUE 96]
8.3.6. A few remarks about the duration of heating and cooling of SMAs

It is crucial to know the response time of active materials in order to use them as actuators. These times are calibrated by integrating the heat equation on a NiTi wire subjected to a constant stress. Comparison with an “imaginary” material exhibiting the same characteristics but without phase transition shows that the response times are longer for SMAs (around 2.7 times longer in terms of heating and around 1.5 times longer with regard to cooling) [CHA 04].

One problem with long cooling times, particularly in confined spaces, has been solved with thermoelectric coolers using bismuth telluride. Thus, a micro-actuator has been created by Abadie et al. [ABA 09] for applications in endoscopy (see Figure 8.16). A multi-stage structure has also been envisaged (see Figure 8.17). The only problem lies in the fragility of the thermoelectrical contacts between the bismuth telluride and the NiTi actuators.

Figure 8.16. Actuator constitution (top); actuator traversed by the electrical current (bottom) [ABA 09]
8.4. Case studies

8.4.1. Study of the flexion of a prismatic bar subjected to a point force

8.4.1.1. Statement

Consider a prismatic bar of NiTi (in view of the constitutive law chosen) with a rectangular section (height $2h$ along $y$; width $b$ along $z$) subjected to a point force $-P y$ at the center of inertia of the end section $x = l$. The section $x = 0$ is anchored (see Figure 8.18).

The material is said to have “perfect pseudo-elastic” behavior (Figure 8.19).

1) As $P$ increases: give the coordinates of the points where the phase transformation begins. Calculate the corresponding value of $P$ which will be denoted $P_{am}$. $P_{am}$ will be calculated on the basis of $\Sigma_{am}$, $b$ and $h$.

2) Let $P \geq P_{am}$, draw the profile of stress at the anchored point $(x = 0)$. Let $2h_p(0)$ be the residual thickness of austenite in $x = 0$. Calculate $P$ as a function of $P_{am}$, $b$, $h$ and of the $h_p(0)/h$ ratio.

3) For a section with fixed $x$ ($0 \leq x \leq l$), calculate $h_p(x)$. From this, deduce the geometric shape of the austenitic domain.
Figure 8.19. Traction curve “without hardening” but with hysteresis

For a fixed \( P \geq P_{am} \), plot \( h_p \) as a function of \( x \).

**NOTE.**– In this problem, we ignore the effect of the shearing force associated with \( P \), and therefore the associated shear stresses. If we take account of these factors, how might the problem be viewed anew?

8.4.1.2. **Brief solution**

“Elastic” flexion stress:

\[
\Sigma_{xx} = \frac{P(l-x)y}{I}
\]

where \( I \) is the quadratic flexion momentum \( I = \frac{2bh^3}{3} \)

\[
\Sigma_{am} = | \Sigma_{xx}(x = 0, y = \pm h) | = \frac{P_{am}h}{I}
\]

\[
\Rightarrow P_{am} = \frac{2bh^2}{3} I \Sigma_{am}
\]

\[
P = \frac{3}{2} P_{am} \left( 1 - \frac{1}{3} \left( \frac{h_p(x = 0)}{h} \right)^2 \right)
\]

\[
h_p(x) = \left( 3h^2 - \frac{2h^2 P}{P_{am}(l-x)} \right)^{\frac{1}{2}}
\]

8.4.2. **Slender tube subject to twisting torques**

8.4.2.1. **Statement**

Consider a slender tube (whose thickness \( e \) is very small in comparison to the average radius \( R \)) of length \( 2l \) (Figure 8.20). At temperature \( T \) and in the stress-free state, the material is in the austenitic state \( (T > A_f) \).
The beam is subjected to a twisting torque $Cz$ at $z = l$; $(-Cz$ at $z = -l$). The threshold stress for the direct transformation is $\tau^am$ for $A \Rightarrow M$ and $\tau^ma$ for $M \Rightarrow A$. Also consider the behavior to be perfect pseudo-elastic (i.e. without hardening) with Coulomb’s modulus $G$ and the shear strain associated with the complete transformation $\gamma_c$ (see Figure 8.21).

1) Classic elastic solution: with the slender tube hypothesis ($e << R$), calculate the quadratic momentum under torsion $I_0$ and the torsion stress $\Sigma_{Z\theta}$ (assumed to be the same throughout the section of the tube). Also find the strain associated with the torsion $E_{z\theta}$. From this, deduce the relation between the torque $C$ and the unitary angle of torsion $\alpha$.

2) Calculate the value of the torque $C^{am}(z = 0)$ corresponding to the start of transformation in the tube and the corresponding angle $\alpha^{am}(z = 0)$ and $\alpha^{am}(z = 1)$.

3) When $C \geq C^{am}(z = 1)$, what is the value of $\alpha$? Plot the evolution of $C$ with the change in $\alpha$. 
4) At this point of operation, give a mechanical and physical explanation of what happens if:

   a) $\alpha$ is kept constant while the tube is heated;

   b) the torque $C$ is eliminated without changing the temperature.

8.4.2.2. Brief solution

$$I_0 = 2\pi R^3 e, \Sigma_2 = \frac{C}{2\pi R^2 e}, E_2 = \frac{\Sigma_2}{2G} = \frac{\alpha R}{2}$$

$$C = GI_0\alpha$$

$$C^{am}(z = 0) = \frac{I_0\tau^{am}}{R} = 2\pi R^2 e\gamma^{am}$$

$$\alpha^{am}(z = 0) = \frac{\tau^{am}}{GR}, \alpha^{am}(z = 1) = \frac{1}{GR} (\tau^{am} + 2G\gamma_c)$$

8.4.3. Study of a “parallel” hybrid structure

8.4.3.1. Statement

Consider a NiTi wire, with pre-deformation $\gamma$ in the martensitic state at temperature $T_0$.

This “straight” wire is covered in epoxy resin: the whole constitutes a hybrid structure (Figure 8.22).

![Figure 8.22. Representation of a “parallel” hybrid structure](image)

Wire: medium A: Young’s modulus $E_A$; volume fraction $f_A$. 
Epoxy resin: medium B, whose behavior is considered to be elastic: Young’s modulus $E_B$; volume fraction $f_B$.

Initial conditions: $t = 0$:
- medium A: $T = T_0$, $E_0 = \gamma$, $z = 1$;
- medium B: considered to be “pre-deformed”: $T = T_0$, $E_0 = \gamma$.

1) If we consider the resin/wire interface to be ideal, very briefly justify the modeling of the hybrid material as two “parallel” bars A and B.

2) Write the equilibrium and compatibility under strain of the combination of the two bars.

2.1) Write the expression of the global strain $\Sigma$ as a function of $f_A$, $\Sigma_A$, $f_B$, $\Sigma_B$.

2.2) Write $d\Sigma_A$, $d\Sigma_B$ and $dE$ (the increment in the total strain) as a function of $E_A$, $E_B$, $f_A$, $f_B$ and $\gamma$, $d\Sigma$, $dz$.

3) At $t = 0^+$, the NiTi wire is heated by the Joule effect. Briefly describe the structure’s physical response.

Give $E(t)$ as a function of the parameters $\gamma$, $E_A$, $E_B$, $f_A$, $f_B$ and $z(t)$.

When $t \to \infty$, give the maximum possible value for $E(t)$.

8.4.3.2. Brief solution

$$dE_A = dE_B = dE$$

$$\Sigma = f_A \Sigma_A + f_B \Sigma_B$$

Incremental constitutive laws:

$$d\Sigma_A = E_A(dE_A - \gamma dz)$$

$$d\Sigma_B = E_B dE_B$$

$$dE = \frac{f_A E_A}{f_A E_A + f_B E_B} \gamma dz$$

$$\int_0^t dE = E(t) - \gamma = \frac{f_A E_A}{f_A E_A + f_B E_B} \gamma \int_0^t dz = \frac{f_A E_A}{f_A E_A + f_B E_B} \gamma (z(t) - 1)$$

$$E(t = +\infty) = \frac{f_b E_b}{f_A E_A + f_B E_B} \gamma$$
8.4.4. Study of a “series” hybrid structure

8.4.4.1. Statement

Consider a hybrid structure comprising two springs connected in a series (the structure is anchored at both ends) (Figure 8.23).

- a NiTi spring, A, pre-deformed in the martensitic state \( z = 1 \), with a value \( \gamma \), length \( l_A \) and section \( S \);
- a spring B with Young’s modulus \( E_B \) and length \( l_B \) and section \( S \).

![Figure 8.23. Representation of a “series” hybrid structure](image)

Initial conditions \( t = 0 \): \( T = T_0 \), A and B in the stress-free state.

1) The NiTi wire is heated. Briefly describe the structure’s physical response.

2) Evaluate \( d\Sigma_A \) as a function of \( d\Sigma_B \).

3) Take \( f_A, f_B \) to be the volumetric proportions of A and B in relation to the total volume of both springs; evaluate \( dE \) as a function of \( f_A, f_B \) and \( dE_A, dE_B \).

4) Write, in incremental form:
   - the constitutive law for spring A;
   - the constitutive law for spring B.

5) From this, deduce \( dE \) as a function of \( d\Sigma \) and \( dz \). What hypothesis can be made about \( dE \)? Deduce \( \Sigma(t) \). As \( t \to \infty \), give the maximum possible value for \( \Sigma(t) \).

6) What might such a setup be used for?
8.4.4.2. Brief solution

\[ d\Sigma_A = d\Sigma_B = d\Sigma \]
\[ dE = f_AdE_A + f_BdE_B \]

where \( dE_A = \frac{d\Sigma_A}{E_A} + \gamma dz \)
\[ dE_B = \frac{d\Sigma_B}{E_B} \implies dE = \left( \frac{f_A}{E_A} + \frac{f_B}{E_B} \right) d\Sigma + \gamma f_A dz \]
\[ dE = 0 \implies d\Sigma = -\frac{\gamma f_A dz}{\left( \frac{f_A}{E_A} + \frac{f_B}{E_B} \right)} \]
\[ \int_0^t d\Sigma = \Sigma(t) - 0 = -\frac{\gamma f_A}{\left( \frac{f_A}{E_A} + \frac{f_B}{E_B} \right)} (z(t) - 1) \]
\[ \Sigma(t = +\infty) = \frac{\gamma f_A}{\left( \frac{f_A}{E_A} + \frac{f_B}{E_B} \right)} \]

8.4.5. Design of an application: breakage of a mechanical link

8.4.5.1. Statement [PAT 01]

A steel rod of diameter \( d = 4 \text{ mm} \) can withstand a load of \( P = 500 \text{ N} \). In order to break this link, we propose to use a SMA ring made of NiTi (Figure 8.24).

![Figure 8.24. Device for breaking a mechanical link](www.iran-mavad.com)
Mechanical properties of the steel rod:

\[ E_{ac} = 200 \text{ GPa} \]
\[ \Sigma_y = 900 \text{ MPa} \]
\[ A = 25\% \text{(elongation before fracture)} \]

Properties of the SMA:

\[ E^* = 100 \text{ GPa} \]
\[ B = 0.32 \text{ MPa.K}^{-1} \]
\[ \varepsilon^m = -4\% \text{ (constant value)} \]
\[ H = 12.8 \text{ MPa} \]
\[ M_f^0 = 0^\circ \text{C}, M_s^0 = 40^\circ \text{C}, A_s^0 = 40^\circ \text{C}, A_f^0 = 80^\circ \text{C} \]

Geometric characteristics of the device:

\[ l_0 = 10 \text{ mm} \]
\[ L = 70 \text{ mm} \]
\[ d = 4 \text{ mm} \]

SMA ring: internal diameter: \( d_{int} = 8 \text{ mm} \), external diameter: \( d_{ext} = 12 \text{ mm} \)

Martensitic transformation occurs if the following criterion is satisfied:

\[ \Sigma \kappa - B \left( T - M_s^0 \right) - Hz = 0 \quad [8.42] \]

The behavior of the steel is considered to be “perfectly elastoplastic”.

The effect of the thermal dilation of the steel and of the SMA is ignored.

1) Conditioning of the setup: determine the temperature to which the ring needs to be cooled in order to obtain a total deformation of \(-4\%\) with a compressive stress of \(-40 \text{ MPa}\).

2) Operation of the device: with the device submitted to a 500 N stress at ambient temperature, the entire system is heated:
a) determine the temperature at which inverse transformation begins in the ring.

b) determine the maximum stress developed by the ring during the course of heating. At what temperature is this stress attained? In light of these findings, what is the volume fraction of martensite in the ring?

c) Verify that heating the ring will indeed lead to the breakage of the link. Determine the temperature at which this breakage will occur.

8.4.5.2. Solution

The choice made is a simplified version of the thermodynamic potential, i.e. a one-dimension version advanced by Chemisky et al. [CHE 11].

Habitat:

\[ G(\Sigma, z, T) = -\frac{\Sigma^2}{2E_a} - \Sigma \kappa z + B(T - M_s^{0})z + \frac{1}{2}Hz^2 \]  

[8.43]

where:

\[ E = -\frac{\partial G}{\partial \Sigma} = \frac{\Sigma}{E_a} + \kappa z = E^{el} + E^{tr} \]  

[8.44]

and:

\[ \Pi_f (z) = -\frac{\partial G}{\partial z} = \Sigma \kappa - B(T - M_s^{0}) - Hz \]  

[8.45]

with, for the initiation of the \( A \Rightarrow M \) transformation:

\[ \Pi_f (z, z = 0) = \Sigma \kappa - B(T - M_s^{0}) = 0 \Rightarrow T = 45^\circ C \]  

[8.46]

Conditioning temperature:

\[ \Pi_f (z, z = 1) = \Sigma \kappa - B(T - M_s^{0}) - H = 0 \Rightarrow T = 5^\circ C \]  

[8.47]

a) \( \Sigma = 0 \), the inverse transformation begins to occur at \( T = A_s^{0} = 40^\circ C \).

NOTE.– Business recovery when the steel rod along is submitted to stretching stress:

\[ P = 500 \text{ N} \Rightarrow \Sigma = P/S = 39.8 \text{ MPa}; \quad E = E^{el} = \Sigma/E_{ac} = 2.10^{-4} = 0.02\%; \quad \Delta l = El_0 = 2.10^{-3} \text{ mm} \]

b) \( F_{ring} + F_{rod} = P \) and \( \Delta l_{ring} = \Delta l_{rod} = \Delta l \)
The rod is rigid if $\Sigma_{rod} < \Sigma_y$:

$$\Sigma_{max} = \frac{1}{S_{ring}} (P - \Sigma_y S_{rod}) = -172 \text{ MPa}$$ \[8.48\]

$$\Delta E = \Delta E^{el} + \Delta \kappa = \frac{\Delta \Sigma}{E^{\star}} + \frac{\kappa}{H} (\kappa \Delta \Sigma - B \Delta T) = 0$$ \[8.49\]

$$\implies \Delta T = \frac{\Delta \Sigma}{B} (\kappa + \frac{H}{E^{\star}} \frac{1}{\kappa}) = 23^\circ C \implies T = 63^\circ C$$ \[8.50\]

Fraction of martensite $z = 0.96$

c) Fracture of the link:

$$\Sigma_{tige} = \Sigma_y \Sigma_{bague} = -172 \text{ MPa and } A = 25\%$$

$$\Delta E = \Delta E^{el} + \Delta E^{tr}$$

Volume fraction of martensite $\Delta E^{tr} = \kappa \Delta z \implies \Delta z = -0.86z = 0.1$

Temperature of the system at fracture:

$$T = A_0 + \frac{1}{B} (\Sigma \kappa - Hz) = 115^\circ C$$ \[8.51\]
Chapter 9

Behavior of Magnetic SMAs

9.1. Introduction

The advantage of magnetic shape-memory alloys (MSMAs) over conventional shape-memory alloys (SMAs), lies in the possibility for their actuation not only by stress or temperature, but also by a magnetic field.

MSMAs have a maximum deformation of around 6–10%, just like conventional SMAs, but the response times they exhibit are similar to those of magnetostrictive materials (around one millisecond). At present, research and usage are largely focused on two main materials. Both were developed in 1995-1996 in the United States, by a team at MIT for Ni-Mn-Ga [ULL 96] and a team at the University of Minnesota for FePd [JAM 98]. Of all the materials which exhibit the properties of MSMAs, the most widely used today is, without contest, Ni-Mn-Ga.

The article by Liang et al. [LIA 06] details the three possibilities for performing magnetic actuation using magnetic shape-memory alloys. The first of these options consists of obtaining a phase transformation induced by a magnetic field; however, this requires very powerful magnetic fields, and proves inappropriate for actuation. The second possibility is martensitic rearrangement induced by a magnetic field. Finally, the third possibility, referred to as the hybrid approach, consists of using a magnetic field gradient to create a sufficient force to engender a phase transformation.

This chapter will be devoted mainly to the modeling of thermo-magneto-mechanical behavior. A literature review will take stock of certain already-existing models.
9.2. Some models of the thermo-magneto-mechanical behavior of MSMAs

The modeling of MSMAs involves two communities: teams of specialists in magnetism – in particular, magnetostrictive materials – and teams grounded in physics and the strength of materials. The original aspect of our studies lies in the joining forces, at FEMTO-ST, of a team in automation engineering (AS2M Department) and one in mechanics (DMA – Department of Applied Mechanics). Amongst other noteworthy publications, this collaboration created the thesis of Jean Yves Gauthier [GAU 07b].

A distinction between models drawn from magnetism and those drawn from mechanics is to be found in the choice of the scale examined. At the microscopic scale, crystallographic examination yields mechanical and spin information, and magnetic results. At the mesoscopic scale, the inter-phase and inter-variant boundaries will be examined, alongside micromagnetic study of the twinned variants and Weiss domains.

Let us now give a brief overview of a number of models. The ones we have chosen are essentially models involving the rearrangement of the martensite platelets. Some publications have been devoted to the “pseudo-elastic” phase transformation, by Chernenko et al. [CHE 04], Pons et al. [PON 03] and Hirsinger et al. [HIR 04b].

As the reorientation of the martensite platelets by a magnetic field is the main actuation force, we shall focus on this effect.

9.2.1. O’Handley and Murray et al.’s model

In their one-dimensional model, the authors [MUR 00, MUR 01b] consider two forms of energy: one mechanical in origin \((\sigma + \sigma_0)\varepsilon_0\) – an affine function of the applied stress \(\sigma\); the other of magnetic origin \(M_S H\) proportional to \(H\); the parameters \(\sigma_0, \varepsilon_0, M_S\) are constants. In addition, the strain can assume one of only two distinct values: 0 or \(\varepsilon_0\). The boundary between these two values is to be found at energetic equilibrium \((\sigma + \sigma_0)\varepsilon_0 = M_S H\).

The same authors put forward a second approach [OHA 00, MUR 01a] based on thermodynamics, with an expression of the free energy, taking account of the Zeeman energy, the energy due to magnetic anisotropy, an elastic energy and an energy due to the external stress. By energy minimization, they obtain the volumetric fraction of martensite as a function of the magnetic field and the stress. They add a magnetic coercive field (negative or positive depending on the direction of variation of the field), dependent upon the stress, in order to be able to take account of the mechanically-generated hysteresis.
9.2.2. Micromagnetism

Tickle and James [TIC 99] consider a three-dimensional model, taking account of the three martensite variants for a cubic-to-quadratic transformation. By addition of the effect of a demagnetizing field, the value of the deformation is obtained by energy minimization.

DeSimone and James [DES 02] extend the theory of micromagnetism, used for purely magnetic and magnetostrictive cases, to MSMAs. The aim of such a model is to characterize the changes in the magnetic microstructure as a function of the magnetic field applied and to deduce from this the macroscopic relations between the deformation and the magnetic field.

9.2.3. Likhachev and Ullakko’s model [LIK 00a, LIK 00b]

Likhachev and Ullako introduce magnetic anisotropy in their model. Two magnetization functions corresponding to the axis of easy magnetization and the axis of difficult magnetization are put forward: respectively $M_a(H)$ and $M_t(H)$. A “stress of magnetic origin” is then deduced. This stress is added to the mechanical stress to give the global stress, which will cause the deformation.

Reversible mechanical behavior is taken into account in [LIK 00a], and a Fermi distribution-type hysteretic behavior is used in [LIK 00b], corresponding to two different exponential functions for the two directions of change in the deformation.

The model advanced by Suorsa et al. [SUO 04] is also based on the Likhachev model from a magnetic point of view. However, the hysteretic mechanical model is an original model developed initially to deal with purely magnetic hysteresis. This model of hysteresis is static, as are all the models presented in this literature review, and takes account of internal loops without memory points. This model has been used for the design of MSMA-based actuators.

9.2.4. Original approaches

Adly et al. [ADL 06] propose a Preisach-type vectorial model to represent the behavior of a MSMA and a magnetostrictive material. The two inputs required by the model are therefore the magnetic field and the mechanical stress. The deformation corresponds to the output variable of the model. This model is by no means based on a physical approach to the material’s behavior. Indeed, the same model has been used for martensitic rearrangement in MSMAs and in conventional magnetostrictive materials, where the phenomena involved are of a very different nature.

Mullner et al. [MUL 02], [MUL 03] put forward an approach based on a microscopic description and magnetoplasticity, and explain that the macroscopic
magneto-mechanical properties depend on the microstructure. According to these authors, mesoscopic or macroscopic approaches are sufficient to predict the magnetic stress, owing to the fact that the properties depend solely on global parameters. On the other hand, the magnetomechanical hysteresis and the threshold of the magnetic field can only be explained on the basis of a microscopic model, because these properties reflect the mutual interaction between the variants and their interactions with the interfaces.

A statistical and probabilistic approach was employed in [GLA 03]. A Gaussian distribution is used to obtain the values of the volumetric fraction of martensite as a function of a magnetic stress. Two functions are taken into account for both directions of change in order to obtain hysteresis. Another probabilistic approach is set out in [BUC 03], where the rearrangement of the variants is taken into account at the same time as phase transformation. A probability of phase transition or rearrangement is calculated on the basis of an energy functional.

The model developed by Couch et al. [COU 07] is an extension of the investigations by Brinson and Tanaka, used in the context of conventional SMAs. This model is typically a model of macroscopic behavior. A constitutive law (constitutive equation) links the variables together in a linear fashion (stress, strain, magnetic field and volumetric fraction of martensite).

9.2.5. Overlaps between these approaches

In [LIK 04], a summary is given as regards the taking into account of magnetism in the models. The influence of two major phenomena needs to be considered: namely the rotation of magnetization due to a magnetocrystalline anisotropy and the variation of the size of the Weiss domains. Some do not take account either of the rotation of magnetization or the variation of the Weiss domains: the magnetization is then considered to be fixed for each of the variants. Others take account of only one or the other of these two factors (either the rotation of magnetization or the variation of the Weiss domains). Finally, certain models take account of both of these phenomena. The concept of magnetically-generated stress is becoming more widely accepted; thus, this stress is used in a purely mechanical model. This technique simplifies the investigation, by separating magnetic and mechanical effects. At the mechanical level, there is a similar range of investigations as is used for conventional SMAs. Most models, however, are based on a globally-elastic or partially-elastic approach, or use a Preisach-type model of hysteresis or another, simpler model, inherited from magnetic materials. True thermodynamic approaches are few and far between, and frequently lack rigorosity in their development. However, this type of approach enables us to properly formalize the concept of magnetically-generated stress, and extend the simulation to dynamics and to the reaction to temperature change. The framework of thermodynamics is certainly the most rigorous means of establishing a complete macroscopic model, albeit relatively complicated in terms of its general formulation.
9.3. Crystallography of Ni-Mn-Ga

As explained by Mullner et al. [MUL 03], the mechanical properties depend on the microstructure of the material. Using X-ray diffraction measurements, coupled with transmission electron microscopy, it is possible to identify the austenitic and martensitic lattices, and thereby discover what crystallographic transformation is taking place, and also to measure the lattice parameters. This was performed on a sample of Ni-Mn-Ga by Ge et al. [GE 06].

We shall draw upon certain lessons learnt in Chapter 3, devoted to martensitic transformation.

9.3.1. The different phases and variants

Here, nickel-manganese-gallium, with a composition similar to the stoichiometry Ni$_2$-Mn-Ga, is studied. At high temperature, the austenitic phase A exhibits a Heusler L$_2^1$ structure, which constitutes an assembly of eight centered cubic lattices (see Figure 3.13). Hereafter, we shall consider a simplified representation: a cube with length of side $a_0$.

In the wake of cooling or of the application of a stress, this material can transform into three other main phases (Figure 9.1):

– quadratic martensite, with an atomic modulation of a periodicity of five atomic layers, referred to as 5 M, characterized by two lattice parameters: $a$ corresponds to the two long axes and $c$ to the short axis;

– centered monoclinic martensite associated with an atomic modulation, with a periodicity of seven atomic layers, referred to as 7 M, characterized by four lattice parameters: $a$ and $b$ associated with the two long axes, $c$ associated with the short axis, and an angle of distortion;

– non-modulated quadratic martensite, also known as NMT (for non-modulated tetragonal structure), characterized by two lattice parameters: $a$ corresponding to the two short axes and $c$ to the long axis.

The values of the lattice parameters vary depending on the composition of the alloy in question. However, the maximum values of deformation with martensitic rearrangement are respectively 5–6%, 10–11% and 15–19% for 5 M, 7 M and NMT martensites. Magnetic field actuation is now a possibility on the first two; however, regarding NMT martensite, only rearrangement by mechanical stress has been observed in experiments.
Figure 9.1. Crystallographic structures of Ni-Mn-Ga: a) L2$_1$ austenite; b) modulated quadratic martensite (5 M); c) modulated monoclinic martensite (7 M); d) non-modulated quadratic martensite (NMT)

With regard to 7 M and NMT martensites, further details are to be found in [SOZ 02], [JIA 02] and [RIC 06]. Hereinafter, we shall focus on 5 M martensite, because this is the most widely used martensitic structure of materials, at present: consequently, there is a more abundant body of experimentation and material is more easily available. Yet the tools used are sufficiently general to be applicable to a different type of MSMA.

A 5 M-type martensite may be present in the form of three variants. This is due to its quadratic structure [CRE 04]. These variants are represented in Figures 9.2 and 9.3. We shall use the notation M1, M2 and M3 to denote the variants which, respectively, have their short axis along the axes $x$, $y$, $z$.

9.3.2. Rearrangement and transformation

Figure 9.4 presents the general behavior of an MSMA. At high temperature, the alloy is in an austenitic state. After cooling, the sample contains the three martensite variants in equal proportions: no macroscopic deformation occurs as a result. The application of a compressive stress favors the formation of the variant whose short axis lies in the direction of that stress (M2 in Figure 9.4) and thereby alters the geometric shape of the sample. The application of a magnetic field favors the variant whose axis of easy magnetization (identical to the short axis) lies in the direction of that field (M1 in Figure 9.4) and also alters the shape of the sample. The balance between these two effects can be used to create actuation.
9.3.3. Calculations of microstructures

The calculations have already been discussed in great detail in Chapter 3, given over to martensitic transformation. Here let us briefly recap a number of elements.
Let $F_k$ be the gradient tensor of the transformation of austenite $A$ into the variant $k$ of martensite $M$:

$$dx(M) = F_k dx_0(A) \quad [9.1]$$

and the Green-Lagrange strain tensor is defined by:

$$E_{tr}^k = \frac{1}{2} (t^{F_k} F_k - 1) = \frac{1}{2} (U^2_k - 1) \quad [9.2]$$

with three variants for the cubic $\rightarrow$ quadratic transformation:

$$U_1 = \begin{bmatrix} \beta & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \alpha \end{bmatrix}, \quad U_2 = \begin{bmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & \alpha \end{bmatrix}, \quad U_3 = \begin{bmatrix} \alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \beta \end{bmatrix} \quad [9.3]$$

and $\alpha = a/a_0$, $\beta = c/a_0$ (see Figure 9.2).

For the reorientation of variant $M_k$ into variant $M_i$, the strain tensor:

$$E_{re}^{ki} = \frac{1}{2} (U_i^2 - U_k^2) \quad [9.4]$$

Note that the interface between austenite and martensite can only exist in the form of “twinned” martensite in opposition to the austenite (see Figure 9.5).

Indeed, the CTM gives the solution to the “twinning equation”:

$$QU_i - U_j = a \otimes \hat{n} \quad [9.5]$$

---

Figure 9.4. Schematic visualization of a transformation and a martensitic rearrangement.
Figure 9.5. “Twinned” martensite forming an interface with austenite

Let us apply this to the cubic $\rightarrow$ quadratic transformation. We shall begin with variants 1 and 2. The calculations are as follows.

Let $R$ be a rotation matrix of 180° around the $\hat{e}$ axis defined by:

$$\hat{e} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$$

[9.6]

It is easy to verify that $R^T U_1 R = U_2$, and we obtain:

1. $a = \frac{\sqrt{2}(\beta^2 - \alpha^2)}{\beta^2 + \alpha^2} \begin{pmatrix} -\beta \\ \alpha \\ 0 \end{pmatrix}, \quad \hat{n} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$

[9.7]

2. $a = \frac{\sqrt{2}(\beta^2 - \alpha^2)}{\beta^2 + \alpha^2} \begin{pmatrix} -\beta \\ -\alpha \\ 0 \end{pmatrix}, \quad \hat{n} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$

[9.8]

Note that these calculations are illustrated in Figure 9.3.

If necessary, $Q$ can be obtained using equation [9.5] (twinning equation).

The equation of compatibility between austenite $A$ and the couple of martensite variants $M_i/M_j$, in proportion $(1-\lambda)$ and $\lambda$ respectively, is:

$$Q^\dagger (\lambda Q U_1 - (1-\lambda)U_1) = 1 + b \otimes m$$

[9.9]
We shall hypothesize that the twinning equation for variants \( i \) and \( j \) has a solution. Once again, Ball and James [BAL 87, BAL 92] give the procedure in order to obtain the solution to the equation for the austenite/martensite interface.

1) Calculate:
\[
\delta = \mathbf{a} \cdot \mathbf{U}_1 (\mathbf{U}_1^2 - 1)^{-1} \mathbf{n}
\]
and:
\[
\eta = tr(\mathbf{U}_1^2) - det(\mathbf{U}_1^2) - 2 + \frac{||\mathbf{a}||^2}{2\delta}
\]

The equation for the austenite/martensite interface has a solution if and only if:
\[
\delta \leq -2 \text{ and } \eta \geq 0
\]

2) To find the solutions, calculate:
\[
\lambda = \frac{1}{2} (1 - \sqrt{1 + \frac{2}{\delta}})
\]

For Ni\textsubscript{2}-Mn-Ga \( \alpha = \alpha_0 = 1.0188 \) and \( \beta = c/a_0 = 0.9589 \), we obtain \( \lambda = 0.3083 \) and:

- for \( M_1 \Rightarrow M_2 \):
\[
E^{tr}_{12} = \frac{1}{2} (\mathbf{U}_2^2 - \mathbf{U}_1^2) = \text{diag}(0.0593, -0.593, 0)
\]

- for \( A \Rightarrow (M_1, M_2) \):
\[
E^{tr} = \frac{1}{2} (\mathbf{U}_{tw}^2 - 1)
\]

where \( \mathbf{U}_{tw} = \lambda \mathbf{U}_2 + (1 - \lambda) \mathbf{U}_1 \), and finally:
\[
E^{tr} = \text{diag}(-0.0224, 0.0004, 0.0190)
\]

9.4. Model of the magneto-thermo-mechanical behavior of a monocrystal of magnetic shape-memory alloy

As usual, we shall conduct our discussion within the context of thermodynamics of irreversible processes (TIP) for models with internal variables – the additional ingredient being magnetism.
9.4.1. Expression of the Gibbs free energy associated with magneto-thermo-mechanical loading

We shall divide the Gibbs free energy $G$ into four expressions: a chemical energy $G_{\text{chem}}$, a thermal energy $G_{\text{therm}}$, a mechanical energy $G_{\text{mech}}$ and finally a magnetic energy $G_{\text{mag}}$. This free energy can therefore be expressed in the following form:

$$
G(\Sigma, T, h, z_0, z_1, \ldots, z_n, \alpha, \theta, \alpha_A) = G_{\text{chem}}(T, z_0) + G_{\text{therm}}(T) + G_{\text{mech}}(\Sigma, z_0, z_1, \ldots, z_n) + G_{\text{mag}}(T, h, z_0, z_1, \ldots, z_n, \alpha, \theta, \alpha_A)
$$  \[9.16\]

where the state variables are as follows:

- $\Sigma$: the stress tensor for the stresses applied to the sample;
- $h = Hx$: the magnetic field applied;
- $T$: the temperature.

The internal variables chosen are:

- $z_0$: the volume fraction of austenite;
- $z_k$: the volume fraction of the variant $M_k$ of martensite ($k = 1 : 3$). We shall consider that the sample allows three martensite variants, which, by the crystallographic calculations demonstrated above, gives us:

$$
\sum_{k=0}^{3} z_k = 1
$$  \[9.17\]

- $\alpha$: the proportion of the Weiss domain within a REV of a martensite variant (see Figure 9.6);
- $\alpha_A$: the proportion of the Weiss domain within the austenite;
- $\theta$: the angle of rotation of the magnetization vector $\mathbf{m}$ under the influence of a magnetic field $h$ within a REV.

It should be noted, here, that no magneto-mechanical or thermo-mechanical energy term is present; the connection between the energies is made by way of an appropriate choice of internal variables.

9.4.2. Choice of the representative elementary volume

Clearly, in order to introduce internal variables, we need to define them. A choice of a representative elementary volume (REV) was made by Hirsinger and Lexcellent [HIR 02] for a sample containing two variants $M_1$ and $M_2$ (see Figure 9.6).
$z$ corresponds to the volume fraction of $M_1$ martensite (and $(1-z)$ to the volume fraction of $M_2$ martensite). Within each of the variants, two Weiss domains are represented, with respective fractions $\alpha$ and $1-\alpha$. $\theta$ corresponds to the angle between the direction of weak magnetization and the real direction of magnetization within $M_2$.

Figure 9.7 illustrates the evolution of the REV under the influence of a magnetic field $h = H_1 x$. For $h = 0$, the total magnetization of the sample is null, because the magnetization of one Weiss domain is compensated by the other domain ($\alpha = 0.5$) (Figure 9.7 (a)). When a relatively weak magnetic field is applied, the size of the Weiss domain whose axis of magnetization lies in the direction of the magnetic field increases, the consequence of which is that the domain size for the other variant also increases, due to the continuity of the magnetic flux. This growth continues until the other Weiss domain disappears completely ($\alpha = 1$) (Figure 9.7 (b)). When the field becomes stronger, two situations may occur. The first, illustrated in Figure 9.7 (c), occurs when the sample is subjected to weak or no stress; a reorientation takes place, increasing the proportion of magnetization along the axis of the magnetic field. The second situation occurs when the sample is mechanically blocked, meaning that the alteration of the respective proportions of the two martensite variants is not possible. We then see a rotation of the magnetization so that it is orientated along the axis of the magnetic field applied [CRE 04, HIR 04a].

However, a problem exists as regards the definition of this REV in terms of the continuity of the magnetic flux when there is a rotation of the magnetization. Indeed, when the angle $\theta$ expands, the magnetic flux at the interface between two variants is reversed in $M_2$, but remains the same in $M_1$.

This detail shows that the REV chosen constitutes a mesoscopic approximation of more complex micromagnetic phenomena.
9.4.3. Expression of chemical energy

This energy relates to the latent heat associated with an $A \implies M$ phase transformation. As all the martensite variants form a single phase in the crystallographic sense of the word, they have the same chemical energy. With reference to $z_0$, the volume fraction of austenite, we can write the chemical contribution to the free energy:

$$G_{chem}(T, z_0) = (u_0^A - Ts_0^A)z_0 + (u_0^M - Ts_0^M)(1 - z_0) = u_0^M - Ts_0^M + \Pi_{0}^{f}(T)z_0$$

[9.18]

with $\Pi_{0}^{f}(T) = \Delta u - T\Delta s$

where $\Delta u = u_0^A - u_0^M; \Delta s = s_0^A - s_0^M$

This formulation is the same as for conventional SMAs.
9.4.4. Expression of thermal energy

If we make the hypothesis that the specific heats are the same, regardless of the state of phase of the material, by definition, we have:

\[ C_p = -T \frac{d^2 G_{\text{therm}}}{dT^2} \]  \[9.19\]

The expression of this energy obtained after integration is written:

\[ G_{\text{therm}} = C_p \left[ (T - T_0) - TLn \left( \frac{T}{T_0} \right) \right] \]  \[9.20\]

9.4.5. Expression of mechanical energy

For a monocrystal comprising an austenitic phase and \( n \) martensite variants, we can use a formulation of \( G_{\text{mech}} \) given in Chapter 5:

\[ \rho G(\Sigma, T, z_0, z_1, \ldots, z_n) = -\Sigma: \sum_{k=3}^{k=3} \sum_{l=1}^{k=1} z_k E_{1}^{k} - \frac{1}{2} \Sigma: M\Sigma + \phi_{\text{it}}(z_0, z_1, \ldots, z_n) \]  \[9.21\]

Here:

\[ \phi_{\text{it}} = Az_0(1 - z_0) + \frac{1}{2} \sum_{k=1}^{k=1} \sum_{l=1}^{n} H_{kl} z_k z_l \]  \[9.22\]

where \( l \) is different to \( k \) and \( z \) is the volume fraction of martensite:

\[ z = \sum_{k=4}^{k=1} z_k = 1 - z_0 \]  \[9.23\]

For what remains of this chapter, we shall limit ourselves to the case where \( h = Hx \) and a uniaxial compression in direction \( y \) (Figure 9.8), meaning that:

\[ \Sigma = diag(0, \sigma, 0) \]  \[9.24\]

In this simple case, equation [9.21] is reduced to:

\[ \rho G_{\text{mech}}(\sigma, z_0, z_1, z_2, z_3) = -\sigma \left[ (z_1 + z_3)(\alpha^2 - 1) + z_2(\beta^2 - 1) \right] - \frac{1}{2} \frac{\sigma^2}{E^*} + Az_0(1 - z_0) + K(z_1z_2 + z_2z_3 + z_3z_1) \]  \[9.25\]

where \( E^* \) is the Young’s modulus, and considering the interactions between the martensite variants which all have the same weight:

\[ K_{ij} = K \ \forall i, j = 1, 2, 3 \]  \[9.26\]
In addition, a restriction needs to be considered:

\[
\sum_{k=0}^{k=3} z_k = 1
\]  

[9.27]

This means that of the four volume fractions, only three are independent.

**9.4.6. Expression of magnetic energy**

**9.4.6.1. General aspects**

As established by Landau *et al.* [LAN 84] and Sommerfeld [SOM 64], magnetic energy is usually expressed by:

\[
U_{mag} = \hat{V} \hat{b}_0 h(b)dbdV
\]  

[9.28]

\( V \) denotes the total volume when the magnetic field is non-null, \( b \) the magnetic induction and \( h \) the magnetic field.

When \( h = Hx \), the energy is defined in scalar form as follows:

\[
U_{mag} = \int_V \int_0^B H(b)dbdV
\]  

[9.29]

We introduce the magnetization term \( M \) such that:

\[
M = \frac{B}{\mu_0} - H
\]  

[9.30]
Note that in order to obtain the magnetic energy, we need to integrate the volume energy on the whole of the volume – that is, on the volume of the MSMA and the volume of air present. In order to obtain a magnetic energy density by integrating on the volume of MSMA, Landau et al. [LAN 84] introduce the field $H_0$ which exists in the absence of material. The real field $H$ can be written:

$$ H = H_0 - N_D m $$  \[9.31\]

where $N_D$ denotes the magnetization coefficient.

In addition, the difference between the total magnetic energy and the magnetic energy in the absence of any material is written as:

$$ U_{mag} - U_{mag}^0 = \int_{V_{m,f}} \int_0^m \mu_0 H_0 dm dV $$  \[9.32\]

Thus, it is this energy which will participate in the energy conversion.

It is more practical to use the magnetic co-energy instead of the magnetic energy when the controlling variable is an electrical current in the coil. This co-energy $\tilde{U}_{mag}$ is obtained by way of the following Legendre transformation:

$$ \tilde{U}_{mag} = \tilde{U}_{mag} - \mu_0 m H $$  \[9.33\]

This gives us:

$$ d\tilde{U}_{mag} = -\mu_0 m dH $$  \[9.34\]

Thus, the expression of $\rho G_{mag}(H)$ will be as follows:

$$ \rho G_{mag}(H) = -\int_0^H \mu_0 m dH $$  \[9.35\]

We shall use the notation $m_1, m_2, m_3$ to represent the magnetizations of the three martensite variants $M_1, M_2, M_3$, and $m_0$ to denote the magnetization of the austenite.

9.4.6.2. Magnetization of martensite: axis of easy magnetization

$$ m_1(H) = m_s (2\alpha(H) - 1) $$  \[9.36\]

where $m_s$ is the saturation magnetization and $\alpha \in [0, 1]$ represents the proportion of the Weiss domain (see Figure 9.6).

Thus, $\alpha$ is chosen as a linear function of $H$:

$$ (2\alpha(H) - 1) = \frac{\chi_a H}{m_s} $$  \[9.37\]

where $m_1(H) = \chi_a H$. 

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9.4.6.3. Magnetization of martensite: axis of difficult magnetization

Magnetization along the axis of difficult magnetization is chosen as corresponding to a rotation of the magnetization within the variant in question. On the basis of the choice of REV made above (see Figure 9.6):

\[ m_2(H) = m_3(H) = m_s \sin(\theta(H)) \]  

where \( \theta \in \left[-\frac{\pi}{2}, \frac{\pi}{2}\right] \) represents the angle of rotation of the magnetization. We shall choose the function \( \sin(\theta(H)) \) as being linear in \( H \) in the form:

\[ \sin(\theta(H)) = \frac{\chi t H}{m_s} \]  

That is to say, \( m_2 = m_3 = \chi t H \).

9.4.6.4. Magnetization of austenite

With an operational temperature lower than the Curie temperature of the material, the behavior is considered to be similar to that of the variant \( M_1 \)

\[ m_0(H) = m_s(2\alpha_A(H) - 1) \]  

where \( \alpha_A \in [0, 1] \) represents the proportion of the Weiss domain in the austenite. \( \alpha_A \) is chosen as a linear function of \( H \):

\[ (2\alpha_A(H) - 1) = \frac{\chi_A H}{m_s} \]  

9.4.6.5. Mixture law

A mixture law then gives the global magnetization of the material:

\[ m(H) = \sum_{k=0}^{k=3} z_k M_k \]  

\[ m(H) = m_s \left( z_0(2\alpha_A(H) - 1) + z_1(2\alpha(H) - 1) + (z_2 + z_3)\sin(\theta(H)) \right) \]  

The curves given by Likhachev et al. [9.9] [LIK 04] show that when \( z = 1, m = M \) is linear in \( H \) with slope \( \chi_t \), and for \( z = 0 \) \( m \) is linear in \( H \) with slope \( \chi_A \) (Figure 9.9).

In this two-variant model \((z_3=0), z_1=z; z_2 = 1-z \) [GAU 07a] we write:

\[ m = m_x = \chi_A H z + \chi t H (1 - z) \]  

[9.44]
Figure 9.9. Magnetization curves for different fractions \( z \) of variant 1 (model with two variants: 1 and 2) model: lines; experiments (o) (Experiments performed by Likhachev et al.) [LIK 04]

Using equation [9.35] and performing integration on different parts of \( m dH \), as done in Gauthier et al. [GAU 07a] and in Gauthier’s thesis [GAU 07b], the expression of \( G_{mag} \) is established:

\[
\begin{align*}
\rho G_{mag}(H, z_0, z_1, z_2, z_3, \alpha, \theta, \alpha_A) &= \\
-\mu_0 m_s &\left[ z_1((2\alpha - 1) H - \frac{m_s}{2\chi_a} (2\alpha - 1)^2) \right] \\
+ (z_2 + z_3) &\left( \sin(\theta) H - \frac{m_s}{2\chi_t} \sin^2(\theta) \right) \\
-\mu_0 m_s &\left[ z_0((2\alpha_A - 1) H - \frac{m_s}{2\chi_A} (2\alpha_A - 1)^2) \right] \\
\end{align*}
\]

Observation of the experimental curves shows that the parameter \( m_s \) is not constant, but rather depends on the temperature [HEC 01]. For ferromagnetic materials, the Weiss theory gives the dependency of \( m_s \) on \( T \) by an implicit equation, made explicit by Zuo et al. [ZUO 98]:

\[
\frac{m_s(T)}{m_s^0} = \tanh \left( \frac{m_s(T) T_c}{m_s^0 T} \right)
\]

where \( T_c \) is the Curie temperature and \( m_s^0 \) the magnetization at 0°C. In order to simplify the calculation, the parameters \( m_s^0 \) and \( T_c \) will be taken to be identical for the austenite and martensite, although in reality they are slightly different.

9.4.7. General expression of the free energy

For a monocrystal containing three martensite variants (for a cubic \( \Rightarrow \) quadratic transformation) and an austenitic phase, under the influence of
magneto-thermo-mechanical stresses (see Figure 9.8, the expression of the Gibbs free energy is written thus:

\[ \rho G(H, \sigma, T, z_0, z_1, z_2, z_3, \alpha, \theta, \alpha_A) = \]

\[ u_o^M - T \sigma_o^M + z_o(\Delta U - T \Delta S) \]

\[ + C_p \left[ (T - T_o) - T \cdot \ln \left( \frac{T}{T_o} \right) \right] \]

\[ - \frac{\sigma^2}{2} \left( (z_1 + z_3)(\beta_a^2 - 1) + z_2(\beta_c^2 - 1) \right) \]

\[ + \frac{1}{2} \frac{\sigma^2}{E} + A z_o(1 - z_o) + K(z_1 z_2 + z_1 z_3 + z_2 z_3) \]

\[ - \mu_0 m_s(T) \left[ z_1 \left( (2\alpha - 1)H - \frac{m_s(T)}{2\chi_a}(2\alpha - 1)^2 \right) \right. \]

\[ + (z_2 + z_3) \left( \sin(\theta)H - \frac{m_s(T)}{2\chi_a}(\sin(\theta))^2 \right) \]

\[ \left. + z_0 \left( (2\alpha_A - 1)H - \frac{m_s(T)}{2\chi_A}(2\alpha_A - 1)^2 \right) \right] \]

with \( \sum_{k=0}^{3} z_k = 1 \)

where \( \beta_a = \alpha \) and \( \beta_c = \beta \).

This expression of \( G \) is a little complicated, but can be subdivided into a number of specific situations (purely magnetic or mechanical or thermal (etc.) loading).

9.4.8. Clausius-Duhem inequality

9.4.8.1. Thermodynamic forces

\[ \text{\textbullet\textbf{E}} = -\rho \frac{\partial G}{\partial \sigma} = \frac{\sigma}{E} \frac{\partial G}{\partial \sigma} + \frac{1}{2} \left[ (z_1 + z_3)(\alpha^2 - 1) + z_2(\beta^2 - 1) \right] \quad [9.49] \]

\[ \text{\textbullet\textbf{m}} = -\rho \frac{\partial G}{\partial H} = \mu_0 m_s \left[ z_0(2\alpha_A - 1) + z_1(2\alpha - 1) + (z_2 + z_3)\sin(\theta) \right] \quad [9.50] \]

\[ \text{\textbullet\textbf{m}} = -\rho \frac{\partial G}{\partial T} = s_o^M - z_o \Delta S + C_p \ln \left( \frac{T}{T_o} \right) \]

\[ + \mu_0 \frac{\partial m_s}{\partial T} \frac{\partial m_s}{\partial T} \left[ z_1 \left( (2\alpha - 1)^2 \right) + (z_2 + z_3) \frac{\sin^2(\theta)}{2\chi} \right] \]

\[ - 2 \mu_0 m_s(T) \frac{\partial m_s}{\partial T} \left[ z_1 \left( (2\alpha - 1)^2 \right) + (z_2 + z_3) \frac{\sin^2(\theta)}{2\chi} \right] \]

\[ + z_0 \left( (2\alpha_A - 1)^2 \right) \]
A magneto-thermal effect is present in the expression of the entropy, due to the temperature dependence of $m_s$.

The thermodynamic forces associated with the variables $\alpha$, $\alpha_A$ and $\theta$ are taken to be equal to zero – i.e.:

$$\rho \frac{\partial G}{\partial \alpha} = 0, \quad \rho \frac{\partial G}{\partial \alpha_A} = 0, \quad \rho \frac{\partial G}{\partial \theta} = 0$$

[9.51]

The choice of the expression of free energy confirms that purely magnetic behavior is considered to be reversible.

Effectively the magnetization curves measured by Heczko et al. [HEC 05] on two samples effectively (one in the stress-free state and the other under a 3 MPa stress) [9.21] do not exhibit hysteresis (Figure 9.10).

![Figure 9.10. Magnetization curves measured in the directions of: easy magnetization (un-stressed sample); difficult magnetization (sample under 3 MPa stress) [HEC 05]](image)

Finally, the thermodynamic forces associated with the fraction and those of the martensite variants are written:

$$\Pi_0 = -\rho \frac{\partial G}{\partial z_0} = -\Delta U - T \Delta S - A(1 - 2z_0)$$

$$+ \mu_0 m_s \left[ (2\alpha_A - 1) H - \frac{m_s}{2\chi_A} (2\alpha_A - 1)^2 \right]$$

[9.52]

$$\Pi_1 = -\rho \frac{\partial G}{\partial z_1} = \frac{\sigma}{2} (\alpha^2 - 1) - K (z_2 + z_3)$$

$$+ \mu_0 m_s(T) \left[ ((2\alpha - 1) H - \frac{m_s}{2\chi_A} (2\alpha - 1)^2) \right]$$

[9.53]
\[ \pi_2^f = -\rho \frac{\partial G}{\partial z_2} = \frac{\sigma}{2} (\beta^2 - 1) - K (z_1 + z_3) \\
+ \mu_0 m_s(T) \left( \sin(\theta) H - \frac{m_s}{2\chi_t}\sin^2(\theta) \right) \tag{9.54} \]

\[ \pi_3^f = -\rho \frac{\partial G}{\partial z_3} = \frac{\sigma}{2} (\alpha^2 - 1) - K (z_1 + z_2) \\
+ \mu_0 m_s(T) \left( \sin(\theta) H - \frac{m_s}{2\chi_t}\sin^2(\theta) \right) \tag{9.55} \]

The behavior is irreversible, so the Clausius-Duhem inequality can be written:

\[ dD = -\rho dG - \mu_0 m dH - \varepsilon d\sigma - s dT \geq 0 \tag{9.56} \]

where \( dD \) constitutes the increment of dissipation. In reference to Chapter 4, its expression is reduced to:

\[ dD = \sum_{i=0}^{3} \pi_i^f dz_i \geq 0 \text{ where } \sum_{i=0}^{3} dz_i = 1 \tag{9.57} \]

### 9.4.9. Kinetics of phase transformation or reorientation

Remember that the choice of transformation kinetics is made on the basis of observations of the growth of a new phase in a parent phase, made by metallurgists such as Koistinen and Marburger in 1959 [KOI 59].

#### 9.4.9.1. Example with two variants (Figures 9.11 and 9.12)

If a sample contains only two martensite variants \( M_1 \) and \( M_2 \), during an isothermal evolution, consider \( z = z_1 = 1 - z_2 \) and the Clausius-Duhem inequality becomes:

\[ dD = \pi_1^f dz_1 + \pi_2^f dz_2 \geq 0 \tag{9.58} \]

\[ dD = (\pi_1^f - \pi_2^f) dz \geq 0 \tag{9.59} \]

An external loop – that is, a complete rearrangement of \( z = 0 \) \( \rightarrow \) \( z = 1 \) (path \( a \)) and the reverse, \( z = 1 \) \( \rightarrow \) \( z = 0 \) (path \( b \)) – is shown in Figure 9.13. Reorientation begins when \( (\pi_1^f - \pi_2^f) \geq \pi_{cr} \) (T) for path \( (a) \) and when \( (\pi_1^f - \pi_2^f) \leq -\pi_{cr} \) (T) for path \( (b) \). After the initiation of reorientation, the behavior is modeled with the following kinetics:

\[ \pi_1^f - \pi_2^f = \lambda \dot{z} \text{ with } \dot{z} = \dot{z}_1 = -\dot{z}_2 \tag{9.60} \]
We can take $\lambda$ as a constant, where the value of $\lambda$ can be taken as dependent upon the previous deformation. Thus, in Gauthier et al. [GAU 07a], the concept of a memory point is introduced, and the distinction is drawn between internal and external loops.

In addition, as previously indicated, $\pi_{cr}(T)$ is a function of the temperature, as shown for conventional SMAs by Brinson [BRI 93] and by Heczko and Straka [HEC 03] for magnetic SMAs. We chose a linear dependency:

$$\pi_{cr}(T) = \pi_{cr}^0 + k_{cr} (A_0^0 - T)$$

[9.61]
9.4.9.2. Equivalence between the actions of the magnetic field $H$ and the stress $\sigma$ [GAU 07a]

Classically, reorientation occurs when the thermodynamic force $\pi^f$ reaches the value $\pi_{cr}$. In the model with two variants $M_1$ and $M_2$:

$$\pi^f(\sigma, H, z = 0) = \pi_{cr}$$ [9.62]

where:

$$\pi_{cr} = \sigma \gamma - K_{12} - \mu_0 m_s^2 \left( \frac{(1 - 2\alpha) \sin\theta}{\chi_t} + \frac{(2\alpha - 1)^2}{2\chi_a} + \frac{\sin^2\theta}{2\chi_t} \right)$$ [9.63]

Three situations must be examined:

- zone I: no saturation in $\alpha$ and $\theta$;
- zone II: saturation in $\alpha$, but not in $\theta$;
- zone III: saturation in $\alpha$ and $\theta$.

In Figure 9.14, we can compare the measured values and predictions with:

$$\mu_0 m_s = 0.65 \, T; \chi_t = 0.82; \chi_a = 4; \pi_{cr} + K_{12} = 2.10^4 \, Pa; \gamma = 0.055$$

9.4.9.3. Generalization to the three variants and the austenitic phase

We generalize the concept of critical force $\pi_{cr}(T)$ and kinetics to all three martensite variants and the austenitic phase. Figure 9.15 represents the phase state of the MSMA and its associated kinetics. $c_{ij}$ represents the rate of transformation from $M_i$ into $M_j$ and $c_{0j}$ that from $A$ into $M_j$, and the following relations are satisfied:

$$\dot{z}_0 = c_{10} + c_{20} + c_{30} - c_{01} - c_{02} - c_{03}$$ [9.64]

$$\dot{z}_1 = c_{01} + c_{21} + c_{31} - c_{10} - c_{12} - c_{13}$$ [9.65]

![Figure 9.13. Thermodynamic force as a function of the fraction of martensite $z$ in $M_1$](image-url)
\[
\dot{z}_2 = c_{02} + c_{12} + c_{22} - c_{20} - c_{21} - c_{23} \tag{9.66}
\]
\[
\dot{z}_3 = c_{03} + c_{13} + c_{23} - c_{30} - c_{31} - c_{32} \tag{9.67}
\]

where the \(c_{ij}\) are defined by

\[
c_{ij} = 0 \text{ if } \pi_f^j - \pi_i^f \leq \pi_{cr}(T) \text{ or } z_i = 0
\]

\[
c_{ij} = \frac{1}{\lambda} \left( \dot{\pi}_f^j - \dot{\pi}_i^f \right) \text{ otherwise}
\]

Figure 9.14. Borderline between \(\sigma\) and \(H\) for the initiation of \(M_2 \Rightarrow M_1\) reorientation. Solid line: simulation; (x) experimental points [GAU 07a]

Figure 9.15. Schematic representation of the kinetics

Different values of \(\lambda\) have to be taken into account: \(\lambda_A\) for the \(A \Rightarrow M_i\) transformation and \(\lambda_M\) for \(M_i \Rightarrow M_j\).

9.4.10. Heat balance equation

As the \(A \Rightarrow M\) transformation is exothermic and the inverse transformation \(M \Rightarrow A\) is endothermic, it is necessary to find the energy balance, which is expressed by an
equation known as the “heat balance equation”:
\[ \rho \dot{e} = -p_i + r - \text{div} \mathbf{q} \quad [9.68] \]
where
\[ p_i = -\sigma : \dot{\varepsilon} - \mu_0 \dot{H} \dot{m} \]
is the power of the forces and \( r \) the external heat sources.

By a Legendre transform, we obtain the free energy:
\[ G = e - Ts - \frac{\sigma \dot{\varepsilon}}{\rho} - \frac{\mu_0 \dot{H} \dot{m}}{\rho} \quad [9.69] \]
where:
\[ \rho \dot{G} = r - \text{div} \mathbf{q} - \rho T \dot{s} - \rho s \dot{T} - \dot{\varepsilon} - \mu_0 \dot{H} m \quad [9.70] \]

Furthermore:
\[ \rho \dot{G} = \rho \frac{\partial G}{\partial \dot{\sigma}} \dot{\sigma} + \rho \frac{\partial G}{\partial \dot{H}} \dot{H} + \rho \frac{\partial G}{\partial \dot{T}} \dot{T} + \sum_{i=0}^{i=3} \rho \frac{\partial G}{\partial z_i} \dot{z}_i \quad [9.71] \]

\[ \rho \dot{G} = -\varepsilon \dot{\sigma} - \mu_0 m \dot{H} - \rho s \dot{T} - \sum_{i=0}^{i=3} \pi_i \dot{z}_i \quad [9.72] \]

The combination of equations [9.70] and [9.72] gives us:
\[ \sum_{i=0}^{i=3} \pi_i \dot{z}_i = -r + \text{div} \mathbf{q} + \rho T \dot{s} \quad [9.73] \]

9.4.11. Identification of the parameters

The material parameters are heavily dependent upon the composition of the alloy. A set of experimental curves is available in the existing literature, but the compositions are often different. The parameters indicated in this chapter are approximations, but give a good idea of the typical order of magnitude of these values. The identification of them requires specific measuring techniques – e.g. X-rays for the lattice parameters, DSC (differential scanning calorimetry) for the phase transformation temperatures, measurements of susceptibility, Curie temperature and finally compression tests in order to obtain the Young’s modulus of the material and the hardness.

9.4.11.1. Differential scanning calorimetry

DSC gives us data about the thermal parameters. The four phase transformation temperatures (in the stress-free state) can be measured: \( M_0^p, M_0^s, A_0^p, A_0^s \). To begin with, the area of the hysteresis curve is equal to \(-\Delta U\). As the model shows, by
verifying that $A_f^0 - A_s^0 \approx M_s^0 - M_f^0$, we can obtain:

\[
\Delta S = \frac{2\Delta U}{A_0^s + M_s^0} \tag{9.74}
\]

\[
A = \frac{-\Delta S (A_s^0 - M_s^0)}{2} \tag{9.75}
\]

\[
\lambda_A = -\Delta S(A_f^0 - M_s^0) \tag{9.76}
\]

9.4.11.2. Crystallographic measurements

The lattice parameters $a_0$, $a$ and $c$ were obtained using X-rays.

9.4.11.3. Magnetic measurements

The curves of $m$ as a function of $H$ for different temperatures may serve to identify $T_c$, $m_s^0$, $\chi_a$, $\chi_t$, $\chi_A$.

9.4.11.4. Mechanical measurements

The curves of reorientation at different temperatures lower than $A_s^0$ can be taken in order to obtain $\pi_{cr}(T)$, $\lambda_M$ and $E^\bullet$.

The parameters selected are reported in Table 9.1.

<table>
<thead>
<tr>
<th>$A_0^S$ = 309.4 K</th>
<th>$M_0^S$ = 301.7 K</th>
<th>$A$ = 5.48105 J/m³</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a_0$ = 5.84 Å</td>
<td>$a = 5.95$ Å</td>
<td>$c = 5.60$ Å</td>
</tr>
<tr>
<td>$E$ = 5.109 Pa</td>
<td>$\lambda_M$ = 4.105</td>
<td>$K = 0$</td>
</tr>
<tr>
<td>$\chi_a = 5$</td>
<td>$\chi_t = 1.05$</td>
<td>$\chi_A = 1.76$</td>
</tr>
<tr>
<td>$T_c$ = 370 K</td>
<td>$m_{s0}$ = 710 kA/m</td>
<td>$\lambda_A = 1.26$ MPa</td>
</tr>
<tr>
<td>$\pi_{cr}^0$ = 12.103 J/m³</td>
<td>$k_{cr}$ = 800 Pa/K</td>
<td></td>
</tr>
</tbody>
</table>

**Table 9.1. List of parameters selected [GAU 11]**

9.4.11.5. Reliability of the model

Just like with the models relating to conventional shape-memory alloys, we are working in the context of the standard generalized mediums described in Chapter 4 [HAL 74, HAL 75]. Thus, the dissipation must be positive regardless of the thermo-magneto-mechanical loading. A digital simulation has been constructed using the software Matlab®/Simulink. This algorithm is presented in Figure 9.16 using S-functions programmed in the computer language C so as to accelerate the execution.
The inputs and outputs of the simulation are shown in Figure 9.17. The power of this model lies in the fact that irrespective of the mechanical (pseudo-elasticity and reorientation), thermal or magnetic loading, the same set of parameters is used. Thus, a number of different cases may be investigated. As our experimental setup is not able to take anisothermal measurements, only predictions will be made.

Figure 9.18 shows the evolution of the deformation $\varepsilon$ and of the volume fractions of the variants $z_i$ with changing temperature $T$. The deformation is around 2% when the magnetic field is applied, and $-4\%$ under the influence of compressive stress. Naturally, there is no deformation in the absence of stress and magnetic field, and at low temperature the fractions $z_i$, $i = 1, 2, 3$ are equal (at $1/3$).

Figure 9.19 presents the deformation when a compressive stress is applied at $T \geq A^f_0$ (where the material is austenitic in the stress-free state) – a pseudo-elastic behavior. One curve with no magnetic field applied and another with a 800 kA/m field are shown together on this figure. Apparently, the effects of the magnetic field on the pseudo-elasticity of the sample are negligible.
Figure 9.18. Results of our simulation of a thermal action, with or without a magnetic field or other stress.

Figure 9.19. Simulation of the mechanical action at high temperature (pseudo-elasticity): $T = 320$ K.
Figure 9.20 represents the evolution of the deformation of the sample subjected to a 800 kA/m magnetic field, when a compressive stress is applied, at low temperature (i.e. in the martensitic state, in the absence of stress), corresponding to the process of reorientation of the martensite variants. Two temperatures are chosen in order to test the effect of temperature on reorientation. Two important results are obtained: the thickness of hysteresis decreases with increasing temperature, and the center of the hysteresis curve shifts towards the top of the diagram when the temperature increases, because the saturation magnetization decreases (see equation [9.48]) and the magnetic action as well.

Figure 9.20. Mechanical action at low temperature giving rise to the reorientation of martensite under $H = 800 \text{kA/m}$

Figure 9.21 shows the influence of the temperature on the curve of magnetization ($m$, $H$). The magnetic field $H$ is first applied with positive values, and then with negative ones. At low temperature, the sample contains all three martensite variants in equal proportions; two changes in direction which appear correspond to the saturation magnetizations of the axes of easy and difficult magnetization. The curve at $T = 0 \text{K}$ constitutes the curve of magnetization of self-accommodating martensite. Since there is no reorientation, there is no hysteresis. At a higher temperature, $T = 280 \text{K}$, but lower than $A_\text{us} = 309.4 \text{K}$, the reorientation of the martensite variants generates hysteresis. Finally, at 320 K the material is austenitic and the curve of magnetization corresponds to this phase state. Note that the magnetization decreases as the temperature increases.

Figure 9.22 represents the evolution of the deformation $\varepsilon$ with the magnetic field applied $H$ with different set levels of compressive stress, at low temperature. It is very helpful to have these curves at our disposal when designing actuators, as done by Gauthier et al. [GAU 07a]. The internal loops are modeled more simply than in...
[GAU 07a]. The influence of the stress $\sigma$ on the strain $\varepsilon$ is as follows. When no stress is being applied, a reorientation takes place along a path when $H$ increases, but not when $H$ decreases. With a compressive stress with modulus greater than 2.5 MPa, no reorientation is possible in view of the magnetic field $H$. Between these two extremes, a partial reorientation occurs for all the paths (increasing or decreasing in $H$).

Figure 9.21. *Curves of magnetization for different isotherms*

Figure 9.22. *Evolution of the deformation $\varepsilon$ with the magnetic field $H$ for different levels of applied stress*

Figure 9.23 illustrates the experimental results obtained by Straka et al. in 2006 [STR 06]. Figure 9.24 shows the simulation of the experiment curves given in Figure 9.23. The curves are obtained with the magnetic field applied with a “negative” and then a “positive” sign in order to show the maximum and minimum deformations for the first cycle and for the repeated cycles (which is very useful for actuators).
Figure 9.23. Evolution of the deformation and magnetization under the influence of the magnetic field with a fixed stress $\sigma = -1$ MPa. Experiments performed by Straka et al. [STR 06]

Figure 9.24. Evolution of the deformation and magnetization under the influence of the magnetic field with a fixed stress $\sigma = -1$ MPa. Modeling of the experiments conducted by Straka et al. [STR 06] by [GAU 11]
At low temperatures ($T = 223$ K), an increase in $H$ generates a deformation which is partly maintained when the magnetic field is removed. At higher temperatures ($T = 288$ K), repeated actuation is possible, and the amplitude of the deformations increases slightly with the temperature ($T = 307$ K). We can note certain differences between the experiment and the simulations, but generally speaking it is correct. Firstly, the magnetic field associated with the start of reorientation decreases with the temperature because of the increasing critical force. Secondly, the maximum deformation that can be attained also decreases, because of the decrease in saturation magnetization.

9.4.12. Application: creation of a “push/pull” actuator

Figure 9.25 presents version V2.2 of this actuator. A horizontal stack is composed of a sample of an MSMA (MSMA A), a moving part made of plastic and another sample of MSMA (MSMA B). This stack is held in position using a non-ferromagnetic material. The total length can be adjusted by way of a screw. Two V2-type magnetic circuits are used to create two magnetic fields $H_a$ and $H_b$, applied respectively to samples MSMA A and MSMA B.

![Figure 9.25. Photograph of the “Push-Pull” actuator](image)

The principle of operation of such an actuator is presented in Figure 9.26. A magnetic field is applied to MSMA A. A martensitic rearrangement occurs, and a deformation appears, causing the moving part to shift to the right. Similarly, if we wish to move it to the left, we apply a field to MSMA B. By modulating the two fields, it is possible to achieve different stable positions.
9.5. Conclusion

The aim of this chapter was to put forward a simulation of a monocrystal of a magnetic shape-memory alloy taking account of the thermo-magneto-mechanical pairing. The attempt has met with success, although the formulation is already complicated (see the expression of the free energy).

For polycrystals, homogenization techniques are envisageable, as are calculations using the finite element method.
Although we have managed to design and develop an actuator, the main obstacle to the industrial use of massive MSMAs is their fragility.

One possible solution lies in the elaboration of thin films of MSMAs applied by RF spraying. These films represent potential materials for micro- and nanosystems. However, their properties are highly dependent on the structures and the internal stresses developed during their manufacture [BER 09] (Figure 9.27).
Chapter 10

Fracture Mechanics of SMAs

10.1. Introduction

As we have attempted to demonstrate, elements made of shape-memory alloys, when subjected to thermomechanical stresses, should be reliable actuators or sensors. One crucial point which falls beyond the remit of this book is that their fatigue resistance must be ensured. Indeed, SMAs are capable of mechanically-reversible phase transformations where large deformations (of around 6–7% for nitinols) can be obtained.

These properties of pseudo-elasticity make SMAs particularly attractive in the biomedical domain (e.g. for stents, catheters, etc.) as mentioned in Chapter 2. For instance, thin or slender structures are subject to rather complex deformations. This gives us an incentive to seek to understand and be able to predict their behavior in terms of fatigue and fracture.

SMAs – magnetic or otherwise – may be considered to be brittle materials. This being the case, brittle fracture may be considered to be governed by the stress field around a crack tip and by parameters which describe the material’s resistance to crack propagation. Thus, crack-tip stress analysis constitutes an essential part of fracture mechanics. For materials with linear elastic behavior, elasticity methods are used to calculate the stresses and the movements in cracked bodies. Here we shall use an analytical approach similar to the complex potential method.

In the case of phase transformation in the vicinity of the crack tip, the behavior is governed by the stress field in that region. Yi and Gao [YI 00] performed a numerical investigation of the fracture of SMAs under mode I loading, and showed that phase transition increases brittleness and decreases the intensity factor $K_I$. 

Wang et al. [WAN 05] examined martensite induced by stress applied to the crack tip on a specimen CT by calculation using the finite element method (FEM). The formation of martensite under stress exhibits similarities with the zone of plasticity at the bottom of a crack for elastoplastic materials.

One of the ingredients in the prediction of phase transformation surfaces is the taking into account of the asymmetry between the traction and compression – a concept which was discussed in some detail in Chapter 7 with regard to the modeling of SMAs.

We shall look at two examples of cracks: those with no curvature at their tip and those with a finite radius of curvature.

At the end of the chapter, a comparison will be made with some experimental results.

10.2. The elastic stress field around a crack tip

This section is borrowed from a section of Chapter 3, of the same name – in the book *Fracture Mechanics* by C.T. Sun and Z.H. Jin [SUN 12].

10.2.1. Basic modes of fracture and stress intensity factors

Conventionally, there are three modes (Figure 10.1).

– Mode I (opening mode): the two lips of the crack make a movement $u_y$, moving symmetrically in relation to the plane $y = 0$.

– Mode II (sliding mode): the two lips of the crack make a movement $u_x$ and the plane of the crack $y = 0$ remains unchanged.

– Mode III (tearing mode): the two lips of the crack make a movement $u_z$, once again on the unchanging plane $y = 0$.

![Figure 10.1. Schematic representation of the three class modes of fracture: a) mode I (opening), b) mode II (in-plane shear) and c) mode III (out-of-plane shear)](image-url)
All three modes can be considered as two-dimensional problems. The stresses around the crack tip in the plane $y = 0$, for all three modes, can be expressed as ($y = 0, x \to 0^+$):

\[
\sigma_{yy} = \frac{K_I}{\sqrt{2\pi x}} + O(\sqrt{x}), \quad \sigma_{xy} = \sigma_{yz} = 0
\]

\[
\sigma_{xy} = \frac{K_{II}}{\sqrt{2\pi x}} + O(\sqrt{x}), \quad \sigma_{yy} = \sigma_{yz} = 0
\]  \[10.1\]

\[
\sigma_{yz} = \frac{K_{III}}{\sqrt{2\pi x}} + O(\sqrt{x}), \quad \sigma_{xy} = \sigma_{yy} = 0
\]

where the $K_I$, $K_{II}$ and $K_{III}$ are called mode I, II and III stress intensity factors.

Note that a long split cylinder with a circular cross-section under torsion stress can produce purely mode III deformation (see Figure 10.2).

Figure 10.2. Mode III deformation of a split tube

10.2.2. Complex potential method for plane elasticity (the Kolosov-Muskheilishvili formulae)

Among the methods for solving a plane elasticity problem, the complex potential method advanced by Kolosov and Muskheilishvili [MUS 53] is the most efficient for solving two-dimensional fracture problems. The form of the potential obtained will obviously depend on the boundary conditions under stress and/or displacement.

10.2.2.1. Basic equations for plane elasticity

In static state (acceleration $\gamma = 0$) and in the absence of volume forces, in plane elasticity (plane stress or plane deformation), the equilibrium equation in terms of stresses is reduced to:

\[
\sigma_{xx,x} + \sigma_{xy,y} = 0
\]

\[
\sigma_{xy,x} + \sigma_{yy,y} = 0
\]  \[10.2\]

where, in the small deformation theory, the strains $(\varepsilon_{xx}, \varepsilon_{yy}, \varepsilon_{xy})$ derive from the displacements $(u_x, u_y)$ in the form:

\[
\varepsilon_{xx} = u_{x,x}, \quad \varepsilon_{yy} = u_{y,y}, \quad 2\varepsilon_{xy} = u_{x,y} + u_{y,x}
\]  \[10.3\]
The elastic constitutive laws are written $\varepsilon \implies \sigma$

\[
\begin{align*}
\sigma_{xx} &= \lambda^* (\varepsilon_{xx} + \varepsilon_{yy}) + 2\mu \varepsilon_{xx} \\
\sigma_{yy} &= \lambda^* (\varepsilon_{xx} + \varepsilon_{yy}) + 2\mu \varepsilon_{yy} \\
\sigma_{xy} &= 2\mu \varepsilon_{xy}
\end{align*}
\]

[10.4]

and inversely $\sigma \implies \varepsilon$:

\[
\begin{align*}
\varepsilon_{xx} &= \frac{1}{2\mu} \left( \sigma_{xx} - \frac{\lambda^*}{2(\lambda^* + \mu)} (\sigma_{xx} + \sigma_{yy}) \right) \\
\varepsilon_{yy} &= \frac{1}{2\mu} \left( \sigma_{yy} - \frac{\lambda^*}{2(\lambda^* + \mu)} (\sigma_{xx} + \sigma_{yy}) \right) \\
\varepsilon_{xy} &= \frac{1}{2\mu} \sigma_{xy}
\end{align*}
\]

[10.5]

where $\mu$ is the shear modulus and $\lambda^* = \frac{3-\kappa}{\kappa-1} \mu$:

\[
\kappa = \begin{cases} 
3 - 4\nu \text{ with planar deformation} \\
\frac{3 - \nu}{1 + \nu} \text{ under planar stress}
\end{cases}
\]

[10.6]

where $\nu$ is obviously the Poisson coefficient. In addition, the compatibility equations in terms of deformations are written:

\[
\varepsilon_{xx,yy} + \varepsilon_{yy,xx} = 2\varepsilon_{xy,xy}
\]

[10.7]

By combination of the constitutive laws and the equilibrium equations, the compatibility equation becomes:

\[
\Delta(\sigma_{xx} + \sigma_{yy}) = 0
\]

[10.8]

where the Laplacian term is expressed in two-dimension by $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$.

For any biharmonic function $A(x, y)$, called the stress function or the Airy function, i.e. such that:

\[
\triangle(\triangle A) = 0
\]

[10.9]

then:

\[
\begin{align*}
\sigma_{xx} &= A_{yy}, \quad \sigma_{yy} = A_{xx}, \quad \sigma_{xy} = -A_{xy}
\end{align*}
\]

[10.10]

is a solution to the equation [10.2] with a biharmonic function $A$.

The problem in mechanics is to find biharmonic functions which satisfy the appropriate boundary conditions.
10.2.2.2. Analytical functions and Cauchy-Riemann equations

In the plane \((x, y)\), we usually define the complex number \(z\):

\[
z = \left\{ \begin{array}{l}
x + iy \\
r \cos \theta + ir \sin \theta = re^{i\theta}
\end{array} \right\} \tag{10.11}
\]

and the complex conjugate:

\[
\bar{z} = \left\{ \begin{array}{l}
x - iy \\
r \cos \theta - ir \sin \theta = re^{-i\theta}
\end{array} \right\} \tag{10.12}
\]

Consider the function \(f\) of a complex number \(z\):

\[
f(z) = u(x, y) + iv(x, y) \tag{10.13}
\]

where \(u(x, y)\) is the real part of \(f(z)\) and \(v(x, y)\) is the imaginary part of \(f(z)\).

\(f(z)\) is analytical if the so-called Cauchy-Riemann equations:

\[
\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \quad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x} \tag{10.14}
\]

are satisfied. This being the case, then consequently, \(\Delta u = \Delta v = 0\).

10.2.2.3. Representation of the Airy function as a complex potential

Let us here introduce a function \(P\) such that:

\[
P = \Delta A \tag{10.15}
\]

so that \(\Delta P = 0\).

Thus, we can construct an analytical function \(f(z) = P + iQ\) with \(\Delta Q = 0\).

Hence:

\[
\psi(z) = \frac{1}{4} \int f(z)dz = p + iq \tag{10.16}
\]

Therefore, \(\psi(z)\) is also analytical and its differential is \(\psi'(z) = \frac{1}{4}f(z)\).

In reference to the Cauchy-Riemann equations, we have:

\[
\psi'(z) = \frac{\partial p}{\partial x} + i \frac{\partial q}{\partial x} = \frac{\partial q}{\partial y} - i \frac{\partial p}{\partial y} \tag{10.17}
\]
A relation between \( P \) and \( p \) (or \( q \)) can therefore be obtained:

\[
P = 4 \frac{\partial p}{\partial x} = 4 \frac{\partial q}{\partial y}
\]

[10.18]

By examining the function \((A - (xp + yq))\), we can show that \(\triangle (A - (xp + yq)) = 0\) and that this function \((A - (xp + yq))\) is the real part of an analytical function \(\chi(z) = 0\).

Using the relation \(xp + yq = Re \{\bar{z}\psi(z)\}\), we obtain the representation in the form of a complex potential of the Airy function \(A\):

\[
A = Re \{\bar{z}\psi(z) + \chi(z)\} = 0
\]

[10.19]

10.2.2.4. Stresses and displacements

Calculation of the stresses using the Airy function (equation [10.10]) gives:

\[
\begin{align*}
\sigma_{xx} + \sigma_{yy} &= 4Re \left[ \psi' (z) \right] \\
\sigma_{yy} - \sigma_{xx} + 2i\sigma_{xy} &= 2 \left[ \bar{z}\psi''(z) + \chi''(z) \right]
\end{align*}
\]

[10.20]

To begin with, the classic formulae used in terms of displacement give us:

\[
\begin{align*}
2\mu \frac{\partial u_x}{\partial x} &= \frac{\partial^2 A}{\partial y^2} - \frac{\lambda}{2(\lambda + \mu)} \Delta A \\
2\mu \frac{\partial u_y}{\partial y} &= \frac{\partial^2 A}{\partial x^2} - \frac{\lambda}{2(\lambda + \mu)} \Delta A \\
\mu \left( \frac{\partial u_x}{\partial y} + \frac{\partial u_y}{\partial x} \right) &= -\frac{\partial^2 A}{\partial x \partial y}
\end{align*}
\]

[10.21]

with \(\Delta A = P = 4\frac{\partial p}{\partial x} = 4\frac{\partial q}{\partial y}\) we obtain:

\[
\begin{align*}
2\mu \frac{\partial u_x}{\partial x} &= -\frac{\partial^2 A}{\partial x^2} + \frac{2(\lambda + 2\mu)}{(\lambda + \mu)} \frac{\partial p}{\partial x} \\
2\mu \frac{\partial u_y}{\partial y} &= -\frac{\partial^2 A}{\partial y^2} + \frac{2(\lambda + 2\mu)}{(\lambda + \mu)} \frac{\partial q}{\partial y}
\end{align*}
\]

[10.22]

By integrating:

\[
\begin{align*}
2\mu u_x &= -\frac{\partial A}{\partial x} + \frac{2(\lambda + 2\mu)}{(\lambda + \mu)} p + f_1(y) \\
2\mu u_y &= -\frac{\partial A}{\partial y} + \frac{2(\lambda + 2\mu)}{(\lambda + \mu)} q + f_2(x)
\end{align*}
\]

[10.23]
We ignore the rigid body displacements, \( f_1(y) \) and \( f_2(x) \) bring the two terms from equation [10.23] in one:

\[
2\mu (u_x + iu_y) = -\left( \frac{\partial A}{\partial x} + i \frac{\partial A}{\partial y} \right) + \frac{2(\lambda \star + 2\mu)}{(\lambda \star + \mu)} \psi(z) \tag{10.24}
\]

With a value of \( \kappa = \frac{\lambda \star + 3\mu}{\lambda \star + \mu} \), we obtain the complex representation of the displacement:

\[
2\mu (u_x + iu_y) = \kappa \psi(z) - (z\bar{\psi}'(z)) - \left( \chi(z) \right) \tag{10.25}
\]

Equations [10.20] and [10.25] are the Kolosov-Muskhelishvili formulae.

10.2.3. Westergaard stress functions method

This method consists of use of the Kolosov-Muskhelishvili formulae in particular conditions.

10.2.3.1. Symmetrical problems (mode I)

Consider an infinite plate with cracks running along the \( x \) axis. If the mechanical loading is symmetrical in reference to the \( x \) axis, then \( \sigma_{xy}(x, y = 0) = 0 \) and equation [10.20] implies:

\[
Im \left\{ z\psi''(z) + \chi''(z) \right\} = 0 \text{ for } y = 0 \tag{10.26}
\]

We can demonstrate that this indicates:

\[
z\psi''(z) + \chi''(z) + B = 0 \tag{10.27}
\]

where \( B \) is a constant real number, so \( \chi''(z) = -z\psi''(z) - B \). By substituting this into equation [10.20], we obtain the stresses:

\[
\begin{align*}
\sigma_{xx} &= 2Re \left\{ \psi' \right\} - 2yIm \left\{ \psi'' \right\} + B \\
\sigma_{yy} &= 2Re \left\{ \psi' \right\} + 2yIm \left\{ \psi'' \right\} - B \\
\sigma_{xy} &= -2yRe \left\{ \psi'' \right\}
\end{align*} \tag{10.28}
\]

and for the displacements:

\[
\begin{align*}
2\mu u_x &= (\kappa - 1) Re \left\{ \psi \right\} - 2yIm \left\{ \psi' \right\} + Bx \\
2\mu u_y &= (\kappa + 1) Im \left\{ \psi \right\} - 2yRe \left\{ \psi' \right\} - By
\end{align*} \tag{10.29}
\]
Let us define $Z_I$ such that:

$$\psi' = \frac{1}{2} (Z_I + B)$$  \[10.30\]

Thus:

$$\psi = \frac{1}{2} (\widehat{Z}_I + Bz), \quad \psi'' = \frac{1}{2} Z'_I$$  \[10.31\]

where $\widehat{Z}_I = \int Z_I dz$. We insert these expressions into the formulation of the stresses and displacements:

$$\sigma_{xx} = \text{Re} \{ Z_I \} - y \text{Im} \{ Z'_I \} + 2B$$
$$\sigma_{yy} = \text{Re} \{ Z_I \} + y \text{Im} \{ Z'_I \}$$  \[10.32\]
$$\sigma_{xy} = -y \text{Re} \{ Z'_I \}$$

$$2\mu u_x = \frac{1}{2} (\kappa - 1) \text{Re} \{ \widehat{Z}_I \} - y \text{Im} \{ Z_I \} + \frac{1}{2} (\kappa + 1) Bx$$
$$2\mu u_x = \frac{1}{2} (\kappa + 1) \text{Im} \{ \widehat{Z}_I \} - y \text{Re} \{ Z_I \} + \frac{1}{2} (\kappa - 3) Bx$$  \[10.33\]

$Z_I$ is called a Westergaard function for “mode I” problems.

We can check, with $\widehat{Z}_I = \int Z_I dz$, that the stresses and displacements derive from the Airy function:

$$A = \text{Re} \{ \widehat{Z}_I \} + y \text{Im} \{ \widehat{Z}_I \} + B y^2$$  \[10.34\]

10.2.3.2. Antisymmetric problems (mode II)

For problems where the loading is antisymmetrical in relation to the x axis, the normal stress $\sigma_{yy}(x, y = 0)$ is equal to 0. This condition gives rise to:

$$\text{Re} \left\{ 2\psi'(z) + z\psi''(z) + \chi'' \right\} = 0, \quad \text{at } y = 0$$  \[10.35\]

Following the same procedure as described for the symmetrical problem, we get:

$$2\psi'(z) + z\psi''(z) + \chi'' + IC = 0$$  \[10.36\]
where $C$ is a constant. By eliminating $\chi (z)$, we obtain:

$$
\sigma_{xx} = 4 \Re \{\psi\} - 2 y \Im \{\psi''\}
$$

$$
\sigma_{yy} = 2 y \Im \{\psi''\}
$$

$$
\sigma_{xy} = - 2 \Im \{\psi'\} - 2 y \Re \{\psi''\} - C
$$

and:

$$
2 \mu u_x = (\kappa + 1) \Re \{\psi\} - 2 y \Im \{\psi'\} - C y
$$

$$
2 \mu u_y = (\kappa - 1) \Im \{\psi\} - 2 y \Re \{\psi'\} - C x
$$

Let us define a function $\Psi(z)$ by $\Psi' = \psi' + i \frac{C}{2}$. Then, $\Psi(z) = \psi(z) + i \frac{C}{2} z$ and $\Psi''(z) = \psi''(z)$.

We get:

$$
\sigma_{xx} = 4 \Re \{\Psi\} - 2 y \Im \{\Psi''\}
$$

$$
\sigma_{yy} = 2 y \Im \{\Psi''\}
$$

$$
\sigma_{xy} = - 2 \Im \{\Psi'\} - 2 y \Re \{\Psi''\}
$$

and:

$$
2 \mu u_x = (\kappa + 1) \Re \{\Psi\} - 2 y \Im \{\Psi'\} + \frac{\kappa + 1}{2} C y
$$

$$
2 \mu u_y = (\kappa - 1) \Im \{\Psi\} - 2 y \Re \{\Psi'\} - \frac{\kappa + 1}{2} C x
$$

The last term in the components of the displacement represents the overall rotation. Let us define the Westergaard function $Z_{II}$ by $Z_{II} = 2i \bar{\Psi} (z)$.

Thus:

$$
\sigma_{xx} = 2 \Im \{Z_{II}\} + y \Re \{Z_{II}'\}
$$

$$
\sigma_{yy} = - y \Re \{Z_{II}'\}
$$

$$
\sigma_{xy} = \Re \{Z_{II}\} - y \Im \{Z_{II}'\}
$$

$$
2 \mu u_x = \frac{1}{2} (\kappa + 1) \Re \{Z_{II}\} + y \Re \{Z_{II}'\} + \frac{1}{2} (\kappa + 1) C y
$$

$$
2 \mu u_y = - \frac{1}{2} (\kappa - 1) \Re \{Z_{II}\} - y \Im \{Z_{II}\} - \frac{1}{2} (\kappa + 1) B x
$$
Hence, $Z_{II}$ gives the solution to the antisymmetric problems. We can give the Airy function:

$$ A = \text{Re} \left\{ \overline{Z_{II}} \right\} + y \text{Im} \left\{ \overline{Z_{II}} \right\} - y \text{Re} \left\{ \overline{Z_{II}} \right\} + Cy^2 \tag{10.43} $$

10.2.4. Solutions by the Westergaard function method

10.2.4.1. Mode I fracture

One of the typical problems is an infinite plate with a crack of length $2a$ along the $x$ axis with loading $\sigma_0$ normal to infinity as shown in Figure 10.3. The problem can be classified as a mode I problem because the stresses are symmetrical in relation to the crack line.

![Figure 10.3. A cracked plate subject to biaxial traction forces at infinity](image)

The boundary conditions in terms of stresses are as follows:

$$ \sigma_{xy} = \sigma_{yy} = 0, \; \text{for} \; |x| \leq a \; \text{and} \; y = 0 $$
$$ \sigma_{xy} = 0, \; \sigma_{xx} = \sigma_0 \; \text{for} \; |x| \Longrightarrow +\infty $$
$$ \sigma_{xy} = 0, \; \sigma_{yy} = \sigma_0 \; \text{for} \; |y| \Longrightarrow +\infty \tag{10.44} $$

The solution satisfying the boundary conditions is given by Westergaard [WES 39] with:

$$ Z_I (z) = \frac{\sigma_0 z}{\sqrt{z^2 - a^2}}, \; B = 0 \tag{10.45} $$
In order to make explicit the expressions of the stress field, we use the polar coordinates shown in Figure 10.4:

\[ z = re^{i\theta} \]
\[ z - a = r_1 e^{i\theta_1} \]
\[ z + a = r_2 e^{i\theta_2} \] [10.46]

The function \( Z_I \) becomes:

\[ Z_I = \frac{\sigma_0 r}{\sqrt{r_1 r_2}} \exp i \left( \theta - \frac{1}{2} \theta_1 - \frac{1}{2} \theta_2 \right) \] [10.47]

The differentiation of \( Z_I \) in relation to \( z \) gives:

\[ Z_I' = -\frac{\sigma_0 a^2}{(z^2 - a^2)^{3/2}} = -\frac{\sigma_0 a^2}{(r_1 r_2)^{3/2}} \exp \left( -\frac{3}{2} (\theta_1 + \theta_2) \right) \] [10.48]

From this, we deduce:

\[ Re \left\{ Z_I \right\} = \frac{\sigma_0 r}{\sqrt{r_1 r_2}} \cos \left( \theta - \frac{1}{2} \theta_1 - \frac{1}{2} \theta_2 \right) \]
\[ Re \left\{ Z_I' \right\} = -\frac{\sigma_0 a^2}{(r_1 r_2)^{3/2}} \cos \left( \frac{3}{2} (\theta_1 + \theta_2) \right) \]
\[ Im \left\{ Z_I' \right\} = \frac{\sigma_0 a^2}{(r_1 r_2)^{3/2}} \sin \left( \frac{3}{2} (\theta_1 + \theta_2) \right) \]
Using these expressions:

\[
\sigma_{xx} = \text{Re} \left\{ Z_1 \right\} - y \text{Im} \left\{ Z_1' \right\}
\]

\[
\sigma_{xx} = \frac{\sigma_0 r}{\sqrt{r_1 r_2}} \left[ \cos \left( \theta - \frac{1}{2} \theta_1 - \frac{1}{2} \theta_2 \right) - \frac{a^2}{r_1 r_2} \sin \theta \sin \frac{3}{2} (\theta_1 + \theta_2) \right] \quad [10.49]
\]

The two other components can be obtained:

\[
\sigma_{yy} = \frac{\sigma_0 r}{\sqrt{r_1 r_2}} \left[ \cos \left( \theta - \frac{1}{2} \theta_1 - \frac{1}{2} \theta_2 \right) + \frac{a^2}{r_1 r_2} \sin \theta \sin \frac{3}{2} (\theta_1 + \theta_2) \right] \quad [10.50]
\]

\[
\sigma_{xy} = \frac{\sigma_0 r}{\sqrt{r_1 r_2}} \sin \frac{\theta_1}{2} \cos \frac{\theta_1}{2} \cos \frac{3}{2} (\theta_1 + \theta_2) \quad [10.51]
\]

It is clear that on the crack \((\theta_1 = \pi, \theta_2 = 0, \theta = 0, \pi)\) we have \(\sigma_{xy} = \sigma_{yy} = 0\).

When \(r \rightarrow \infty\), we can observe that \(r_1 \approx r_2 \approx r \Rightarrow \infty\) and \(\theta_1 \approx \theta_2 \approx \theta\), and consequently:

\[
\sigma_{xy} = 0, \quad \sigma_{xx} = \sigma_0 \text{ for } |x| \Rightarrow +\infty \quad \sigma_{xy} = 0, \quad \sigma_{yy} = \sigma_0 \text{ for } |y| \Rightarrow +\infty
\]

10.2.4.2. The solution near to the crack tip

If we examine the tip A \((r = a, \theta = 0)\), we see that in the vicinity of A:

\[
r_1 \ll a \theta \approx 0 \theta_2 \approx 0 r \approx a r_2 \approx 2a \sin \theta \approx \frac{r_1}{a} \sin \theta_1
\]

Therefore:

\[
\sigma_{xx} = \frac{\sigma_0 a}{\sqrt{2\pi r_1}} \cos \frac{\theta_1}{2} \left( 1 - \sin \frac{\theta_1}{2} \sin \frac{3\theta_1}{2} \right)
\]

\[
\sigma_{yy} = \frac{\sigma_0 a}{\sqrt{2\pi r_1}} \cos \frac{\theta_1}{2} \left( 1 + \sin \frac{\theta_1}{2} \sin \frac{3\theta_1}{2} \right)
\]

\[
\sigma_{xy} = \frac{\sigma_0 a}{\sqrt{2\pi r_1}} \sin \frac{\theta_1}{2} \cos \frac{\theta_1}{2} \cos \frac{3\theta_1}{2}
\]

Along the crack propagation direction \((\theta = \theta_1 = \theta_2 = 0)\):

\[
\sigma_{yy} = \frac{\sigma_0 \sqrt{\pi a}}{\sqrt{2\pi r_1}} \sigma_{xy} = 0
\]
Fracture Mechanics of SMAs

A comparison with the basic modes (equation 10.1) yields the Mode I stress intensity factor:

$$ K_I = \sigma_0 \sqrt{\pi a} \quad [10.52] $$

If we change the coordinate axes and take the origin to be $A$ then $\theta_1 \implies \theta$ and $r_1 \implies r$ (Figure 10.8) and:

$$ \sigma_{xx} = \frac{K_I}{\sqrt{2\pi r}} \cos \frac{\theta}{2} \left( 1 - \sin \frac{\theta}{2} \sin \frac{3\theta}{2} \right) $$

$$ \sigma_{yy} = \frac{K_I}{\sqrt{2\pi r}} \cos \frac{\theta}{2} \left( 1 + \sin \frac{\theta}{2} \sin \frac{3\theta}{2} \right) \quad [10.53] $$

$$ \sigma_{xy} = \frac{K_I}{\sqrt{2\pi r}} \sin \frac{\theta}{2} \cos \frac{\theta}{2} \cos \frac{3\theta}{2} $$

We obtain the classic formulae for the Mode I stress field at the crack tip from the existing body of literature.

Following the same procedures, we obtain the displacements around the crack tip:

$$ u_x = \frac{K_I}{8\pi \mu} \sqrt{2\pi r} \left[ (2\kappa - 1) \cos \frac{\theta}{2} - \cos \frac{3\theta}{2} \right] $$

$$ u_y = \frac{K_I}{8\pi \mu} \sqrt{2\pi r} \left[ (2\kappa + 1) \sin \frac{\theta}{2} - \sin \frac{3\theta}{2} \right] \quad [10.54] $$

There is a singularity in $1/\sqrt{r}$ for the stresses; the stress intensity factor can be defined by:

$$ K_I = \lim_{r \to 0} \sqrt{2\pi r} \sigma_{yy} (\theta = 0) \quad [10.55] $$

10.2.4.3. Mode II fracture

Consider a plate cracked along a length $2a$ on the $x$ axis, subjected to uniform shear $\tau_0$ in infinity (Figure 10.5).

The boundary conditions in terms of stresses are as follows:

$$ \sigma_{xy} = \sigma_{yy} = 0, \ for \mid x \mid \leq a \text{ and } y = 0 $$

$$ \sigma_{xy} = \tau_0, \ \sigma_{xx} = 0 \ for \mid x \mid \implies +\infty $$

$$ \sigma_{xy} = \tau_0, \ \sigma_{yy} = 0 \ for \mid y \mid \implies +\infty \quad [10.56] $$

We can show that the Westergaard function:

$$ Z_{II} (z) = \frac{\tau_0 z}{\sqrt{z^2 - a^2}} \quad [10.57] $$
is a solution to the problem. Given that the same procedures produce the same effects, we calculate the stress intensity factor \( K_{II} \):

\[
K_{II} = \tau_0 \sqrt{\pi a}
\]  

[10.58]

**Figure 10.5. Cracked plate subject to pure shear at infinity**

The stresses around the crack tip \( A \), taking \( A \) to be the origin of the axes:

\[
\begin{align*}
\sigma_{xx} &= - \frac{K_{II}}{\sqrt{2\pi r}} \sin \frac{\theta}{2} \left( 2 + \cos \frac{\theta}{2} \cos \frac{3\theta}{2} \right) \\
\sigma_{yy} &= \frac{K_{II}}{\sqrt{2\pi r}} \sin \frac{\theta}{2} \cos \frac{\theta}{2} \cos \frac{3\theta}{2} \\
\sigma_{xy} &= \frac{K_{II}}{\sqrt{2\pi r}} \cos \frac{\theta}{2} \left( 1 - \sin \frac{\theta}{2} \sin \frac{3\theta}{2} \right)
\end{align*}
\]  

[10.59]

and the displacements around the crack tip:

\[
\begin{align*}
u_x &= K_{II} \frac{\sqrt{2\pi r}}{8\pi \mu} \left[ (2\kappa + 3) \sin \frac{\theta}{2} + \sin \frac{3\theta}{2} \right] \\
u_y &= -K_{II} \frac{\sqrt{2\pi r}}{8\pi \mu} \left[ (2\kappa - 3) \cos \frac{\theta}{2} + \cos \frac{3\theta}{2} \right]
\end{align*}
\]  

[10.60]

The Mode II stress intensity factor can be obtained by:

\[
K_{II} = \lim_{r \to 0} \sqrt{2\pi r} \sigma_{xy} (\theta = 0)
\]  

[10.61]
10.2.4.4. Mode III fracture

Mode III is associated with an antiplane deformation such that the displacement is given by:

\[ u_x = u_y = 0, \ u_z = w(x, y) \]  \[10.62\]

where:

\[ \varepsilon_{xz} = \frac{1}{2} \frac{\partial w}{\partial x}, \ \varepsilon_{yz} = \frac{1}{2} \frac{\partial w}{\partial y}, \ \varepsilon_{xx} = \varepsilon_{yy} = \varepsilon_{xy} = \varepsilon_{zz} = 0 \]  \[10.63\]

and the corresponding stresses:

\[ \sigma_{xz} = 2\mu \varepsilon_{xz}, \ \sigma_{yz} = 2\mu \varepsilon_{yz}, \ \sigma_{xx} = \sigma_{yy} = \sigma_{xy} = \sigma_{zz} = 0 \]  \[10.64\]

The equilibrium equations are reduced to:

\[ \triangle w = 0 \]  \[10.65\]

Hence:

\[ w = \frac{1}{\mu} I m \{ Z_{III}(z) \} \]  \[10.66\]

where \( Z_{III}(z) \) is an analytical function. The stresses can be represented by:

\[ \sigma_{xz} - i\sigma_{yz} = -iZ'_{III}(z) \]  \[10.67\]

Consider a cracked infinite plate under antiplane shear stress \( S \) in infinity represented by Figure 10.6:

![Cracked plate subject to antiplane stress in infinity](www.iran-mavad.com)
The boundary conditions are as follows:

\[
\begin{align*}
\sigma_{xy} &= \sigma_{yy} = \sigma_{yz} = 0, \text{ for } |x| \leq a \text{ et } y = 0 \\
\sigma_{xx} &= \sigma_{xy} = \sigma_{xz} = 0, \text{ for } |x| \rightarrow +\infty \\
\sigma_{xy} &= \sigma_{yy} = 0, \sigma_{yz} = S \text{ for } |y| \rightarrow +\infty
\end{align*}
\]  

[10.68]

We choose:

\[Z_{III} = S \sqrt{\frac{a^2}{2} - a^2}\]  

[10.69]

Consider the Mode III stress intensity factor:

\[K_{III} = S \sqrt{\pi a}\]  

[10.70]

and the stresses around the crack tip:

\[
\begin{align*}
\sigma_{yz} &= \frac{K_{III}}{\sqrt{2\pi r}} \cos \frac{\theta}{2} \\
\sigma_{xz} &= -\frac{K_{III}}{\sqrt{2\pi r}} \sin \frac{\theta}{2}
\end{align*}
\]  

[10.71]

The other components of the stress tensor are null, meaning that \(\sigma_{xx} = \sigma_{yy} = \sigma_{xy} = \sigma_{zz} = 0\).

The antiplane displacement \(w\) is equal to:

\[w = u_z = \sqrt{\frac{2}{\pi}} \frac{K_{III}}{\mu} \sqrt{r \sin \frac{\theta}{2}}\]  

[10.72]

10.2.4.5. Case study: specimen of finite dimensions: effects of size

Consider a cracked plate of height \(2H\) and width \(2b\). The length of the crack is still \(2a\) (see Figure 10.7).

In Mode I, the intensity factor \(K_I\) can be expressed as:

\[K_I = \sigma \sqrt{\pi a} F\left(\frac{a}{b}, \frac{a}{H}\right)\]  

[10.73]

where \(F\left(\frac{a}{b}, \frac{a}{H}\right)\) constitutes a dimensionless function of \(\frac{a}{b}\) and \(\frac{a}{H}\). When \(H \gg b\), the plate is considered to be semi-infinite and the parameter \(\frac{a}{H}\) must be subtracted from the expression \(F\left(\frac{a}{b}, \frac{a}{H}\right)\). In equation [10.74], Irwin [IRW 57] proposes the approximate formula:

\[F\left(\frac{a}{b}\right) = 1 + 0.128 \left(\frac{a}{b}\right) - 0.288 \left(\frac{a}{b}\right)^2 + 1.525 \left(\frac{a}{b}\right)^3\]  

[10.74]
We can find more sophisticated empirical formulae, e.g. in [MUR 87]:

\[ F\left(\frac{a}{b}\right) = 1.122 - 0.231 \left(\frac{a}{b}\right) + 10.55 \left(\frac{a}{b}\right)^2 + 21.72 \left(\frac{a}{b}\right)^3 + 30.39 \left(\frac{a}{b}\right)^4 \]  \[10.75\]

Now, knowing the stresses and the displacements, we have all the tools we need to predict the shape of the transformation surfaces around the crack tip.

10.3. Prediction of the phase transformation surfaces around the crack tip (no curvature at the crack tip) [LEX 11]

The aim here is to find the geometric shape of the phase transformation surfaces for the three modes and also for mixed modes.

Consider a second-order symmetrical tensor \( \sigma \) and \( S_\sigma \) its deviatoric part:

\[ S_\sigma \equiv \sigma - \frac{1}{3} \text{tr}(\sigma) 1 \]

Conventionally, the equivalent stress, also known as the Huber–von Mises stress, is defined by:

\[ \bar{\sigma} \equiv \kappa |S_\sigma|, \]

where \( \kappa \equiv \sqrt{\frac{2}{3}} \) is a normalization parameter and \( |\sigma| \equiv \sqrt{\text{tr}(\sigma^T \sigma)} \) the norm of a tensor \( \sigma \).

In order to take account of the skewness between the traction and compression in the prediction of surfaces [VAC 91], [ORG 98a], as in Chapter 7, we introduce the Lode parameter:

\[ y_\sigma \equiv \frac{6\kappa}{|S_\sigma|^3} \det S_\sigma \]  \[10.76\]
Irrespective of the mode in question, the tensor considered in this study is of the form:

\[
\sigma = \chi(r) q(\theta)
\]

where \( A \), the crack tip, constitute the origin of the system of polar coordinates (Figure 10.8):

\[
\chi(r) = \frac{K_t}{\sqrt{2\pi r}} > 0
\]

The factor \( K_t \) can be found in the form \( K_I, K_{II}, K_{III} \) depending on the mode of loading of the crack.

The same is true as regards the stress deviator tensor:

\[
S_\sigma = \chi(r) S_q(\theta)
\]

and consequently, the Lode parameter is independent of \( r \). \( y_\sigma(\theta) \) and the Huber–von Mises stress can be written:

\[
y_\sigma(\theta) \equiv \frac{6\kappa}{|S_q(\theta)|^2} \det S_q(\theta)
\]

\[
\tau = \kappa \chi(r)|S_q(\theta)| = \kappa \frac{K_t}{\sqrt{2\pi r}} |S_q(\theta)|.
\]

From this, we deduce that:

\[
r(\theta) = \frac{1}{2\pi} \left( \frac{K_t}{\tau} \right)^2 \kappa^2 |S_q(\theta)|^2
\]
Consider the phase transformation boundary surface $F(\sigma)$ defined, as in Chapter 7, by:

$$F(\sigma) = \sigma f(y_\sigma) - \sigma_c(T) = 0$$

where $f(y_\sigma) > 0$ is a regular function (of a continuous second derivative).

We get the following expression of the boundary radius:

$$r(\theta) = \frac{1}{4\pi} \left( \frac{K_t}{\sigma_c} \right)^2 \left( \frac{2\kappa^2 |S_q(\theta)|^2}{R(\theta)} \right) f^2(y_\sigma).$$

Hence, finally, we obtain a dimensionless term $r_L$:

$$r_L(\theta) \equiv \frac{r(\theta)}{L_{Am,f}} = R(\theta) f^2(y_\sigma)$$

for:

$$R(\theta) = 3 |S_q(\theta)|^2$$

$$L_{Am,f} = \frac{1}{4\pi} \left( \frac{K_t}{\sigma_c} \right)^2$$

Finally, we introduce the parameter $\beta$ in order to draw the distinction between the plane stress plane (PS) and the plane deformation (PD):

$$\beta = \begin{cases} 1 & \text{under PS} \\
1 - 2\nu & \text{under PD} \end{cases}$$

The choice of $f(y_\sigma)$ is important. The criterion function $F(\sigma)$ must be convex in the stress space.

In reference to the works of Bouvet et al. [BOU 02], we have already chosen:

$$f(y_\sigma) = \cos \left( \frac{1}{3} \arccos \left( 1 - a (1 - y_\sigma) \right) \right)$$

which ensures that $F(\sigma)$ is convex for $0 \leq a \leq 1$, as demonstrated by Laydi andLexcellent [LAY 10].

A simple expression of $f(y_\sigma)$ can be chosen in the form $f(y_\sigma) = 1 + by_\sigma$ and once again the convexity of $F(\sigma)$ can be assured if and only if $0 \leq a \leq 1/8$.

Let us now examine the different modes for the conditions of plane stress or plane deformation.
10.3.1. Mode I

As established above (equation [10.53]), the tensor \( q_I (\theta) \) is written:

\[
q_I (\theta) = \cos \left( \frac{\theta}{2} \right) \begin{pmatrix}
1 - \sin \left( \frac{\theta}{2} \right) \sin \left( \frac{3\theta}{2} \right) & \sin \left( \frac{\theta}{2} \right) \cos \left( \frac{3\theta}{2} \right) & 0 \\
\sin \left( \frac{\theta}{2} \right) \cos \left( \frac{3\theta}{2} \right) & 1 + \sin \left( \frac{\theta}{2} \right) \sin \left( \frac{3\theta}{2} \right) & 0 \\
0 & 0 & 1 - \beta
\end{pmatrix}
\]

\[
S_{q_I} (\theta) = \cos \left( \frac{\theta}{2} \right) \begin{pmatrix}
\frac{1}{3} \beta - \sin \left( \frac{\theta}{2} \right) \sin \left( \frac{3\theta}{2} \right) & \sin \left( \frac{\theta}{2} \right) \cos \left( \frac{3\theta}{2} \right) & 0 \\
\sin \left( \frac{\theta}{2} \right) \cos \left( \frac{3\theta}{2} \right) & \frac{1}{3} \beta + \sin \left( \frac{\theta}{2} \right) \sin \left( \frac{3\theta}{2} \right) & 0 \\
0 & 0 & 1 + \beta \cos \left( \frac{\theta}{2} \right) \sin \left( \frac{3\theta}{2} \right)
\end{pmatrix}
\] [10.80]

\[
\det(S_{q_I}) = \frac{1}{3} \beta \cos^3 \left( \frac{\theta}{2} \right) \left( 1 - \cos \theta - \frac{2}{9} \beta^2 \right)
\]

\[
|S_{q_I}|^2 = \cos^2 \left( \frac{\theta}{2} \right) \left( 1 - \cos \theta + \frac{2}{3} \beta^2 \right)
\] [10.81]

\[
R (\theta) = 3 |S_{q_I}|^2 = 2 \cos^2 \left( \frac{\theta}{2} \right) \left( \frac{3}{2} (1 - \cos \theta) + \beta^2 \right) = \frac{3}{2} \sin^2 \theta + \beta^2 (1 + \cos \theta)
\]

\[
y_\sigma = 2 \kappa \beta \frac{1 - \cos \theta - \frac{2}{9} \beta^2}{(1 - \cos \theta + \frac{2}{3} \beta^2)^2}
\]

Finally, the dimensionless radius \( r_L (\theta) \) can be calculated using equation [10.78] for each correction \( f (y_\sigma) \).

As presented in Figures 10.9 and 10.10, \( r_L (\theta) \) was traced for the two expressions of \( f \) with \( \beta = 1 \) under plane stress and \( \nu = 0.4 \) under plane deformation.

– Under PS, the size of the surfaces is approximately double what it is under PD.

– The effect of skewness between the traction and compression is more manifest under PS than under PD.

– The refined correction function in \( y_\sigma \) predicts a slightly more extensive domain of transformation than does the Bouvet function.

10.3.2. Mode II

As established in equation [10.59], the tensor \( q_{II} (\theta) \) is written:

\[
q_{II} (\theta) = \begin{pmatrix}
- \sin \left( \frac{\theta}{2} \right) (2 + \cos \left( \frac{\theta}{2} \right) \cos \left( \frac{3\theta}{2} \right)) & \cos \left( \frac{\theta}{2} \right) (1 - \sin \left( \frac{\theta}{2} \right) \sin \left( \frac{3\theta}{2} \right)) & 0 \\
\cos \left( \frac{\theta}{2} \right) (1 - \sin \left( \frac{\theta}{2} \right) \sin \left( \frac{3\theta}{2} \right)) & \sin \left( \frac{\theta}{2} \right) \cos \left( \frac{3\theta}{2} \right) & 0 \\
0 & 0 & (\beta - 1) \sin \left( \frac{\theta}{2} \right)
\end{pmatrix}
\]
Figure 10.9. Mode I: phase transformation surface under plane stress

Figure 10.10. Mode I: phase transformation surface under plane deformation condition

and the deviator tensor $S_{q_2} (\theta)$:

$$S_{q_11} (\theta) = \begin{pmatrix} -\sin \left( \frac{\theta}{2} \right) \left( 1 + \frac{\theta}{2} + \cos \left( \frac{\theta}{2} \right) \cos \left( \frac{\theta^2}{2} \right) \right) & \cos \left( \frac{\theta}{2} \right) \left( 1 - \sin \left( \frac{\theta}{2} \right) \sin \left( \frac{\theta^2}{2} \right) \right) & 0 \\ \cos \left( \frac{\theta}{2} \right) \left( 1 - \sin \left( \frac{\theta}{2} \right) \sin \left( \frac{\theta^2}{2} \right) \right) & \sin \left( \frac{\theta}{2} \right) \left( 1 - \frac{\theta}{2} + \cos \left( \frac{\theta}{2} \right) \cos \left( \frac{\theta^2}{2} \right) \right) & 0 \\ 0 & 0 & \frac{3}{4} \beta \sin \left( \frac{\theta}{2} \right) \end{pmatrix}$$ [10.82]
Finally, $R(\theta)$, $y_\sigma$ are calculated:

\[
R(\theta) = \frac{1}{3} \beta^2 (1 - \cos \theta) + \frac{9}{4} \cos 2\theta + \frac{15}{4}
\]

\[
y_\sigma = 2\kappa \beta \sin \left( \frac{\theta}{2} \right) \frac{\frac{1}{4} \beta^2 (1 - \cos \theta) - \frac{3}{4} \cos 2\theta - \frac{5}{4}}{\left( \frac{1}{4} \beta^2 (1 - \cos \theta) + \frac{9}{4} \cos 2\theta + \frac{15}{4} \right)^2}
\]

As presented in Figures 10.11 and 10.12, the $r_L(\theta)$ are calculated with $\beta = 1$ under PS and $\nu = 0.4$ under PD.

\textbf{Figure 10.11.} Mode II: phase transformation surface under plane stress condition

The main observations are as follows:

– the size of the transformation surfaces is slightly smaller under plane deformation than under plane stress;
the sizes of the surfaces are governed by the skewness parameters $a$ or $b$. Similarly as for Mode I, their influence is greater under plane stress than under plane deformation;

– the two choices of the functions $f(y_\sigma)$ give equivalent boundary surfaces.

### 10.3.3. Mode III

In this case, the tensor $\mathbf{q}_{III}$ is equal to its deviator $\mathbf{s}_{q_{III}}$:

$$\mathbf{s}_{q_{III}} = \mathbf{q}_{III} = \begin{pmatrix} 0 & 0 & -\sin^{\frac{\theta}{2}} \\ 0 & 0 & \cos^{\frac{\theta}{2}} \\ -\sin^{\frac{\theta}{2}} \cos^{\frac{\theta}{2}} & 0 \end{pmatrix}$$

[10.84]

$$\det(\mathbf{s}_{q_{III}}) = 0, \quad |\mathbf{S}_{q_{III}}|^2 = 2, \quad R(\theta) = 6, \quad y_\sigma = 0$$

The distinction between plane stress and plane deformation is meaningless here.

The parameter $b$ no longer has a bearing on the size of the surface, whereas for the correction surface initiated by Bouvet $f(y_\sigma = 0) = \cos \left( \frac{1}{2} \arccos (1 - a) \right)$ determines the size of the domain by the intervention of the choice of $a \in [0, 1]$ (see Figure 10.13).

To conclude this study on the classic modes: for a given mode, the geometric shape of the transformation boundary surfaces exhibits great similarity to that for an...
elastoplastic material, which is not, in itself, surprising. Before unloading, the traction curves in both cases have the same shape.

Let us now look at the effect of a mixed load: mode I + mode II, on the fracture behavior.

![Figure 10.13. Mode III phase transformation surface](image)

**10.3.4. Mixed Mode I + II: analytical prediction of the transformation surfaces**

Take a plate presenting a crack inclined at an angle $\alpha$ in relation to the $y$ axis (Figure 10.14).

![Figure 10.14. Cracked plate inclined at an angle $\alpha$](image)
Murakami et al.'s book about stress intensity factors [MUR 87] gives the following factors:

\[
K_I = \sigma_0 \sqrt{\pi \sin^2 (\alpha)} = K_0 k_1 (\alpha) \tag{10.85}
\]
\[
K_{II} = \sigma_0 \sqrt{\pi \cos (\alpha)} = K_0 k_2 (\alpha)
\]

where \( K_0 = \sigma_0 \sqrt{\pi a} \) and \( k_1 = \sin^2 (\alpha) \) and \( k_2 = \sin (\alpha) \cos (\alpha) \).

For mode I, we have defined the stress state by:

\[
\sigma_I (r, \theta) = \frac{K_I}{\sqrt{2\pi r}} q_I (\theta)
\]

By superposition, the stress tensor around the crack tip is defined by:

\[
\sigma (r, \theta, \alpha) = \frac{K_0}{\sqrt{2\pi r}} (k_1 (\alpha) q_I (\theta) + k_2 (\alpha) q_{II} (\theta)) = \chi_0 (r) q (\theta, \alpha) \tag{10.86}
\]

where \( \chi_0 (r) = \frac{K_0}{\sqrt{2\pi r}} \) and \( q (\theta, \alpha) = k_1 (\alpha) q_I (\theta) + k_2 (\alpha) q_{II} (\theta) \).

The Lode invariant and the deviator tensor become:

\[
y_{\sigma} (\theta, \alpha) \equiv \frac{6\kappa}{|S_q (\theta, \alpha)|^2} \det S_q (\theta, \alpha) \tag{10.87}
\]
\[
S_q (\theta, \alpha) = k_1 (\alpha) S_{qI} (\theta) + k_2 (\alpha) S_{qII} (\theta)
\]

The stress \( \sigma \) is written:

\[
\sigma (r, \theta, \alpha) = \kappa \chi_0 |S_q (\theta, \alpha)| \tag{10.88}
\]

Considering the transformation surface equation, we deduce the radius of the domain boundary:

\[
r(\theta, \alpha) = \frac{1}{4\pi} \left( \frac{K_0}{\sigma_c} \right)^2 \left( \frac{2\kappa^2 |S_q (\theta, \alpha)|^2}{R(\theta, \alpha)} \right)^2 f^2 (y_{\sigma}) \tag{10.89}
\]

where:

\[
|S_q (\theta, \alpha)|^2 = \sin^4 (\alpha) |S_{qI} (\theta)|^2 + \sin^2 (\alpha) \cos^2 (\alpha) |S_{qII} (\theta)|^2 + \sin^3 (\alpha) \cos (\alpha) |S_{qI} (\theta); S_{qII} (\theta)| \tag{10.90}
\]

While we know the expressions of \(|S_{qI} (\theta)|^2\) and \(|S_{qII} (\theta)|^2\) (see equations [10.81] and [10.83]), we still need to calculate \(|S_{qI} (\theta); S_{qII} (\theta)|\), which gives us:

\[
|S_{qI} (\theta); S_{qII} (\theta)| = \sin (\theta) \left( \cos (\theta) - \frac{\beta^2}{3} \right) \tag{10.91}
\]
and also:

\[ r_L(\theta, \alpha) \equiv \frac{r(\theta, \alpha)}{L_{Amf}} = R(\theta, \alpha) f^2(y_\sigma) \]  \[ \tag{10.92} \]

where:

\[ R(\theta, \alpha) = 3\sin^2(\alpha) \]  \[ \tag{10.93} \]

\[ X\left(\frac{\beta^2}{3} (1 - \cos(\theta - 2\alpha)) + \frac{3}{4} + \frac{1}{4} \cos(2\theta) + \frac{1}{2} (\cos(2\alpha) + \cos(2\theta - 2\alpha))\right) \]

and:

\[ y_\sigma(\theta, \alpha) \equiv \frac{6\kappa}{\det S_q(\theta, \alpha)} \]  \[ \tag{10.94} \]

where:

\[ \det S_q(\theta, \alpha) = \frac{\beta}{108} \sin^3(\alpha) \sin(\theta - \alpha) \]

\[ X(8\beta^2 \sin^2\left(\frac{\theta}{2} - \alpha\right) - 9 \cos(2\theta)) \]

\[ + 2 \cos(2\alpha) + 2 \cos(2\theta - 2\alpha) + 3 \]  \[ \tag{10.95} \]

\( r_L \) is traced for a fixed value of \( \alpha \), namely \((\alpha = 30^\circ, 60^\circ)\) and variable \( \theta \) under plane stress \((\beta = 1)\) (see Figures 10.15 and 10.17) and under plane deformation \((\nu = 0.4)\) (Figures 10.16 and 10.18).

Figure 10.15. Mixed mode under plane stress: \( \alpha = 30^\circ \)
Figure 10.16. Mixed mode under plane deformation: $\alpha = 30^\circ$

Figure 10.17. Mixed mode under plane stress: $\alpha = 60^\circ$
10.4. Prediction of the phase transformation surfaces around the crack tip (curvature $\rho$ at the crack tip)

For Mode I, for a crack with curvature radius $\rho$, Creager and Paris propose the following stress field around the crack tip:

$$
\sigma_{xx} = \frac{K_I}{\sqrt{2\pi r}} \cos \theta \left( 1 + \frac{\sin^2 \frac{3\theta}{2}}{2} \right) - \frac{K_I}{\sqrt{2\pi r}} \left( \frac{\rho}{2r} \right) \cos \frac{3\theta}{2} \\
\sigma_{yy} = \frac{K_I}{\sqrt{2\pi r}} \cos \theta \left( 1 + \frac{\sin^2 \frac{3\theta}{2}}{2} \right) + \frac{K_I}{\sqrt{2\pi r}} \left( \frac{\rho}{2r} \right) \cos \frac{3\theta}{2} \tag{10.96} \\
\sigma_{xy} = \frac{K_I}{\sqrt{2\pi r}} \sin \theta \cos \theta \left( \frac{3\theta}{2} \right) - \frac{K_I}{\sqrt{2\pi r}} \left( \frac{\rho}{2r} \right) \sin \frac{3\theta}{2}
$$

Note that $r$ is finite on the crack tip: $r = \frac{\rho}{2}$ and therefore, the stresses have a finite value, so there is no singularity.

Remember that:

$$
\sigma_{yz} = \sigma_{zx} = 0 \\
\sigma_{zz} = 0 \text{ under PS} \tag{10.97} \\
\sigma_{zz} = \nu (\sigma_{xx} + \sigma_{yy}) \text{ under PD}
$$

For a given boundary value $\sigma_c(T) > 0$, we seek to calculate the function:

$$
r: \theta \in [0, 2\pi] \rightarrow r(\theta) \geq \frac{1}{2} \rho > 0 \tag{10.98}
$$
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a solution of the nonlinear equation:

\[ F(\sigma) = \sigma f(y) - \sigma_c(T) = 0 \]  

[10.99]

If we look at the particular case of von Mises, i.e. where \( f = 1 \):

\[ \sigma = \sigma_c \]  

[10.100]

we introduce an auxiliary variable:

\[ z = \frac{\rho}{2r} \]  

[10.101]

We can find a solution:

\[ z = \psi_p(\chi) = \left( \sqrt{\chi^2 + p^2} + \chi \right)^{\frac{1}{2}} - \left( \sqrt{\chi^2 + p^2} - \chi \right)^{\frac{1}{2}} \]  

[10.102]

and thereby show that:

\[ r = \frac{1}{2} \frac{\rho}{\psi_p(\chi)} \]  

[10.103]

is a solution to equation [10.100] if and only if:

\[ \chi \leq \frac{1}{2} \]  

[10.104]

In general, we replace \( \sigma_c \) from equation [10.100] with \( \frac{\sigma_c}{f(y)} \), or simpler still, with \( \sigma_c f(y) \), because:

\[ \sigma = \frac{K_f}{\sqrt{\sigma_p}} z^{\frac{1}{2}} \sum \text{ and } y_\sigma = y_\Sigma \]  

[10.105]

i.e. \( \frac{K_f}{\sqrt{\sigma_p}} z^{\frac{1}{2}} \sum = \sigma = \frac{\sigma_c}{f(y)} \).

More specifically, we have the equivalences:

\[ G(\sigma) = \sigma f(y_\Sigma) = \sigma_c \iff \sqrt{\sum} G(\Sigma) = 2 \kappa \chi^{\frac{1}{2}} \iff z = \psi_p(\chi \alpha_\theta(z)) \]  

[10.106]

where \( \alpha_\theta \) is a continuous function of \( z \) and of \( \theta \) defined by \( \alpha_\theta(z) \equiv |f(y_\Sigma)|^{-2} \).

Its expression is easy to obtain, by using equation [10.76] to combine the value of \( S_\Sigma \) with that of:

\[ det(S_\Sigma) = \frac{2\beta}{3} \cos \frac{\theta}{2} \left( z^2 + \frac{1}{4} \sin^2 \theta - \left| \frac{\beta}{3} \cos \frac{\theta}{2} \right|^2 \right) \]
In addition, we have the frame:

\[
\frac{1}{8} \eta^3 \leq \chi_{\alpha \theta}(z) \leq \frac{1}{2} \eta^3 \quad \text{where} \quad \eta = (6 \chi | f(0)|^{-2})^{\frac{1}{2}}
\]  \[10.107\]

This result is a direct consequence of the convexity of \( G \) (see [LAY 12]) which imposes the following necessary condition on \( f \):

\[
3^{-\frac{1}{2}} f(0) \leq f(y) \leq 2.3^{-\frac{1}{2}} f(0) \quad \forall y \in [-1, 1]
\]  \[10.108\]

Finally, in order to solve the problem \[10.99\] we need to find \( \hat{z} \) that solves one of the following equivalent equations:

\[
\varphi_p(\hat{z}) = \chi_{\alpha \theta}(\hat{z}) \iff \hat{z} = \psi_p(\chi_{\alpha \theta}(\hat{z}))
\]  \[10.109\]

Consider that:

\[
\xi \equiv \psi_p\left(\frac{1}{8} \eta^3\right)
\]  \[10.110\]

The following theorem can be demonstrated (personal communication from M.R. Laydi).

Consider \( \eta \in [0, 1] \). In this case, equation \[10.99\] can accept at least one solution \( r = \frac{L}{2\pi} \) such that:

\[
\xi \leq \psi_p\left(\frac{1}{8} \eta^3\right) \leq z \leq \psi_p\left(\frac{1}{2} \eta^3\right) \leq \eta \quad \forall \theta
\]  \[10.111\]

In addition, if:

\[
\eta \leq 0.34
\]  \[10.112\]

then the solution to the problem is unique.

10.4.1. Applications

We consider the following physical parameters:

\[
\nu = 0.3, \quad \rho = 0.5 \text{ mm}, \quad K_f = 50 \text{ MPa}\sqrt{m},
\]

phase transformation start stress \( \sigma_s = 30 \text{ MPa} \) phase transformation end stress \( \sigma_f = 60 \text{ MPa} \).
10.4.1.1. Application I (Figure 10.19)

Take \( f(y) = 1 + by, b \in [0, \frac{1}{8}] \).

Satisfaction of the condition 10.112:

\[
\eta = (6\chi|f(0)|^{-2})^{\frac{1}{2}} = \left( \pi \rho \left( \frac{\sigma_c}{K_I} \right)^2 |f(0)|^{-2} \right)^{\frac{1}{2}}
\]

\[
= \left\{ \begin{array}{l}
0.08 \text{ at the start of the transformation} \\
0.013 \text{ at the end of the transformation}
\end{array} \right\} < 0.34
\]

In both cases, the unicity condition is satisfied.

![Figure 10.19. Cracked plate with a Mode I curvature radius (application I)](image)

10.4.1.2. Application II (Figure 10.20)

Take:

\[
f(y) = \cos \left( \frac{1}{3} \arccos (1 - a (1 - y)) \right), \forall a \in [0, 1]
\]

The condition 10.112 depends on the value of \( a \), but it is still satisfied.

10.5. Some experimental results about fracture of SMAs

Coupled thermomechanical problems can be solved by digital image correlation (DIC). Thus, Daly et al. [DAL 07] measured the deformations at the crack tip by DIC on thin plates of nitinol. This \textit{in situ} optical method provide information about
the phase transformation zones by locating deformations. The choice of the “linear elastic fracture mechanics” (LEFM) theory seems justified by the small size of the transformation zone, as shown in Figure 10.21.

![Cracked plate with a Mode I curvature radius (application II)](image)

**Figure 10.20.** Cracked plate with a Mode I curvature radius (application II)

**Figure 10.21.** Measurement of $\varepsilon_{yy}$ obtained by DIC at the crack tip for $K_I = 44 \text{ MPa}\sqrt{m}$ [DAL 07]

The shape of the lobes of the transformation surface, inclined at around 60°, validates the taking into account of the asymmetry between the traction and compression in the calculations.

In addition, local temperature measurements can be taken using infrared cameras. The evolution of the local temperature can be considered to be an indicator of the start
of crack propagation, as attested by Figure 10.22. The measurements show an increase in temperature of around 40° associated with the phase transformation – which, it must be remembered, is highly exothermic.

![Figure 10.22](image)

**Figure 10.22.** Change in temperature during a fracture test: a) at the start of propagation; b) during propagation; c) at fracture [LEX 11]

Isotherms appear in the form of a boomerang in Figure 10.22b), with an orientation of ±50° in relation to the original direction of the crack.

Traction tests have been performed in the SYMME Lab in Annecy on samples exhibiting different radii of curvature. Depending on the dimensions of the sample and on the radius of curvature, we can calculate the stress intensity factors by making use of the correction coefficient from equation [10.75]:

\[
\rho (\text{mm}) \quad 0.25 \quad 0.5 \quad 1 \quad 1.5
\]

\[
K_{1c} (\text{MPa}\sqrt{\text{m}}) \quad 91 \quad 102 \quad 108 \quad 115
\]

[10.113]

An overall view of Figure 10.23 indeed shows the areas of the beginning and end of transformation, and their geometric shape conforms to our calculations.

![Figure 10.23](image)

**Figure 10.23.** Overall image of a plate with a radius of curvature under mechanical loading
To go into a little more detail, Figures 10.24, 10.25 and 10.26 show the deformation $\varepsilon_{yy}$ ($y$ being the normal to the crack with a radius of curvature $\rho = 1$ mm and for different applied loads). The two inclined lobes spread out around the crack as the applied load increases [TAI 12].

**Figure 10.24.** Deformation $\varepsilon_{yy}$ for $K_I = 69 \text{ MPa}\sqrt{m}$

**Figure 10.25.** Deformation $\varepsilon_{yy}$ for $K_I = 88 \text{ MPa}\sqrt{m}$
10.6. Problem of delamination between a SMA and an elastic solid [LAY 12]

In the wake of the work of Rice et al. [RIC 90], we investigate elasto-brittle fracture between two different materials. The upper layer is formed of a shape-memory alloy (material 1) and the lower layer of an isotropic elastic solid (material 2), as shown in Figure 10.27.

A crack at $y = 0$, $x < 0$ denoted $\Gamma_-$ and an interface at $y = 0$, $x > 0$ denoted $\Gamma_+$ separate the two materials. Material 1 is a shape-memory alloy which may be either in the austenitic state (Young’s modulus $E_A$, Poisson coefficient $\nu_1$) or in the martensitic state (Young’s modulus $E_M$, Poisson coefficient $\nu_1$) depending on the mechanical
loading applied at the geographic zone considered. Material 2 has elastic moduli $E_2$ and $\nu_2$.

As usual, the stresses around the crack tip are in $(1/\sqrt{r})$, implying that they are limitless. Consequently, a phase transformation induced by this stress (or a reorientation of the martensite plates) occurs around the crack tip, at the very beginning of mechanical loading.

The primary objective is to calculate the boundary surfaces of the beginning and end of phase transformations around the crack tip.

Using a von Mises-type approach, Freed et al. [FRE 08] constructed these surfaces. Here, we integrate the skewness between the traction and compression into the estimation.

In the context of the elastic linear theory of continuous media, the stress field around the crack tip, for a crack at the interface between two isotropic materials, assumes the following singular form:

$$\Sigma = \frac{1}{\sqrt{2\pi r}} \left( Re \left( K r^{ie} \right) \Sigma^I + Im \left( K r^{ie} \right) \Sigma^{II} \right)$$

Here, the tensors $\Sigma$ with the superscripts I and II correspond to Modes I and II (mode III is not examined).

Rice et al. [RIC 90] gave the stress field for material 1. For material 2, it is sufficient to change $\pi \epsilon n - \pi$ in the expressions $\Sigma^I (\Sigma^I)$ and $\Sigma^{II} (\Sigma^{II})$:

$$\Sigma^I = \frac{1}{\cosh (\pi \epsilon)} \Sigma^I (\theta, \epsilon, \nu)$$
$$\Sigma^{II} = \frac{1}{\cosh (\pi \epsilon)} \Sigma^{II} (\theta, \epsilon, \nu)$$

[10.115]

The tensors $\hat{\Sigma}^I (\theta, \epsilon, \nu)$ et $\hat{\Sigma}^{II} (\theta, \epsilon, \nu)$ exhibit the following form:

$$\hat{\Sigma}^I = \begin{pmatrix} \Sigma^I_{rr} & \Sigma^I_{r\theta} & 0 \\ \Sigma^I_{\theta r} & \Sigma^I_{\theta\theta} & 0 \\ 0 & 0 & \nu (\Sigma^I_{rr} + \Sigma^I_{\theta\theta}) \end{pmatrix}$$
$$\hat{\Sigma}^{II} = \begin{pmatrix} \Sigma^{II}_{rr} & \Sigma^{II}_{r\theta} & 0 \\ \Sigma^{II}_{\theta r} & \Sigma^{II}_{\theta\theta} & 0 \\ 0 & 0 & \nu (\Sigma^{II}_{rr} + \Sigma^{II}_{\theta\theta}) \end{pmatrix}$$

[10.116]
with the components of $\Sigma I \Sigma^{II}$:

\[
\begin{pmatrix}
\Sigma_{rr}^I &= -\sinh(\varepsilon(\pi - \theta)) \cos\left(\frac{\theta}{2}\right) + \exp(-\varepsilon(\pi - \theta)) \cos\left(\frac{\theta}{2}\right) \left(1 + \sin^2\left(\frac{\theta}{2}\right)\right) + \varepsilon \sin(\theta)
\Sigma_{\theta\theta}^I &= \sinh(\varepsilon(\pi - \theta)) \cos\left(\frac{\theta}{2}\right) + \exp(-\varepsilon(\pi - \theta)) \sin\left(\frac{\theta}{2}\right) \cos^2\left(\frac{\theta}{2}\right) - \varepsilon \sin(\theta)
\Sigma_{r\theta}^I &= -\sinh(\varepsilon(\pi - \theta)) \sin\left(\frac{\theta}{2}\right) + \exp(-\varepsilon(\pi - \theta)) \sin\left(\frac{\theta}{2}\right) \left(1 + \cos^2\left(\frac{\theta}{2}\right)\right) - \varepsilon \sin(\theta)
\Sigma_{rr}^{II} &= \cosh(\varepsilon(\pi - \theta)) \sin\left(\frac{3\theta}{2}\right) - \exp(-\varepsilon(\pi - \theta)) \sin\left(\frac{\theta}{2}\right) \cos\left(\frac{\theta}{2}\right) \cos^2\left(\frac{\theta}{2}\right) + \varepsilon \sin(\theta)
\Sigma_{\theta\theta}^{II} &= -\cosh(\varepsilon(\pi - \theta)) \sin\left(\frac{3\theta}{2}\right) - \exp(-\varepsilon(\pi - \theta)) \sin\left(\frac{\theta}{2}\right) \sin^2\left(\frac{\theta}{2}\right) - \varepsilon \sin(\theta)
\Sigma_{r\theta}^{II} &= \cosh(\varepsilon(\pi - \theta)) \cos\left(\frac{3\theta}{2}\right) + \exp(-\varepsilon(\pi - \theta)) \cos\left(\frac{\theta}{2}\right) \sin^2\left(\frac{\theta}{2}\right) + \varepsilon \sin(\theta)
\end{pmatrix}
\]

We define an “equivalent Poisson coefficient” $\nu = 0$ under $CP$; $\nu = \nu_1$ under $DP$.

The introduction of the parameter $\varepsilon$, called the oscillation parameter, enables us to take into account the ratio of the elastic properties of the two materials in the expression of the stresses $\Sigma I$ and $\Sigma^{II}$.

This parameter is given by:

\[
\varepsilon = \frac{1}{2\pi} \log \left(\frac{1 - \beta}{1 + \beta}\right)
\]

where $\beta$ is Dundurs’ second parameter [DUN 70]. For an interface between two linear isotropic elastic materials, $\beta$ takes the following form:

\[
\beta = \frac{\mu_1 (K_2 - 1) - \mu_2 (K_1 - 1)}{\mu_1 (K_2 + 1) + \mu_2 (K_1 + 1)}
\]

where $\mu_i = \frac{E_i}{2(1+\nu_i)}$ and $\nu_i \in [0, 0.5]$ $(i = 1, 2)$ are the shear moduli and the Poisson coefficients, and $K_i$ is the volumetric expansion:

\[
K_i = \left(\frac{3 - \nu_i}{1 + \nu_i}\right)
\]

The problem is to find an angle:

\[
\psi = \arctan \left(\frac{\sigma_{xy}}{\sigma_{yy}}\right) \text{ on } \Gamma^+
\]

such that:

\[
G(\sigma) = \pi f(y_\sigma) = \sigma_\varepsilon \text{ on } \Gamma^+
\]
Thus, Rice et al. [RIC 90] gave the definition of the local phase angle $\dot{\psi}$ as:

$$\dot{\psi} = \psi + \log \left( \frac{\hat{r}}{\hat{L}} \right)$$  \[10.123\]

where $\hat{r} = r (\theta = 0)$ is the radius of $\Gamma_+$, $\hat{L}$ is a characteristic length (that is, the length of a crack, the thickness of a layer, etc.) and $\psi$ is a given which depends on the direction of loading.

In addition:

$$K = |K| \exp \left( i \dot{\psi} \right)$$  \[10.124\]

and stress tensor $\sigma$:

$$\sigma (r, \theta, \varepsilon, \nu) = \frac{|K|}{\sqrt{2\pi} r} \sum \left( \dot{\psi}, \theta, \varepsilon, \nu \right)$$  \[10.125\]

where:

$$\sum \left( \dot{\psi}, \theta, \varepsilon, \nu \right) = \cos \left( \dot{\psi} \right) \sum_1 \left( \theta, \varepsilon, \nu \right) + \sin \left( \dot{\psi} \right) \sum_2 \left( \theta, \varepsilon, \nu \right)$$  \[10.126\]

The determination of the particular values of $\dot{\psi}$ corresponding firstly to the beginning of phase transformation $\psi_s$ and secondly to the end of that transformation $\psi_f$ is important.

For an interface between austenite (Young’s modulus $E_1 = E_A$) and material 2:

$$\psi_s = \dot{\psi} (\hat{r}, \varepsilon_A) = \psi + \varepsilon_A \log \left( \frac{\hat{r}}{\hat{L}} \right)$$  \[10.127\]

For an interface between martensite (Young’s modulus $E_1 = E_M$) and material 2:

$$\psi_f = \dot{\psi} (\hat{r}, \varepsilon_M) = \psi + \varepsilon_M \log \left( \frac{\hat{r}}{\hat{L}} \right)$$  \[10.128\]

The transformation boundary surface is written as usual:

$$G (\sigma) = \sigma f (y_\sigma) = \sigma_c$$  \[10.129\]

where:

$$\sigma_c = \begin{cases} C_M (T - M_0^0) & \text{for the beginning of the transformation} \\ C_M (T - M_f^0) & \text{for the end of the transformation} \end{cases}$$  \[10.130\]
Because $y_\sigma$ is independent of $r$, we have:

$$\frac{|K|}{\sqrt{2\pi r}} G(\Sigma) = C_M (T - M_0^f) \rho^{-1}$$  \[10.131\]

where:

$$\rho \equiv \left\{ \begin{array}{l} \rho_s = \frac{T - M_0^f}{T - M_f^0} > 1 \\ \rho_f = 1 \end{array} \right\}$$  \[10.132\]

By introducing a reference value $L$ called the standardization parameter:

$$L = \frac{1}{2\pi} \left( \frac{|K|}{C_M (T - M_f^0)} \right)^2$$  \[10.133\]

This leads to a simple expression of $r$:

$$r = L\rho^2 |G(\Sigma)|^2$$  \[10.134\]

The value of $\hat{\psi}$ is obtained by solving the system:

$$\begin{cases} \hat{\psi} = \psi + \varepsilon \log \left( \frac{\hat{r}}{L} \right) \\ \hat{r} = L \rho^2 |G(\Sigma(\hat{\psi}))|^2 \end{cases}$$  \[10.135\]

where $\Sigma(\hat{\psi}) = \Sigma(\hat{\psi}; \theta = 0, \varepsilon, \bar{\nu})$.

For the applications, we take $\nu_1 = \nu_2 = \nu$ and the values of the Young’s moduli of the two materials:

- material 1: austenite $E_1 = E_A = 70$ GPa; material 2: $E_2 = 30$ GPa;
- material 1: martensite $E_1 = E_M = 30$ GPa; material 2: $E_2 = 30$ GPa;

and:

$$f (y_\sigma) = \cos \left( \frac{1}{3} \arccos (1 - a (1 - y_\sigma)) \right), \forall a \in [0, 1]$$  \[10.136\]

Finally, we assume the same values $\nu, \rho_s, L, \hat{L}$ as Freed et al. [FRE 08]:

$$\nu = 0.3, \rho_s = 2, \hat{L} = 5.10^{-3} \text{m}, L = 4.10^{-2} \text{m}$$
We obtain:

\[ \varepsilon_M = 0 \Rightarrow \psi_f (a) = \psi \forall a \in [0, 1] \]

and

\[ \varepsilon_A = \begin{cases} -0.045 \text{ under PS} \\ -0.037 \text{ under PD} \end{cases} \]

Figures 10.28 show the effect of the skewness parameter \( a \) on the value of \( (\psi - \psi_s (a)) \) for different angles \( \psi \) applied under plane stresses and plane deformations. The impact of the skewness is greater under PS than under PD (for instance \( (\psi - \psi_s (a)) = 1.7^\circ \) under PS; \( 0.2^\circ \) under PD for \( \psi = 15^\circ \)).

![Figure 10.28](image)

**Figure 10.28. Effect of the parameter \( a = \frac{i}{10}, i = 0, 1, 2, \ldots, 10 \) on the difference between \( \psi \) and \( \psi_s (a) \). Left: plane stress. Right: plane deformation**

The observation of the different curves (Figures 10.29 and 10.30) shows that the size and shape of the boundary curves is practically the same for the symmetry \( a = 0 \) as for the maximal dissymmetry \( a = 1 \).

Experimental tests, which remain tricky to execute, will be necessary in order to validate our calculations.
Figure 10.29. Zones of phase tranformation under conditions of plane deformations with $\psi = 60^\circ, 45^\circ, 30^\circ$

Figure 10.30. Zones of phase tranformation under conditions of plane stresses with $\psi = 60^\circ, 45^\circ, 30^\circ$
Chapter 11

General Conclusion

This book gives a fairly broad treatment of the thermomechanical behavior of SMAs, and to a lesser extent the magnetic part of MSMAs.

As usual, there are gaps in this coverage; for instance, the part devoted to the elaboration of these alloys, which is crucial as regards their long-term usage.

We shall divide this conclusion into two parts – one dealing with resolved problems and the other with unresolved problems, before going on to suggest a number of possible paths for the future.

11.1. Resolved problems

Nowadays in the existing body of literature, there is a fairly wide-ranging and fairly comprehensive range of models describing pseudo-elasticity, the shape-memory effect, taking account of internal loops, of the asymmetry between traction and compression, and of the saturation of phase transformation. The approaches are based either on micromechanics (these approaches are better adapted to the understanding of the physical mechanisms at work and the optimization of the transformation properties) or macroscopics (better adapted to finite element method calculations regarding structure).

This book, however, represents an attempt to explain martensitic transformation on the crystallographic scale, followed by a homogenization (see Chapter 3). A description of other approaches such as that of Preisach and statistical physics is given in Chapter 6. Finally, a phenomenological approach, on the macroscopic scale, brings the investigation to a close.
Some of these macroscopic models are formulated in finite transformations; most of them in the small strain hypothesis. A number of them have been implemented in finite element method computer coding (e.g. ABAQUS, MARC).

Models integrating the coupling between plasticity and phase transformation are also beginning to emerge, with different motivations (cyclical behavior, iron-based SMAs, high-temperature SMAs, the precipitates effect, etc.).

Examples of finite element-aided design of applications including SMA elements are beginning to come to light.

11.2. Unresolved problems

The modeling of the R phase (premartensite in NiTi) remains marginal. However, a specially designed $R_L$ model has been successfully used to express this reversible mechanical behavior [LEX 94] and calculate the recovering stress. As we have seen, this anhysteretic (i.e. without mechanical dissipation) premartensitic transformation is very useful for biomedical applications.

The validation of these models is based essentially on tests on wires or tubes with a “plateau-like” behavior for NiTi alloys, caused by localization of the transformation. It is therefore vital to have a more reliable database of experimental results on samples that do not exhibit localization. There has also hitherto been a lack of testing carried out on structures made of SMAs for the validation of the implantation in FEM computer codes, or at least on samples with heterogeneous stress or strains.

With the exception of a very early version of the Aurrichio model, describing only pseudo-elasticity and available as a standard on ABAQUS, no appropriate model has been advanced which could be adopted by a commercial FEM software package as an immovable reference point.

The effects of size and localization in wires or thin films warrants a more in-depth investigation.

SMAs other than NiTi and copper-based materials deserve more attention from the community of model-makers (e.g. iron-based SMAs, high temperature SMAs, etc.).

The attempts at collaboration with big industry, even those which have been successful, have unfortunately not opened the way to “mass” development of applications for SMAs.

At present, we are unable to offer a “made-to-measure SMA”, created to respond to a clear set of technical specifications, for a specific usage. For instance, what are we to say to an industrialist who wants an SMA with fairly high transformation...
temperatures, a rather large thickness of hysteresis and a considerably high recovering stress or strain?

In spite of the very significant potential applications in civil engineering (cables for bridge dampings, seismic monitoring of historic buildings in Italy), the dynamic and damping properties of SMAs have not been sufficiently well studied; the same is true of the internal heat source relating to the exothermic and endothermic nature of the direct and inverse transformations.

The command and control of structures made of SMAs should be able to bring together automation engineers (who sometimes use SMAs as a “black box”) and material mechanical engineers (who are supposed to bring “physics” to the table).

11.3. Suggestions for future directions

We need to take into account thermo-magneto-mechanical coupling, but also the coupling between phase transformation and plasticity (iron-based SMAs, porous SMAs, SMAs with precipitates, high-temperature SMAs).

It is essential to make certain models more convivial, with perhaps an instruction booklet (see Chapter 7)!

Ideas for the beneficial use of SMAs still need to be found. In parallel, we need to construct design-support tools, in order to create prototypes.
Appendix 1

Intrinsic Properties of Rotation Matrices
(see Chapter 3)

In Chapter 3, on the subject of “martensitic transformation”, we wish to show with:

\[
\begin{aligned}
R(\tilde{u},\delta \theta) &= R(\delta \tilde{u}, \theta) \\
R(\tilde{u},\delta \theta) - (R(\tilde{u},\delta \theta))^T &= 2\delta \sin(\theta) \mathbf{Q}_{\tilde{u}} \\
\forall \delta R, R \in \{-1,1\}
\end{aligned}
\]

that for any rotation \( R \), there is at least one couple \((\tilde{u}_R, \theta_R)\), such that:

\[
R = R(\tilde{u}_R, \delta R \theta_R) \text{ for a certain } \delta R \in \{-1,1\}
\]

where \( \tilde{u}_R \) denotes a unitary vector, such that:

\[
\begin{aligned}
R(\tilde{u},\delta \theta) &= R(\delta \tilde{u}, \theta) \\
R(\tilde{u},\delta \theta) - (R(\tilde{u},\delta \theta))^T &= 2\delta \sin(\theta) \mathbf{Q}_{\tilde{u}} \\
\forall \delta R, R \in \{-1,1\}
\end{aligned}
\]

\[
R\tilde{u}_R = \tilde{u}_R
\]

and \( \theta_R \) is the angle defined in \([0, \pi]\) by:

\[
\theta_R = \arccos(\kappa_R) \text{ with } \kappa_R = \frac{1}{2} (\text{tr}(R) - 1)
\]
A1.1. Characterization of rotations

For the purpose of defining what we mean by a rotation, let us first establish the following intermediary result $\mathbf{R, R}$. 

- Let $\mathbf{R}$ be a rotation and $j$ the complex number such that $j^2 = -1$. Thus, the set of eigenvalues of $\mathbf{R}$ is equal to the compound set of the values:

$$\lambda_3 = 1, \lambda_2 = \exp(-j\theta_R), \lambda_1 = \exp(j\theta_R)$$

where $\theta_R \in [0, \pi]$ is defined solely by:

$$\theta_R = \arccos(\kappa_R)$$

PROOF.– We know that $\varrho(A) \leq \sqrt{\varrho(A^T A)} \forall A$, where $\varrho(B)$ denotes the greatest modulus of the eigenvalues of a matrix $B$. Hence $\varrho(\mathbf{R}) \leq \sqrt{\varrho(\mathbf{R}^T \mathbf{R})} = 1$. In addition, the characteristic polynomial of $\mathbf{R}$, using the fact that $\mathbf{R} - \lambda \mathbf{I} = \text{cof}(\mathbf{A})$, has the explicit expression:

$$\text{det} (\mathbf{R} - \lambda \mathbf{I}) = (1 - \lambda) (\lambda^2 - 2\kappa \lambda + 1).$$

Lfi,0) Thus, the eigenvalues of $\mathbf{R}$ are $\lambda_3 = 1$ and the two roots $\lambda_2, \lambda_1$ of the equation $\lambda^2 - 2\kappa \lambda + 1 = 0$. However:

$$|\kappa_R| = \frac{1}{2} |(\lambda_1 + \lambda_2 + \lambda_3 - 1)| = \frac{1}{2} |\lambda_1 + \lambda_2| \leq \varrho(\mathbf{R}) \leq 1$$

so we can write:

$$\lambda_2 = \kappa_R - j\sqrt{1 - \kappa_R^2} = \exp(-j\theta_R), \lambda_1 = \kappa_R + j\sqrt{1 - \kappa_R^2} = \exp(j\theta_R)$$

Hereafter, $\mathbf{u}_R$ will be used to denote any unitary vector, such that:

$$\mathbf{R} \mathbf{u}_R = \mathbf{u}_R$$

- Consider a rotation $\mathbf{R}$. Thus:

$$\mathbf{R} = \mathbf{R} (\mathbf{u}_R, \delta_R \theta_R)$$

for $\delta_R$ such that:

$$\delta_R = 1 \text{ or } \delta_R = -1$$

PROOF.– Case $|\kappa_R| = 1$ (i.e. $\cos \theta_R = \kappa_R$ and $\sin \theta_R = 0$). The eigenvalues are all real, with:

$$\lambda_1 = \lambda_2 = \kappa_R \text{ and } \lambda_3 = 1$$
As the matrix $R$ is orthogonal, there is a direct orthonormal trihedron $(\hat{e}_1, \hat{e}_2, \hat{e}_3 = \hat{u}_R)$ formed of the eigenvectors of $R$. Hence, for any value of $x$, we can write that:

$$x = \alpha_1 \hat{e}_1 + \alpha_2 \hat{e}_2 + \alpha_3 \hat{e}_3$$

where $\alpha_i = x_\hat{e}_i$, $i = 1, 2, 3$

with:

$$\alpha_3 \hat{e}_3 = (x_\hat{e}_3) \hat{e}_3 = (\hat{e}_3 \odot \hat{e}_3) x = P_{\hat{u}_R} x$$

By applying $R$, we find:

$$\begin{align*}
Rx &= \alpha_1 \underbrace{R\hat{e}_1 + \alpha_2 R\hat{e}_2}_{\kappa_R \hat{e}_1} + \underbrace{\alpha_3 R\hat{e}_3}_{\kappa_R \hat{e}_3} \\
    &= \kappa_R \left( \alpha_1 \hat{e}_1 + \alpha_2 \hat{e}_2 \right) + \alpha_3 \hat{e}_3 \\
    &= \kappa_R \left( \alpha_1 \hat{e}_1 + \alpha_2 \hat{e}_2 \right) + \alpha_3 \hat{e}_3 \\
    &= \kappa_R \left( \frac{x - \alpha_3 \hat{e}_3}{\cos \theta_R} \right) + \alpha_3 \hat{e}_3 \\
    &= \kappa_R \left( \frac{x - \alpha_3 \hat{e}_3}{\cos \theta_R} \right) + \alpha_3 \hat{e}_3
\end{align*}$$

thus giving us the result.

Consider the case $|\kappa_R| \neq 1$ (therefore $\sin \theta_R \neq 0$). Let $\hat{e}_3 = \hat{u}_R$ and $(v_1, v_2)$ be a couple of vectors, such that:

$$\begin{align*}
\begin{cases}
Rv_1 &= \cos \theta_R v_1 - \sin \theta_R v_2 \\
Rv_2 &= \sin \theta_R v_1 + \cos \theta_R v_2
\end{cases}
\end{align*}$$

so that $v = v_1 + j v_2$ is an eigenvector associated with the eigenvalue $\lambda_1 = \exp (j \theta_R)$. An elementary calculation on the basis of the identities:

$$v_1 \cdot v_2 = (\cos \theta_R v_1 \cdot v_2) + (\sin \theta_R v_1 \cdot v_2)$$

shows that for any and every rotation $R$, there is at least one couple $(\hat{u}_R, \theta_R)$, such that:

$$R = R (\hat{u}_R, \delta_R \theta_R) \text{ for a certain } \delta_R \in \{-1, 1\}$$
Appendix 2

“Twinning Equation” Demonstration
(see Chapter 3)

A2.1. Question

Given two Bain matrices \( U_i \) and \( U_j \) (symmetrical and positive definite) corresponding to two martensite variants, is there a rotation \( Q \), a vector \( a \) and a unitary vector \( \hat{n} \) such that:

\[
QU_i - U_j = a \otimes \hat{n}
\]  \[A2.1\]

What conditions must be fulfilled in order for the plane interface \( M_i/M_j \) to exist?

Knowns: \( U_i \) and \( U_j \); unknowns: \( Q \), \( \hat{n} \) and \( a \).

A2.2. Solution

Convenient notation:

\[
a \otimes \hat{n} = a\hat{n}^T, \hat{n} \otimes a = \hat{n}a^T
\]

\[
QU_i - U_j = a\hat{n}^T
\]  \[A2.2\]

where:

\[
QU_i = U_j + a\hat{n}^T
\]  \[A2.3\]
Calculate $Q$ and then $Q^T$:

$$Q = U_j U_i^{-1} + a\tilde{n}^T U_i^{-1}$$

$$Q^T = U_i^{-1} U_j + U_i^{-1} \tilde{n} a^T$$ \[A2.4\]

followed by $Q^T Q$:

$$Q^T Q = U_i^{-1} U^2_i U_i^{-1} + U_i^{-1} U_j a\tilde{n}^T U_i^{-1} + U_i^{-1} \tilde{n} a^T U_j U_i^{-1} + U_i^{-1} \tilde{n} a^T a\tilde{n}^T U_i^{-1}$$ \[A2.5\]

$Q^T Q$ will be the identity matrix $1$ if:

$$1 = U_i^{-1} U^2_i U_i^{-1} + U_i^{-1} U_j a\tilde{n}^T U_i^{-1} + U_i^{-1} \tilde{n} a^T U_j U_i^{-1} + U_i^{-1} \tilde{n} a^T a\tilde{n}^T U_i^{-1}$$ \[A2.6\]

We multiply the right-hand side by $U_i$, then multiply the left-hand terms by $U_i$ as well, and we obtain:

$$U_i^2 = U_i^2 + U_j a\tilde{n}^T + \tilde{n} a^T U_j + \tilde{n} a^T a\tilde{n}^T$$ \[A2.7\]

$$U_i^2 = (U_j + \tilde{n} a^T)(U_j + a\tilde{n}^T)$$ \[A2.8\]

Calculate $C = U_i^{-1} U^2_i U_i^{-1}$ as suggested in the instructions for using the twinning equation.

We obtain:

$$C = (1 + b \otimes a)(1 + a \otimes b)$$ \[A2.9\]

by introducing the vector $b = U_j^{-1} \tilde{n} \neq 0$.

This symmetrical, positive definite matrix $C$ accepts $a \wedge b$ as an eigenvector, with the eigenvalue $\lambda_2 = 1$.

For convenience’s sake, we introduce the coefficients $\lambda'_i = \lambda_i - 1$, where obviously $\lambda_i$, $i = 1, 2, 3$ the eigenvalues of $C$.

Thus, we calculate:

$$tr(C - 1) = 2a^T b + (a^T a)(b^T b) = \lambda'_1 + \lambda'_3$$ \[A2.10\]
We can calculate the determinant of the $2 \times 2$ matrix named $C - 1$, in the plane perpendicular to $a \wedge b$ with a base $\vec{e}_1, \vec{e}_3$ such as $b = |b| \vec{e}_3$

Thus:

$$
\frac{C - 1}{|b|} = \begin{bmatrix} a^1 & 0 \\ a^3 & 1 \end{bmatrix} + \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} a^1 a^2 \\ |b| \end{bmatrix} + |b| a^2 \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}
$$

[A2.11]

$$
\frac{C - 1}{|b|} = \begin{bmatrix} 0 & a^1 \\ a^1 2a^3 + b \ |a|^2 \\ b \end{bmatrix}
$$

[A2.12]

where, evidently:

$$
\det (C - 1) = \lambda_1 \lambda_3 = (\lambda_1 - 1) (\lambda_3 - 1)
$$

[A2.13]

This determinant is negative, so we choose $\lambda_1 \leq 1$ and $\lambda_3 \geq 1$ where of course, $\lambda_2 = 1$.

Furthermore:

$$
a^1 = \sqrt{\frac{(1 - \lambda_1) (\lambda_3 - 1)}{|b|}}
$$

[A2.14]

We still need to find $\hat{n}, a, Q$, knowing that $U_i$ and $U_j$, i.e. the type of transformation, are given, which means that $\lambda_1$ and $\lambda_3$ are known.

Let us place ourselves in the not-insignificant case where $C \neq 1$.

Thus, equation [A2.9] is equivalent to:

$$
\begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_3 \end{bmatrix} = \begin{bmatrix} 1 + 2a_1 b_1 + a_1^2 |b|^2 & a_1 b_3 + b_1 a_3 + a_1 a_3 |b|^2 \\ a_1 b_3 + b_1 a_3 + a_1 a_3 |b|^2 & 1 + 2a_3 b_3 + a_3^2 |b|^2 \end{bmatrix}
$$

[A2.15]

An elementary calculation shows that:

$$
\lambda_1 \lambda_3 = (1 + a.b)^2 \Rightarrow 1 + a.b = \pm \frac{1}{\sqrt{\lambda_1 \lambda_3}}
$$

[A2.16]

and:

$$
\begin{bmatrix} \lambda_1 & 0 \\ 0 & \lambda_3 \end{bmatrix} \begin{bmatrix} b_1 \\ b_3 \end{bmatrix} = (1 + a.b) \begin{bmatrix} b_1 + a_1 |b|^2 \\ b_3 + a_3 |b|^2 \end{bmatrix}.
$$

[A2.17]
Hence:

\[
\begin{pmatrix}
  a_1 \\
  a_2
\end{pmatrix}
= \frac{1}{|b|^2} \begin{pmatrix}
  \kappa \frac{1}{\sqrt{\lambda_1 \lambda_3}} (\lambda_1 - 1) b_1 \\
  \kappa \frac{1}{\sqrt{\lambda_1 \lambda_3}} (\lambda_3 - 1) b_3
\end{pmatrix}
\]  \quad \text{with } \kappa = \pm 1  \quad [A2.18]

By substitution of \( a_1 \) and \( a_2 \) into equation [A2.15], we get:

\[
\begin{pmatrix}
  \lambda_1 - 1 & 0 \\
  0 & \lambda_3 - 1
\end{pmatrix}
= \frac{1}{|b|^2} \begin{pmatrix}
  \frac{\lambda_1 - \lambda_3}{\lambda_3} b_1^2 & 0 \\
  0 & \frac{\lambda_3 - \lambda_1}{\lambda_1} b_3^2
\end{pmatrix}
\]  \quad [A2.19]

so:

\[
b = \rho \left( \sqrt{\frac{\lambda_3(1 - \lambda_1)}{\lambda_3 - \lambda_1}} \hat{e}_1 + \sqrt{\frac{\lambda_1(\lambda_3 - 1)}{\lambda_3 - \lambda_1}} \hat{e}_3 \right)
\]  \quad [A2.20]

and by inserting the \( b_i \) values from equation [A2.20] into equation [A2.18] we obtain the \( a_i \) values:

\[
\begin{pmatrix}
  a_1 \\
  a_2
\end{pmatrix}
= \frac{1}{\rho} \begin{pmatrix}
  \kappa \frac{1}{\sqrt{\lambda_1 \lambda_3}} (\lambda_1 - 1) \sqrt{\frac{\lambda_3(1 - \lambda_1)}{\lambda_3 - \lambda_1}} \\
  \kappa \frac{1}{\sqrt{\lambda_1 \lambda_3}} (\lambda_3 - 1) \sqrt{\frac{\lambda_1(\lambda_3 - 1)}{\lambda_3 - \lambda_1}}
\end{pmatrix}
\]  \quad [A2.21]

Note that in the calculation, we have taken \( b \) for \( a \); thus, \( \hat{n} \) becomes the standardized value of the new \( a \) given in expression [A2.21].

\( Q \) can be obtained using equation [A2.4].
Appendix 3

Calculation of the Parameters $a$, $n$ and $Q$ from the “Twinning” Equation (see Chapter 3)

A3.1. Problem

Consider $\alpha$ and $\beta$, such that:

$$\alpha \beta \neq 0; |\alpha| > |\beta|$$

We set:

$$Q = \begin{pmatrix} \cos \theta & -\sin \theta & 0 \\ \sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix}; \quad U_1 = \begin{pmatrix} \beta & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \alpha \end{pmatrix}; \quad U_2 = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & \alpha \end{pmatrix}; \quad \hat{n} = \begin{pmatrix} n_1 \\ n_2 \\ n_3 \end{pmatrix}, |\hat{n}| = 1$$

The problem is to find $\hat{n}$, $a$ and $Q$ (on the basis of the demonstration of the twinning equation).

A3.2. Statement

Given two Bain matrices $U_i$ and $U_j$ (symmetrical and positive definite) corresponding to two martensite variants, is there a rotation $Q$, a vector $a$ and a unitary vector $\hat{n}$ such that:

$$Q U_i - U_j = a \otimes \hat{n} \quad \text{[A3.1]}$$
What conditions must be fulfilled in order for the plane interface \( M_i/M_j \) to exist?

**Knowns:** \( U_i \) and \( U_j \); unknowns: \( Q, \hat{n} \) and \( a \).

**Solution:**

Convenient notation

\[
a \otimes \hat{n} = a\hat{n}^T, \hat{n} \otimes a = \hat{n}a^T
\]

\[
QU_i - U_j = a\hat{n}^T \tag{A3.2}
\]

or:

\[
QU_i = U_j + a\hat{n}^T \tag{A3.3}
\]

Calculate \( Q \) and then \( Q^T (\alpha \text{ and } \beta) \) in the knowledge that:

\[
QU_1 - U_2 = a \otimes \hat{n}. \tag{A3.4}
\]

**A3.3. Solution**

\( \alpha \beta \neq 0 \), so (A3.4) is equivalent to:

\[
Q = (U_2 + a \otimes \hat{n}) U_1^{-1}
\]

\[
= \begin{pmatrix}
\frac{\alpha}{\beta} + \frac{1}{\beta}a_1n_1 & \frac{1}{\alpha}a_1n_2 & \frac{1}{\alpha}a_1n_3 \\
\frac{1}{\beta}a_2n_1 & \frac{1}{\alpha} - \frac{1}{\beta} + \frac{1}{\alpha}a_2n_2 & \frac{1}{\alpha}a_2n_3 \\
\frac{1}{\beta}a_3n_1 & \frac{1}{\alpha}a_3n_2 & \frac{1}{\alpha}a_3n_3 + 1
\end{pmatrix}
\]

In view of the expression of \( Q \), we have a demonstration of the twinning equation.

**Statement:** given two Bain matrices \( U_i \) and \( U_j \) (symmetrical and positive definite) corresponding to two martensite variants, is there a rotation \( Q \), a vector \( a \) and a unitary vector \( \hat{n} \) such that:

\[
QU_i - U_j = a \otimes \hat{n} \tag{A3.5}
\]
Calculation of the Parameters $a$, $n$ and $Q$

What conditions must be fulfilled in order for the plane interface $M_i/M_j$ to exist?

**Knowns:** $U_i$ and $U_j$; unknowns: $Q, \hat{n}$ and $a$.

**Solution:**

Convenient notation:

$$a \otimes \hat{n} = an^T, \hat{n} \otimes a = \hat{n}a^T$$

$$QU_i - U_j = an^T \quad [A3.6]$$

or:

$$QU_i = U_j + an^T \quad [A3.7]$$

Calculate $Q$ and then $Q^T$:

$$\begin{cases}
a_1 n_3 = a_2 n_3 = a_3 n_2 = a_3 n_1 = 0 \\
\frac{1}{\alpha} a_3 n_3 + 1 = 1 \\
\frac{1}{\beta} a_1 n_1 = \frac{1}{\alpha} \beta + \frac{1}{\alpha} a_2 n_2 = \cos \theta \\
\frac{1}{\beta} a_2 n_1 = -\frac{1}{\alpha} a_1 n_2 = \sin \theta
\end{cases}$$

This is equivalent to:

$$a_3 n_3 = 0 \quad \text{and} \quad \begin{cases}
a_1 n_3 = a_2 n_3 = 0 \\
\frac{1}{\alpha} \beta a_1 n_1 = \frac{1}{\alpha} \beta + \frac{1}{\alpha} a_2 n_2 = \cos \theta \\
\frac{1}{\beta} a_2 n_1 = -\frac{1}{\alpha} a_1 n_2 = \sin \theta
\end{cases} \quad [A3.8]$$

The case of $n_3 \neq 0$ is absurd, because:

$$(A3.8) \Leftrightarrow \begin{cases}
a_1 = a_2 = 0 \\
\frac{\alpha}{\beta} = \frac{\beta}{\alpha} = \cos \theta \Rightarrow |\alpha| = |\beta| \\
0 = \sin \theta
\end{cases}$$
Hence, necessarily, \( n_3 = 0 \) and:

\[
\begin{aligned}
\frac{\alpha}{\beta} + \frac{1}{\beta} a_1 n_1 &= \frac{1}{\alpha} \beta + \frac{1}{\alpha} a_2 n_2 = \cos \theta \\
\frac{1}{\beta} a_2 n_1 &= -\frac{1}{\alpha} a_1 n_2 = \sin \theta 
\end{aligned}
\]

This gives us:

\[
\begin{pmatrix}
\alpha_1 \\
\alpha_2 
\end{pmatrix} = \begin{pmatrix}
n_1 \\
\beta n_2 \\
\alpha \frac{n_1}{\beta} 
\end{pmatrix}^{-1} \begin{pmatrix}
\frac{\beta}{\alpha} - \frac{\alpha}{\beta} \\
0
\end{pmatrix} = \frac{\alpha^2 - \beta^2}{\alpha^2 n_1^2 + \beta^2 n_2^2} \begin{pmatrix}
(n_1 n_2 + \beta n_2) \\
(n_1 n_2 + \beta n_2)
\end{pmatrix} > 0 \\
\]

Thus:

\[
\begin{pmatrix}
\cos \theta \\
\sin \theta 
\end{pmatrix} = \frac{2}{\alpha^2 + \beta^2} \begin{pmatrix}
\alpha \beta \\
(n_1 n_2 - \beta^2)
\end{pmatrix}
\]

However:

\[
\{ \cos^2 \theta + \sin^2 \theta = 1 \text{ and } n_1^2 + n_2^2 = 1 \} \\
\Rightarrow \left( \frac{\alpha^2 - \beta^2}{>0} \right) (2n_1^2 - 1) \left( (\alpha^2 - \beta^2) n_1^2 + \beta^2 \right) = 0
\]

which implies:

\[
n_1^2 = \frac{1}{2} \text{ and subsequently } n_2^2 = \frac{1}{2}
\]

This gives us the following four possible cases, where \( a_3 \) can assume any arbitrary value.

\[
\begin{pmatrix}
\cos \theta \\
\sin \theta 
\end{pmatrix} = \begin{pmatrix}
\frac{\alpha}{\beta} + \frac{1}{\beta} a_1 n_1 = \frac{\alpha}{\beta} - \alpha n_1 \frac{\alpha^2 - \beta^2}{\alpha^2 n_1^2 + \beta^2 n_2^2} n_1 = \frac{\alpha}{\alpha^2 n_1^2 + \beta^2 n_2^2} \\
\frac{1}{\beta} a_2 n_1 = \frac{1}{\beta} \frac{(\alpha^2 - \beta^2)}{\alpha^2 n_1^2 + \beta^2 n_2^2} \beta n_2 n_1 = \frac{\alpha^2 - \beta^2}{\alpha^2 n_1^2 + \beta^2 n_2^2} n_2 n_1
\end{pmatrix}
\]
A3.3.1. Case 1

\[ \hat{n} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \Rightarrow \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} 2 \left( \alpha^2 - \beta^2 \right) \\ -\alpha n_1 \\ \beta n_2 \end{pmatrix} = \frac{\sqrt{2} \left( \alpha^2 - \beta^2 \right)}{\alpha^2 + \beta^2} \begin{pmatrix} -\alpha \\ \beta \end{pmatrix} \]

\[ \Rightarrow \begin{pmatrix} \cos \theta \\ \sin \theta \end{pmatrix} = \frac{2}{\alpha^2 + \beta^2} \begin{pmatrix} \alpha \beta \\ \frac{\alpha n_2 (\alpha^2 - \beta^2)}{2} \end{pmatrix} \]

\[ \alpha = 1.0188; \beta = 0.9589 \]

\[ \begin{pmatrix} \cos \theta \\ \sin \theta \end{pmatrix} = \frac{2}{(1.0188)^2 + (0.9589)^2} \begin{pmatrix} 1.0188 \times 0.9589 \\ \frac{1}{2} \left( (1.0188)^2 - (0.9589)^2 \right) \end{pmatrix} = \frac{0.99817}{6.0520 \times 10^{-2}} \]

\[ \theta = \arctan \left( \frac{6.0520 \times 10^{-2}}{0.99817} \right) = 6.055 \times 10^{-2} \]

\[ \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \sqrt{2} \begin{pmatrix} (1.0188)^2 - (0.9589)^2 \\ 0.9589 \end{pmatrix} \begin{pmatrix} -1.0188 \\ 0.08207 \end{pmatrix} \]

A3.3.2. Case 2

\[ \hat{n} = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix} \Rightarrow \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} 2 \left( \alpha^2 - \beta^2 \right) \\ -\alpha n_1 \\ \beta n_2 \end{pmatrix} = \frac{\sqrt{2} \left( \alpha^2 - \beta^2 \right)}{\alpha^2 + \beta^2} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \]

\[ \Rightarrow \begin{pmatrix} \cos \theta \\ \sin \theta \end{pmatrix} = \frac{2}{\alpha^2 + \beta^2} \begin{pmatrix} \alpha \beta \\ \frac{\alpha n_2 (\alpha^2 - \beta^2)}{2} \end{pmatrix} \]

A3.3.3. Case 3

\[ \hat{n} = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ -1 \\ 0 \end{pmatrix} \Rightarrow \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} = \begin{pmatrix} 2 \left( \alpha^2 - \beta^2 \right) \\ -\alpha n_1 \\ \beta n_2 \end{pmatrix} = \frac{\sqrt{2} \left( \alpha^2 - \beta^2 \right)}{\alpha^2 + \beta^2} \begin{pmatrix} \alpha \\ -\beta \end{pmatrix} \]

\[ \Rightarrow \begin{pmatrix} \cos \theta \\ \sin \theta \end{pmatrix} = \frac{2}{\alpha^2 + \beta^2} \begin{pmatrix} \alpha \beta \\ \frac{\alpha n_2 (\alpha^2 - \beta^2)}{2} \end{pmatrix} \]
A3.3.4. Case 4

\[ \hat{\mathbf{n}} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} \Rightarrow \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = \frac{2 (\alpha^2 - \beta^2)}{\alpha^2 + \beta^2} \begin{pmatrix} -\alpha n_1 \\ \beta n_2 \end{pmatrix} = -\sqrt{2} \frac{(\alpha^2 - \beta^2)}{\alpha^2 + \beta^2} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} \]

\[ \Rightarrow \begin{pmatrix} \cos \theta \\ \sin \theta \end{pmatrix} = \frac{2}{\alpha^2 + \beta^2} \begin{pmatrix} \alpha n_1 n_2 (\alpha^2 - \beta^2) \\ -\frac{1}{2} \end{pmatrix} \]
Appendix 4

“Twinned” Austenite/Martensite Equation
(see Chapter 3)

A4.1. Proposition 1

Let \( U_0 = U_0^T \) be a \( 3 \times 3 \) non-singular matrix such that:

\[
RU_0\hat{R} = U_0 + a \otimes n
\]  \hspace{1cm} \text{[A4.1]}

where \( R, \hat{R} \) are rotations \( a \neq 0 \) and \( |n| = 1 \), which are solutions to the twinning equation [A4.1].

Consider:

\[
C_0(\lambda) = (U_0 + \lambda a \otimes n)(U_0 + \lambda n \otimes a)
\]  \hspace{1cm} \text{[A4.2]}

and also:

\[
g(\lambda) = \det(C_0(\lambda) - 1).
\]  \hspace{1cm} \text{[A4.3]}

Thus, \( g(\lambda) \) is a quadratic function of \( \lambda \), which satisfies \( g(\lambda) = g(1 - \lambda) \).

Demonstration in the publication by Ball and James [BAL 87].

A4.2. Proposition 2

Suppose that for a value of \( \lambda \), \( C_0(\lambda) \) with three eigenvalues \( 1, \lambda_1, \lambda_3 \), then:

\[
(1 - \lambda_1) (\lambda_3 - 1) = \text{tr}U_0^2 - \det U_0^2 - 2 + (\lambda^2 - \lambda) |a|^2
\]  \hspace{1cm} \text{[A4.4]}
A triplet \( \{\tilde{R}, \lambda, b \otimes m\} \) consisting of a rotation \( \tilde{R} \), a scalar \( \lambda \in [0, 1] \) and a rank 1 matrix: \( b \otimes m \) such that:

\[
U_0 + \lambda a \otimes n = \tilde{R}^T (1 + b \otimes m) \tag{A4.5}
\]

will be a solution to equation \([A4.5]\).

**A4.3. Theorem**

Let \( U_0 \) be a symmetrical, positive definite matrix satisfying the twinning equation \([A4.1]\):

\[
RU_0 \tilde{R} = U_0 + a \otimes n \tag{A4.6}
\]

for some pairs of rotation matrix \( R, \tilde{R} \) and vectors \( a \neq 0 \) and \( |n| = 1 \).

1. Assume that \( U_0 \) has no eigenvalue equal to 1, a necessary and sufficient condition for equation \([A4.5]\) to have a solution is:

\[
1 + \frac{1}{2} \delta^* \leq 0 \tag{A4.7}
\]

and that:

\[
tr U_0^2 - det U_0^2 - 2 + \frac{1}{2\delta^*} |a|^2 \geq 0 \tag{A4.8}
\]

where:

\[
\delta^* = a U_0 (U_0^2 - 1)^{-1} n \tag{A4.9}
\]

If, in addition:

\[
1 + \frac{1}{2} \delta^* < 0 \tag{A4.10}
\]

when the strict inequality lies in equation \([A4.8]\), there are exactly four distinct solutions to equation \([A4.5]\), which take the form:

\[
\begin{align*}
\{\tilde{R}_1, \lambda^*, b_1^+ \otimes m_1^+\} \\
\{\tilde{R}_2, \lambda^*, b_1^- \otimes m_1^-\} \\
\{\tilde{R}_3, 1-\lambda^*, b_2^+ \otimes m_2^+\} \\
\{\tilde{R}_4, 1-\lambda^*, b_2^- \otimes m_2^-\}
\end{align*}
\]
where:

\[
\lambda^* = \frac{1}{2} \left( 1 - \sqrt{1 + \frac{2}{\delta^*}} \right),
\]  

[A4.12]

so 0 < \lambda^* < 1/2.

Without going into too great an amount of detail, the above offers some elements of comprehension on the procedure of calculation used for the “twinning austenite/martensite” microstructure.
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