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Modélisation du Comportement Thermomécanique des Couches Minces en Alliages à Mémoire de Forme

(Modeling of the Thermomechanical Behavior of Shape
Memory Alloys Thin Layers)

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DEDICATION

This work is dedicated to those who believed in me long before I
believed in
myself.

To my parents, whose quiet strength, unwavering patience, and
countless
sacrifices built the path I walk today. Your faith has been my compass in
moments of doubt.

To my family and loved ones, who stood beside me with kindness,
understanding, and encouragement, turning challenges into
possibilities.

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this
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ABSTRACT

Shape memory alloys (SMAs) are functional materials widely used in actuation and adaptive applications due to their ability to undergo reversible phase transformations under mechanical and thermal loading. When employed in the form of thin layers, their thermomechanical behavior is strongly influenced by geometric constraints and loading conditions, which can significantly affect functional performance. Accurate prediction of this behavior therefore requires dedicated and reliable numerical modeling approaches.

The main objective of this thesis is to develop a reliable numerical framework capable of predicting the thermomechanical behavior of shape memory alloy thin layers subjected to mechanical and thermal loading. Such structures are increasingly used in microactuators, MEMS, and adaptive systems, where accurate prediction of their response is essential for design, optimization, and performance assessment.

This thesis presents a numerical model for the analysis of the thermomechanical behavior of shape memory alloy thin layers. A thermodynamically consistent constitutive model is developed to describe stress-induced pseudoelasticity and thermally driven shape memory effects, with phase transformation mechanisms captured through the evolution of internal variables.

The constitutive model is first implemented in independent numerical environments using MATLAB and Python. These implementations provide a controlled and flexible numerical approach for analyzing the model, analyzing its physical response, and performing standalone simulations without reliance on commercial finite element software. This stage enables an efficient investigation of representative loading paths and facilitates physical interpretation of the material behavior.

The numerically verified model is then implemented as a user material subroutine (UMAT) and integrated into the finite element software Abaqus. Two-dimensional plane stress simulations are performed to investigate the response of SMA thin layers under mechanical and thermomechanical loading conditions. Particular attention is given to biaxial pseudoelastic loading and thermoelastic actuation under mechanical constraint.

The numerical results using developed algorithms were in a good agreement with experimental data available in literature. Also the numerical simulation using UMAT of Abaqus, in one dimensional case, gave good results compared to experimental data, validating and confirming the reliability of the developed model.

Overall, this work delivers a computational model that can be used as a predictive tool for the analysis and design of shape memory alloy thin layers subjected to thermomechanical loading.

Keywords: Shape Memory Alloys; Thin Layers; UMAT; Finite Element Method; Thermoelasticity.

RÉSUMÉ

Les alliages à mémoire de forme (AMF) sont des matériaux fonctionnels largement utilisés dans les applications d'actionnement et de structures adaptatives, en raison de leur capacité à subir des transformations de phase réversibles sous sollicitations mécaniques et thermiques. Lorsqu'ils sont employés sous forme de couches minces, leur comportement thermomécanique est fortement influencé par les contraintes géométriques et les conditions de chargement, ce qui peut affecter de manière significative leurs performances fonctionnelles. La prédiction fiable de ce comportement nécessite donc des approches de modélisation numérique dédiées et robustes.

L'objectif principal de cette thèse est de développer un cadre numérique fiable pour prédire le comportement thermomécanique des couches minces en alliages à mémoire de forme soumises à des sollicitations mécaniques et thermiques. Ces structures sont largement utilisées dans les micro-actionneurs, les MEMS et les systèmes adaptatifs, où une prédiction précise de leur réponse est essentielle pour la conception et l'optimisation.

Cette thèse présente un cadre numérique pour l'analyse du comportement thermomécanique de couches minces en alliages à mémoire de forme. Un modèle constitutif thermodynamiquement cohérent est développé afin de décrire la pseudoélasticité induite par les contraintes mécaniques ainsi que les effets de mémoire de forme activés thermiquement, en tenant compte des mécanismes de transformation de phase à travers l'évolution de variables internes.

Le modèle constitutif est d'abord implémenté dans des environnements numériques indépendants utilisant MATLAB et Python. Ces implémentations offrent un cadre contrôlé et flexible permettant la vérification numérique du modèle, l'analyse de sa réponse physique et la réalisation de simulations autonomes sans recours à des logiciels commerciaux de calcul par éléments finis. Cette étape permet une étude efficace de trajectoires de chargement représentatives et facilite l'interprétation physique du comportement du matériau.

Le modèle numériquement vérifié est ensuite implémenté sous forme de sous-programme utilisateur (UMAT) et intégré au logiciel de calcul par éléments finis Abaqus. Des simulations bidimensionnelles en état de contrainte plane sont réalisées afin d'étudier la réponse des couches minces en AMF sous chargements mécaniques et thermomécaniques. Une attention particulière est portée aux chargements pseudoélastiques biaxiaux ainsi qu'à l'actionnement thermoélastique sous contrainte mécanique.

Les résultats numériques obtenus grâce aux algorithmes développés concordent bien avec les données expérimentales disponibles dans la littérature. De même, la simulation numérique réalisée avec UMAT d'Abaqus, dans le cas unidimensionnel, a fourni de bons résultats en comparaison avec les données expérimentales, validant et confirmant la fiabilité du modèle développé.

Dans l'ensemble, ce travail aboutit à un cadre de calcul numériquement vérifié et polyvalent, pouvant servir d'outil prédictif pour l'analyse et la conception de couches minces en alliages à mémoire de forme soumises à des sollicitations thermomécaniques.

Mots Clés: Alliages à mémoire de forme ; Couches minces ; UMAT ; Méthode des éléments finis ; Thermoélasticité.

الملخص

تُعدّ السبائك ذات الذاكرة الشكلية من المواد الوظيفية واسعة الاستخدام في تطبيقات التشغيل والأنظمة التكيفية، وذلك بفضل قدرتها على الخضوع لتحويلات طورية قابلة للعكس تحت تأثير الأحمال الميكانيكية والحرارية. وعند استخدامها على شكل طبقات رقيقة، يتأثر سلوكها الترمو-ميكانيكي بشكل كبير بالقيود الهندسية وشروط التحميل، مما قد يؤثر بصورة مباشرة على أدائها الوظيفي. لذلك فإن التنبؤ الدقيق بهذا السلوك يتطلب اعتماد نماذج عددية مخصصة وموثوقة.

يتمثل الهدف الرئيسي لهذه الأطروحة في تطوير إطار عددي موثوق قادر على التنبؤ بالسلوك الترمو-ميكانيكي للطبقات الرقيقة المصنوعة من السبائك ذات الذاكرة الشكلية والخاضعة لأحمال ميكانيكية وحرارية. وتزداد أهمية هذه البنى في تطبيقات المشغلات الدقيقة (Microactuators) وأنظمة MEMS والأنظمة التكيفية، حيث يُعدّ التنبؤ الدقيق باستجابتها أمرًا أساسيًا لتحقيق التصميم الأمثل وتقييم الأداء.

تقدم هذه الأطروحة إطارًا عدديًا لدراسة السلوك الترمو-الميكانيكي للطبقات الرقيقة المصنوعة من السبائك ذات الذاكرة الشكلية. وقد تم تطوير نموذج سلوكي متسق ترموديناميكياً لوصف كلٍّ من السلوك شبه المرن الناتج عن التحميل الميكانيكي وتأثيرات الذاكرة الشكلية المحفزة حراريًا، مع أخذ آليات التحول الطوري بعين الاعتبار من خلال تطور المتغيرات الداخلية.

في المرحلة الأولى، تم تنفيذ النموذج السلوكي في بيئات عددية مستقلة باستخدام برنامجي MATLAB و Python، حيث وُفّرت هذه البيئات إطارًا مرناً ومضبوطاً للتحقق العددي من النموذج، وتحليل استجابته الفيزيائية، وإجراء محاكاة مستقلة دون الاعتماد على برامج العناصر المحدودة التجارية. وقد أتاح ذلك دراسة فعالة لمسارات تحميل ممثلة، إلى جانب تقديم تفسير فيزيائي أوضح لسلوك المادة.

بعد التحقق العددي، تم تنفيذ النموذج على شكل روتين مادة مستخدم (UMAT) ودمجه ضمن برنامج العناصر المحدودة Abaqus. وقد أُجريت محاكاة ثنائية الأبعاد بافتراض حالة الإجهاد المستوي لدراسة استجابة الطبقات الرقيقة من السبائك ذات الذاكرة الشكلية تحت الأحمال الميكانيكية والترموميكانيكية، مع التركيز بشكل خاص على التحميل شبه المرن ثنائي المحور وعلى التشغيل الترمو-مرن تحت قيود ميكانيكية.

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كلمات مفتاحية: السبائك ذات الذاكرة الشكلية، الطبقات الرقيقة، UMAT، طريقة العناصر المحدودة، السلوك الترمو-ميكانيكي.

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NOMENCLATURE

Symbol	Description	Unit
Roman Symbols		
A_s, A_f	Austenite Start and Finish Temperatures	°C or K
M_s, M_f	Martensite Start and Finish Temperatures	°C or K
E_a, E_m	Young's Modulus of Austenite and Martensite	MPa
C	Clausius–Clapeyron coefficient	MPa/K
H	Transformation hardening modulus	MPa
G	Gibbs Free Energy	J/m ³
Ψ	Helmholtz free energy density	J/m ³
F_{ext}	Global External Force Vector	N
K	Global Stiffness Matrix	N/m
U	Global Nodal Displacement Vector	m
T	Temperature	°C or K
t	Time	s
Δt	Time increment	s
Greek Symbols		
f	Martensite Volume Fraction	—
ε	Total Strain Tensor	—
ε^e	Elastic Strain Tensor	—
ε^m	Martensitic Strain Tensor	—
ε_{tr}	Transformation Strain Tensor	—
ε_L	Maximum Transformation Strain	—
ν	Poisson's Ratio	—
σ	Cauchy Stress Tensor	MPa
σ_{eq}	Equivalent (Von Mises) Stress	MPa
σ_{bias}	Bias Stress (Constant Applied Load)	MPa
σ_{cr}	Critical Stresses for Start/Finish	MPa
Φ	Transformation Function (Yield Surface)	—
Abbreviations		
<i>AM</i>	Additive Manufacturing	—
<i>CVD</i>	Chemical Vapor Deposition	—
<i>FEM</i>	Finite Element Method	—
<i>MEMS</i>	Micro-Electro-Mechanical Systems	—
<i>OWSME</i>	One-Way Shape Memory Effect	—
<i>PVD</i>	Physical Vapor Deposition	—
<i>RMA</i>	Return Mapping Algorithm	—
<i>SMA</i>	Shape Memory Alloy	—
<i>SME</i>	Shape Memory Effect	—
<i>TWSME</i>	Two-Way Shape Memory Effect	—
<i>UMAT</i>	User Material Subroutine (Abaqus)	—

GENERAL INTRODUCTION

GENERAL INTRODUCTION

Thin layers have become an essential component in many modern engineering systems due to their ability to provide functional properties while maintaining compact geometries and reduced material usage. By exploiting reduced thickness, thin layers enable lightweight designs, efficient energy transfer, and enhanced surface-related performance. As a result, they are widely used in applications where size, weight, and functional efficiency are critical factors [1].

When materials are employed in the form of thin layers, their mechanical and thermomechanical behavior may differ significantly from that observed in conventional structural configurations. Geometric constraints, reduced thickness, residual stresses, and specific boundary conditions often lead to complex stress states that strongly influence the overall response. Consequently, thin layers require dedicated analysis approaches that account for their particular geometry, interface effects, and loading conditions [2].

Among functional materials, Shape Memory Alloys (SMAs) are of special interest due to their unique thermomechanical characteristics. SMAs can undergo reversible solid-state phase transformations between austenite and martensite phases, giving rise to two remarkable effects: pseudoelasticity, characterized by large recoverable strains under mechanical loading, and the shape memory effect, in which deformation recovery is driven by temperature variations under mechanical constraint. These properties allow SMAs to generate significant actuation forces and reversible deformations, making them attractive for adaptive and responsive engineering systems [3, 4].

The combination of thin layer technology with shape memory alloys has opened new perspectives for the development of compact and efficient functional devices. When SMAs are used as thin layers, their response is governed not only by intrinsic material behavior but also by geometric constraints, substrate interaction, and thermomechanical coupling effects. This interaction plays a crucial role in phase transformation mechanisms, stress distribution, and overall functional performance. Understanding these effects is essential for the reliable design and optimization of SMA-based thin-layer systems, particularly in microactuators, MEMS, and biomedical microdevices [5–7].

Despite the important progress made in the modeling of shape memory alloys, predicting the thermomechanical behavior of SMA thin layers remains a difficult task. This difficulty is

mainly related to the interaction between phase transformation mechanisms, the small thickness of the layer, mechanical constraints, and the applied loading conditions. For this reason, developing reliable numerical tools is necessary to better understand the response of these structures and to support the design and optimization of miniaturized devices such as microactuators, MEMS, and adaptive microsystems [4, 6, 7].

Numerical modeling provides an effective approach for analyzing the complex behavior of SMA thin layers. Finite element methods, in particular, allow the investigation of coupled thermomechanical responses under controlled loading paths and boundary conditions. For thin-layer configurations, two-dimensional modeling under plane stress assumptions offers a relevant and efficient representation of the physical behavior while maintaining reasonable computational cost [2, 4].

The objective of this thesis is to develop and apply a numerical model dedicated to the analysis of shape memory alloy thin layers subjected to thermomechanical loading. The proposed approach relies on a two-dimensional finite element formulation combined with a user material subroutine, enabling an accurate description of phase transformation mechanisms and the evolution of internal variables. Pseudoelastic and thermoelastic responses are investigated through representative numerical simulations to ensure physical and numerical consistency.

This thesis is organized as follows. Chapter 1 introduces the general context of thin layers and highlights their importance and applications. Chapter 2 is dedicated to the fundamental thermomechanical behavior of shape memory alloys. Chapter 3 presents the constitutive model describing the response of SMAs. Chapter 4 details the numerical implementation and verification of the proposed model. Finally, Chapter 5 focuses on two-dimensional finite element simulations to investigate pseudoelastic and thermoelastic behaviors of SMA thin layers under controlled loading conditions, with emphasis on physical interpretation and numerical consistency.

References

- [1] M. Ohring, *Materials Science of Thin Films: Deposition and Structure*, 2nd ed.; Academic Press: San Diego, CA, USA, 2002.
- [2] L. B. Freund and S. Suresh, *Thin Film Materials: Stress, Defect Formation and Surface Evolution*; Cambridge University Press: Cambridge, UK, 2003.
- [3] K. Otsuka and C. M. Wayman, Eds., *Shape Memory Materials*; Cambridge University Press: Cambridge, UK, 1998.
- [4] D. C. Lagoudas, Ed., *Shape Memory Alloys: Modeling and Engineering Applications*; Springer: New York, NY, USA, 2008. doi: 10.1007/978-0-387-47685-8.
- [5] M. A. Zainal, S. Sahlan, and M. S. M. Ali, “Micromachined shape-memory-alloy microactuators and their application in biomedical devices,” *Micromachines*, vol. 6, no. 7, pp. 879–901, 2015. doi: 10.3390/mi6070879.
- [6] N. Choudhary and D. Kaur, “Shape memory alloy thin films and heterostructures for MEMS applications: A review,” *Sensors and Actuators A: Physical*, vol. 242, pp. 162–181, 2016. doi: 10.1016/j.sna.2016.02.026.
- [7] I. Stachiv, E. Alarcon, and M. Lamac, “Shape memory alloys and polymers for MEMS/NEMS applications: Review on recent findings and challenges in design, preparation, and characterization,” *Metals*, vol. 11, no. 3, p. 415, 2021. doi: 10.3390/met11030415.

CHAPTER I
A BIBLIOGRAPHIC OVERVIEW
OF THIN LAYERS

I.1 Introduction

Thin layers are formally defined as films of material with thicknesses in the range of nanometers to a few micrometers, which are deposited onto a substrate material. The primary purpose of depositing such layers is to achieve specific functionalities, such as providing a protective coating against environmental degradation, creating a decorative finish, or strategically modifying the electrical, optical, and mechanical properties of the substrate. A thin layer may be composed of a single layer or, more complexly, a multilayer stack designed to achieve enhanced performance. Despite their minimal volume, these layers can fundamentally alter the surface characteristics of the underlying material (Fig. I.1). [1-4].

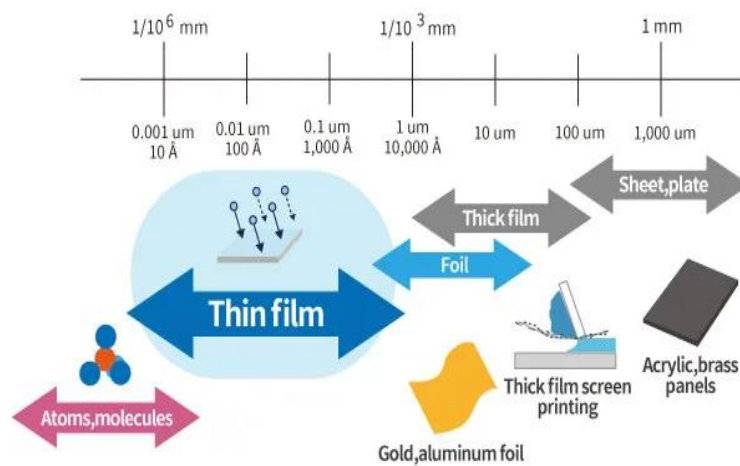


Figure I.1. Thickness Range of Thin Layers [5].

I.2 Types and Classifications

Thin layers are categorized based on several key criteria. A primary classification distinguishes between inorganic thin layers, such as metals, oxides, and semiconductors, and organic thin layers, which include polymer and molecular layers [6, 7]. They are also commonly categorized by their atomic structure (crystalline, polycrystalline, or amorphous) and by their thickness scale. Within materials science, a critical distinction is made between ultrathin layers, which may be only a few atomic layers thick, and thicker layers that begin to exhibit bulk material properties, as layer thickness profoundly influences a material's characteristics [8]. A further major classification is based on the deposition method, broadly divided into physical and chemical techniques [9]. It is noteworthy that regardless of their type, the majority of thin layers are fabricated using vacuum-based processes to ensure high purity and controlled growth conditions [10].

I.3 Applications of Thin Layers

Thin layers are a cornerstone of modern technology, with ubiquitous applications across numerous industries due to their ability to tailor surface and interface properties. Key application areas include (Fig. I.2):

- **Electronics and Semiconductors:** Thin layers form the fundamental building blocks of integrated circuits and microelectronic devices. Nanometer-scale dielectric and conductive layers are essential for creating transistors, resistors, and interconnects in modern microchips [11, 12].
- **Optics:** In optical applications, thin-layer coatings are indispensable for manufacturing anti-reflective surfaces on lenses, as well as fabricating mirrors, optical filters, and waveguides for telecommunications and displays [13, 14].
- **Energy and Photovoltaics:** Thin-layer photovoltaics, which utilize semiconductor layers such as amorphous silicon or CdTe, represent a critical class of solar cells. These devices convert sunlight to electricity with significantly reduced material usage and cost compared to traditional bulk cells [15, 16].
- **Protective and Tribological Coatings:** Hard thin layers, such as metallic nitrides, oxides, or diamond-like carbon, are applied to industrial tools and mechanical components. These coatings significantly improve wear and corrosion resistance without altering the bulk properties of the underlying material [17].
- **Sensing and Biomedical Devices:** In sensing and biomedical applications, thin layers provide functionalized surfaces that can be chemically or biologically active. They leverage their high surface-to-volume ratio and tunable conductivity for the detection of specific gases, chemicals, or biomolecules [18, 19].
- **Flexible Electronics:** This emerging field relies heavily on the deposition of functional thin layers onto flexible polymer substrates. This technology enables the creation of bendable circuits, wearable sensors, and foldable displays [20].

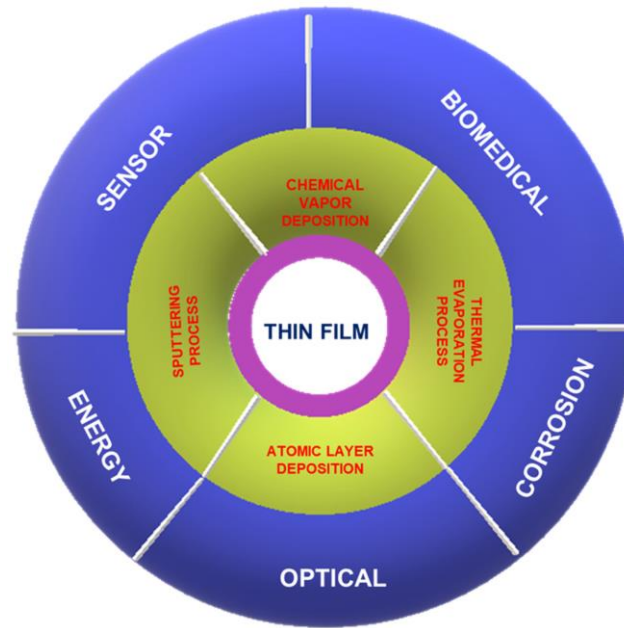


Figure I.2. Thin-layer preparations and their different fields of application. [21]

I.4 Deposition Methods (Physical vs. Chemical)

The fabrication of thin layers is accomplished through a variety of techniques that can be broadly classified into two main categories: physical methods and chemical methods. The selection of a specific technique is critical as it directly influences the microstructure, properties, and ultimate performance of the layer [22].

I.4.1. Physical Deposition Methods

In **physical vapor deposition (PVD)**, material is physically transferred from a source to the substrate, typically within a high-vacuum environment, without undergoing a chemical reaction in the vapor phase. This transport is achieved through mechanical, electromechanical, or thermodynamic processes [23, 24]. The most prevalent PVD techniques include:

- **Thermal Evaporation:** This method involves heating a source material (often in a crucible) within a high-vacuum chamber until it evaporates. The resulting vapor then travels in a line-of-sight path and condenses onto a cooler substrate, forming a thin layer [25, 26].
- **Sputtering:** In this process, a target made of the desired coating material is bombarded with high-energy ions, typically from an inert gas plasma like Argon. This bombardment physically ejects, or "sputters," atoms from the target, which then deposit onto the

substrate to form the layer. Sputtering is highly versatile and allows for excellent control over layer properties [27, 28].

- **Advanced Techniques:** Other sophisticated PVD methods, such as **pulsed laser deposition (PLD)** and **molecular beam epitaxy (MBE)**, are employed for fabricating high-purity, complex, or single-crystal (epitaxial) thin layers [24].

I.4.2. Chemical Deposition Methods

In contrast to PVD, **chemical deposition** techniques utilize chemical reactions, either at the substrate surface or within the precursor solution, to form the layer material (Fig. I.3).

- **Chemical Vapor Deposition (CVD):** This is a widely used process where volatile precursor gases are introduced into a reaction chamber. These gases decompose or react on a heated substrate surface to produce a non-volatile solid layer. CVD is highly valued for its ability to produce uniform, conformal coatings on complex geometries and is a cornerstone of the semiconductor industry (Table. 1.1) [29, 30].
- **Solution-Based Deposition:** This category encompasses a range of lower-cost, non-vacuum techniques where the layer is formed from a liquid phase. Common methods include **sol-gel processing**, **spin coating**, and **electrodeposition (electroplating)**. A liquid precursor solution is applied to the substrate, and the layer is formed either by chemical reaction or by the evaporation of the solvent, often followed by a thermal annealing step to crystallize the material and remove residual organics [31, 32].

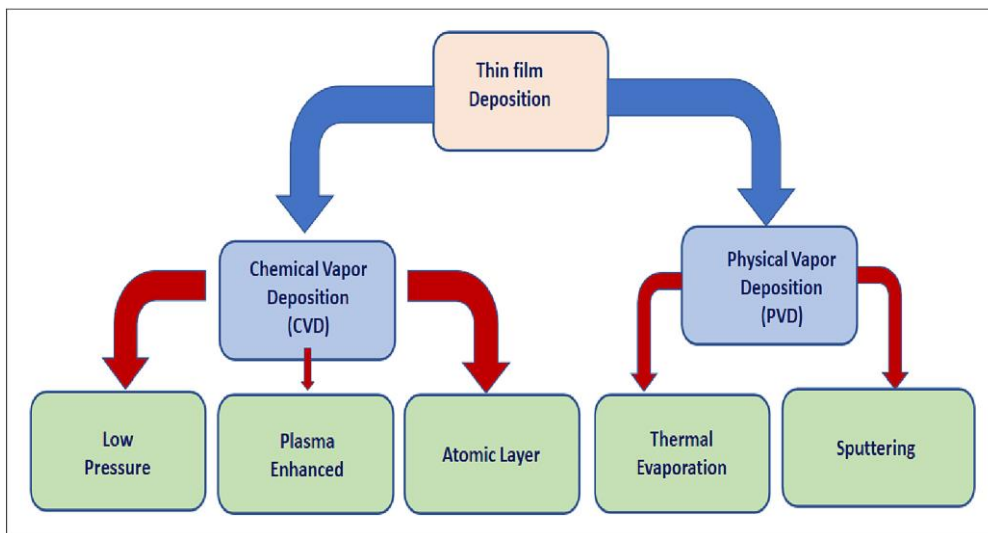


Figure I.3. Thin layer deposition techniques. [33]

Table I.1. Summary of the Advantages and Limitations of the Thermal Evaporation Technique. [34]

SL	Aspect	Advantages	Limitations
1	Deposition Efficiency	Highly suitable for semiconductor manufacturing, especially for high-volume production of microelectronic components.	Limited compatibility with certain materials due to thermal sensitivity.
2	Vaporization Method	Employs tungsten filament heating for efficient and rapid material evaporation.	Achieving uniform layer thickness across large substrates can be difficult.
3	Environmental Interference	Vacuum operation significantly reduces contamination from atmospheric particles during deposition.	The technique demands high energy input, which may increase operational costs.
4	Vacuum Control	Functions effectively under high-vacuum conditions, allowing precise deposition control.	Process complexity increases with the need for sustained vacuum environments.

I.5. Thin Layers in Shape Memory Alloys (SMAs)

Shape memory alloys (SMAs) are a unique class of functional materials renowned for their ability to recover a pre-deformed shape upon heating, a phenomenon known as the shape memory effect. They can also exhibit a large, reversible deformation under load within a specific temperature range, referred to as pseudoelasticity or superelasticity. These remarkable properties are governed by a reversible, solid-state martensitic phase transformation between a high-temperature parent phase (austenite) and a low-temperature product phase (martensite) (Fig. I.4). [35, 36].

Among the various SMA systems, alloys of nickel and titanium (NiTi), commonly known as Nitinol, are the most commercially significant and widely researched. This is due to their superior combination of large recoverable strain (up to 8%), high actuation stress, and excellent fatigue and corrosion resistance [36]. The integration of SMA materials into thin-layer form opens significant opportunities for the development of micro-scale actuators and sensors, particularly for applications in microelectromechanical systems (MEMS) and biomedical devices [37, 38].

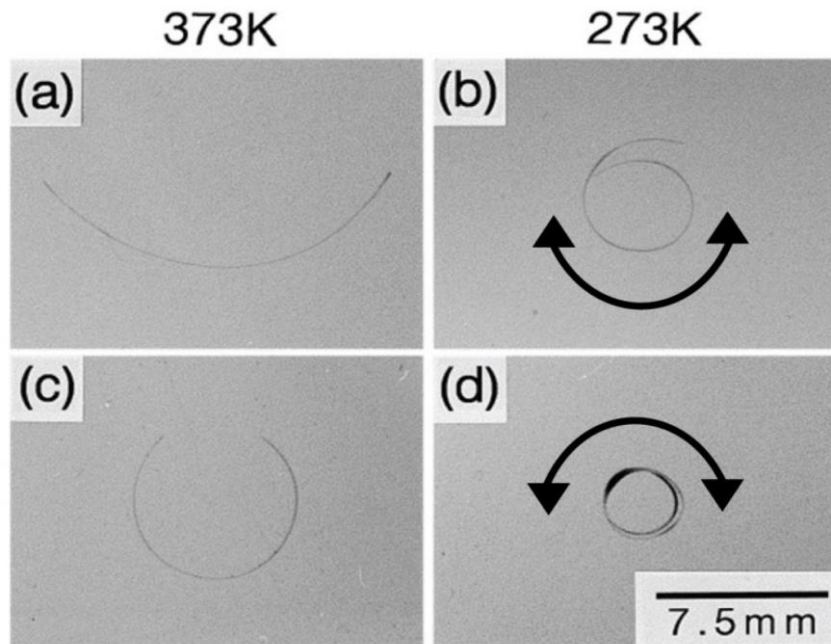


Figure I.4. Spontaneous shape change of $\text{Ti}_{51.3}$ at %Ni thin layers after different aging treatments. The images show the layer's shape in (a, c) boiling water and (b, d) iced water. Adapted from Ishida et al. [39].

This section will review the state-of-the-art in SMA thin layers, focusing on their unique properties, established deposition methods, fabrication challenges, and key applications.

I.6 Unique Properties of SMA Thin Layers

SMA thin layers retain the primary functional properties of their bulk counterparts—shape memory and superelasticity but in a miniaturized form factor that enables novel device architectures. Their properties can be significantly influenced by layer-specific factors such as thickness, grain size, and substrate interaction.

I.6.1 Work Output and Actuation

One of the most significant advantages of SMAs is their exceptionally high work output per unit volume, which is among the highest of all actuator material classes [35]. Even as layers of only a few micrometers in thickness, NiTi can generate substantial force and displacement when undergoing its thermally induced phase transformation. A key advantage at this scale is the layer's small thermal mass, which allows for extremely rapid thermal cycling. Researchers have demonstrated that thin-layer NiTi actuators can be heated and cooled in milliseconds, enabling high-frequency actuation that is unachievable with conventional SMA components due to thermal inertia [38].

I.6.2 Mechanical Properties and Superelasticity

When held above their transformation temperature, SMA thin layers exhibit superelastic behavior, meaning they can accommodate large strains (several percent) and fully recover their original shape upon unloading. However, the mechanical response of thin layers can differ from bulk materials due to scale effects. Studies have shown that nanograined or ultrafine-grained NiTi layers can exhibit a modified stress-strain response, which is attributed to factors like grain size constraints and high intrinsic layer stress [40]. Furthermore, because the layer is often attached to a substrate, the substrate can impose mechanical constraints that influence the martensitic transformation, affecting properties such as the apparent modulus and the transformation hysteresis.

I.6.3 Tuning via Ternary Alloys

The properties of binary NiTi thin layers can be precisely tailored by incorporating a third alloying element. The addition of copper to form Ni-Ti-Cu alloys is a well-established strategy to modify the transformation characteristics. Copper substitution in NiTi has been shown to lower the martensitic transformation temperatures and, most importantly, reduce the thermal hysteresis of the transformation. This reduced hysteresis (a narrower temperature range between the forward and reverse transformations) is highly desirable for actuator applications, as it allows for faster, more efficient, and more repeatable cycling. While this often comes with a slight trade-off in maximum transformation strain, the ability to tune properties via composition—by adjusting the Ni:Ti ratio or adding elements like Cu, Hf, or Pd is a powerful tool for designing layers for specific operating temperatures and mechanical responses [40].

I.6.4 High-Temperature SMA Layers

While standard NiTi-based alloys are typically limited to operating temperatures below approximately 100 °C, there is a growing demand for actuators that can function in harsher environments [40]. To meet this need, Cu-based shape memory alloys, such as Cu-Al-Ni, have emerged as promising candidates for high-temperature applications. Cu-Al-Ni thin layers can be engineered to have transformation temperatures well above 150 °C [41]. Furthermore, recent research suggests that at the micro- and nano-scales, Cu-Al-Ni layers can exhibit excellent superelastic stability over many cycles, potentially outperforming NiTi in certain high-temperature scenarios (Table I.2) [40]. This makes them highly attractive for applications in aerospace, automotive, or industrial MEMS actuators.

Table I.2. Nominal thickness of each elemental metallic layer according to the nominal composition of the Cu-Al-Ni thin layer. [40]

Metallic Layer	Nominal Thickness (Å)	Nominal Comp. (wt.%)
Al	1160	11.0
Ni	132/66 *	4.1
Cu	1354	84.9

* Ni layer at the top and bottom.

I.7 Deposition Techniques for SMA Thin Layers

The deposition of shape memory alloys as thin layers presents unique challenges, primarily related to achieving precise control over the layer's chemical composition and crystalline structure. The functional properties of SMAs are critically sensitive to stoichiometry, and thus, the deposition process must be meticulously controlled. The most prevalent methods for fabricating SMA thin layers are based on PVD techniques.

The most common and industrially relevant method for SMA thin-layer fabrication is sputter deposition [36, 42]. For binary NiTi, deposition is typically performed using radio-frequency (RF) or direct-current (DC) magnetron sputtering from a pre-alloyed NiTi target. A significant characteristic of this process is that as-deposited NiTi layers are often amorphous or nanocrystalline due to the relatively low substrate temperatures involved. Consequently, a post-deposition annealing step (typically in the range of 450–600 °C) is essential to crystallize the layer into the B2 austenite phase, which is required to exhibit the shape memory effect [43].

For ternary systems like Ni-Ti-Cu or Cu-based SMAs such as Cu-Al-Ni, sputtering from a multi-component alloy target is also a common approach [40]. However, this can present challenges, as the constituent elements may have different sputtering yields, potentially leading to a layer composition that deviates from that of the target. To circumvent this, an alternative and highly controllable approach is the sequential deposition of elemental layers followed by an interdiffusion anneal. In this method, nanometer-thick layers of the pure constituent metals (e.g., Cu, Al, and Ni) are deposited in a specific sequence. A subsequent high-temperature annealing treatment is then used to promote interdiffusion and form the desired single-phase alloyed layer [40]. This multilayer approach offers exceptional control over the final stoichiometry by precisely adjusting the thickness of each individual layer (Fig. I.5).

While sputtering is dominant, other PVD techniques have also been successfully applied. Pulsed laser deposition (PLD) and electron-beam evaporation have been used to deposit NiTi-based layers, including ternary variants. These methods often produce amorphous layers that also require post-annealing and can offer benefits such as high purity due to the ultra-high vacuum conditions [35].

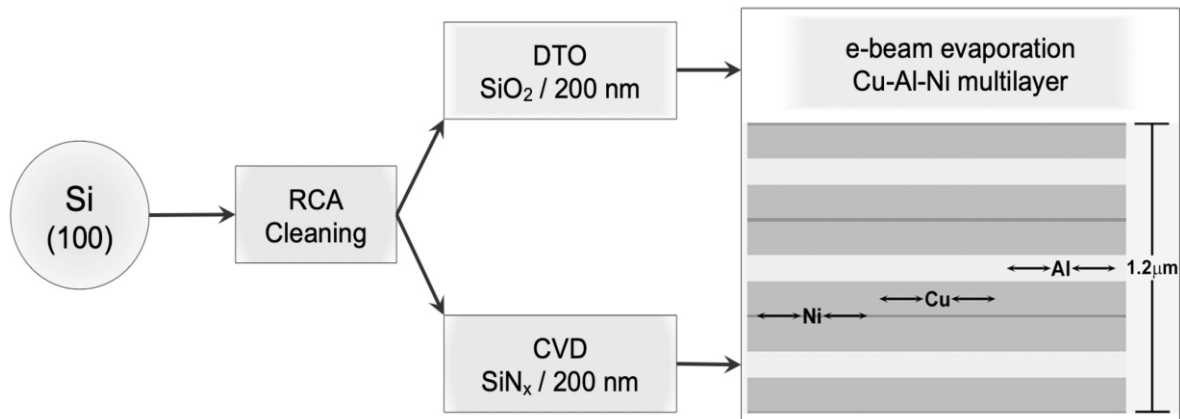


Figure I.5. Flow diagram for obtaining a set of Cu, Al, and Ni metallic multilayers deposited by the e-beam evaporation technique on Si substrates with two types of coatings, SiO₂ and SiN_x, both 200 nm thick, referred to as samples CAN/SO and CAN/SN, respectively. The final step illustrates the stacking order of the metallic layers and their nominal thickness (1.2 μm). [40]

I.8 Challenges in Fabrication and Performance

Producing high-quality, reliable SMA thin layers involves overcoming several significant challenges that extend beyond those of conventional thin-layer deposition. The functional properties of these materials are exceptionally sensitive to processing parameters, requiring meticulous control at every stage of fabrication.

I.8.1 Stoichiometry Control

Achieving the correct chemical composition is arguably the most critical challenge in SMA thin layer fabrication. The transformation temperatures and mechanical properties of SMAs are highly sensitive to stoichiometry. In NiTi alloys, for instance, a deviation of just 1 at. % in the nickel content can shift the transformation temperatures by tens of degrees Celsius [42]. During sputter deposition, this requires careful calibration of the process, as preferential sputtering of one element from the target can occur over time, leading to a drift in layer composition. Advanced techniques, such as the sequential evaporation of elemental layers, offer more precise control but add complexity to the process [40].

I.8.2 Crystallization and Phase Formation

As-deposited SMA layers are typically amorphous and require a post-deposition annealing step to induce crystallization into the functional phase (e.g., the B2 austenite phase for NiTi). This thermal treatment must be carefully optimized. Improper annealing conditions, such as excessively high temperatures or long durations, can lead to the precipitation of undesirable and brittle intermetallic phases (e.g., Ni_4Ti_3 in Ni-rich NiTi), which degrade the shape memory effect. Furthermore, in multilayer deposition, the stacking order of the elemental layers must be designed to prevent the formation of highly stable but non-functional intermetallics, such as NiAl, during the interdiffusion anneal [40].

I.8.3 Layer Stress and Adhesion

Intrinsic stress, a common issue in thin layers, is particularly significant for SMA layers. High stresses can arise from the deposition process itself (e.g., energetic particle bombardment in sputtering) and from the thermal mismatch between the layer and the substrate during annealing and cooling. If the total stress is too high, it can suppress the martensitic transformation, alter the transformation temperatures, or even lead to catastrophic mechanical failure, such as layer delamination or cracking [38]. To mitigate this, careful selection of substrate materials and the use of adhesion-promoting buffer layers are often necessary. In many MEMS applications, the layer is partially or fully released from the substrate (creating a freestanding structure) to eliminate substrate clamping and allow the layer to actuate freely [43].

I.8.4 Scaling, Uniformity, and Contamination

For practical device manufacturing, achieving uniform layer properties across large-area substrates (e.g., silicon wafers) and ensuring batch-to-batch repeatability are major concerns. Any gradients in layer thickness or composition can result in non-uniform performance across an array of devices. Industrial-scale challenges include target degradation over long-term use and minimizing contamination from residual gases like oxygen in the deposition chamber, as impurities can significantly alter the phase transformation behavior [41]. Both NiTi and Cu-based SMAs are also susceptible to surface oxidation during high-temperature annealing, which necessitates processing in a high-vacuum or inert gas environment to preserve the functional surface (Fig. I.6).

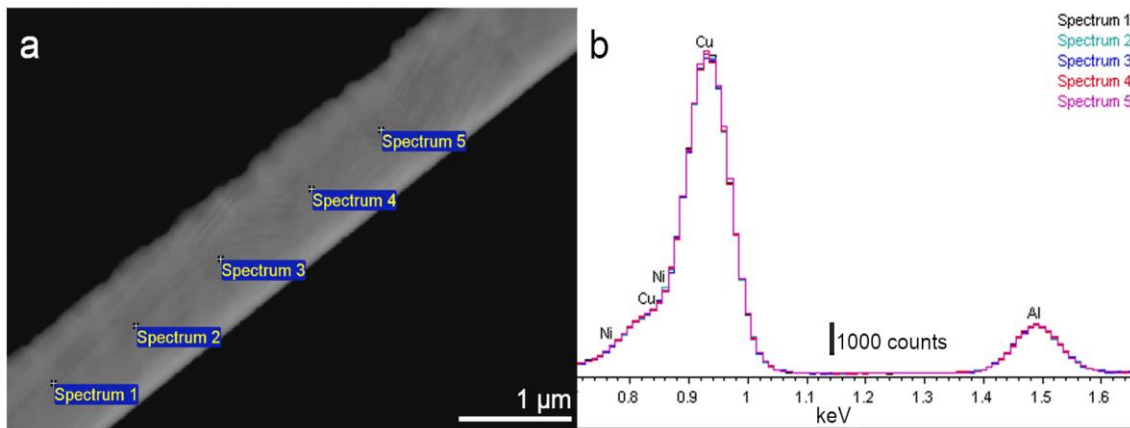


Figure I.6. EDX analysis of the CAN/SN sample. (a) SEM image with Backscattered electron (BSE) of a cross-section analyzed in five points; (b) intensity maxima for Cu ($L\alpha$) and Al ($K\alpha$) overlap in five spectra, denoting a high compositional homogeneity. [40]

I.9 Applications of SMA Thin Layers

The unique combination of high work output, small form factor, and integrability with semiconductor fabrication processes has enabled SMA thin layers to be applied in a variety of innovative micro-scale devices. Their applications span across multiple engineering and scientific domains.

I.9.1 Microactuators and MEMS

This is the primary application area for SMA thin layers. Their ability to produce large forces and displacements relative to their size makes them ideal actuators for microelectromechanical systems (MEMS) [37]. Notable examples demonstrated in the literature include:

1. **Micropumps:** Where a sputtered NiTi layer bonded to a silicon diaphragm is thermally cycled to drive fluid flow for lab-on-a-chip or microfluidic systems [45].
2. **Microgrippers:** In which NiTi layers are deposited onto micro-machined fingers. When heated, the NiTi contracts and closes the gripper, allowing for the precise manipulation of microscopic objects in fields like microsurgery or micro-assembly [46].
3. **Microvalves and Microswitches:** Freestanding NiTi thin-layer bridges or cantilevers can bend or deflect when electrically heated, functioning as compact, high-force switches or valves that are much smaller than traditional electromagnetic counterparts [37].

I.9.2 Sensing Applications

SMA thin layers can also function as sensors. The sensing mechanism typically relies on the sharp change in electrical resistance that accompanies the martensitic phase transformation, allowing the layer to act as a sensitive temperature switch. Additionally, the stress-induced phase transformation can be exploited. An applied force or pressure can induce martensite, altering the layer's mechanical resonance or electrical properties, which has been used to develop pressure and resonant mass sensors [35].

I.9.3 Flexible Electronics and Micro-Origami

Due to their ability to undergo large, reversible deformations, NiTi thin layers are being explored for use in flexible and stretchable electronics. When patterned onto compliant polymer sheets, SMA layers can act as "actuating hinges." By selectively heating these hinges, a flat sheet can be programmed to fold itself into a complex spatial structure, a concept known as micro-origami. This has been demonstrated for creating deployable mini-robots and adaptive optical systems. [37]

I.9.4 Biomedical Devices

The excellent biocompatibility of Nitinol makes SMA thin layers highly suitable for minimally invasive medical tools and implants. Building on the success of bulk Nitinol in devices like cardiovascular stents, thin-layer SMAs are being developed for applications such as micro-scale surgical instruments (e.g., biopsy microgrippers) that can be delivered via catheter. Other potential applications include dynamically actuated stent covers, micro-valves for controlling fluid flow in shunts, and on-demand drug delivery micropumps [37].

I.9.5 High-Temperature Microactuators

With the development of Cu-Al-Ni and other high-temperature SMA thin layers, new possibilities are emerging for MEMS devices that must operate in harsh environments, such as in aerospace or automotive engine components. A Cu-Al-Ni thin-layer actuator could function reliably at temperatures of 150–200 °C, where conventional NiTi-based devices would fail. This enables the development of high-temperature micro-valves, latches, or sensor components for demanding industrial applications (Fig. I.7) [41].

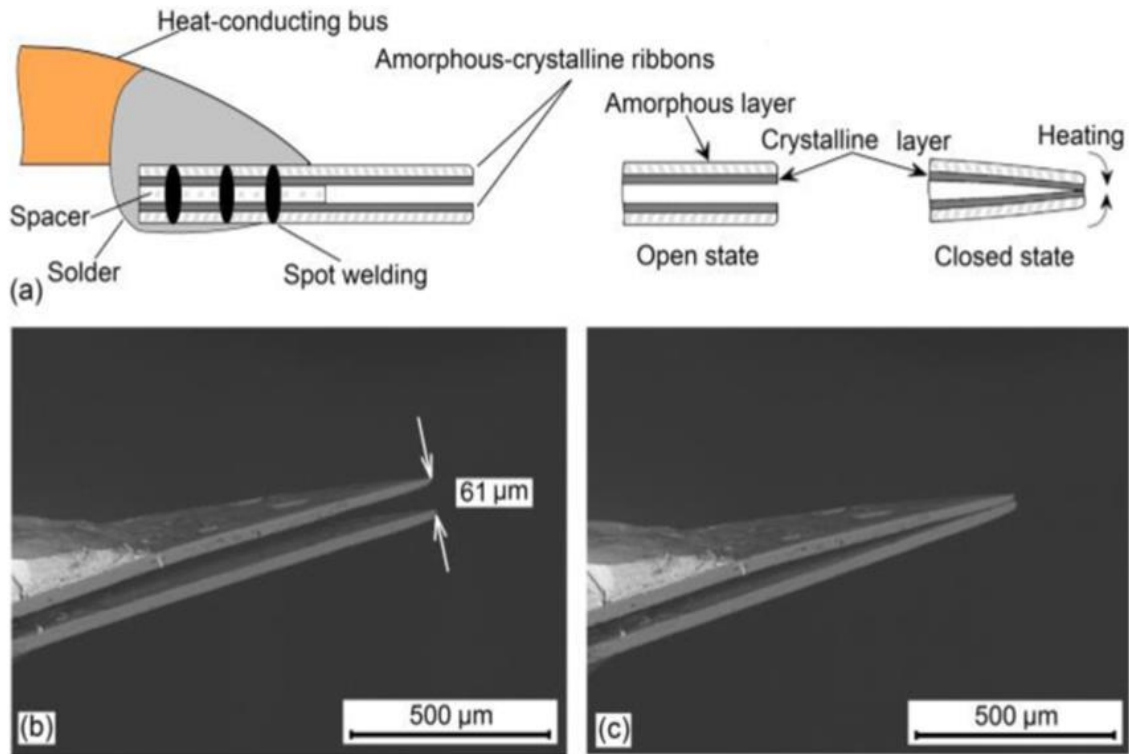


Figure I.7. Schematic and SEM Images of a Bistable TiNiCu-Based Microgripper in Open and Closed States. [46]

I.10 Conclusion

This chapter has reviewed the fundamental characteristics of thin layers, their main deposition techniques, and their growing importance in advanced functional applications. Particular attention was given to deposition methods such as sputtering and evaporation, highlighting both their technological capabilities and the associated fabrication challenges, including composition control, crystallization phenomena, and residual stresses.

Special emphasis was placed on shape memory alloy thin layers, whose unique thermomechanical properties have enabled innovative applications in MEMS technology, biomedical devices, and flexible electronics. Owing to their reduced dimensions, the functional performance of these layers is strongly governed by size effects and by mechanical interactions with the underlying substrate.

The literature survey further indicates that, although fabrication processes for NiTi-based SMA thin layers have reached a high level of maturity, the predictive modeling of their constrained thermomechanical behavior remains limited, particularly under multiaxial loading conditions and strong layer–substrate coupling. This observation motivates the present thesis, which aims to develop and validate a thermodynamically consistent constitutive framework for

SMA thin layers, implement it in numerical environments, and apply it to representative thin-layer configurations in order to analyze actuation performance, constraint effects, and potential failure mechanisms.

I.11 References

- [1] Abou-Ras, D.; Kirchartz, T.; Rau, U., Eds. *Advanced Characterization Techniques for Thin Layer Solar Cells*; Wiley-VCH Verlag GmbH & Co. KGaA: Weinheim, Germany, 2016.
- [2] McDonnell, S. J.; Wallace, R. M. Atomically-thin layered materials for device applications based upon 2D TMDC materials. *Thin Solid Films* 2016, 616, 482–501.
- [3] Hasim, S. N. F.; Hamid, M. A. A.; Shamsudin, R.; Jalar, A. Synthesis and characterization of ZnO thin layers by thermal evaporation. *Journal of Physics and Chemistry of Solids* 2009, 70, 1501–1504.
- [4] Garg, R.; Gonuguntla, S.; Saddam, S. K.; Iqbal, M. S.; Dada, A. O.; Pal, U.; Ahmadipour, M. Sputtering thin layers: Materials, applications, challenges and future directions. *Advances in Colloid and Interface Science* 2024, 330, 103203.
- [5] Kunene, T.; Tartibu, L.; Ukoba, K.; Jen, T.-C. Review of atomic layer deposition process, application and modeling tools. *Materials Today: Proceedings* 2022, 62. doi: 10.1016/j.matpr.2022.02.094.
- [6] Chen, X.; Dai, W.; Wu, T.; Luo, W.; Yang, J.; Jiang, W.; Wang, L. Thin layer thermoelectric materials: Classification, characterization, and potential for wearable applications. *Coatings* 2018, 8, 244.
- [7] Cranston, R. R.; Lessard, B. H. Metal phthalocyanines: Thin-layer formation, microstructure, and physical properties. *RSC Advances* 2021, 11, 21716–21737.
- [8] Zhang, Z.; Lagally, M. G. Atomistic processes in the early stages of thin-layer growth. *Science* 1997, 276, 377–383.
- [9] Gaspari, F. Thin Layers. In *Comprehensive Energy Systems*; Elsevier: Amsterdam, The Netherlands, 2018; pp. 88–116.
- [10] Stoian, M.; Maurer, T.; Lamri, S.; Fechet, I. Techniques of preparation of thin layers: Catalytic combustion. *Catalysts* 2021, 11, 1530.
- [11] Franssila, S. *Introduction to Microfabrication*, 2nd ed.; John Wiley & Sons: Chichester, UK, 2010; pp. 265–288.
- [12] Lee, S. D.; Lee, Y. J.; Nam, K. S.; Jeong, Y.; Kim, D. H.; Kim, C. S.; Park, S. G.; Kwon, S. H.; Kwon, J. D.; Park, J. S. Characterization of microcrystalline silicon thin layer solar cells prepared by high working pressure plasma-enhanced chemical vapor deposition. *Journal of Electroceramics* 2014, 33, 149–154.

- [13] Raut, H. K.; Ganesh, V. A.; Nair, A. S.; Ramakrishna, S. Anti-reflective coatings: A critical, in-depth review. *Energy & Environmental Science* 2011, 4, 3779.
- [14] Yao, Z. J. Single crystal silicon supported thin layer micromirrors for optical applications. *Optical Engineering* 1997, 36, 1408–1413.
- [15] Shah, A. *Thin-Layer Silicon Solar Cells*; CRC Press: Boca Raton, FL, USA, 2010.
- [16] Maruyama, T.; Arai, S. Titanium dioxide thin layers prepared by chemical vapor deposition. *Solar Energy Materials and Solar Cells* 1992, 26, 323–329.
- [17] Rahmati, B.; Zangeneh, S.; Zangeneh-Madar, K. Improving the corrosion and wear properties of Ti–6Al–4V alloy by ceramic tantalum oxide thin layer. *Ceramics International* 2016, 42, 16298–16304.
- [18] Elanjeitsenni, V. P.; Vadivu, K. S.; Prasanth, B. M. A review on thin layers and conducting polymers as sensor devices. *Materials Research Express* 2022, 9, 022001.
- [19] Sberveglieri, G. Recent developments in semiconducting thin-layer gas sensors. *Sensors and Actuators B: Chemical* 1995, 23, 103–109.
- [20] Chen, Y.; Chuang, W. Flexible thin-layer transistors for wearable electronics. *Electronics* 2020, 9, 997.
- [21] Sakthinathan, S.; Meenakshi, G. A.; Vinothini, S.; Yu, C.-L.; Chen, C.-L.; Chiu, T.-W.; Vittayakorn, N. A review of thin-layer growth, properties, applications, and future prospects. *Processes* 2025, 13, 587.
- [22] Martin, P. M. *Deposition Technologies: An Overview*. In *Handbook of Deposition Technologies for Films and Coatings: Science, Applications and Technology*, 3rd ed.; Martin, P. M., Ed.; William Andrew: Norwich, NY, USA, 2009; pp. 1–31.
- [23] Budida, J.; Srinivasan, K. Review of thin layer deposition and techniques. *Materials Today: Proceedings* 2023, 92, 1030–1033.
- [24] Reichelt, K.; Jiang, X. The preparation of thin layers by physical vapour deposition methods. *Thin Solid Films* 1990, 191, 91–126.
- [25] Fouad, O. A.; Ismail, A. A.; Zaki, Z. I.; Mohamed, R. M. Zinc oxide thin layers prepared by thermal evaporation deposition and their photocatalytic activity. *Applied Catalysis B: Environmental* 2006, 62, 144–149.
- [26] Safarian, J.; Engh, T. A. Vacuum evaporation of pure metals. *Metallurgical and Materials Transactions A* 2013, 44, 747–753.
- [27] Li, J.; Ren, G.-K.; Chen, J.; Chen, X.; Wu, W.; Liu, Y.; Chen, X.; Song, J.; Lin, Y.-H.; Shi, Y. Facilitating complex thin film deposition by using magnetron sputtering: A review. *JOM* 2022, 74, 3069–3081. doi: 10.1007/s11837-022-05294-0.

- [28] Bi, Z.; Zhang, Z.; Fan, P. Effect of sputter deposition parameters on the characteristics of PZT ferroelectric thin layers. *Journal of Physics: Conference Series* 2007, 61, 115–119.
- [29] Sun, L.; Yuan, G.; Gao, L.; Yang, J.; Chhowalla, M.; Gharahcheshmeh, M. H.; Gleason, K. K.; Choi, Y. S.; Hong, B. H.; Liu, Z. Chemical vapour deposition. *Nature Reviews Methods Primers* 2021, 1, 5.
- [30] Hitchman, M. L.; Tian, F. Studies of TiO₂ thin layers prepared by chemical vapor deposition for photocatalytic and photoelectrocatalytic degradation of 4-chlorophenol. *Journal of Electroanalytical Chemistry* 2002, 538, 165–172.
- [31] Yu, C. L.; Sakthinathan, S.; Lu, M. T.; Yu, S. T.; Kuo, C. Y.; You, Y. F.; Chiu, T. W. CuAlO₂/AlN double-layer thin layer prepared by the spin coating approach. *Thin Solid Films* 2022, 753, 139260.
- [32] Yuk, J.; Troczynski, T. Sol-gel BaTiO₃ thin layer for humidity sensors. *Sensors and Actuators B: Chemical* 2003, 94, 290–293.
- [33] Thabit, N. Y. A.; Makhoulf, A. S. H. Chapter 1 — Fundamentals of smart coatings and thin layers: Synthesis, deposition methods, and industrial applications. In *Advances in Smart Coatings and Thin Layers for Future Industrial and Biomedical Engineering Applications*; Elsevier: Amsterdam, The Netherlands, 2020; pp. 3–35.
- [34] Toma, F. T. Z.; Rahman, M. S.; Hussain, K. M. A.; Ahmed, S. A comprehensive review on thin layer deposition techniques. *Journal of Modern Nanotechnology* 2024, 4, 1–16.
- [35] Nimalan, T.; Begam, M. R. Physical and chemical methods: A review on the analysis of deposition parameters of thin layer preparation methods. *International Journal of Thin Layer Science and Technology* 2024, 13, 59–66.
- [36] Behera, A.; Rajak, D. K.; Kolahchi, R.; et al. Current global scenario of sputtered deposited NiTi smart systems. *Journal of Materials Research and Technology* 2020, 9, 14582–14598.
- [37] Zainal, M. A.; Sahlan, S.; Ali, M. S. M. Micromachined shape-memory-alloy microactuators and their application in biomedical devices. *Micromachines* 2015, 6, 879.
- [38] Muniraj, L. Development of NiTi-Based Microactuators: Stress Analysis and Thermal Cycling. Ph.D. Thesis, Heriot-Watt University, Edinburgh, UK, 2016.
- [39] Ishida, A.; Sato, M.; Takei, A.; Nomura, K.; Miyazaki, S. Effect of heat treatment on shape memory behavior of Ti-rich Ti-Ni thin layers. *Metallurgical and Materials Transactions A* 1998, 29, 2779–2784.
- [40] Gómez-Cortés, J. F.; San Juan, J.; Ortiz, A. L.; et al. Thermal stability of Cu–Al–Ni shape memory alloy thin layers obtained by nanometer multilayer deposition. *Nanomaterials* 2023, 13, 2605.
- [41] López-Ferreño, I.; Gómez-Cortés, J. F.; Breczewski, T.; Ruiz-Larrea, I.; Nó, M. L.; San Juan, J. M. High-temperature shape memory alloys based on the Cu–Al–Ni system: Design and

thermomechanical characterization. *Journal of Materials Research and Technology* 2020, 9, 9972–9984. doi: 10.1016/j.jmrt.2020.07.002.

[42] Fontes, A. V.; Rodrigues, P.; Santo, D.; et al. Influence of deposition parameters on sputtered NiTi shape memory alloy thin layers. *Surface and Coatings Technology* 2020, 381, 125136.

[43] Christoph, B.; Chluba, C.; Zamponi, C.; Quandt, E.; Miranda, R. L. Fabrication and characterization of freestanding NiTi-based thin layer materials for shape memory micro-actuator applications. *Shape Memory and Superelasticity* 2019, 5, 327–335.

[44] Xu, D.; Wang, L.; Ding, G.; Zhou, Y.; Yu, A. Characteristics and fabrication of NiTi/Si diaphragm micropump. *Sensors and Actuators A: Physical* 2001, 93, 87–92.

[45] Sun, Y. B.; Wang, Q. M.; Hirakawa, K. Design and fabrication of a MEMS microgripper using thin-layer NiTi. *Journal of Micromechanics and Microengineering* 2005, 15, 1125–1132.

[46] Shelyakov, A.; Sitnikov, N.; Borodako, K.; et al. Design of microgrippers based on amorphous-crystalline TiNiCu alloy with two-way shape memory. *Journal of Micro-Bio Robotics* 2020, 16, 129–135.

CHAPTER II

**A COMPREHENSIVE REVIEW
OF SHAPE MEMORY ALLOYS**

II.1 Introduction

The current era in materials science has witnessed a clear transition from conventional passive materials toward active and intelligent systems, capable of sensing and responding to external environmental variations in a controlled and predictable manner [1]. This intrinsic responsiveness originates from reversible modifications at the microstructural level, leading to measurable changes in macroscopic properties such as deformation, stiffness, viscosity, or optical behavior.

Within this class of smart materials, Shape Memory Alloys (SMAs) occupy a prominent position due to their exceptional ability to recover predefined shapes upon heating and to accommodate large reversible deformations under mechanical loading [2, 3]. The shape memory effect (SME) was first observed in the 1930s in Au–Cd and In–Tl alloys; however, it was the discovery of this phenomenon in nickel–titanium alloys by the Naval Ordnance Laboratory (NOL) in the early 1960s that triggered widespread scientific and industrial interest [4]. This equiatomic Ni–Ti alloy, commonly known as Nitinol, demonstrated a combination of high strain recovery, mechanical stability, and biocompatibility.

This chapter provides a bibliographic review of Shape Memory Alloys, beginning with their positioning within the broader framework of smart materials. The fundamental mechanisms governing SMA behavior are then introduced, with particular emphasis on the crystallographic and thermodynamic aspects of martensitic phase transformations. The principal thermomechanical responses—namely pseudoelasticity and the shape memory effect—are subsequently examined. Recent developments and representative applications in aerospace, biomedical, and industrial domains are also discussed. Finally, special attention is devoted to SMA thin layers and their integration into micro-scale systems, where geometric constraints and size effects play a dominant role, thereby motivating further developments in modeling approaches aimed at accurately describing their constrained behavior in MEMS applications.

II.2 Smart Materials: An Overview

II.2.1 Definition of Smart Materials

Smart materials, also known as responsive or adaptive materials, refer to engineered substances whose physical or chemical properties undergo measurable and predictable changes upon exposure to external stimuli such as mechanical stress, temperature fluctuations, or

electromagnetic fields [5]. Distinct from traditional materials, smart materials inherently integrate sensory and actuating functions within their microstructure, eliminating the requirement for external sensors or actuators in numerous applications [6]. Their intrinsic responsiveness enables the design of efficient, compact, and highly reliable systems [7].

II.2.2 Categories of Smart Materials

Smart materials can be classified based on their specific responses and the type of stimuli that trigger these responses. Although this chapter primarily focuses on SMAs, a brief overview of other smart material categories is beneficial for understanding the distinctive position SMAs occupy (Fig. II.1).

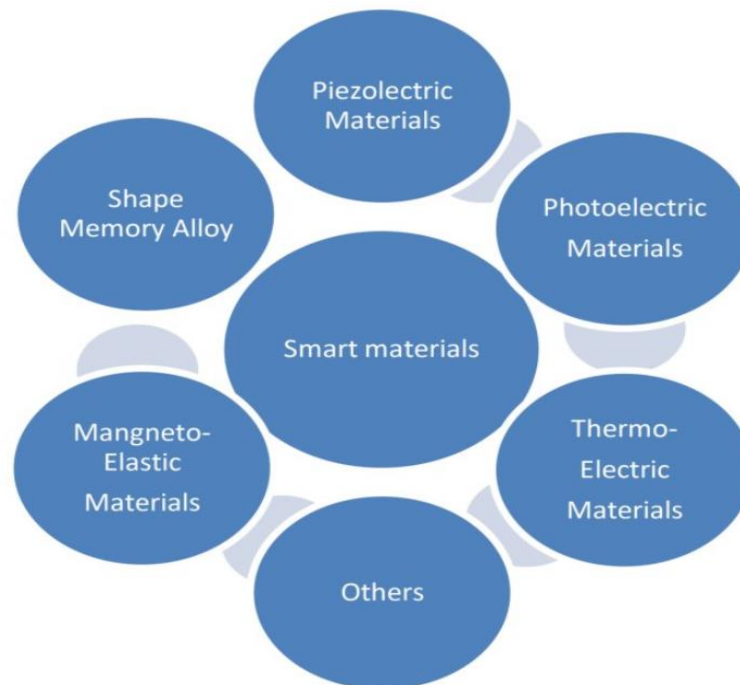


Figure II.1. Smart Materials and their classification. [8]

- **Shape Memory Materials:** This category predominantly includes Shape Memory Alloys (SMAs), as well as Shape Memory Polymers (SMPs) and Shape Memory Ceramics (SMCs). These materials exhibit significant shape alterations primarily induced by temperature or mechanical stress [9].
- **Piezoelectric and Electrostrictive Materials:** Piezoelectric materials generate electrical charges in response to applied mechanical stresses and conversely deform upon the application of electrical fields. A prominent example, Lead Zirconate Titanate (PZT), is extensively used in sensors, actuators, and transducers [10, 11].

- **Magnetostrictive Materials:** Materials in this group undergo dimensional changes in response to applied magnetic fields. Terfenol-D, an alloy comprising terbium, dysprosium, and iron, is notably employed in high-performance sonar and acoustic actuators [12].
- **Thermochromic and Photochromic Materials:** These materials reversibly alter their color with changes in temperature (thermochromic) or upon exposure to light (photochromic). They find applications in temperature indicators, smart windows, and adaptive optical devices [13].
- **Electrorheological (ER) and Magnetorheological (MR) Fluids:** These fluids exhibit significant and rapid viscosity changes upon exposure to electric fields (ER fluids) or magnetic fields (MR fluids). Their swift transition from liquid-like to semi-solid states has made them invaluable in damping and control devices, such as clutches, dampers, and shock absorbers [14, 15].

Within this broad spectrum, SMAs distinguish themselves by offering substantial shape recovery magnitudes and generating high recovery stresses. These unique capabilities position SMAs as ideal candidates for actuation and structural control applications [16].

II.3 Shape Memory Alloys (SMAs): Fundamental Principles

The unique characteristics of Shape Memory Alloys are not purely chemical but rather stem from their physical behavior, specifically a reversible solid-state phase transformation between a high-temperature parent phase known as Austenite and a low-temperature product phase called Martensite [2, 17].

II.3.1 Crystallography and the Martensitic Transformation

The martensitic transformation, fundamental to SMAs, involves an atomic rearrangement occurring in a coordinated manner without long-range atomic diffusion. Unlike diffusional transformations, atoms shift collectively through shear mechanisms, allowing the crystalline lattice to rapidly reconfigure while maintaining its original composition (Fig. II.2) [18].

- **Austenite Phase:** Austenite, the high-temperature stable phase, generally exhibits a highly ordered and symmetric crystal structure. In the widely-used Ni-Ti alloys, this phase possesses a Body-Centered Cubic (BCC) structure, specifically the B2 (CsCl-

type) structure [4, 19]. Austenite is stable at elevated temperatures under minimal mechanical stress.

- **Martensite Phase:** When the temperature decreases below a critical threshold (M_s), austenite transforms into the martensite phase. Martensite exhibits lower symmetry, typically adopting a monoclinic (B19') or orthorhombic (B19) structure in Ni-Ti alloys [20]. To accommodate internal strains without overall macroscopic deformation, martensite initially forms as internally twinned variants—regions sharing identical crystal structures but differing crystallographic orientations—separated by highly mobile twin boundaries [21].

Applying mechanical stress to twinned martensite induces a detwinning process. Under stress, favorable martensitic variants grow by the movement of twin boundaries, enabling the alloy to sustain large deformation (up to 8-10%) at relatively low, stable stress levels. Upon completion of the detwinning, the material fully consists of a single martensitic variant, preserving the "memory" of its deformation [22].

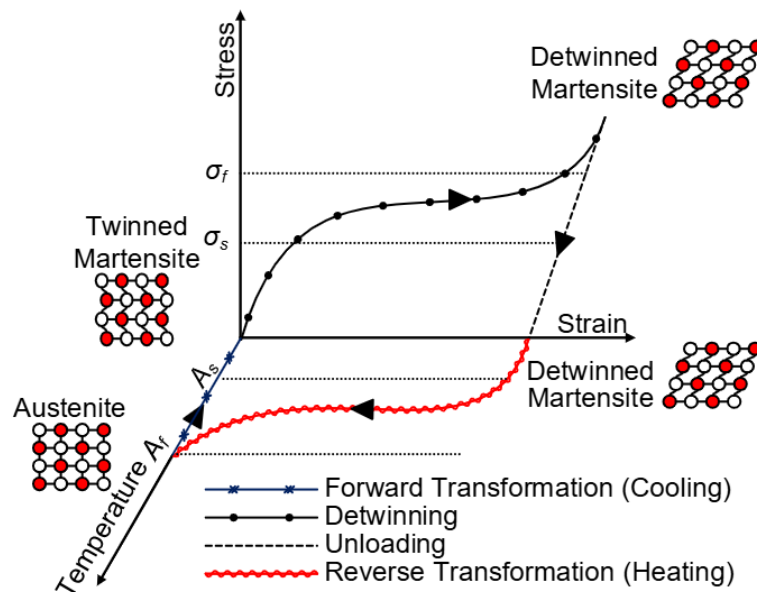


Figure II.2. Diagram illustrating crystallographic transformations of Austenite and Martensite. [23]

- (a) High-temperature Austenite (B2 structure).
- (b) Low-temperature, self-accommodated twinned Martensite upon cooling.
- (c) Detwinned Martensite after mechanical loading.
- (d) Shape recovery to original Austenite structure upon heating [17].

II.3.2 Thermodynamics of the Phase Transformation

The reversible transformation between Austenite and Martensite phases is governed by both temperature and applied stress, characterized by four critical transformation temperatures:

- Martensite start temperature M_s
- Martensite finish temperature M_f
- Austenite start temperature A_s
- Austenite finish temperature A_f

Transformation typically occurs over a temperature range, exhibiting hysteresis defined as $A_f > M_s$. This thermal hysteresis ($A_f - M_s$) quantifies energy dissipation throughout a complete thermal cycle, representing a key design parameter in SMA actuators [24]. The critical transformation stress-temperature relation follows a linear trend described by the Clausius–Clapeyron equation used for solid-state phase changes [25]:

$$\frac{dT}{d\sigma_{cr}} = -\frac{\varepsilon_t T_0}{\Delta H} = -\frac{\varepsilon_t}{\Delta S}$$

Where ΔH and ΔS are the enthalpy and entropy of transformation, respectively, ε_t denotes transformation strain; and T_0 represents the equilibrium temperature. equation explains stress-induced stabilization of martensite above typical transformation temperatures, central to the superelastic behavior. The stress-temperature phase relationship in SMAs is often visualized by a schematic phase diagram (Fig. II.3), outlining the stable regions for Austenite, twinned Martensite, and detwinned (stress-induced) Martensite [25].

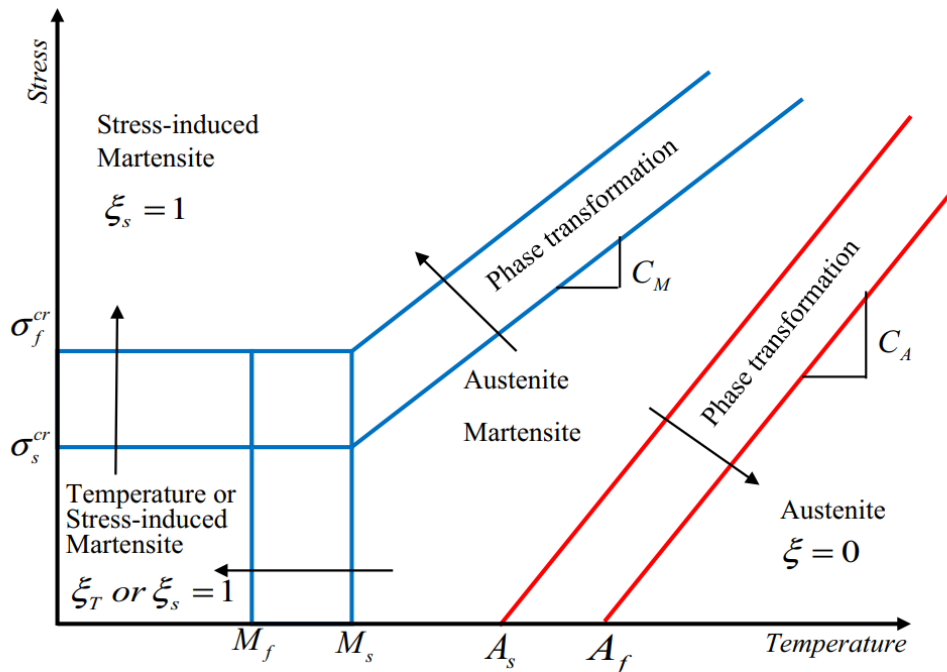


Figure II.3. Illustrative stress-temperature phase diagram representing stable regions for Austenite, twinned Martensite, and detwinned (stress-induced) Martensite in Shape Memory Alloys. The linear relationship between stress and temperature, depicted by the inclined boundary lines, follows the Clausius–Clapeyron equation. [26]

II.3.3 Common SMA Systems

While numerous alloys demonstrate the shape memory phenomenon, only a select few have achieved significant commercial success due to optimal combinations of performance, cost-effectiveness, and manufacturability.

- **Nickel-Titanium Alloys (Nitinol):** Nitinol, consisting typically of 49-51 atomic % nickel, remains the most extensively utilized SMA. Its distinctive properties include significant recoverable strains (up to ~8%), high recovery stress, excellent corrosion resistance, and remarkable biocompatibility, making it particularly suitable for biomedical applications [27, 28]. Nevertheless, its relatively high cost and manufacturing challenges limit wider use.
- **Copper-Based SMAs (Cu-Zn-Al, Cu-Al-Ni):** Copper-based alloys are among the earliest-studied SMAs, offering advantages of lower cost and ease of manufacturing compared to Ni-Ti alloys [29]. However, they suffer from issues such as grain boundary brittleness and martensite stabilization over time, negatively impacting their shape memory performance and restricting their application to less critical tasks [30].
- **Iron-Based SMAs (Fe-Mn-Si, Fe-Ni-Co-Ti):** These alloys promise significantly reduced costs due to compatibility with conventional steel production methods. Despite

this advantage, iron-based SMAs typically show incomplete shape memory recovery relative to Nitinol [31]. They primarily find applications requiring substantial clamping forces, such as pipe couplings or reinforcement components in civil engineering [32].

Below, a summary of key properties of major SMA systems (Table II.1) :

Table II.1: Summarized key properties of major SMA systems. [4, 25], [29-32]

Properties	Ni-Ti (Nitinol)	Cu-Based (Cu-Al-Ni)	Fe-Based (Fe-Mn-Si)
Max. Recoverable Strain	~8%	~4-5%	~2-4%
Recovery Stress	High (~800 MPa)	Medium (~300 MPa)	High (~500 MPa)
Hysteresis (Temp.)	20-50 °C	10-20 °C	100-200 °C
Cost	High	Low	Very Low
Biocompatibility	Excellent	Poor	Fair
Stability/Fatigue Life	Excellent	Fair to Poor	Good

II.4 Thermomechanical Properties and Effects

The fundamental martensitic transformation inherent in Shape Memory Alloys leads to several distinctive macroscopic phenomena, extensively leveraged in various engineering applications.

II.4.1 The One-Way Shape Memory Effect (OWSME)

The One-Way Shape Memory Effect represents the fundamental property exhibited by SMAs. It refers to the alloy's ability to recover its original predetermined shape when heated, after undergoing deformation in its low-temperature martensitic phase. The typical process illustrating this effect is as follows (Fig. II.4):

- An SMA component is initially formed to its desired "parent" geometry in the Austenitic phase.
- The alloy is then cooled below the Martensite finish temperature M_f , causing full transformation into twinned Martensite.
- A mechanical load is subsequently applied, inducing deformation by detwinning the martensitic structure. Upon removal of the load, the component retains its deformed shape.

- Heating the component above its Austenite finish temperature A_f initiates the reverse transformation, reverting the material to its original Austenitic geometry.

This phenomenon is referred to as "one-way," since the material retains memory only of its high-temperature shape and does not spontaneously revert to the deformed low-temperature state upon cooling [2, 33].

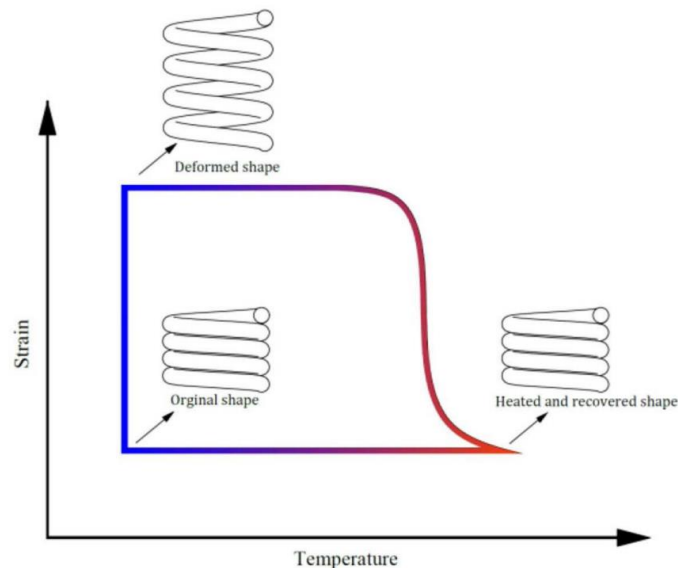


Figure II.4. Representation of the One-Way Shape Memory Effect (OWSME). [34]

II.4.2 The Two-Way Shape Memory Effect (TWSME)

The Two-Way Shape Memory Effect (Fig. II.5) is a less common yet particularly valuable property wherein the alloy retains memory of two distinct configurations: one at high temperature and another at low temperature. Through thermal cycling, the SMA can autonomously alternate between these shapes without the application of external mechanical loads [35]. Unlike the OWSME, the TWSME is not an inherent property and must be introduced through specific thermomechanical "training" methods. Typically, these involve applying constrained deformation during repeated phase transformations, leading to the formation of internal stress fields and dislocation arrays. These internal changes preferentially promote the formation of particular martensitic variants upon subsequent cooling [36], [37]. While the recoverable strain achievable with TWSME is generally lower compared to OWSME, the alloy's ability to perform mechanical work in both heating and cooling cycles makes it highly advantageous for cyclic actuation applications [38].

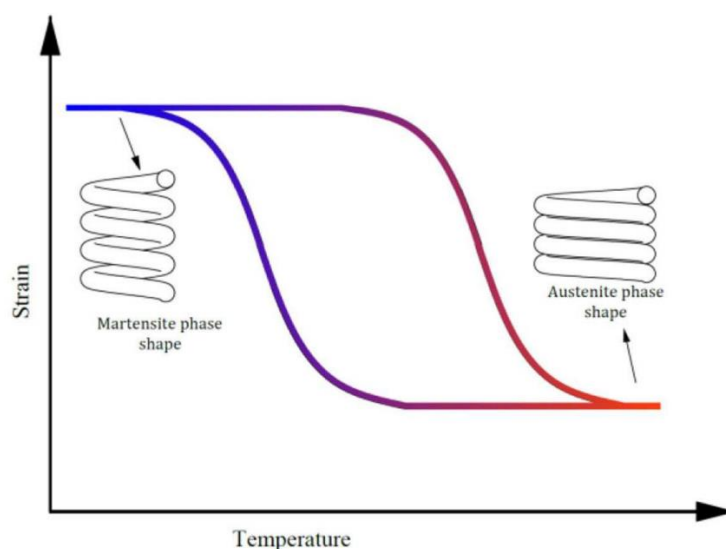


Figure II.5. Representation of the Two-Way Shape Memory Effect (TWSME). [34]

II.4.3 Superelasticity (Pseudoelasticity)

Superelasticity also referred to as pseudoelasticity is a remarkable phenomenon exhibited by SMAs when operating above the Austenite finish temperature A_f (Fig. II.6). In this regime, the alloy remains fully Austenitic at rest. Upon mechanical loading, the material initially deforms elastically; however, once a critical stress level is surpassed, a stress-induced martensitic (SIM) transformation is initiated. This transformation allows for large, reversible strains without permanent deformation.

During loading, a characteristic stress plateau appears in the stress-strain curve, corresponding to the phase transformation from Austenite to martensite. When the applied stress is removed, the stress-induced martensite reverts spontaneously back to Austenite, resulting in complete recovery of the original shape [39]. This behavior leads to a closed hysteresis loop in the stress-strain response an energy-dissipative feature that is characteristic of superelastic materials [40].

The term "superelasticity" is used because the strain recovery far exceeds the conventional elastic limit of metals, reaching up to 8% in NiTi alloys. This unique property forms the basis for several biomedical and consumer applications such as eyeglass frames, orthodontic archwires, and self-expanding vascular stents [41].

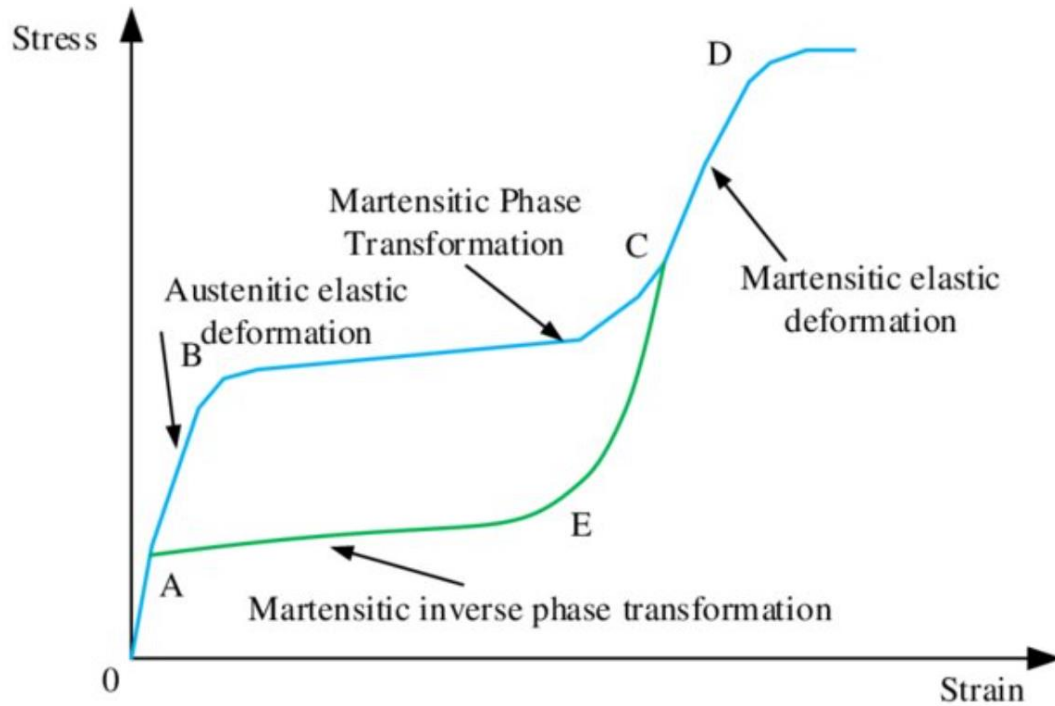


Figure II.6. Representative stress–strain response of a superelastic SMA at a temperature exceeding the Austenite finish temperature ($T > A_f$), highlighting the characteristic transformation behavior. [42]

The stress plateau observed during loading corresponds to the forward phase transformation from Austenite to Martensite ($A \rightarrow M$), while the unloading plateau represents the reverse transformation back to Austenite ($M \rightarrow A$). The enclosed area within the hysteresis loop signifies the mechanical energy dissipated per unit volume during the transformation cycle. [43]

II.4.4 Damping Capacity

Shape Memory Alloys are renowned for their high damping capability, particularly within the temperature range encompassing the martensitic transformation [44]. Damping, in this context, refers to the material's ability to dissipate mechanical energy typically as heat under cyclic loading conditions.

The principal mechanisms responsible for this energy dissipation in SMAs include:

- **Phase Transformation Hysteresis:**

The thermal and mechanical hysteresis loops associated with martensitic transformations contribute significantly to damping.

- **Interface Mobility:**

The movement of twin boundaries within the martensitic phase, along with Austenite–Martensite interface motion during phase transformations, serves as a major source of energy dissipation [45].

Thanks to this behavior, SMAs are highly attractive for applications requiring passive energy dissipation, such as vibration control in mechanical systems, noise reduction, and structural damping in civil engineering especially in seismic isolators and dampers [46, 47].

II.4.5 Rubber-Like Effect (EC)

The so-called “rubber-like” effect refers to a peculiar behavior observed in certain SMA systems particularly in aged Cu-based alloys where the material demonstrates substantial flexibility at low stress levels, without undergoing a phase transformation. This mechanical response resembles the elasticity of rubber, hence the nomenclature.

This effect is believed to result from the reversible reorganization of martensitic variants surrounding nano-scale precipitates or defect zones introduced during thermal aging [48].

Although the strain levels involved are generally small and the commercial relevance is currently limited, this phenomenon remains an active area of academic interest due to its potential implications in flexible SMA systems [49].

II.4.6 Thermoelastic (superthermal) strain-temperature effect

Also known as the superthermal or thermoelastic effect (Fig. II.7), this property describes the behavior of SMAs under constant mechanical stress during thermal cycling. When an SMA initially in the Austenitic phase is subjected to a steady mechanical load and heated beyond its A_f temperature, it retains its shape. However, upon cooling, the formation of detwinned martensite under stress induces significant deformation.

The transformation begins at a stress-dependent temperature known as M_s^σ and continues until complete martensitic transformation at M_f^σ . Conversely, on heating, the reverse transformation begins at A_s^σ and completes at A_f^σ . The strain–temperature cycle traces a closed hysteresis loop, typical of thermoelastic materials, and is fully reversible due to the diffusionless nature of the transformation [50].

This effect underpins many SMA-based thermal actuators and is fundamental to shape recovery behavior under thermal cycling. It also enables energy storage and dissipation, making it useful in sensors and adaptive systems.

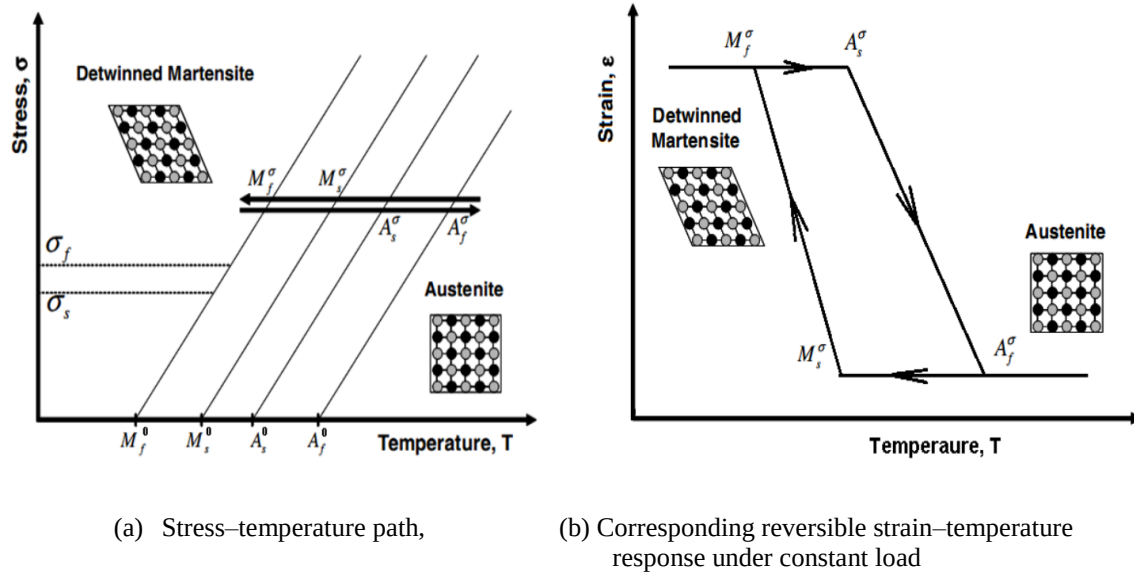


Figure II.7. Visualization of the thermoelastic effect in shape memory alloys [50].

II.5 A Review of Recent Advances in SMA Research (2015-2025)

The field of SMAs is far from static. The last decade has seen significant progress aimed at overcoming the limitations of conventional SMAs and expanding their functional envelope. This section summarizes key trends, drawing from recent dissertations and high-impact journal articles.

II.5.1 High-Temperature Shape Memory Alloys (HTSMAs)

A major limitation of commercial Ni-Ti alloys is their relatively low transformation temperature, typically below 100 °C. This precludes their use in high-temperature environments such as jet engines, automotive exhaust systems, and downhole oil and gas applications [51]. Research into HTSMAs, defined as those with transformation temperatures above 100 °C, has therefore been a major focus (Fig. II.8). The primary strategies involve ternary or quaternary additions to the Ni-Ti system:

Ni-Ti-X (X = Hf, Zr, Pd, Pt, Au): Adding a third element (X) that substitutes for either Ni or Ti can significantly increase transformation temperatures. Ni-Ti-Hf and Ni-Ti-Zr systems have shown promise, achieving transformation temperatures up to 300-500 °C while maintaining good shape memory properties [52, 53]. A 2021 doctoral thesis by Smith explored

the phase stability and cyclic performance of Ni-Ti-Hf alloys, demonstrating stable actuation up to 250 °C but also highlighting challenges with precipitate formation that can degrade performance over time [54]. Ni-Ti-Pd and Ni-Ti-Pt can reach even higher temperatures (>500 °C) but are prohibitively expensive for most applications [55].

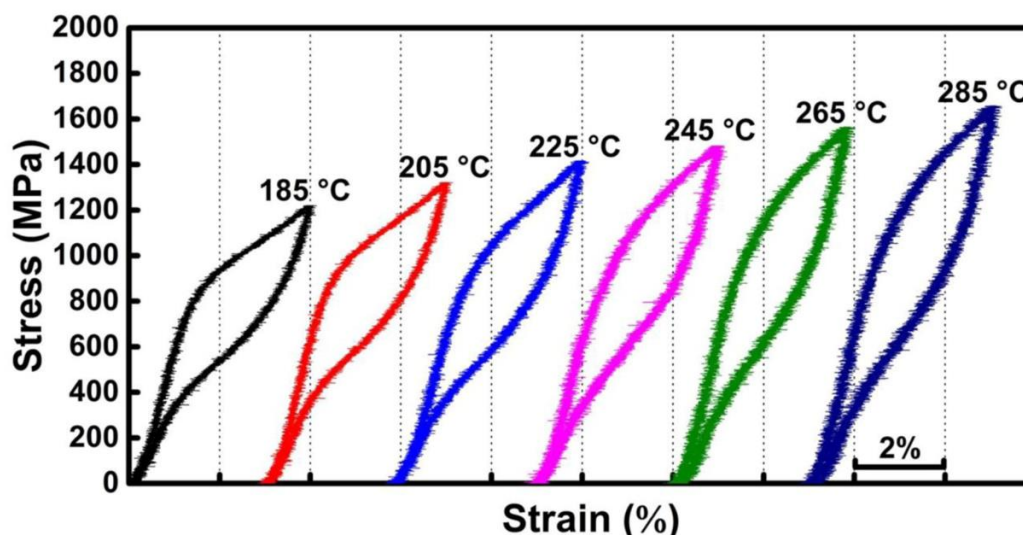


Figure II.8. Representative stress–strain curves for a high-temperature shape memory alloy recorded at constant temperatures between 185 °C and 285 °C, illustrating the alloy’s actuation capability and mechanical stability at elevated temperatures. [56]

II.5.2 Magnetic Shape Memory Alloys (MSMAs)

A notable advancement in the field is the emergence of magnetic shape memory alloys (MSMAs) (Fig. II.9), which respond to magnetic fields rather than temperature changes. The prototypical MSMA, Ni-Mn-Ga, can produce significant, rapid strains through the reorientation of martensitic variants under an applied magnetic field [57]. These materials are particularly appealing for applications requiring high-frequency actuation, since they offer actuation bandwidths that far exceed those of thermally activated SMAs [58, 59]. Research in the last decade has focused on improving the ductility of these alloys and reducing the required magnetic field strength, while also investigating alternative compositions such as Fe-Pd and Ni-Co-Al systems [60].

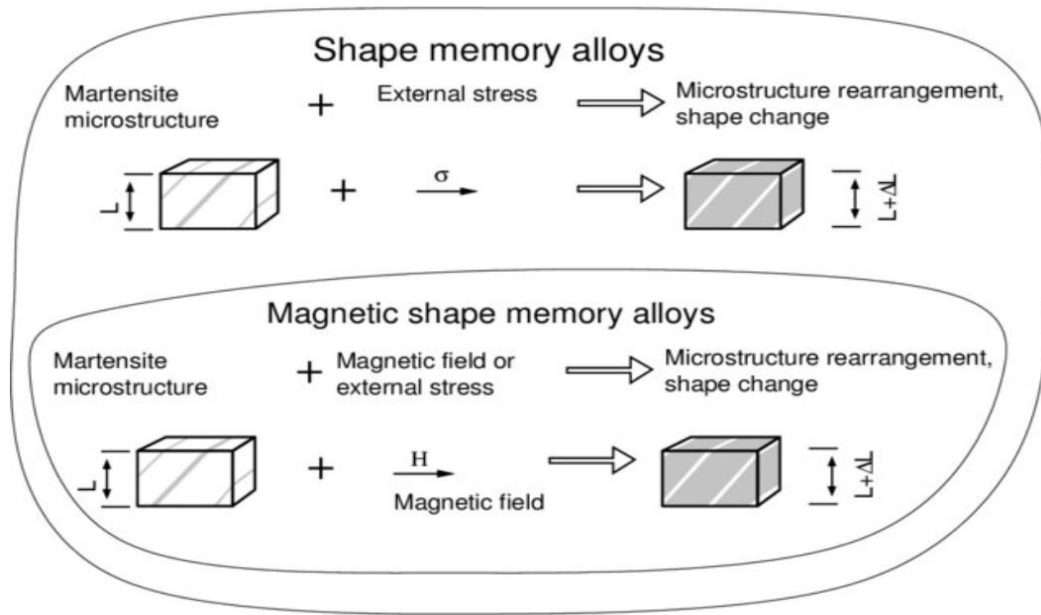


Figure II.9. Schematic comparing classical and magnetic. [61]

II.5.3 Additive Manufacturing of SMAs

Additive manufacturing (AM) techniques (Fig. II.10), particularly selective laser melting (SLM) and laser powder bed fusion (L-PBF), have revolutionized the fabrication of SMAs by enabling the production of components with intricate geometries and tailored architectures [62]. The ability to precisely control the composition and microstructure allows for the creation of functionally graded SMA parts, monolithic devices with integrated hinges, and custom biomedical implants [63]. However, significant challenges remain, as detailed in a 2023 dissertation by Chen [64]. These include:

- **Composition Control:** Evaporation of titanium during the high-temperature laser process can alter the Ni/Ti ratio, which has a profound effect on transformation temperatures.
- **Defects:** Porosity, lack of fusion, and residual stresses are common defects that can degrade the mechanical and memory properties.
- **Anisotropy:** The directional nature of the printing process can lead to anisotropic microstructures and properties.

Overcoming these challenges through process optimization and post-processing heat treatments is a very active area of current research [65, 66].

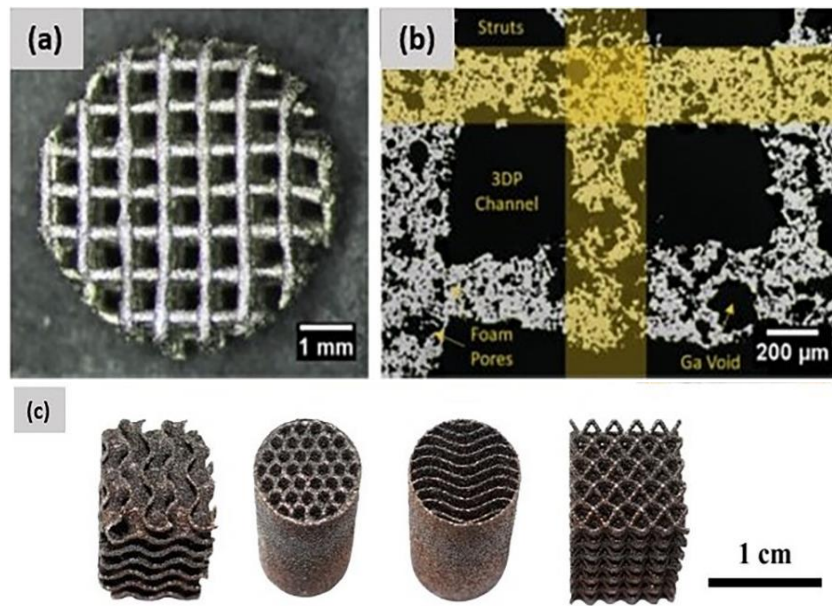


Figure II.10. Examples of Additive Manufacturing of SMAs: (a) Simple lattice structure, (b) Cross-sectional analysis of the microstructure, (c) Advanced architected designs. [67]

II.5.4 Porous and Foam SMAs

Creating porous or foam-like structures from SMAs combines the unique properties of the alloy with the benefits of a cellular structure, such as low density, high surface area, and the ability to accommodate fluid flow. Porous Ni-Ti has garnered significant interest for biomedical applications, particularly as orthopedic implants for bone replacement (Fig. II.11) [68]. The porous structure, with a stiffness similar to bone, can reduce stress shielding, while the interconnected pores promote bone ingrowth and integration [69]. Recent work has focused on using AM to precisely control the pore size, shape, and distribution to optimize both mechanical and biological performance [70].

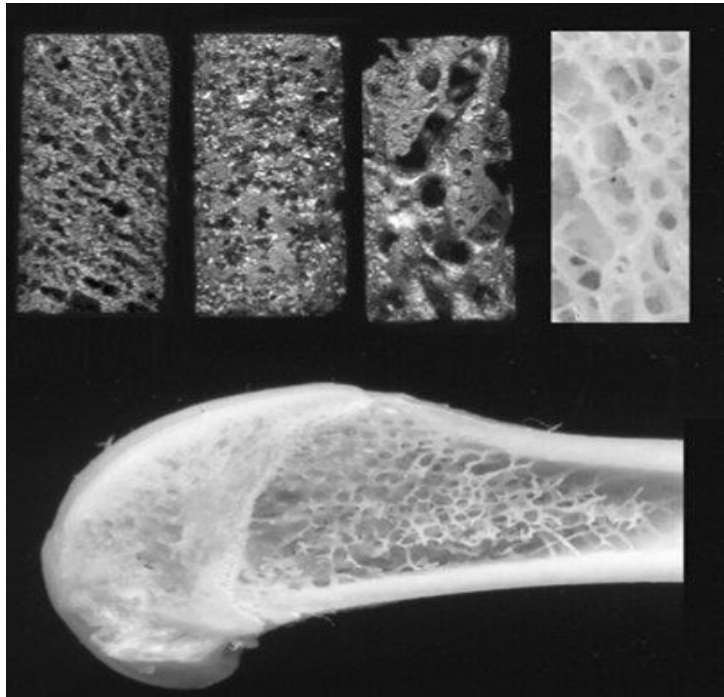


Figure II.11. Biomimetic Design of Porous NiTi to Replicate Trabecular Bone and Mitigate Stress Shielding. [71]

II.6 Applications of Shape Memory Alloys

The unique properties of SMAs have led to a diverse range of successful commercial applications across multiple industries. This section highlights key areas with project-based examples (Fig. II.12).

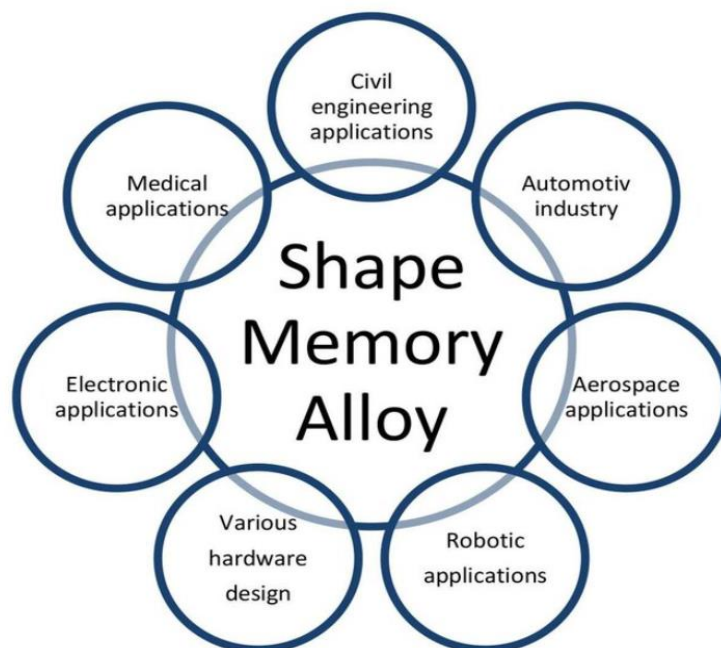


Figure II.12. Overview of the main application fields for Shape Memory Alloys. [34]

II.6.1 Aerospace and Space Applications

The aerospace industry values SMAs for their high power-to-weight ratio, reliability, and ability to perform actuation without pyrotechnics or complex motors.

- **Case Study: NASA's Variable Geometry Chevron (VGC):** Jet engine noise during takeoff and landing is a major environmental concern. NASA, in collaboration with Boeing, developed VGCs using SMAs to reduce this noise. The chevrons are tabs on the trailing edge of the engine nacelle. At low speeds, SMA actuators bend the chevrons into the exhaust stream, promoting mixing with ambient air and reducing noise. As the aircraft gains altitude and speed, the engine heat activates the SMA, causing the chevrons to retract to their undeformed, aerodynamically efficient shape [72, 73]. This passive, lightweight system improves fuel efficiency during cruise while reducing community noise.
- **Non-Explosive Release Mechanisms:** SMAs are used to create highly reliable, shock-free release devices for deploying solar panels, antennas, and scientific instruments on satellites. A common design uses a pre-stretched, superelastic Nitinol ring to hold a payload in place. To release the payload, a small heater is activated, triggering the OWSME in a separate SMA component that expands and breaks the ring, releasing the payload smoothly and without the debris or shock associated with explosive bolts [74]. The Frangibolt® is a well-known commercial example of this technology (Fig. II.13 and Fig. II.14) [75].

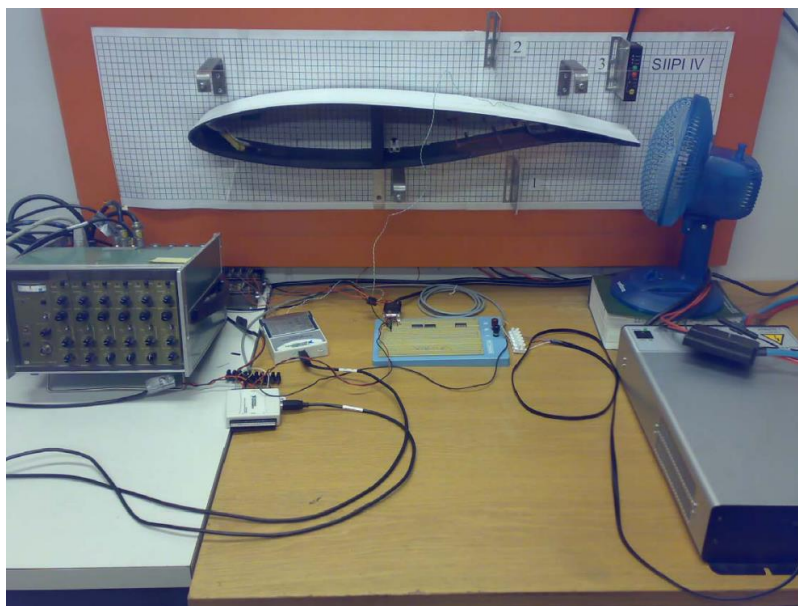


Figure II.13. Adaptive Aircraft Airfoil [76]

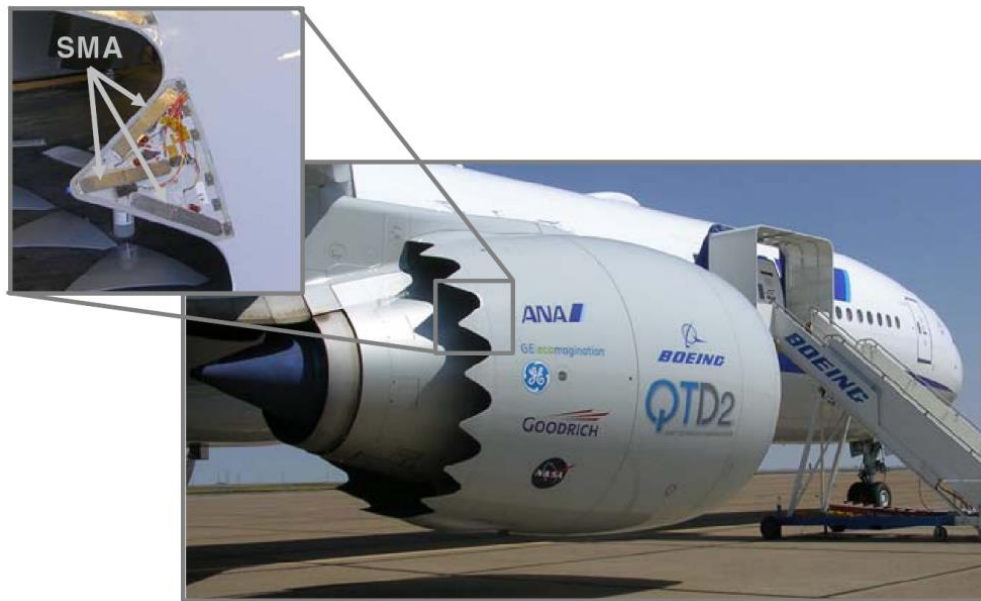


Figure II.14. Variable Geometry Jet Engine [76]

II.6.2 Biomedical Applications

The combination of superelasticity, biocompatibility, and shape memory effect makes Nitinol an ideal material for medical implants and instruments.

- **Case Study: The Self-Expanding Stent:** Coronary artery stents are mesh-like tubes used to prop open blocked arteries. SMA stents are delivered to the site of the blockage in a compressed, martensitic state via a catheter. Once in position, the catheter sheath is retracted, and the stent warms to body temperature (37°C). This temperature is above the stent's A_f , causing it to transform to austenite and expand to its predetermined, larger diameter with a constant, gentle outward force (due to the superelastic plateau), opening the artery [28, 77]. The superelasticity of Nitinol also allows the stent to flex with the natural movement of the artery without kinking or breaking. This has revolutionized interventional cardiology (Fig. II.15).

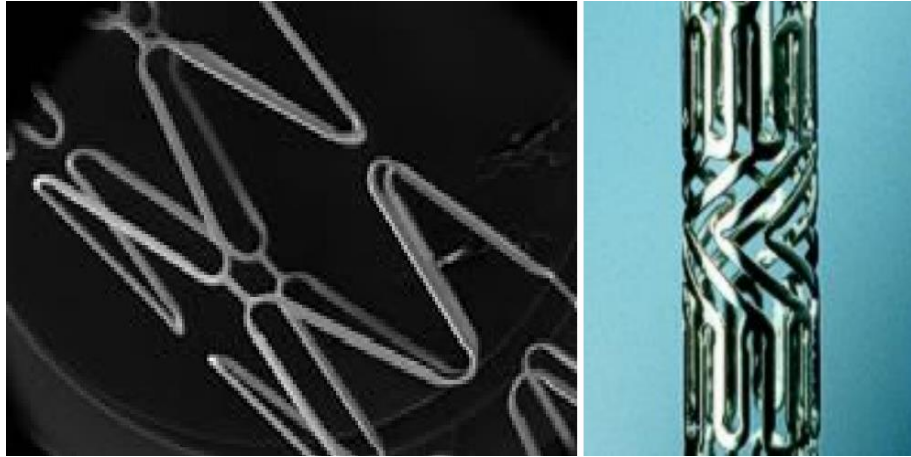


Figure II.15. Examples of Ni-Ti Stents [78]

- **Orthodontic Archwires:** Superelastic Nitinol wires exert a constant, gentle force on teeth over a wide range of deflection. This is in contrast to traditional stainless steel wires, which exert a high initial force that decays rapidly. The constant force from SMA wires moves teeth more efficiently and with less patient discomfort [41].
- **Surgical Instruments:** SMAs play a pivotal role in the design of endoscopic and laparoscopic tools. A prime example is the stone retrieval basket, which relies on the material's flexibility to maneuver through complex anatomical tracks before expanding into its functional shape [79]. Beyond these soft tissue applications, NiTi alloys are essential in dentistry and orthopedics. The endodontic files presented in Figure II.16 are used for root canal therapy, exploiting the alloy's superior flexibility and fatigue life [78]. Furthermore, Figure II.17 depicts NiTi osteosynthesis staples; these implants use the shape memory effect to apply sustained compression across fracture lines, effectively promoting bone consolidation [78].



Figure II.16. Example of Ni-Ti Endodontic Tools [78]



Figure II.17. Ni-Ti Osteosynthesis (Bone) Staples [78]

II.6.3 Automotive and Civil Engineering Applications

- **Automotive:** SMAs are used in actuators for engine temperature control, mirror folding mechanisms, and climate control vents. Their silent, reliable operation is a key advantage (Fig. II.18) [16].

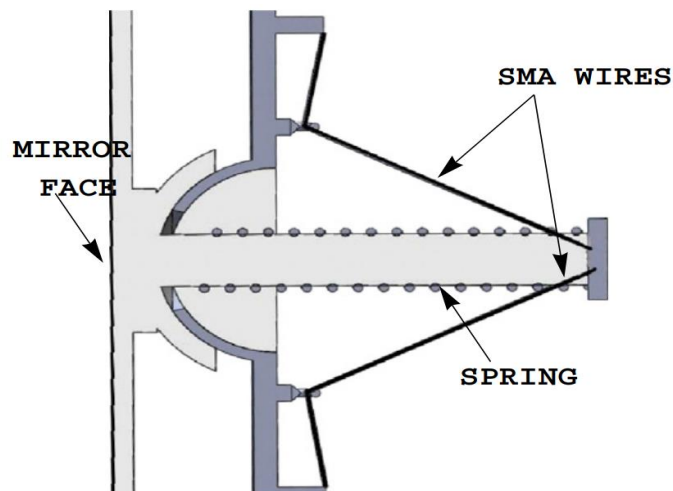


Figure II.18. SMA Side Mirror Actuator [80]

- **Civil Engineering:** Fe-based SMAs are being developed and used for pre-stressing and retrofitting concrete structures. SMA bars or strips can be installed on a structure, heated to induce recovery stress (creating a clamping force), and then act as passive

reinforcements. Their superelastic properties also provide excellent energy dissipation for seismic damping (Fig. II.19) [32, 47].

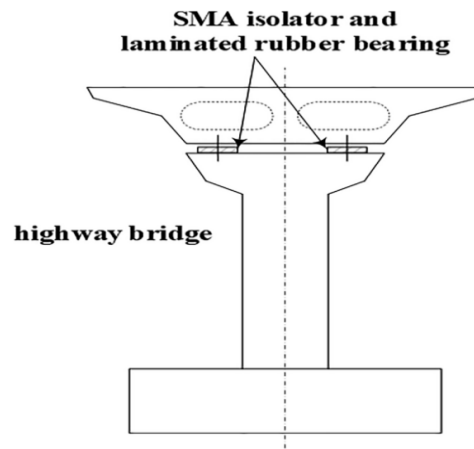


Figure II.19. SMA Isolator in a highway bridge. [81]

II.7 SMA Thin Layers: Fabrication and Properties

The continuous miniaturization of technological systems has positioned shape memory alloy (SMA) thin layers at the forefront of materials innovation for microscale and nanoscale devices. These layers are increasingly critical in micro-electromechanical systems (MEMS) and nano-electromechanical systems (NEMS), where conventional bulk materials often fall short in terms of integration, response time, and actuation precision [82].

II.7.1 Fabrication Techniques

The synthesis of SMA thin layers demands a high level of control over composition and microstructure to preserve the functional properties characteristic of their bulk counterparts. Among the available deposition methods, magnetron sputtering is considered the gold standard for fabricating Ni-Ti based SMA layers. In this process, a target composed of the desired alloy is bombarded with energetic ions within a controlled vacuum environment, resulting in the ejection and subsequent deposition of atoms onto a substrate such as silicon or glass. This enables the formation of homogeneous, well-adhered layers typically ranging from a few hundred nanometers up to several microns in thickness [83]. Achieving the desired shape memory behavior in thin layers is not trivial. The as-deposited layers are usually amorphous or exhibit limited crystallinity, necessitating subsequent thermal annealing. This heat treatment step facilitates the formation of the B2 austenite phase, which is indispensable for the manifestation of both shape memory and superelastic effects [84]. Furthermore, the precise regulation of deposition parameters including sputtering power, substrate bias, and chamber

pressure is critical to minimizing compositional deviations and ensuring the reproducibility of transformation temperatures.

II.7.2 Unique Properties and Applications

Thin layers of shape memory alloys retain the essential functional behaviors characteristic of bulk materials, yet their reduced dimensions make them exceptionally well-suited for actuation at the microscale. Due to their minimal thermal mass, these layers respond to heating and cooling much more quickly than conventional SMA components, enabling actuation at frequencies reaching several hundred hertz—performance that far exceeds what is achievable with larger-scale counterparts [85].

Key applications include (Fig. II.20):

- **Microvalves:** Thin layer SMA diaphragms can be integrated onto silicon chips to create microvalves for precise fluid control in microfluidic "lab-on-a-chip" devices [86].
- **Microgrippers:** Miniature grippers powered by SMA thin layer actuators can be used for manipulating microscopic objects, such as biological cells or micro-assembly components [87].
- **Micropumps:** SMA layers can be used to drive the diaphragms of micropumps, offering high power density in a small package [88].

The primary challenge in thin layer research is managing the influence of the substrate, which can constrain the layer's deformation and affect its fatigue life [89].

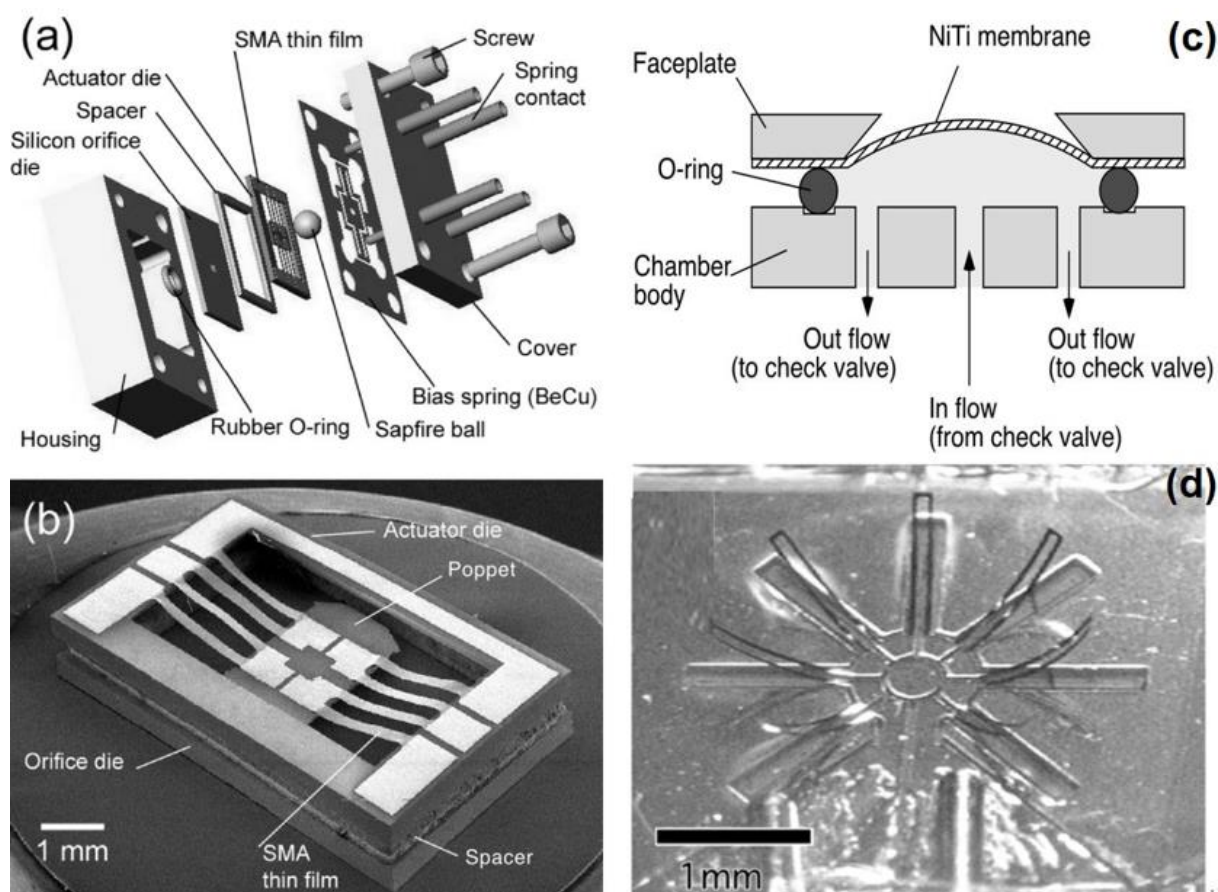


Figure II.20. Microvalve driven by SMA layer: (a) Exploded view and (b) Subassembly of micromachined parts; (c) Micropump; (d) Microgripper [90]

II.8 Conclusion

Shape Memory Alloys form a unique class of smart materials whose functional behavior is governed by a reversible martensitic phase transformation. This transformation enables large recoverable strains through the shape memory effect, as well as pseudoelastic behavior under mechanical loading. In this chapter, the fundamental physical mechanisms controlling SMA behavior have been reviewed, from crystallographic aspects and thermodynamic driving forces to the macroscopic responses observed under coupled thermal and mechanical stimuli.

The review has highlighted the diversity of SMA systems and applications, with particular emphasis on NiTi-based alloys due to their favorable combination of functional performance and technological maturity. At the same time, the literature clearly shows that SMA behavior is characterized by strong nonlinearity, hysteresis, and pronounced thermomechanical coupling, especially when subjected to complex loading paths and mechanical constraints.

These features pose significant challenges for predictive modeling and simulation. Accurate description of phase transformation mechanisms, internal variable evolution, and

energy dissipation requires robust constitutive formulations grounded in thermodynamic principles. The physical concepts and material characteristics discussed in this chapter therefore provide the necessary foundation for the constitutive modeling framework developed in the following chapter.

II.9 References

- [1] Y. Wu, X. Liu, B. Zhang, Y. Liang, and Y. Li, "Design of mechanically intelligent structures: Review of modelling stimuli-responsive materials for adaptive structures," *Heliyon*, vol. 10, no. 5, p. e34026, 2024, doi: 10.1016/j.heliyon.2024.e34026.
- [2] K. Otsuka and C. M. Wayman, Eds., *Shape Memory Materials*. Cambridge, UK: Cambridge University Press, 1998.
- [3] D. C. Lagoudas, Ed., *Shape Memory Alloys: Modeling and Engineering Applications*. New York, NY, USA: Springer, 2008.
- [4] W. J. Buehler, J. V. Gilfrich, and R. C. Wiley, "Effect of low-temperature phase changes on the mechanical properties of alloys near composition TiNi," *Journal of Applied Physics*, vol. 34, no. 5, pp. 1475-1477, 1963.
- [5] M. V. Gandhi and B. S. Thompson, *Smart Materials and Structures*. London, UK: Chapman & Hall, 1992.
- [6] B. Culshaw, "Smart structures and materials,". Boston, MA, USA: Artech House, 1996.
- [7] Y. Wu, Q. Zhang, Z. Zhang, and Q. Wang, "Multifunctional magnetic soft composites: a review," *Multifunctional Materials*, vol. 3, no. 4, p. 042003, 2020, doi: 10.1088/2399-7532/abb79e.
- [8] D. Pinheiro and T. Deivarajan, "A Concise Review Encircling Lead Free Porous Piezoelectric Ceramics," *Acta Physica Polonica A*, vol. 136, Sep. 2019, doi: 10.12693/APhysPolA.136.555.
- [9] A. Lendlein and S. Kelch, "Shape-memory polymers," *Angewandte Chemie International Edition*, vol. 41, no. 12, pp. 2034-2057, 2002.
- [10] K. Uchino, "Piezoelectric actuators and ultrasonic motors," Kluwer Academic Publishers, 1997.

- [11] B. Jaffe, W. R. Cook, and H. Jaffe, *Piezoelectric Ceramics*. London, UK: Academic Press, 1971.
- [12] A. E. Clark, "Magnetostrictive rare earth-Fe₂ compounds," in *Ferromagnetic Materials*, vol. 1, E. P. Wohlfarth, Ed. North-Holland, 1980, pp. 531-589.
- [13] Seeboth et al., "Thermochromic Polymers – Function by Design," *Chemical Reviews*, 114(5):3037–3068, 2014.
- [14] T. G. Ginder, "Rheology of magnetorheological fluids: Models and measurements," *MRS Bulletin*, vol. 23, no. 8, pp. 26-29, 1998.
- [15] W. M. Winslow, "Induced fibrillation of suspensions," *Journal of Applied Physics*, vol. 20, no. 12, pp. 1137-1140, 1949.
- [16] T. W. Duerig, K. N. Melton, D. Stöckel, and C. M. Wayman, Eds., *Engineering Aspects of Shape Memory Alloys*. London, UK: Butterworth-Heinemann, 1990.
- [17] J. Van Humbeeck, "Shape memory alloys: a material and a technology," *Advanced Engineering Materials*, vol. 3, no. 11, pp. 837-850, 2001.
- [18] K. Bhattacharya, *Microstructure of Martensite: Why it Forms and how it Gives Rise to the Shape-Memory Effect*. New York, NY, USA: Oxford University Press, 2003.
- [19] K. Otsuka and X. Ren, "Physical metallurgy of Ti–Ni-based shape memory alloys," *Progress in Materials Science*, vol. 50, no. 5, pp. 511-678, 2005.
- [20] T. Tadaki, Y. Nakata, and K. Shimizu, "Crystal structure of the martensite in Ti-Ni-Fe alloys," *Transactions of the Japan Institute of Metals*, vol. 28, no. 11, pp. 883-890, 1987.
- [21] H. Sehitoglu, I. Karaman, X. Zhang, and H. J. Maier, "On the shape memory and superelasticity of NiTi," *Materials Science and Engineering: A*, vol. 314, no. 1-2, pp. 67-75, 2001.
- [22] Y. Liu and P. G. McCormick, "Thermodynamic analysis of the martensitic transformation in NiTi," *Acta Metallurgica et Materialia*, vol. 42, no. 7, pp. 2401-2406, 1994.
- [23] H. Rojob, "Innovative Near-Surface Mounted Iron-Based Shape Memory Alloy for Strengthening Structures," 2017, Accessed: Jun. 28, 2025. [Online]. Available: <http://hdl.handle.net/11023/3583>

- [24] C. M. Friend, "The thermal and mechanical hysteresis in the shape memory alloy NiTi," *Journal de Physique IV*, vol. 5, no. C2, pp. C2-385, 1995.
- [25] D. C. Lagoudas, *Shape Memory Alloys: Modeling and Engineering Applications*, Springer, pp. 25-28, 2008.
- [26] M. Nekouei, M. Raghebi, and M. Mohammadi, "Free vibration analysis of laminated composite conical shells reinforced with shape memory alloy fibers," *Acta Mechanica*, vol. 230, Dec. 2019, doi: 10.1007/s00707-019-02501-z.
- [27] S. A. Shabalovskaya, "Surface, corrosion and biocompatibility aspects of Nitinol," *Biomedical Materials Engineering*, vol. 12, no. 1, pp. 69-109, 2002.
- [28] T. Duerig, A. Pelton, and D. Stöckel, "An overview of nitinol medical applications," *Materials Science and Engineering: A*, vol. 273–275, pp. 149-160, 1999.
- [29] J. M. Guilemany, J. Fernández, and R. M. T. L. Pons, "Advances in copper shape memory alloys," *Materials Science Forum*, vol. 327-328, pp. 177-184, 2000.
- [30] J. Dutkiewicz, "Phase transformations in β Cu-based shape memory alloys," *Journal of Materials Processing Technology*, vol. 50, no. 1-4, pp. 255-268, 1995.
- [31] A. Sato, E. Chishima, K. Soma, and T. Mori, "Shape memory effect in $\gamma \rightleftharpoons \epsilon$ transformation in Fe-30Mn-1Si alloy single crystals," *Acta Metallurgica*, vol. 30, no. 6, pp. 1177-1183, 1982.
- [32] J. L. A. Ortega, "Development and characterization of Fe-Mn-Si-based shape memory alloys for civil engineering applications," Ph.D. dissertation, Dept. of Mech. Eng., University of Texas at Austin, Austin, TX, 2019.
- [33] H. Funakubo, Ed., *Shape Memory Alloys*. Gordon and Breach Science Publishers, 1987.
- [34] I. Özkul, M. Kurgun, E. Kalay, C. Aksu Canbay, and K. Aldas, "Shape memory alloys phenomena: classification of the shape memory alloys production techniques and application fields," *The European Physical Journal Plus*, vol. 134, Nov. 2019, doi: 10.1140/epjp/i2019-12925-2.
- [35] R. Stalmans, J. Van Humbeeck, and L. Delaey, "Training of the two-way memory effect in copper-based shape memory alloys," *Journal de Physique IV*, vol. 1, no. C4, pp. C4-403, 1991.

- [36] Y. Liu, Y. Liu, and J. Van Humbeeck, "Two-way shape memory effect in a cold-drawn NiTi alloy," *Acta Materialia*, vol. 47, no. 1, pp. 199-209, 1999.
- [37] P. G. Perkins, "The mechanism of the 'two-way' shape memory effect," *Scripta Metallurgica*, vol. 8, no. 12, pp. 1469-1471, 1974.
- [38] D. Miller, "Design and performance of two-way shape memory alloy actuators," Ph.D. dissertation, Dept. of Aerospace Eng., Massachusetts Institute of Technology, Cambridge, MA, 2018.
- [39] L. C. Brinson, "One-dimensional constitutive behavior of shape memory alloys: thermomechanical derivation with non-constant material functions," *Journal of Intelligent Material Systems and Structures*, vol. 4, no. 2, pp. 229-242, 1993.
- [40] H. Tobushi, K. Tanaka, K. Kimura, T. Hori, and T. Sawada, "Stress-strain-temperature relationship associated with the R-phase transformation in TiNi shape memory alloy," *JSME International Journal, Series I*, vol. 35, no. 3, pp. 278-284, 1992.
- [41] F. Miura, M. Mogi, Y. Ohura, and H. Hamanaka, "The super-elastic property of the Japanese Ni-Ti alloy wire for use in orthodontics," *American Journal of Orthodontics and Dentofacial Orthopedics*, vol. 90, no. 1, pp. 1-10, 1986.
- [42] X. Chen and H. Zheng, "Application and Performance Evaluation of Superelastic Shape Memory Alloys in Building Vibration Isolation Systems," *Applied Mathematics and Nonlinear Sciences*, vol. 9, Jun. 2024, doi: 10.2478/amns-2024-1455.
- [43] P. Kumar, "Thermomechanical characterization and modeling of superelasticity in Nickel-Titanium alloys," Ph.D. dissertation, School of Materials Eng., Purdue University, West Lafayette, IN, 2016.
- [44] J. Van Humbeeck, "Damping capacity of shape memory alloys," *Journal de Physique IV*, vol. 6, no. C8, pp. C8-371, 1996.
- [45] V. G. Gavriljuk, V. V. Nemoshkalenko, J. Van Humbeeck, and P. C. M. Gubbels, "High damping capacity of NiTi and Ni-Ti-based alloys," *Scripta Materialia*, vol. 44, no. 11, pp. 2505-2510, 2001.
- [46] R. DesRoches, B. Fell, M. Delemont, and S. M. J. G. Futurum, "Application of shape memory alloys in seismic resistant design," *Proceedings of the 13th World Conference on Earthquake Engineering*, Vancouver, B.C., Canada, 2004, Paper No. 1092.

- [47] M. Dolce, D. Cardone, and R. Marnetto, "Implementation and testing of passive control devices based on shape memory alloys," *Earthquake Engineering & Structural Dynamics*, vol. 29, no. 7, pp. 945-968, 2000.
- [48] S. K. Wu, H. C. Lin, and T. S. Chou, "A study of the rubber-like behavior in a Cu-Zn-Al alloy," *Acta Metallurgica et Materialia*, vol. 38, no. 1, pp. 95-102, 1990.
- [49] G. S. Firstov, J. Van Humbeeck, Y. N. Koval, "Anelasticity and rubber-like behavior in martensitic alloys," *Materials Science and Engineering: A*, vol. 378, no. 1-2, pp. 2-10, 2004.
- [50] B. Meddour, *Modélisation et simulation du comportement thermomécanique des alliages à mémoire de forme*, Ph.D. dissertation, Dept. Génie Mécanique, Univ. Hadj Lakhdar de Batna, Batna, Algeria, 2016.
- [51] J. Ma, I. Karaman, and R. D. Noebe, "High-temperature shape memory alloys," *International Materials Reviews*, vol. 55, no. 5, pp. 257-315, 2010.
- [52] D. R. Johnson, "Development of NiTiHf high temperature shape memory alloys," Ph.D. dissertation, Dept. of Materials Science and Eng., The Ohio State University, Columbus, OH, 2017.
- [53] D. M. Norfleet, P. M. Sarosi, M. J. Mills, and M. J. Mills, "Precipitation in Ni-rich NiTiHf high-temperature shape-memory alloys," *Acta Materialia*, vol. 57, no. 12, pp. 3539-3553, 2009.
- [54] L. Smith, "Cyclic stability and microstructural evolution of NiTiHf high temperature shape memory alloys for aerospace actuation," Ph.D. dissertation, College of Eng., University of Michigan, Ann Arbor, MI, 2021.
- [55] S. C. Vogel, D. M. Teter, R. B. Schwarz, and J. F. Bingert, "Phase stability and transformation temperatures of NiTi-based high-temperature shape-memory alloys," *Metallurgical and Materials Transactions A*, vol. 33, no. 8, pp. 2545-2556, 2002.
- [56] S. Li et al., "A high-entropy high-temperature shape memory alloy with large and complete superelastic recovery," *Materials Research Letters*, vol. 9, no. 6, pp. 263–269, Jun. 2021, doi: 10.1080/21663831.2021.1893233.
- [57] K. Ullakko, J. K. Huang, C. Kantner, R. C. O'Handley, and V. V. Kokorin, "Large magnetic-field-induced strains in Ni₂MnGa single crystals," *Applied Physics Letters*, vol. 69, no. 13, pp. 1966-1968, 1996.

- [58] O. Heczko, "Magnetic shape memory alloys," *Materials Science and Technology*, vol. 27, no. 4, pp. 789-803, 2011.
- [59] R. D. James and M. Wuttig, "Magnetostriction of martensite," *Philosophical Magazine A*, vol. 77, no. 5, pp. 1273-1299, 1998.
- [60] L. Straka, A. Sozinov, and O. Heczko, "A review of magnetic shape memory alloys: From Ni-Mn-Ga to new systems," *Journal of Magnetism and Magnetic Materials*, vol. 547, p. 168869, 2022.
- [61] M. Chmielus, "Structure and Magneto-Mechanical Properties of NiMnGa Magnetic Shape-Memory Alloys," Verlag: Logos Verlag Berlin GmbH, Jan. 2010.
- [62] S. M. Speirs, M. S. B. bin, C. Dadbakhsh, S. V. D. Voorde, J. P. Kruth, and J. Van Humbeeck, "Selective laser melting of NiTi: an overview of the state-of-the-art and a review of the processing window," *Additive Manufacturing*, vol. 1, pp. 7-18, 2014.
- [63] M. Elahinia, "Fabrication and processing of NiTi implants: A review," *Progress in Materials Science*, vol. 83, pp. 630-663, 2016.
- [64] B. Chen, "Process-structure-property relationships in additively manufactured Nickel-Titanium," Ph.D. dissertation, Dept. of Mechanical Eng., Carnegie Mellon University, Pittsburgh, PA, 2023.
- [65] W. J. S. de Klerk, "The effect of post-processing on the properties of additively manufactured NiTi shape memory alloys," Ph.D. dissertation, University of Twente, Enschede, Netherlands, 2020.
- [66] H. L. Wei, T. T. T. Nguyen, Y. Zhang, and Z. C. Liu, "A review of additive manufacturing of NiTi shape memory alloys: processing, properties, and applications," *Journal of Materials Engineering and Performance*, vol. 30, pp. 3177–3208, 2021.
- [67] M. Mehrpouya et al., "Additive manufacturing of architected shape memory alloys: a review," *Virtual and Physical Prototyping*, vol. 19, no. 1, p. e2414395, Dec. 2024, doi: 10.1080/17452759.2024.2414395.
- [68] D. C. Dunand, "Processing of titanium foams," *Advanced Engineering Materials*, vol. 6, no. 6, pp. 369-376, 2004.

- [69] A. R. Pelton, V. Schroeder, M. Mitchell, L. Gong, and M. Barney, "Medical applications of porous Nitinol," *Materials Science Forum*, vol. 638-642, pp. 433-438, 2010.
- [70] H. P. Tang, F. P. Zhao, Y. Y. Zhao, N. Jia, and G. Y. Wang, "Porous NiTi alloys with tailored pore characteristics by selective laser melting," *Materials & Design*, vol. 99, pp. 101-107, 2016.
- [71] M. Bahraminasab, B. B. Sahari "(PDF) NiTi Shape Memory Alloys, Promising Materials in Orthopedic Applications," ResearchGate. Accessed: Jun. 29, 2025. [Online]. Available:
https://www.researchgate.net/publication/255179284_NiTi_Shape_Memory_Alloys_Promising_Materials_in_Orthopedic_Applications.
- [72] T. L. Turner, "NASA Shape Memory Alloy (SMA) Research Overview," NASA Technical Memorandum, NASA/TM-2009-215771, 2009.
- [73] R. G. Culley and J. H. Mabe, "Flight test of a shape memory alloy actuated variable geometry chevron," 45th AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit, Denver, CO, 2009, AIAA-2009-5147.
- [74] M. B. Pope, "Use of shape memory alloys for spacecraft mechanisms," *Proceedings of the 38th Aerospace Mechanisms Symposium*, NASA/CP-2006-214294, 2006.
- [75] TiNi Aerospace Inc., "Frangibolt® Non-Explosive Release Actuator," Product Datasheet, San Leandro, CA.
- [76] A. Duval, "Modélisation du comportement thermomécanique d'alliages à mémoire de forme. Application au dimensionnement de microsystèmes et extension en non local," Jan. 2009.
- [77] A. R. Pelton, D. Stöckel, and T. W. Duerig, "Medical uses of Nitinol," *Materials Science Forum*, vol. 327-328, pp. 63-70, 2000.
- [78] K. L. Taillard, "Étude du comportement thermomécanique des Alliages à Mémoire de Forme sous sollicitations multiaxiales complexes," phdthesis, École normale supérieure de Cachan - ENS Cachan, 2006. Accessed: Jun. 29, 2025. [Online]. Available:
<https://theses.hal.science/tel-00200906>
- [79] G. H. H. T. Song, "Applications of shape memory alloys in medicine," *Materials Science and Engineering: A*, vol. 273-275, pp. 755-766, 1999.

- [80] E. A. Williams, G. Shaw, and M. Elahinia, "Control of an automotive shape memory alloy mirror actuator," *Mechatronics*, vol. 20, no. 5, pp. 527–534, Aug. 2010, doi: 10.1016/j.mechatronics.2010.04.002.
- [81] S. Zareie, A. S. Issa, R. J. Seethaler, and A. Zabihollah, "Recent advances in the applications of shape memory alloys in civil infrastructures: A review," *Structures*, vol. 27, pp. 1535–1550, Oct. 2020, doi: 10.1016/j.istruc.2020.05.058.
- [82] M. Kohl, *Shape Memory Actuators*, Springer, 2004.
- [83] S. Miyazaki and A. Ishida, "Martensitic transformation and shape memory behavior in sputter-deposited TiNi-base thin layers," *Materials Science and Engineering: A*, vol. 273–275, pp. 106–133, 1999.
- [84] Y. Fu, H. Du, and S. Zhang, "Sputter-deposited TiNi thin layers: Effects of deposition temperature on microstructure and transformation behavior," *Materials Letters*, vol. 57, no. 18, pp. 2707–2713, 2003.
- [85] R. H. Wolf and A. H. Heuer, "TiNi (shape memory) layers for MEMS applications," *Journal of Microelectromechanical Systems*, vol. 4, no. 4, pp. 206–212, 1995.
- [86] P. Krulevitch, A. P. Lee, P. B. Ramsey, J. C. Trevino, J. Hamilton, and M. A. Northrup, "Thin layer shape memory alloy microactuators," *Journal of Microelectromechanical Systems*, vol. 5, no. 4, pp. 270–282, 1996.
- [87] M. Kohl, E. Just, W. Pfleging, and S. Miyazaki, "A novel thermo-magnetic-bias SMA microgripper with large gripping force," *Sensors and Actuators A: Physical*, vol. 93, no. 3, pp. 182–190, 2001.
- [88] C. L. Shih, B. K. T. Ho, C. J. Kim, and J. L. Judy, "A robust, high-speed, high-force, and low-voltage MEMS microactuator using a thin-layer shape memory alloy," *Journal of Microelectromechanical Systems*, vol. 10, no. 1, pp. 69–79, 2001.
- [89] Q. He, "Fatigue and fracture of TiNi shape memory alloy thin layers for MEMS applications," Ph.D. dissertation, Dept. of Mechanical and Aerospace Eng., University of California, Irvine, CA, 2018.
- [90] M. A. Zainal, S. Sahlan, and M. S. M. Ali, "Micromachined Shape-Memory-Alloy Microactuators and Their Application in Biomedical Devices," *Micromachines*, vol. 6, no. 7, Art. no. 7, Jul. 2015, doi: 10.3390/mi6070879.

CHAPTER III

**CONSTITUTIVE MODELING OF
SMA THERMOMECHANICAL
BEHAVIOR**

III.1 Thermodynamic Recalls

The behavior of shape memory alloys is governed by mechanical or thermal loadings, which necessitates the application of the laws of thermodynamics.

a. First Principle of Thermodynamics: It states that the change in internal energy, dU , is the sum of the energies exchanged with the exterior in the form of work, δW , and heat, δQ .

$$dU = \delta W + \delta Q \dots\dots\dots (III-1)$$

b. Second Principle of Thermodynamics: The entropy, dS , created by the exchange of heat is always greater than or equal to the quantity $\delta Q/T$, where T is the absolute temperature.

$$dS \geq \frac{\delta Q}{T} \dots\dots\dots (III-2)$$

c. Thermodynamic Potential: A thermodynamic potential is a function of state variables that describes the thermodynamic state of a system. The four common potentials are:

- ✓ Internal Energy: U
- ✓ Enthalpy: $H = U - \sigma: \epsilon$
- ✓ Helmholtz Free Energy: $\psi = U - sT$
- ✓ Gibbs Free Energy: $FED = H - sT = U - \sigma: \epsilon - sT$

For problems where stress (σ) and temperature (T) are the primary control variables, the Gibbs Free Energy is the most appropriate potential.

III.2 State Laws Derived from a Thermodynamic Potential

Considering a representative elementary volume (REV), the first principle (law of conservation of energy) can be expressed in its local form as:

$$du = \sigma: d\epsilon - \text{div}(q) + r \dots\dots\dots (III-3)$$

where u is the internal energy density, ϵ is the strain tensor, q is the heat flux vector, and r is an internal heat source. The second principle can be written locally as:

$$ds \geq \frac{r}{T} - \frac{\text{div}(q)}{T} \dots\dots\dots (III-4)$$

By combining these principles and using the definition of the Helmholtz free energy ($\psi = u - sT$), we arrive at the fundamental Clausius-Duhem inequality, which governs the energy dissipation within the material:

$$\sigma : d\varepsilon - d\psi - sdT \geq 0 \quad \text{..... (III-5)}$$

If we consider the Gibbs Free Energy, $FED(\sigma, T, f)$, where f is the internal variable representing the martensite fraction, the Clausius-Duhem inequality takes the form:

$$-\varepsilon : d\sigma - dFED - sdT \geq 0 \quad \text{..... (III-6)}$$

The total differential of FED is:

$$dFED = \left(\frac{\partial FED}{\partial \sigma} \right) : d\sigma + \left(\frac{\partial FED}{\partial T} \right) dT + \left(\frac{\partial FED}{\partial f} \right) df \quad \text{..... (III-7)}$$

Substituting this into the inequality yields:

$$\left(-\varepsilon - \frac{\partial FED}{\partial \sigma} \right) : d\sigma + \left(-s - \frac{\partial FED}{\partial T} \right) dT - \left(\frac{\partial FED}{\partial f} \right) df \geq 0 \quad \text{..... (III-8)}$$

For this inequality to hold true for any process, the terms associated with the non-dissipative variables (σ and T) must be zero. This gives us the state laws:

$$\varepsilon = - \frac{\partial FED}{\partial \sigma} \quad \text{..... (III-9)}$$

$$s = - \frac{\partial FED}{\partial T} \quad \text{..... (III-10)}$$

The inequality then reduces to the term representing the energy dissipated during the phase transformation:

$$- \left(\frac{\partial FED}{\partial f} \right) * df \geq 0 \quad \text{..... (III-11)}$$

This is the fundamental constraint that will be used to build our model.

III.3 One-Dimensional Modeling of SMA Behavior

We now apply the general thermodynamic framework to the one-dimensional case. We consider a Representative Elementary Volume (REV) that contains a mixture of austenite and martensite phases, as shown previously in Figure III-1.

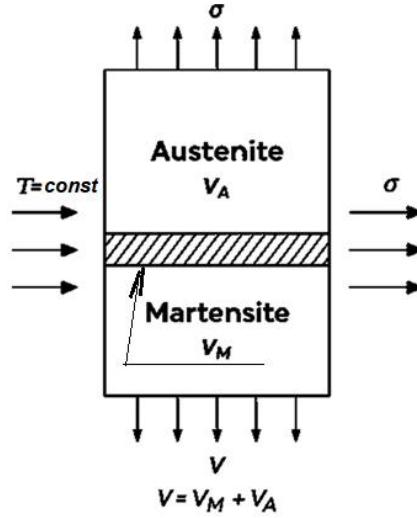


Figure III.1. Representative elementary volume. [1]

III.3.1 Gibbs Free Energy Potential

The specific form of the Gibbs Free Energy density, FED, for the 1D two-phase mixture is formulated as a sum of energetic contributions, consistent with the reference model¹:

$$\text{FED}(\sigma, T, f) = -\sigma^2/2 * [(1-f)/E_A + f/E_M] - \sigma \cdot f \cdot \varepsilon_0 + f \cdot B \cdot (f + 1)(T - T_0) + C \cdot f \cdot (f - 1) \quad \text{..... (III-12)}$$

Where:

$\frac{\sigma^2}{2} \cdot \left[\frac{1-f}{E_A} + \frac{f}{E_M} \right]$: Elastic strain energy density.

$\sigma \cdot f \cdot \varepsilon_0$: Mechanical energy associated with martensitic phase transformation.

$B \cdot f \cdot (f + 1) \cdot (T - T_0)$: Energy density due to the phase change.

$C \cdot f \cdot (f - 1)$: Interaction energy between the two phases (austenite and martensite).

Other parameters:

f: The martensite fraction can be expressed as: $f = \frac{V_M}{V_A + V_M}$

E_M and E_A : Elastic moduli (Young's modulus) of austenitic and martensitic phases respectively.

ε_0 : Maximum axial strain.

T_0 : Reference temperature.

B, C: Material constants to be identified.

From this potential, we can derive the law of behavior using the state law for strain:

$$\varepsilon = -\frac{\partial FED}{\partial \sigma} = \sigma \cdot \left(\frac{1-f}{E_A} + \frac{f}{E_M} \right) + f \cdot \varepsilon_0 \quad (III-13)$$

This expression highlights that the total strain consists of a linear mixture of the elastic strain contributions from austenite and martensite, augmented by the transformation-induced strain.

III.3.2 Thermodynamic and Dissipative Forces

The thermodynamic driving force for the phase transformation, F_{th} , is derived from the potential as

$$-\frac{\partial FED}{\partial f} \cdot \frac{df}{dt} \geq 0 \quad (III-14)$$

The driving force derived from FED is presented by:

$$-\frac{\partial FED}{\partial f} = THD^F \quad (III-15)$$

Due to energy dissipation, a pseudo-potential is assumed, denoted as:

$$PTH^D = -K \left(\frac{f^3}{3} + \frac{f^2}{2} \right) - Hf \quad (III-16)$$

From this pseudo-potential, the dissipative force can be derived as (PTH^D):

$$-\frac{dPTH^D}{df} = DIS^F \quad (III-17)$$

Therefore, it results in:

$$DIS^F = Kf(f + 1) + H \quad (III-18)$$

III.3.3 Transformation Criteria

For a transformation to proceed, the thermodynamic driving force must be equal to the dissipative force. This establishes the general criteria for the forward ($A \rightarrow M, f^* > 0$) and reverse ($M \rightarrow A, f^* < 0$) transformations⁸:

- Forward Transformation ($A \rightarrow M$): $THD^F = DIS^F$
- Reverse Transformation ($M \rightarrow A$): $THD^F = -DIS^F$

These conditions can be written using a transformation function, Ω , which must be equal to zero for the transformation to occur. For the forward transformation:

$$\Omega^{FOR}(\sigma, f, T) = THD^F - DIS^F = 0 \quad (III-19)$$

And for the reverse transformation:

$$\Omega^{REV}(\sigma, f, T) = THD^F + DIS^F = 0 \quad (III-20)$$

The consistency condition requires that the rate of change of the transformation function is zero during the transformation (i.e., $\frac{d\Omega}{dt} = 0$). Applying this condition allows us to derive the evolution law for the martensite fraction. For the forward transformation, this yields:

$$\Omega^{FOR}(\sigma, f, T) = \frac{\sigma^2}{2} \left[\left(\frac{1}{E_M} \right) - \left(\frac{1}{E_A} \right) \right] + \sigma \varepsilon_0 - B(2f + 1)(T - T_0) - C(2f - 1) - Kf(f + 1) - H = 0 \quad (III-21)$$

where K and H are material constants representing the hardening and the threshold for dissipation, respectively.

This fundamental equation governs the evolution of the material's internal state and forms the basis for simulating all the specific SMA phenomena.

As the function remains zero, its time derivative should also be null:

$$\frac{d\Omega}{dt} = \frac{\partial \Omega}{\partial \sigma} \cdot \frac{d\sigma}{dt} + \frac{\partial \Omega}{\partial T} \cdot \frac{dT}{dt} + \frac{\partial \Omega}{\partial f} \cdot \frac{df}{dt} = 0 \quad (III-22)$$

Hence, it can be deduced that:

$$\left[\sigma \cdot \left(\frac{1}{E_M} - \frac{1}{E_A} \right) + \varepsilon_0 \right] \dot{\sigma} - B \cdot (2f + 1) \dot{T} + [-2B(T - T_0) - 2C - K(2f + 1)] \cdot \dot{f} = 0 \quad (III-23)$$

$$\dot{f} = \frac{\left[\sigma \cdot \left(\frac{1}{E_M} - \frac{1}{E_A} \right) + \varepsilon_0 \right] \cdot \dot{\sigma} - B \cdot (2f + 1) \cdot \dot{T}}{-2B \cdot (T - T_0) - 2C - K \cdot (2f + 1)} \quad (III-24)$$

In the specific case of an isothermal condition, equation (14) simplifies to:

$$\dot{f} = - \frac{\left[\sigma \cdot \left(\frac{1}{E_M} - \frac{1}{E_A} \right) + \varepsilon_0 \right] \cdot \dot{\sigma}}{-2B \cdot (T - T_0) - 2C - K \cdot (2f + 1)} \quad (III-25)$$

For reverse transformation, similarly, the following condition applies:

$$THD^F = -DIS^F \quad (III-26)$$

The transformation criterion Ω is now expressed by:

$$\Omega^{REV}(\sigma, f, T) = THD^F + DIS^F \quad (III-27)$$

Hence, we derive:

$$\Omega^{REV}(\sigma, T, f) = \frac{\sigma^2}{2} \left[\left(\frac{1}{E_M} \right) - \left(\frac{1}{E_A} \right) \right] + \sigma \varepsilon_0 - B(2f + 1)(T - T^0) - C(2f - 1) + Kf(f + 1) + H$$

In analogy to equation (14), the fraction rate of martensite becomes:

$$\dot{f} = \frac{\left[\sigma \cdot \left(\frac{1}{E_M} - \frac{1}{E_A} \right) + \varepsilon^0 \right] \cdot \dot{\sigma} - B \cdot (2f + 1) \cdot \dot{T}}{-2B \cdot (T - T^0) - 2C + K \cdot (2f + 1)} \quad \text{..... (III-28)}$$

Under isothermal conditions (constant temperature):

$$\dot{f} = - \left[\sigma \cdot \left(\frac{1}{E_M} - \frac{1}{E_A} \right) + \varepsilon^0 \right] \cdot \frac{\dot{\sigma}}{\{-2B \cdot (T - T^0) - 2C + K \cdot (2f + 1)\}} \quad \text{..... (III-29)}$$

III.4 Modeling The Pseudoelasticity Effect

The pseudoelastic effect is observed when an SMA is mechanically loaded and unloaded at a constant temperature T_1 which is superior to the austenite finish temperature ($T_1 > A_f^0$). The material, initially in its austenitic state, undergoes a stress-induced transformation to martensite upon loading and spontaneously reverts to austenite upon unloading (Fig. III.2).

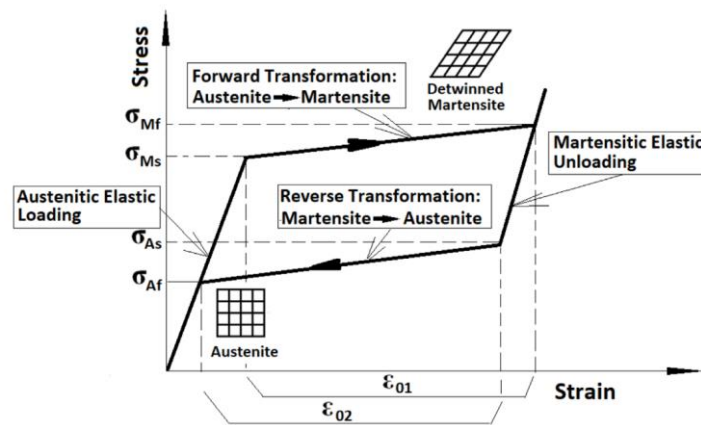


Figure III.2. Diagram illustrating pseudoelasticity effect.

III.4.1 Transformation Criteria Under Isothermal Conditions

This behavior is modeled by specializing the general transformation criteria for an isothermal process ($\frac{dT}{dt} = 0$).

The forward transformation ($A \rightarrow M$) during loading is governed by the criterion $\Omega^{FOR} = 0$:

$$\Omega^{FOR}(\sigma, f, T_1) = THD^F - DIS^F = 0 \quad \text{..... (III-30)}$$

Expanding this using the previously defined forces yields:

$$\frac{\sigma^2}{2} \left(\frac{1}{E_M} - \frac{1}{E_A} \right) + \sigma \varepsilon_0 - B(T_1 - T_0) - C(2f - 1) - Kf(f + 1) - H = 0 \quad \text{..... (III-31)}$$

The reverse transformation ($M \rightarrow A$) during unloading is governed by the criterion $\Omega^{REV} = 0$:

$$\Omega^{REV}(\sigma, f, T_1) = THD^F + DIS^F = 0 \quad \text{..... (III-32)}$$

Which expands to:

$$\frac{\sigma^2}{2} \cdot \left(\frac{1}{E_M} - \frac{1}{E_A} \right) + \sigma \cdot \varepsilon_0 - B \cdot (T_1 - T_0) - C \cdot (2f - 1) + K \cdot f \cdot (f + 1) + H = 0 \quad \text{..... (III-33)}$$

III.4.2 Determination of Material Constants

The four material constants that define the dissipative behavior (B, C, K, H) can be uniquely determined from a single experimental pseudoelastic stress-strain curve. This is achieved by evaluating the transformation criteria at the four critical points of the hysteresis loop:

- ✓ At the start of forward transformation: ($\sigma = \sigma_M^S, f = 0$)
- ✓ At the end of forward transformation: ($\sigma = \sigma_M^f, f = 1$)
- ✓ At the start of reverse transformation: ($\sigma = \sigma_A^S, f = 1$)
- ✓ At the end of reverse transformation: ($\sigma = \sigma_A^f, f = 0$)

Substituting these four conditions into the Ω_{FOR} and Ω_{REV} equations creates a solvable system of four linear equations for the four unknown constants.

III.4.3 Evolution Laws For The Isothermal Case

For an isothermal process, the general evolution laws simplify significantly. The rate of martensite formation during loading is given by:

$$\dot{f} = \frac{\left(\left[\sigma \cdot \left(\frac{1}{E_M} - \frac{1}{E_A} \right) + \varepsilon_0 \right] \cdot \dot{\sigma} \right)}{(2B \cdot (T_1 - T_0) + 2C + K \cdot (2f + 1))} \quad \text{..... (III-34)}$$

And for the reverse transformation during unloading:

$$\dot{f} = \frac{\left(\left[\sigma \cdot \left(\frac{1}{E_M} - \frac{1}{E_A} \right) + \varepsilon_0 \right] \cdot \dot{\sigma} \right)}{(2B \cdot (T_1 - T_0) + 2C - K \cdot (2f + 1))} \quad \text{..... (III-35)}$$

These equations provide the complete theoretical description of the pseudoelastic effect within the unified thermodynamic framework.

III.4.4 Determination of constants (B, C, K, H)

To determine the material constants, B, C, K and H , experimental tests performed on NiTi tubes at distinct constant temperatures (46°C, 56°C, 65°C, and 70°C) by Ng and Sun. [2] have been utilized. Specifically, experimental data at 65°C (summarized in Table III.1) were selected as reference to calculate these constants:

Table III.1. Experimental data at $T = 65^\circ\text{C}$, adapted from Ng and Sun [2].

σ_M^S (MPa)	268	E_M (MPa)	18442
σ_M^f (MPa)	275	M_s^0 (K)	279
σ_A^S (MPa)	62	ε_{01}	0.06106
σ_A^f (MPa)	37	ε_{02}	0.05903
E_A (MPa)	25775		

Reference temperature is fixed as:

$$T^0 = M_s^0$$

✓ At the beginning of forward transformation, the conditions are given by:

$$\sigma = \sigma_{MS}; T = T_1; f = 0$$

$$\Omega^{FOR}(\sigma = \sigma_{MS}, T = T_1, f = 0) = \left(\frac{\sigma_{MS}^2}{2}\right) * \left(\frac{1}{E_M} - \frac{1}{E_A}\right) + \sigma_{MS} * \varepsilon_{01} - B * (T_1 - M_s^0) + C - H = 0 \quad \text{..... (III-36)}$$

✓ At the end of forward transformation:

$$\sigma = \sigma_{MF}, T = T_1, f = 1$$

$$\Omega^{FOR}(\sigma = \sigma_{MF}, T = T_1, f = 1) = \left(\frac{\sigma_{MF}^2}{2}\right) * \left(\frac{1}{E_M} - \frac{1}{E_A}\right) + \sigma_{MF} * \varepsilon_{01} - 3B * (T_1 - M_s^0) - C - H = 0 \quad \text{..... (III-37)}$$

✓ At the start of reverse transformation:

$$\sigma = \sigma_{AS}, T = T_1, f = 1$$

$$\Omega^{REV}(\sigma = \sigma_{AS}, T = T_1, f = 1) = \left(\frac{\sigma_{AS}^2}{2}\right) * \left(\frac{1}{E_M} - \frac{1}{E_A}\right) + \sigma_{AS} * \varepsilon_{02} - 3B * (T_1 - M_s^0) + 2 * K + H = 0 \quad \text{..... (III-38)}$$

✓ At the end of reverse transformation:

$$\sigma = \sigma_{AF}, T = T_1, f = 0$$

$$\Omega^{REV}(\sigma = \sigma_{AF}, T = T_1, f = 0) = \left(\frac{\sigma_{AF}^2}{2} \right) * \left(\frac{1}{E_M} - \frac{1}{E_A} \right) + \sigma_{AF} * \varepsilon_{02} - B * (T_1 - M_s^0) + C + H = 0 \dots \dots \dots (III-39)$$

Resolving the equations system from (III-36) to (III-39), we obtained the values of constants B, C, K, H shown in Table III-2

Table III.2. Model parameters.

Value	Constant
0.08491	B (MPa. K -1)
-4.53424	C (MPa)
-0.25953	K (MPa)
7.36171	H (MPa)

III.5 Modeling of The Thermoelastic Effect (Superthermal)

The thermoelastic effect, also known as the superthermal effect, describes the behavior of an SMA under a constant mechanical stress ($\sigma = \sigma_0$) while subjected to a thermal cycle. The phase transformation is driven entirely by the change in temperature, resulting in a characteristic hysteresis loop in the strain-temperature diagram (Fig. III.3). This phenomenon is the basis for most thermally-activated SMA actuators.

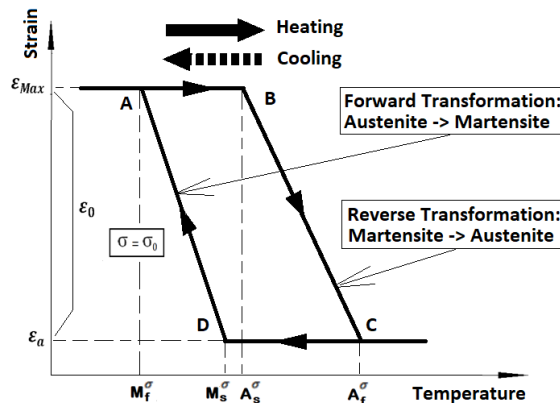


Figure III.3. Diagram showing the superthermal effect.

III.5.1 Transformation Criteria

This behavior is modeled by specializing the general transformation criteria for an isobaric process, where the stress is constant ($\frac{d\sigma}{dt} = 0$).

The forward transformation ($A \rightarrow M$) occurs upon cooling and is governed by the criterion:

$$\Omega^{\text{FOR}}(\sigma_0, f, T) = \text{THD}^F - \text{DIS}^F = 0 \quad \text{(III-40)}$$

Expanding this for the constant stress case yields:

$$\frac{\sigma^2}{2} \left[\left(\frac{1}{E_M} \right) - \left(\frac{1}{E_A} \right) \right] + \sigma \varepsilon_0 - B(2f + 1)(T - T_0) - C(2f - 1) - Kf(f + 1) - H = 0 \quad \text{(III-41)}$$

The reverse transformation (M $\rightarrow$ A) occurs upon heating and is governed by:

$$\Omega^{\text{REV}}(\sigma_0, f, T) = \text{THD}^F + \text{DIS}^F = 0 \quad \text{(III-42)}$$

Which expands to:

$$\frac{\sigma^2}{2} \left[\left(\frac{1}{E_M} \right) - \left(\frac{1}{E_A} \right) \right] + \sigma \varepsilon_0 - B(2f + 1)(T - T_0) - C(2f - 1) + Kf(f + 1) + H = 0 \quad \text{(III-43)}$$

III.5.2 Determination of Material Constants

The material constants (B, C, K, H) can also be determined from a single experimental strain-temperature curve conducted at a known constant stress, σ_0 . This is achieved by evaluating the criteria at the four critical transformation temperatures:

- ✓ At the start of forward transformation: ($T = M_s^\sigma, f = 0$)
- ✓ At the end of forward transformation: ($T = M_f^\sigma, f = 1$)
- ✓ At the start of reverse transformation: ($T = A_s^\sigma, f = 1$)
- ✓ At the end of reverse transformation: ($T = A_f^\sigma, f = 0$)

Substituting these four conditions into the Ω_{FOR} and Ω_{REV} equations creates a solvable system of four linear equations for the four unknown constants.

III.5.3 Evolution Laws for the Isobaric Case

For an isobaric process ($\frac{d\sigma}{dt} = 0$), the general evolution laws simplify. The rate of martensite formation during cooling ($\frac{dT}{dt} < 0$) is given by:

$$\frac{d\phi^{\text{For}}(\sigma, T, f)}{dt} = \left(\frac{\partial \phi^{\text{For}}}{\partial \sigma} \right) \cdot \left(\frac{d\sigma}{dt} \right) + \left(\frac{\partial \phi^{\text{For}}}{\partial T} \right) \cdot \left(\frac{dT}{dt} \right) + \left(\frac{\partial \phi^{\text{For}}}{\partial f} \right) \cdot \left(\frac{df}{dt} \right) = 0 \quad \text{(III-44)}$$

$$\dot{f} = - \frac{(B \cdot (2f + 1) \cdot \dot{T})}{(2B \cdot (T - T_0) + 2C + K \cdot (2f + 1))} \quad \text{(III-45)}$$

And for the reverse transformation during heating ($\frac{dT}{dt} > 0$):

$$\frac{d\phi^{Rev}(\sigma, T, f)}{dt} = \left(\frac{\partial \phi^{Rev}}{\partial \sigma}\right) \cdot \left(\frac{d\sigma}{dt}\right) + \left(\frac{\partial \phi^{Rev}}{\partial T}\right) \cdot \left(\frac{dT}{dt}\right) + \left(\frac{\partial \phi^{Rev}}{\partial f}\right) \cdot \left(\frac{df}{dt}\right) = 0 \quad \text{III-46}$$

$$\dot{f} = -\frac{(B \cdot (2f + 1) \cdot \dot{T})}{(2B \cdot (T - T_0) + 2C - K \cdot (2f + 1))} \quad \text{III-47}$$

These equations provide the complete theoretical description of the thermoelastic effect within the unified framework.

III.5.4 Determination of constants B, C, K and H

The phenomenological model contains four parameters (B, C, K, H) that must be identified from experimental data. In this study, calibration was performed independently for two different stress levels to assess the model's performance and parameter consistency. The parameters are determined by solving the system of four constitutive equations (Eq. III-44 to III-47) using the characteristic transformation temperatures ($M_s^\sigma, M_f^\sigma, A_s^\sigma, A_f^\sigma$) for each case.

III.5.4.1. Calibration at 65 MPa

For the 65 MPa stress level, the required experimental values were sourced from the study conducted by Bourbon et al. on a Cu-Zn-Al alloy. The characteristic values used for the calibration are presented in Table III.3.

Table III.3. Experimental data for Cu-Zn-Al at 65 MPa (Source: Bourbon et al.) [3].

M_s^σ (K)	324	A_s^σ (K)	330
M_f^σ (K)	311	A_f^σ (K)	340
E_A (MPa)	72000	ϵ_0	0.0255
E_M (MPa)	70000	ϵ_a	0.001063

III.5.4.2. Calibration at 100 MPa

To validate the model at a different condition, experimental data for a Cu-Zn-Al alloy (Cu – 25.57% Zn – 4.09% Al) under a constant stress of 100 MPa was sourced from the study by Bourbon et al. The characteristic transformation temperatures extracted from this data are listed in Table III.4. These values were subsequently used to solve the system of equations and determine the model parameters specific to this stress level.

Table III.4. Experimental data for Cu-Zn-Al at 100 MPa.

M_s^σ (K)	323	A_s^σ (K)	330
M_f^σ (K)	317	A_f^σ (K)	338
E_A (MPa)	72000	ε_0	0.0341
E_M (MPa)	70000	ε_a	0.00139

Applying equations (III-41) and (III-43), we obtain the conditions at each phase transformation stage:

✓ At the initiation of forward (direct) transformation:

$$\sigma = \sigma_0; T = M_s^\sigma; f = 0$$

$$\left(\frac{\sigma^2}{2}\right)\left(\frac{1}{E_M} - \frac{1}{E_A}\right) + \sigma\varepsilon_0 - B(M_s^\sigma - M_s^0) + C - H = 0 \quad \text{..... (III-48)}$$

✓ Upon completion of forward transformation:

$$\sigma = \sigma_0; T = M_f^\sigma; f = 1$$

$$\left(\frac{\sigma^2}{2}\right)\left(\frac{1}{E_M} - \frac{1}{E_A}\right) + \sigma\varepsilon_0 - 3B(M_f^\sigma - M_s^0) - C - 2K - H = 0 \quad \text{..... (III-49)}$$

✓ At the initiation of reverse transformation:

$$\sigma = \sigma_0; T = A_s^\sigma; f = 1$$

$$\left(\frac{\sigma^2}{2}\right)\left(\frac{1}{E_M} - \frac{1}{E_A}\right) + \sigma\varepsilon_0 - 3B(A_s^\sigma - M_s^0) - C + 2K + H = 0 \quad \text{..... (III-50)}$$

✓ Upon completion of reverse transformation:

$$\sigma = \sigma_0; T = A_f^\sigma; f = 0$$

$$\left(\frac{\sigma^2}{2}\right)\left(\frac{1}{E_M} - \frac{1}{E_A}\right) + \sigma\varepsilon_0 - B(A_f^\sigma - M_s^0) + C + H = 0 \quad \text{..... (III-51)}$$

To evaluate the accuracy of the simulations, the model was calibrated and compared with experimental data reported in the literature. Due to the phenomenological nature of the model, calibration was performed independently for each stress level.

For both the 65 MPa and 100 MPa cases, the model was calibrated using experimental data from Bourbon et al. [3]. The distinct sets of model parameters (B, C, K, H) derived for each case are listed in Table III.5 and Table III.6, respectively.

Table III.5. Calibrated model parameters for Cu-Zn-Al at $\sigma=65$ MPa.

B (MPa. K ⁻¹)	0.027128
C (MPa)	-0.047474
K (MPa)	0.27806
H (MPa)	-0.297643

Table III.6. Calibrated model parameters for Cu-Zn-Al at $\sigma = 100 \text{ MPa}$.

$B \text{ (MPa.K}^{-1}\text{)}$	0.175083
$C \text{ (MPa)}$	1.531983
$K \text{ (MPa)}$	-0.437709
$H \text{ (MPa)}$	2.188547

III.6 Modeling The One-Way Shape Memory Effect (SME)

III.6.1 General Description

The One-Way Shape Memory Effect (SME) refers to the ability of a Shape Memory Alloy (SMA) to recover a previously imposed strain when subjected to a heating cycle, after being deformed at low temperatures (Fig. III.4). This effect is classically characterized by three successive thermomechanical phases:

Step 1 – Mechanical loading at low temperature ($T < M_f^0$): The SMA is initially in a self-accommodated martensitic state. Upon increasing mechanical stress, martensitic variants reorient, producing a residual macroscopic strain.

Step 2 – Heating under zero stress ($\sigma = 0$): Upon heating beyond the critical temperature A_f^0 , the oriented martensite transforms back into austenite, recovering the initial shape.

Step 3 – Cooling under zero stress ($\sigma = 0$): The material transforms again into a self-accommodated martensitic phase. No external strain is generated due to variant self-cancellation.

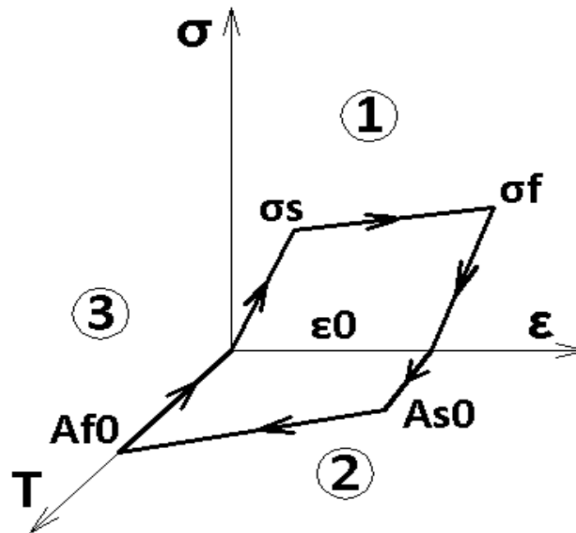


Figure III-4: Representation of the simple SME in the (ϵ, T, σ) space.

Each stage is modeled using the specific thermodynamic potential for this work.

III.6.2 Step 1: Reorientation of Martensite under Stress ($T < M_f^0$)

At low temperatures, the material is fully martensitic, and the elastic modulus is assumed constant and equal to E_M . Under increasing stress, reorientation of variants leads to an irreversible transformation strain. We consider the following Gibbs Free Energy Density for this specific configuration:

$$FED_1(\sigma, T, f) = -\frac{\sigma^2}{2E_M} - \sigma \cdot f \cdot \varepsilon_0 + f \cdot B \cdot (f + 1) \cdot (T - T_0) + C \cdot f \cdot (1 - f) \dots \dots \dots (III-52)$$

The Thermodynamic Driving Force for martensitic reorientation is given by:

$$THD_1^F = -\frac{\partial FED_1}{\partial f} = \sigma \cdot \varepsilon_0 - B \cdot (2f + 1) \cdot (T - T_0) - C \cdot (2f - 1) \dots \dots \dots (III-53)$$

The Dissipative Force is:

$$DIS^F = K \cdot f \cdot (f + 1) + H \dots \dots \dots (III-54)$$

The reorientation process follows the forward transformation criterion $\Omega^{FOR} = THD_1^F - DIS^F = 0$, which governs the evolution of the internal variable f as the stress increases during this stage.

III.6.3 Stage 2: Shape Recovery by Heating ($\sigma = 0$)

At the end of Stage 1, the material is in a fully oriented martensitic state ($f = 1$), exhibiting a remanent transformation strain. In Stage 2, the material is subjected to a thermal cycle at zero stress, i.e., $\sigma = 0$. The aim is to model the reverse transformation from oriented martensite to austenite, leading to complete strain recovery.

We use the general form of the Gibbs Free Energy Density defined in section III.3.1, with $\sigma = 0$:

$$FED_2(T, f) = f \cdot B \cdot (f + 1) \cdot (T - T_0) + C \cdot f \cdot (1 - f) \dots \dots \dots (III-55)$$

The driving force is calculated as:

$$THD_2^F = -\frac{\partial FED_2}{\partial f} = -B \cdot (2f + 1) \cdot (T - T_0) - C \cdot (2f - 1) \dots \dots \dots (III-56)$$

As the transformation is reverse ($M \rightarrow A$), the criterion becomes:

$$\Omega^{REV_2} = THD_2^F + DIS^F = 0 \dots\dots\dots (III-57)$$

Applying the consistency condition $\frac{d\Omega_{REV}}{dt} = 0$, we obtain the evolution law for the martensite fraction during heating:

$$\dot{f} = \frac{(B \cdot (2f+1) \cdot \dot{T})}{(2B \cdot (T-T_0) + 2C - K \cdot (2f+1))} \dots\dots\dots (III-58)$$

This equation governs the decrease of the internal variable f from 1 to 0 as the material is heated. The macroscopic strain recovery is expressed by:

$$\varepsilon = f \cdot \varepsilon_0 (\text{since } \sigma = 0) \dots\dots\dots (III-59)$$

Hence, when $f \rightarrow 0$, $\varepsilon \rightarrow 0$, which confirms the full shape recovery.

III.6.4 Stage 3: Martensitic Phase Reformation by Cooling ($\sigma = 0$)

Once the austenitic phase is fully restored ($f = 0$) at the end of Stage 2, the alloy is subjected to cooling under zero external stress. As the temperature decreases below the martensitic finish temperature M_f^0 , the austenite transforms into self-accommodated martensite.

A key physical distinction of this transformation is that, despite the internal phase change, no macroscopic strain is observed. To capture this behavior, we consider that the effective transformation strain is zero ($\epsilon_0 = 0$) at the macroscopic scale. The Gibbs Free Energy Density reduces to:

$$FED_3(T, f) = f \cdot B \cdot (f + 1) \cdot (T - T_0) + C \cdot f \cdot (1 - f) \dots\dots\dots (III-60)$$

The Thermodynamic Driving Force is therefore:

$$THD_3^F = -\frac{\partial FED_3}{\partial f} = -B \cdot (2f + 1) \cdot (T - T_0) - C \cdot (2f - 1) \dots\dots\dots (III-61)$$

This is a forward transformation ($A \rightarrow M$), so the criterion is:

$$\Omega^{FOR_3} = THD_3^F - DIS^F = 0 \dots\dots\dots (III-62)$$

Using $\frac{d\Omega_{FOR}}{dt} = 0$, we derive the evolution law for the martensite fraction during cooling:

$$\dot{f} = \frac{(B \cdot (2f+1) \cdot \dot{T})}{(2B \cdot (T-T_0) + 2C + K \cdot (2f+1))} \quad \text{..... (III-63)}$$

This equation governs the increase of the internal variable f from 0 to 1 as temperature decreases, while the macroscopic strain remains zero, thus providing a complete and thermodynamically consistent description of the SME.

III.7 Two-Dimensional Modeling of SMA Behavior

III.7.1 Introduction

The two-dimensional modeling of Shape Memory Alloys (SMAs) extends the thermodynamic formulation developed in the one-dimensional case to structures where a plane stress (PS) or plane strain (PE) assumption is valid. This framework aims to capture the mechanical response of thin SMA elements, such as plates and membranes, while maintaining thermodynamic consistency.

The derivation starts from the general Gibbs free energy density, adapted to 2D Voigt notation, and leads to the constitutive equations, transformation criteria, and evolution laws for the internal variable — the volume fraction of detwinned martensite f .

III.7.2 Compliance Tensors

A) Plane Stress (PS)

Austenite:

$$S_A^{PS} = \begin{bmatrix} \frac{1}{E_A} & -\frac{\nu}{E_A} & 0 \\ -\frac{\nu}{E_A} & \frac{1}{E_A} & 0 \\ 0 & 0 & \frac{1}{G_A} \end{bmatrix} \quad \text{..... (III-64)}$$

Martensite:

$$S_M^{PS} = \begin{bmatrix} \frac{1}{E_M} & -\frac{\nu}{E_M} & 0 \\ -\frac{\nu}{E_M} & \frac{1}{E_M} & 0 \\ 0 & 0 & \frac{1}{G_M} \end{bmatrix} \quad \text{..... (III-65)}$$

Where :

$$G_A = \frac{E_A}{2 \cdot (1 + \nu)} \quad \text{..... (III-66)}$$

$$G_M = \frac{E_M}{2 \cdot (1 + \nu)} \quad \text{..... (III-67)}$$

B) Plane Strain (PE)

The PE form is obtained from the full 3D compliance by enforcing $\varepsilon_{\{zz\}} = 0$. Reduced form:

Austenite:

$$S_A^{PE} = \begin{bmatrix} \frac{1-\nu^2}{E_A} & -\frac{\nu(1+\nu)}{E_A} & 0 \\ -\frac{\nu(1+\nu)}{E_A} & \frac{1-\nu^2}{E_A} & 0 \\ 0 & 0 & \frac{1}{G_A} \end{bmatrix} \dots\dots\dots (III-68)$$

Martensite:

$$S_M^{PE} = \begin{bmatrix} \frac{1-\nu^2}{E_M} & -\frac{\nu(1+\nu)}{E_M} & 0 \\ -\frac{\nu(1+\nu)}{E_M} & \frac{1-\nu^2}{E_M} & 0 \\ 0 & 0 & \frac{1}{G_M} \end{bmatrix} \dots\dots\dots (III-69)$$

III.7.3 Transformation Direction Vector

For equibiaxial transformation in Voigt notation:

$$R = \left[\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0 \right]^T \dots\dots\dots (III-70)$$

III.7.4 Pseudoelastic Effect

The pseudoelastic effect (superelasticity) occurs when an SMA is loaded–unloaded at a constant temperature $T_1 > A_f$. The transformation from Austenite to Martensite is induced by stress and is fully reversible. Gibbs free energy density is written as follows:

$$FED(\sigma, T, f) = -0.5\sigma^T \cdot S_{eff(f)} \cdot \sigma - \varepsilon_0 f \cdot \sigma^T \cdot R + B \cdot f \cdot (f + 1) \cdot (T - T_0) + Cf(f - 1) \dots\dots\dots (III-71)$$

with:

$$S_{eff(f)} = (1 - f) \cdot S_A + f \cdot S_M \dots\dots\dots (III-72)$$

$$\Delta S = S_M - S_A \dots\dots\dots (III-73)$$

The constitutive law:

$$\varepsilon = S_{eff(f)} \cdot \sigma + \varepsilon_0 \cdot f \cdot R \dots\dots\dots (III-74)$$

The thermodynamic driving force:

$$THD^{F(\sigma, T, f)} = 0.5\sigma^T \cdot \Delta S \cdot \sigma + \varepsilon_0 \sigma^T R - B \cdot f \cdot (f + 1) \cdot (T - T_0) - Cf(f - 1) \dots \dots \dots (III-75)$$

The dissipative force:

$$DIS^{F(f)} = K \cdot (2 \cdot f - 1) + H \dots \dots \dots (III-76)$$

Both transformation functions:

Forward transformation ($A \rightarrow M$):

$$\Omega^{FOR} = THDF - DISF = 0 \dots \dots \dots (III-77)$$

Reverse transformation ($M \rightarrow A$):

$$\Omega^{REV} = THDF + DISF = 0 \dots \dots \dots (III-78)$$

The partial derivatives:

Forward:

$$PTH_{\sigma FOR}^D = \Delta S \cdot \sigma + \varepsilon_0 \cdot R \dots \dots \dots (III-79)$$

$$PTH_{T FOR}^D = -B \cdot f \cdot (f + 1) \dots \dots \dots (III-80)$$

$$PTH_{f FOR}^D = -B \cdot (2 \cdot f + 1) \cdot (T - T_0) - 2 \cdot C \cdot f + C - 2 \cdot K \dots \dots \dots (III-81)$$

Reverse:

$$PTH_{\sigma REV}^D = \Delta S \cdot \sigma + \varepsilon_0 \cdot R \dots \dots \dots (III-82)$$

$$PTH_{T REV}^D = -B \cdot f \cdot (f + 1) \dots \dots \dots (III-83)$$

$$PTH_{f REV}^D = -B \cdot (2 \cdot f + 1) \cdot (T - T_0) - 2 \cdot C \cdot f + C + 2 \cdot K \dots \dots \dots (III-84)$$

Evolution Laws (Isothermal, $dT = 0$):

Forward:

$$\dot{f}_{FOR} = - \frac{\left[(PTH_{\sigma FOR}^D)^T \cdot d\sigma \right]}{\left[PTH_{f FOR}^D \right]} \dots \dots \dots (III-85)$$

Reverse:

$$\dot{f}_{REV} = - \frac{\left[(PTH_{\sigma REV}^D)^T \cdot d\sigma \right]}{\left[PTH_{f REV}^D \right]} \dots \dots \dots (III-86)$$

III.7.5 Thermoelastic Effect

The thermoelastic effect occurs when an SMA is subjected to a constant mechanical stress σ_0 while undergoing a thermal cycle (cooling/heating). In this case, the phase transformation is driven

by temperature rather than by stress, generating a recoverable macroscopic strain. This phenomenon is at the core of many SMA actuator applications.

Gibbs free energy density

For constant stress $\sigma = \sigma_0$:

$$FED(\sigma_0, T, f) = -0.5\sigma_0^T \cdot S_{eff(f)} \cdot \sigma_0 - \varepsilon_0 \cdot f \cdot \sigma_0^T \cdot R + B \cdot f \cdot (f + 1) \cdot (T - T_0) + C \cdot f \cdot (f - 1) \dots (III-87)$$

with:

$$S_{eff(f)} = (1 - f) \cdot S_A + f \cdot S_M \dots (III-88)$$

$$\Delta S = S_M - S_A \dots (III-89)$$

Constitutive Law:

$$\varepsilon = S_{eff(f)} \cdot \sigma_0 + \varepsilon_0 \cdot f \cdot R \dots (III-90)$$

Thermodynamic Driving Force:

Identical in form to the pseudoelastic case:

$$THD^F(\sigma_0, T, f) = 0.5 \cdot \sigma_0^T \cdot \Delta S \cdot \sigma_0 + \varepsilon_0 \cdot \sigma_0^T \cdot R - B \cdot f \cdot (f + 1) \cdot (T - T_0) - C \cdot f \cdot (f - 1) \dots (III-91)$$

Dissipative Force:

$$DIS^F = K \cdot (2 \cdot f - 1) + H \dots (III-92)$$

Transformation Functions

Forward (cooling, $A \rightarrow M$):

$$\Omega^{FOR} = THDF - DISF = 0 \dots (III-93)$$

Reverse (heating, $M \rightarrow A$):

$$\Omega^{REV} = THDF + DISF = 0 \dots (III-94)$$

Partial Derivatives

Forward:

$$PTH_{T_{FOR}}^D = -B \cdot f \cdot (f + 1) \dots (III-95)$$

$$PTH_{f_{FOR}}^D = -B \cdot (2 \cdot f + 1) \cdot (T - T_0) - 2 \cdot C \cdot f + C - 2 \cdot K \dots (III-96)$$

Reverse:

$$PTH_{T_{REV}}^D = -B \cdot f \cdot (f + 1) \dots (III-97)$$

$$PTH_{f_{REV}}^D = -B \cdot (2 \cdot f + 1) \cdot (T - T_0) - 2 \cdot C \cdot f + C + 2 \cdot K \dots (III-98)$$

Evolution Laws (Isobaric, $d\sigma = 0$)

Forward (cooling):

$$\dot{f}_{FOR} = - \frac{[PTH_{T_{FOR}}^D \cdot dT]}{[PTH_{f_{FOR}}^D]} \dots (III-99)$$

Reverse (heating):

$$\dot{f}_{REV} = - \frac{[PTH_{T_{REV}}^D \cdot dT]}{[PTH_{f_{REV}}^D]} \dots (III-100)$$

III.7.6 One-Way Shape Memory Effect (SME)

The One-Way SME describes the ability of an SMA, after being deformed at low temperature, to recover its original shape upon heating.

Stage 1: Low-Temperature Mechanical Loading (Orientation)

At $T_1 < M_f$, the material is fully martensitic. Mechanical stress reorients the martensite variants.

Gibbs free energy density:

$$FED_1(\sigma, T, f) = -0.5 \cdot \sigma^T \cdot S_M \cdot \sigma - \varepsilon_0 \cdot f \cdot \sigma^T \cdot R + B \cdot f \cdot (f + 1) \cdot (T - T_0) + C \cdot f \cdot (f - 1) \dots (III-101)$$

Thermodynamic driving force:

$$THD^F_1 = \varepsilon_0 \cdot \sigma^T \cdot R - B \cdot f \cdot (f + 1) \cdot (T - T_0) - C \cdot f \cdot (f - 1) \dots (III-102)$$

Dissipative force:

$$DIS^F = K \cdot (2 \cdot f - 1) + H \dots (III-103)$$

Transformation function:

$$\Omega^{FOR} = THDF_1 - DISF = 0 \dots (III-104)$$

Evolution Law (isothermal, $dT = 0$):

$$\dot{f} = - \frac{[(\varepsilon_0 \cdot R)^T \cdot d\sigma]}{[-B \cdot (2 \cdot f + 1) \cdot (T_1 - T_0) - 2 \cdot C \cdot f + C - 2 \cdot K]} \quad \text{(III-105)}$$

Stage 2: Heating under Zero Stress

After unloading from Stage 1, the material retains residual strain. Heating above A_f^0 transforms martensite into austenite.

Gibbs Free Energy Density:

$$FED_2(T, f) = B \cdot f \cdot (f + 1) \cdot (T - T_0) + C \cdot f \cdot (f - 1) \quad \text{(III-106)}$$

Transformation Function (reverse):

$$\Omega^{REV} = -B \cdot f \cdot (f + 1) \cdot (T - T_0) - C \cdot f \cdot (f - 1) + K \cdot (2 \cdot f - 1) + H = 0 \quad \text{(III-107)}$$

Evolution Law (isobaric, $\sigma = 0$):

$$\dot{f} = - \frac{[-B \cdot f \cdot (f + 1) \cdot dT]}{[-B \cdot (2 \cdot f + 1) \cdot (T - T_0) - 2 \cdot C \cdot f + C + 2 \cdot K]} \quad \text{(III-108)}$$

Stage 3: Cooling under Zero Stress

The fully austenitic material cools below M_s , transforming into self-accommodated martensite (no macroscopic strain).

Gibbs free energy density:

$$FED_3(T, f) = B \cdot f \cdot (f + 1) \cdot (T - T_0) + C \cdot f \cdot (f - 1) \quad \text{(III-109)}$$

Transformation function (forward):

$$\Omega^{FOR} = -B \cdot f \cdot (f + 1) \cdot (T - T_0) - C \cdot f \cdot (f - 1) - K \cdot (2 \cdot f - 1) - H = 0 \quad \text{(III-110)}$$

Evolution law (isobaric, $\sigma = 0, \varepsilon_0 = 0$):

$$\dot{f} = - \frac{[-B \cdot f \cdot (f + 1) \cdot dT]}{[-B \cdot (2 \cdot f + 1) \cdot (T - T_0) - 2 \cdot C \cdot f + C - 2 \cdot K]} \quad \text{(III-111)}$$

III.7.7 Identification of Material Parameters

The four material parameters (B, C, K, H) are determined experimentally from characteristic transformation points measured on stress–strain or strain–temperature curves. For each phenomenon, the identification procedure is based on evaluating the transformation functions Ω^{FOR} and Ω^{REV} at four critical points of the hysteresis loop.

III.7.7.1 Pseudoelasticity

The four characteristic points at constant temperature $T_1 > A_f$ are:

Start of forward transformation:

$$f = 0, \sigma = \sigma_M^s, T = T_1$$

$$\Omega^{FOR}(\sigma_M^s, T_1) = 0 \quad \text{..... (III-112)}$$

End of forward transformation:

$$f = 1, \sigma = \sigma_M^f, T = T_1$$

$$\Omega^{FOR}(\sigma_M^f, T_1) = 0 \quad \text{..... (III-113)}$$

Start of reverse transformation:

$$f = 1, \sigma = \sigma_A^s, T = T_1$$

$$\Omega^{REV}(\sigma_A^s, T_1) = 0 \quad \text{..... (III-114)}$$

End of reverse transformation:

$$f = 0, \sigma = \sigma_A^f, T = T_1$$

$$\Omega^{REV}(\sigma_A^f, T_1) = 0 \quad \text{..... (III-115)}$$

From the general expressions of Ω^{FOR} and Ω^{REV} :

Forward:

$$\Omega^{FOR} = 0.5 \cdot \sigma^T \cdot \Delta S \cdot \sigma + \varepsilon_0 \cdot \sigma^T \cdot R - Bf(f+1)(T-T_0) - Cf(f-1) - K(2f-1) - H \quad \text{..... (III-116)}$$

Reverse:

$$\Omega^{REV} = 0.5 \cdot \sigma^T \cdot \Delta S \cdot \sigma + \varepsilon_0 \cdot \sigma^T \cdot R - Bf(f+1)(T-T_0) - Cf(f-1) + K \cdot (2 \cdot f - 1) + H \quad \text{..... (III-117)}$$

By substituting the four sets (σ, f, T) into the above, we obtain a linear system of four equations in the four unknowns B, C, K, H . Solving this system yields the material parameters for the pseudoelastic effect.

III.7.7.2 Thermoelastic Effect

The four characteristic points at constant stress σ_0 are:

Start of forward transformation:

$$f = 0, T = M_s^\sigma, \sigma = \sigma_0$$

$$\Omega^{FOR}(\sigma_0, M_s^\sigma, 0) = 0 \quad \text{..... (III-118)}$$

End of forward transformation:

$$f = 1, T = M_f^\sigma, \sigma = \sigma_0$$

$$\Omega^{FOR}(\sigma_0, M_f^\sigma, 1) = 0 \quad \text{..... (III-119)}$$

Start of reverse transformation:

$$f = 1, T = A_s^\sigma, \sigma = \sigma_0$$

$$\Omega^{REV}(\sigma_0, A_s^\sigma, 1) = 0 \dots\dots\dots (III-120)$$

End of reverse transformation:

$$f = 0, T = A_f^\sigma, \sigma = \sigma_0$$

$$\Omega^{REV}(\sigma_0, A_f^\sigma, 0) = 0 \dots\dots\dots (III-121)$$

Substituting these four (σ, f, T) sets into the forward/reverse transformation functions provides another linear system in B, C, K, H . This procedure uses strain–temperature data instead of stress–strain data.

III.7.7.3 One-Way Shape Memory Effect (SME)

For SME, parameters are identified separately for each stage:

Stage 1 (Reorientation):

Constants C, K, H specific to reorientation are extracted from a low-temperature tensile test ($T < M_f$), using the start σ_s and finish σ_f of reorientation:

$$\Omega^{FOR}(\sigma_s, T, f = 0) = 0 \dots\dots\dots (III-122)$$

$$\Omega^{FOR}(\sigma_f, T, f = 1) = 0 \dots\dots\dots (III-123)$$

These two equations, combined with independent calibration of B from Stage 2, determine K and H .

Stage 2 (Reverse transformation) and Stage 3 (Forward transformation):

Parameters B, C, K, H are calibrated using strain–temperature curves under $\sigma = 0$, following the same four-point procedure as in the thermoelastic effect.

III.8 Conclusion

This chapter has presented the development of a unified thermomechanical constitutive model for Shape Memory Alloys (SMAs). Starting from the fundamental principles of thermodynamics and a carefully selected Gibbs free energy potential, a phenomenological framework was established to describe the complex mechanisms associated with martensitic phase transformations.

The originality of the proposed model lies in its specific mathematical formulation, particularly in the non-linear expression of the interaction potential energy and the associated dissipative forces. This formulation enables an accurate representation of the characteristic hysteresis behavior observed in SMAs. One of the main contributions of this work is the successful extension of the constitutive formulation from a one-dimensional representation to a two-dimensional plane stress framework, demonstrating the consistency and reliability of the proposed theoretical foundations for engineering-scale analyses.

The capability of this unified framework is further illustrated by its ability to reproduce the principal thermomechanical responses of SMAs, including pseudoelasticity and thermally driven shape memory effects, within a single and coherent set of constitutive equations. This unified description highlights the flexibility of the model and its suitability for capturing history-dependent material behavior under coupled loading conditions.

Overall, this chapter establishes a solid constitutive basis that enables advanced numerical implementations and detailed simulations of SMA-based components. The proposed model provides the foundation for the numerical analyses presented in the following chapters, where its performance is assessed under representative mechanical and thermomechanical loading scenarios. Future extensions of this work may include the incorporation of cyclic effects or functional fatigue, further enhancing the predictive capabilities of the model for long-term applications.

III.9 References

- [1] I. Zidane and B. Meddour, “On modelling of the one-dimensional pseudoelastic effect of shape memory alloys,” *Mechanics & Industry*, vol. 26, p. 6, 2025, doi: 10.1051/meca/2024040.
- [2] K.L. Ng, Q.P. Sun, “Stress-induced phase transformation and detwinning in NiTi polycrystalline shape memory alloy tubes,” *Mechanics of Materials*, vol. 38, pp. 41–56, 2006. doi:10.1016/j.mechmat.2005.05.008
- [3] G. Bourbon, “Contribution à l'étude isotherme et anisotherme du comportement cyclique des AMF,” PhD dissertation, Université de Franche-Comté, 1994.

CHAPTER IV
NUMERICAL IMPLEMENTATION
AND SIMULATION

Chapter IV: Numerical Implementation and Simulation

The theoretical constitutive models developed in Chapter 3 are now translated into a functional computational framework. This chapter details the implementation strategy and presents systematic simulations of the models by comparing their numerical predictions with reference thermomechanical responses reported in the literature for the major SMA phenomena. The objective is to verify the numerical implementation and assess the model response under controlled loading conditions.

IV.1 Implementation Strategy

The thermomechanical constitutive models formulated in Chapter 3 including Gibbs free energy definitions, transformation criteria, and stress–strain relationships were translated into computational tools for engineering applications. The parameter sets identified in Tables III-2, III-5, and III-6 provide the calibrated material constants used in all simulations. This section outlines the numerical platforms and simulation workflow, ensuring no repetition of the theoretical derivations presented in Chapter 3.

IV.1.1 Computational Platforms

MATLAB and Python – Primary Development Environment

In-house numerical codes developed in MATLAB and Python were used for representative one-dimensional and two-dimensional simulations presented in this chapter. These platforms offered:

- Rapid prototyping without compilation delays;
- Full algorithmic transparency for tracing state variables and debugging transformation behavior;
- Integrated optimization tools for parameter identification using literature datasets;
- Advanced visualization of stress–strain–temperature–martensite fraction relationships.

Abaqus/UMAT – Industrial Interface

In addition to the in-house MATLAB/Python numerical implementations used for systematic verification, a FORTRAN UMAT was developed for Abaqus/Standard to ensure compatibility with commercial finite element workflows. The UMAT was first verified under one-dimensional uniaxial pseudoelastic loading at the material-point level, and it was subsequently exercised in numerical simulations two-dimensional Abaqus simulations (reported in Chapter V) to assess field

homogeneity, post-processing consistency (contours and local histories), and stable numerical response under multiaxial loading conditions.

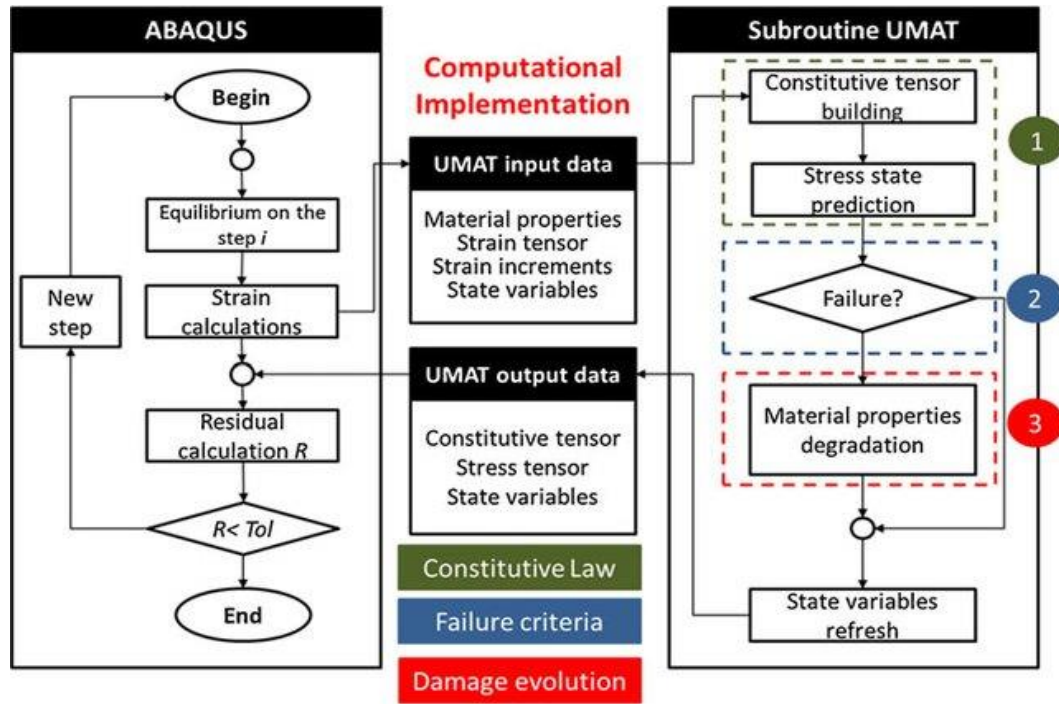


Figure IV.1. Data flow and computational sequence between Abaqus/Standard and the UMAT at each integration point, highlighting the constitutive update (state variables, stress update, and consistent tangent where applicable). [1]

IV.1.2 Dimensional Scope

- ✓ 1D (Uniaxial) – Scalar stress–strain formulation used for initial algorithm verification and parameter calibration at the material-point level;
- ✓ 2D (Planar) – Plane-stress formulations expressed in Voigt notation, with stress and strain vectors $\sigma, \varepsilon \in \mathbb{R}^3 \times 1$ and associated 3×3 compliance and stiffness matrices, enabling the description of in-plane multiaxial loading conditions relevant to thin-layer configurations.

In the adopted one- and two-dimensional formulations, the framework consistently tracks the martensite fraction f , the transformation strain magnitude ε_0 , and the transformation direction R , while the equivalent compliance $S_{eq(f)}$ governs the recoverable elastic response throughout the transformation process.

IV.1.3 Material Systems and Data Sources

The numerical simulations are based on three experimental datasets introduced in Chapter 3:

- ✓ **Pseudoelasticity** – NiTi specimens subjected to isothermal mechanical loading (Ng and Sun, 2006);
- ✓ **Thermoelasticity** – Cu–Zn–Al alloys under constant applied stress (65 MPa and 100 MPa, Bourbon);
- ✓ **Shape Memory Effect** – Three-stage thermomechanical cycling (orientation, recovery, cooling) under uniaxial and multiaxial loading conditions (Ng K. L. et al.).

IV.1.4 Numerical Integration Scheme

The computational sequence for model implementation was organized into two complementary levels:

- Numerical algorithm (predictor–corrector):

1. Parameter calibration in one-dimensional loading using MATLAB/Python optimization routines;
2. Elastic predictor based on the current equivalent compliance;
3. Transformation predictor derived from thermodynamic driving forces;
4. Stress corrector ensuring equilibrium and consistency;
5. State update including the evolution of internal variables.

- Development stages:

1. Algorithm prototyping and debugging in one-dimensional configurations;
2. Extension to multiaxial two-dimensional formulations;
3. Simulation against reference experimental datasets;
4. Parameter sensitivity analysis;
5. Performance optimization for computational efficiency.

IV.1.5 Verification and Simulation Workflow

The verification and simulation process followed a structured sequence:

1. Acquisition of experimental stress–strain–temperature datasets from the literature;
2. Calibration of material parameters in one-dimensional configurations using MATLAB/Python routines, followed by cross-simulation in two-dimensional formulations under matched loading conditions;

3. Quantitative assessment of accuracy using hysteresis loop characteristics and consistency of material-parameter effects on phase transformation;
4. Verification of industrial compatibility through one-dimensional UMAT integration in Abaqus;
5. Assessment of numerical consistency through mesh refinement and boundary-condition variations analyses in two-dimensional configurations.

IV.1.6 Development of Standalone Computational Tools

Dedicated standalone computational tools were developed in MATLAB and Python to enable independent use of the constitutive models outside commercial finite element software. These implementations provide:

1. Transparent algorithmic access for research and education;
2. Efficient parameter calibration and numerical testing under various loading paths;
3. Compatibility with Abaqus UMAT, verified under one-dimensional pseudoelastic loading;
4. A modular structure allowing extension toward advanced two-dimensional and multiaxial formulations.

These tools ensure flexibility for academic studies and industrial-oriented analyses, while maintaining full consistency with the numerical framework described above.

IV.2 Simulation of the Pseudoelastic Model

The simulation of the constitutive framework begins with the pseudoelastic effect. This phenomenon is examined hierarchically, starting from the fundamental 1D case and progressing from one-dimensional to two-dimensional numerical simulations. The material and model parameters used for this study are summarized in Table IV.1.

Table IV.1. Material and model parameters used for the pseudoelasticity Simulation, calibrated from [2].

Parameter	Description	Value	Unit
E_A	Young's Modulus (Austenite)	25775	MPa
E_M	Young's Modulus (Martensite)	18442	MPa
ν	Poisson's Ratio	0.3	-
ϵ^0	Max. Transformation Strain	0.06106	-
T	Operating Temperature	343.15	K
M_S^0	Martensite Start Temp. (Zero Stress)	279	K
B	(Constant)	0.18746	MPa/K
C	(Constant)	-0.88082	MPa
K	(Constant)	1.44134	MPa
H	(Constant)	8.007499	MPa

IV.2.1 1D Uniaxial Simulation

The model was calibrated and verification against experimental data from NiTi tubes reported by Ng and Sun. [2] at temperatures ranging from 46°C to 70°C. The simulated stress–strain hysteresis loops (Figures IV-2 to IV-6) reproduce the main features of pseudoelastic behavior, including forward and reverse transformation, loop shape and the material constant associated with the phase transformation.

A slight deviation is observed at 46°C due to non-ideal elastic response in the austenite, while simulations at 65°C and above exhibit excellent agreement with experiments, confirming the consistency of the 1D formulation.

*Pseudoelasticity Algorithm (1D)

A. Forward transformation (Loading, A $\rightarrow$ M)

1. Initialization:

Variables: σ^k (stress), f^k (martensite fraction), T (temperature)

2. Ω^{FOR} Calculation:

$$\Omega^{FOR}(\sigma, f, T) = \frac{\sigma^2}{2} \left[\left(\frac{1}{E_M} \right) - \left(\frac{1}{E_A} \right) \right] + \sigma \epsilon^0 - B (2f + 1) (T - T^0) - C(2f - 1) - K f(f + 1) - H$$

3. **If austenitic:**

$$\Delta \varepsilon = \frac{\Delta \sigma}{E_A}$$

$$\Delta f = 0$$

4. **If martensitic:**

$$\Delta \varepsilon = \frac{\Delta \sigma}{E_M}$$

$$\Delta f = 0$$

5. **If a forward martensitic transformation occurs:**

$$\Delta f = \frac{(\varepsilon_{01} \cdot \Delta \sigma)}{(2B \cdot (T - T^0) + 2C + K \cdot (2 \cdot f^k + 1))}$$

$$\Delta \varepsilon = \varepsilon_{01} \cdot \Delta f$$

(Apply only if $\Delta f > 0$ and $\Delta \sigma > 0$)

6. **Update state variables :**

$$\sigma^{k+1} = \sigma^k + \Delta \sigma$$

$$f^{k+1} = f^k + \Delta f$$

$$\varepsilon^{k+1} = \varepsilon^k + \left(\frac{\Delta \sigma}{E_{eq^k}} \right) + \varepsilon_{01} \cdot \Delta f$$

where:

$$E_{eq^k} = \frac{1}{\left[\frac{1-f^k}{E_A} + \frac{f^k}{E_M} \right]}$$

B. Reverse Transformation (Unloading, $M \rightarrow A$)

1. **Same variables as forward step:**

$$\sigma^k, f^k, T$$

2. **Ω^{REV} Calculation**

$$\Omega^{REV}(\sigma, T, f) = \frac{\sigma^2}{2} \left[\left(\frac{1}{E_M} \right) - \left(\frac{1}{E_A} \right) \right] + \sigma \varepsilon^0 - B(2f + 1)(T - T^0) - C(2f - 1) + Kf(f + 1) + H$$

3. If austenitic:

$$\Delta \varepsilon = -\frac{\Delta \sigma}{E_A}$$

$$\Delta f = 0$$

3. If martensitic:

$$\Delta \varepsilon = -\frac{\Delta \sigma}{E_M}$$

$$\Delta f = 0$$

4. If a reverse transformation occurs :

$$\Delta f = \frac{(\varepsilon_{01} \cdot \Delta \sigma)}{(2B \cdot (T - T^0) + 2C - K \cdot (2f^k + 1))}$$

$$\Delta \varepsilon = \varepsilon_{01} \cdot \Delta f$$

(Apply only if $\Delta f < 0$ and $\Delta \sigma < 0$)

5. Update state variable :

$$\sigma^{k+1} = \sigma^k + \Delta \sigma$$

$$f^{k+1} = f^k + \Delta f$$

$$\varepsilon^{k+1} = \varepsilon^k + \left(\frac{\Delta \sigma}{E_{eq^k}} \right) + \varepsilon_{01} \cdot \Delta f$$

This algorithm is repeated for the entire loading and unloading path to generate the complete pseudoelastic hysteresis loop.

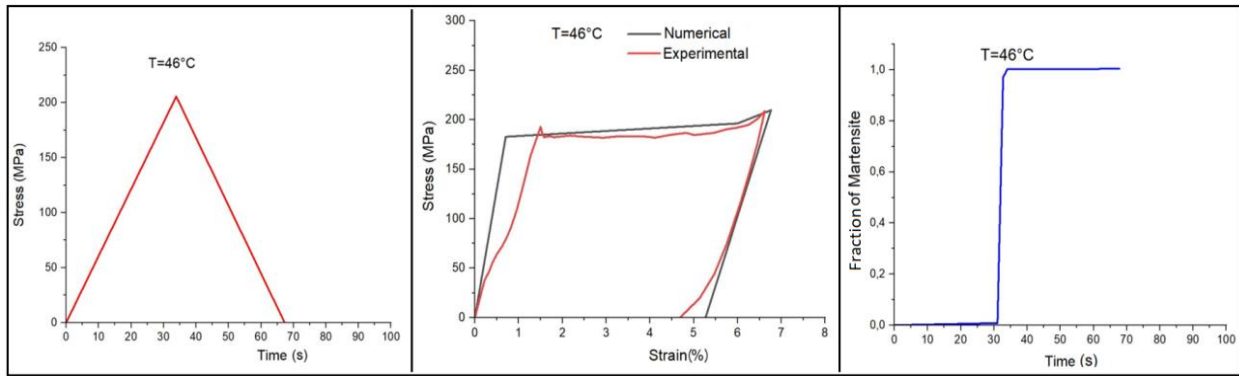


Figure IV.2. At $T=46^{\circ}\text{C}$: (a) Mechanical loading history; (b) Stress-strain relationship; (c) Martensite fraction evolution.

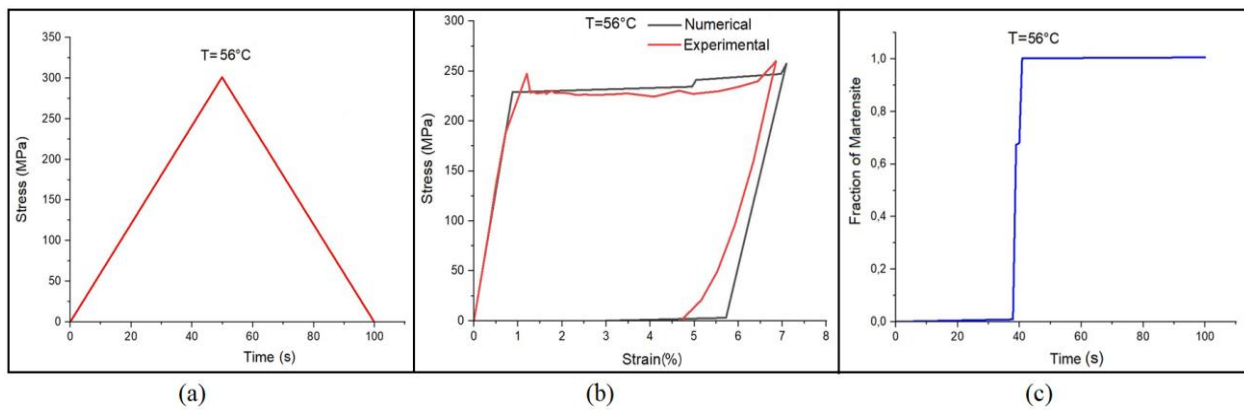


Figure IV.3. At $T=56^{\circ}\text{C}$: (a) Mechanical loading history; (b) Stress-strain relationship; (c) Martensite fraction evolution.

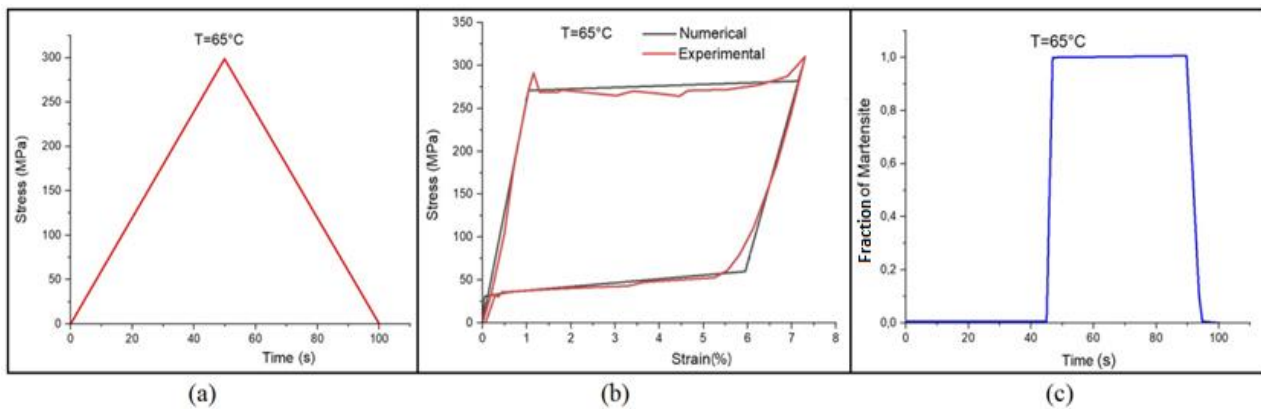


Figure IV.4. At $T=65^{\circ}\text{C}$: (a) Mechanical loading history; (b) Stress-strain relationship; (c) Martensite fraction evolution.

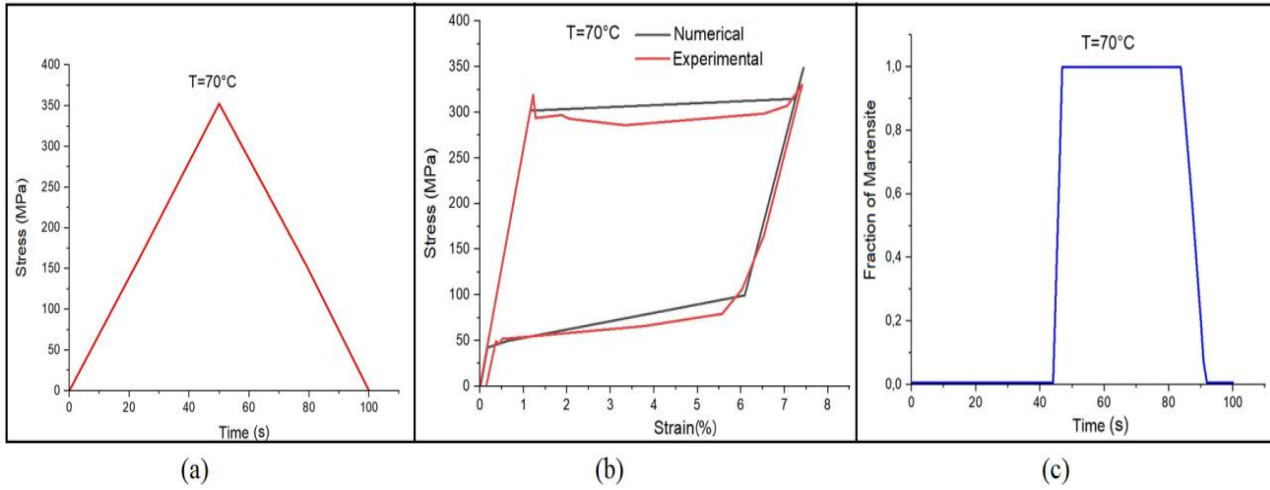


Figure IV.5. At $T=70^{\circ}\text{C}$: (a) Mechanical loading history; (b) Stress-strain relationship; (c) Martensite fraction evolution.

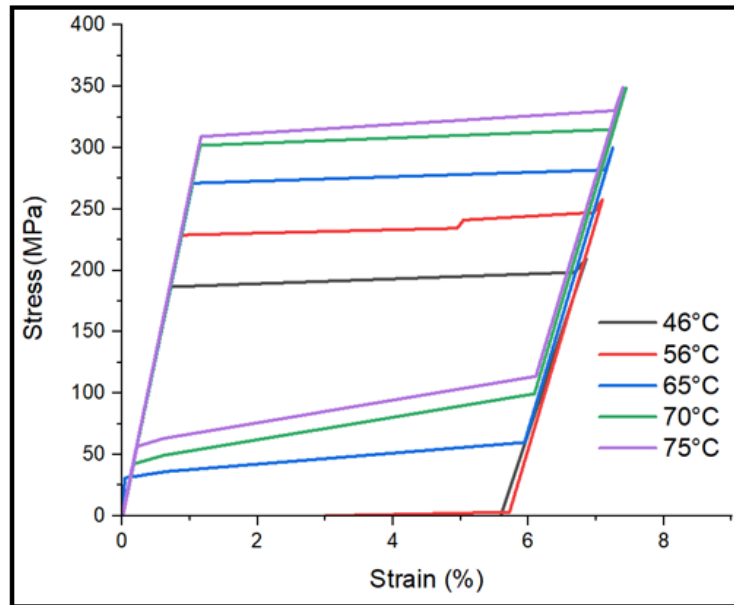


Figure IV.6. Response of the developed model across multiple temperatures.

The loading histories for each numerical scenario are illustrated in Figures IV. (2a, 3a, 4a, 5a). At $T=46^{\circ}\text{C}$, Fig. IV. 2(b) indicates an observable deviation resulting from non-ideal elastic behavior of the NiTi alloy in the austenitic state. On the other hand, Figures IV. (3b, 4b, 5b) demonstrate satisfactory conformity between simulation and experimental data, particularly evident at temperatures equal to or higher than 65°C . Additionally, the evolution of martensite fraction illustrated in Figures IV. (2c, 3c, 4c, 5c) aligns accurately with the constitutive model, highlighting its consistency with the predicted phase transformation mechanisms.

Ultimately, Figure IV.6 emphasizes the model's ability to reproduce the pseudoelastic response of SMAs over varying temperature ranges.

IV.2.2 Two-Dimensional Pseudoelastic Simulation (Voigt notation, 3×1)

General incremental evolution (isothermal, T fixed):

$$\Delta f = \frac{[\varepsilon_{01}(\mathbf{R} : \Delta \sigma)]}{[2B(T - T^0) + 2C \pm K(2f^k + 1)]}$$

(Use “+” for forward $A \rightarrow M$, “-” for reverse $M \rightarrow A$)

A) Forward transformation (Loading, $A \rightarrow M$)

1- Inputs: $\sigma^k(3 \times 1)$, f^k , $T = T_1$ (constant), $\mathbf{R}(3 \times 1)$, S_A and $S_M(3 \times 3)$, ε_{01} .

2- Forward potential:

$$\Omega^{FOR}(\sigma, T_1, f^k) = 0.5 \cdot \sigma^T (S_A - S_M) \sigma + \varepsilon_{01} \cdot \sigma^T \mathbf{R} - B(2f^k + 1)(T_1 - T^0) - C(2f^k - 1) - K f^k(f^k + 1) - H$$

3- Elastic branches (no transformation):

- Austenite: $\Delta \varepsilon = S_A : \Delta \sigma$, $\Delta f = 0$
- Martensite: $\Delta \varepsilon = S_M : \Delta \sigma$, $\Delta f = 0$

4- Martensitic transformation ($A \rightarrow M$):

$$\Delta f = \frac{[\varepsilon_{01}(\mathbf{R} : \Delta \sigma)]}{[2B(T_1 - T^0) + 2C + K(2f^k + 1)]}$$

(apply if $\Delta f > 0$ and $\mathbf{R} : \Delta \sigma > 0$)

$$\Delta \varepsilon = S_{eq}^k : \Delta \sigma + \varepsilon_{01} \mathbf{R} \cdot \Delta f$$

5- Update:

$$\sigma^{k+1} = \sigma^k + \Delta \sigma$$

$$f^{k+1} = f^k + \Delta f$$

$$\varepsilon^{k+1} = \varepsilon^k + \Delta \varepsilon$$

where:

$$S_{eq}^k = (1 - f^k)S_A + f^k S_M$$

B) Reverse transformation (Unloading, $M \rightarrow A$)

1- Inputs: $\sigma^k(3 \times 1)$, f^k , $T = T_1$ (constant), $\mathbf{R}(3 \times 1)$, S_A and $S_M(3 \times 3)$, ε_{01} .

2- Reverse potential:

$$\Omega^{REV}(\sigma, T_1, f^k) = 0.5 \cdot \sigma^T (S_A - S_M) \sigma + \varepsilon_{01} \cdot \sigma^T R - B (2f^k + 1)(T_1 - T^0) - C (2f^k - 1) + K f^k (f^k + 1) + H$$

3- Elastic branches (no transformation):

- Austenite: $\Delta \varepsilon = S_A : \Delta \sigma, \Delta f = 0$
- Martensite: $\Delta \varepsilon = S_M : \Delta \sigma, \Delta f = 0$

4- Martensitic reverse transformation (M $\rightarrow$ A):

$$\Delta f = \frac{[\varepsilon_{01}(R : \Delta \sigma)]}{[2B(T_1 - T^0) + 2C - K(2f^k + 1)]} \quad (IV-1)$$

(Apply if $\Delta f < 0$ and $R : \Delta \sigma < 0$)

$$\Delta \varepsilon = S_{eq}^k : \Delta \sigma + \varepsilon_{01} R \cdot \Delta f$$

5- Update:

$$\sigma^{k+1} = \sigma^k + \Delta \sigma$$

$$f^{k+1} = f^k + \Delta f$$

$$\varepsilon^{k+1} = \varepsilon^k + \Delta \varepsilon$$

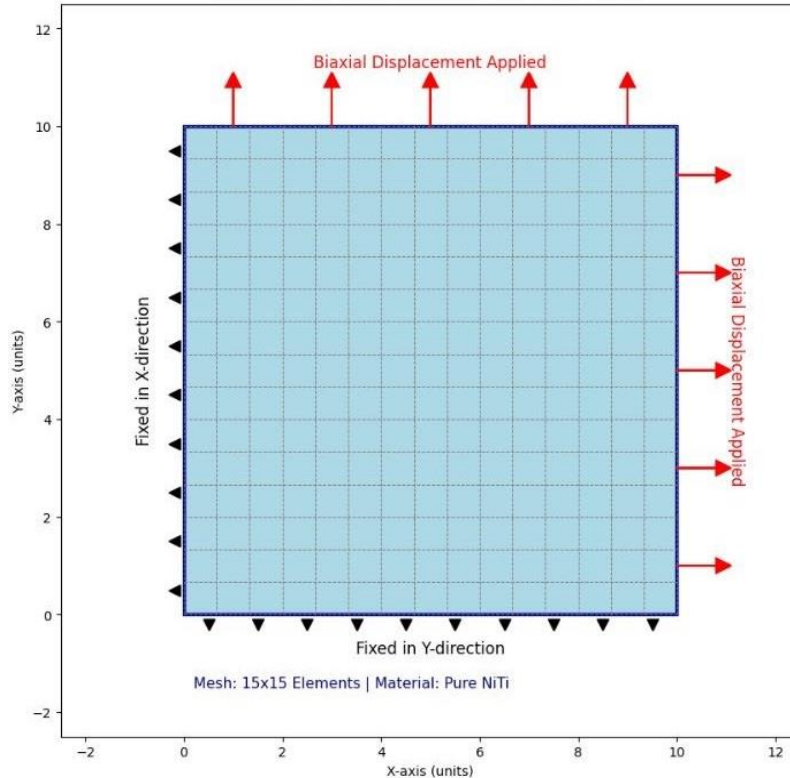


Figure IV.7. 2D Biaxial Simulation. Model setup showing mesh and boundary conditions.

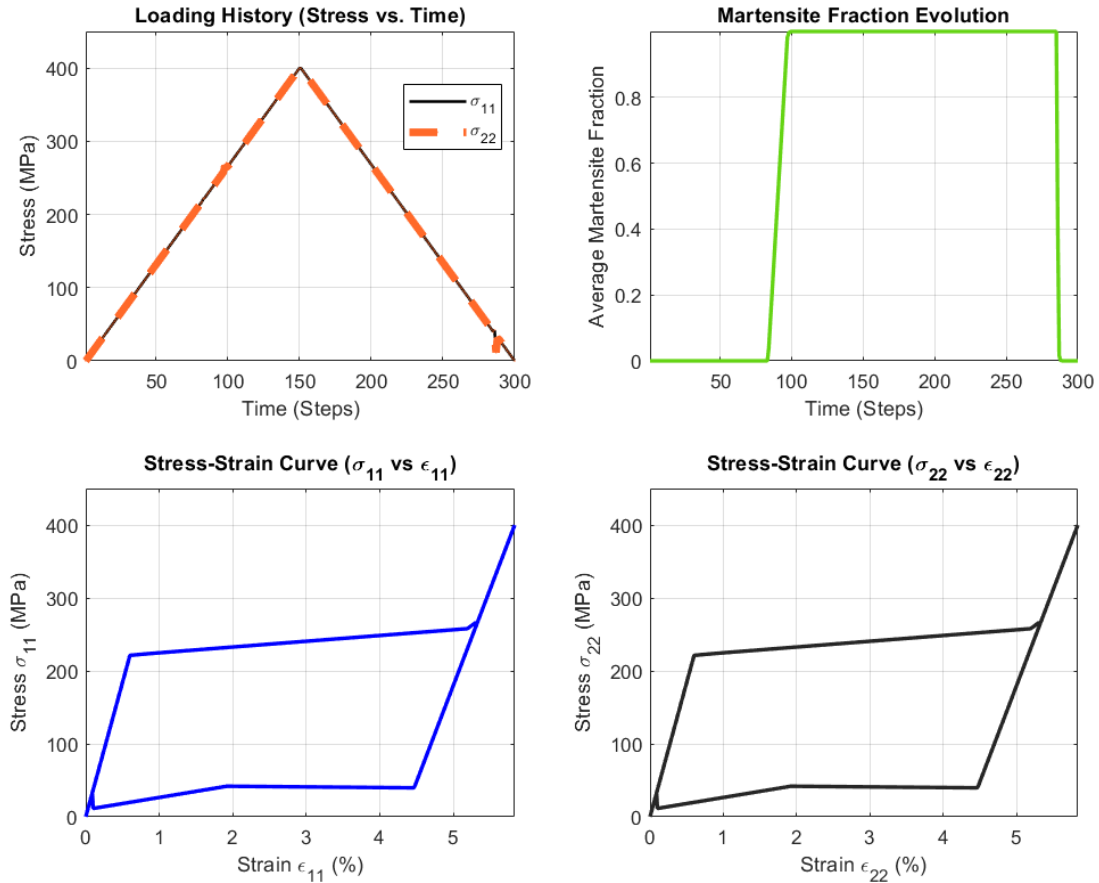


Figure IV.8. Two-dimensional biaxial pseudoelastic simulation showing the prescribed loading history, martensite fraction evolution, and stress–strain responses.

The results, presented in Figure IV.8, confirm the model's accuracy.

The stress-strain curves for both principal directions exhibit the characteristic pseudoelastic hysteresis loops. The martensite fraction evolves from 0 to 1 during loading and fully reverts to 0 upon unloading, in precise correlation with the transformation plateaus. This successful Simulation in 2D confirms the model's correct implementation for planar problems.

IV.3 Simulation of the Thermoelastic Model

This section examines the behavior of the proposed constitutive model under non-isothermal loading conditions, with particular focus on the thermoelastic effect. In this case, phase transformation is driven by temperature variations under a constant applied stress, a mechanism that is fundamental to the operation of most SMA-based actuators. The material and model parameters used for this numerical assessment are summarized in Table IV.2.

Table IV.2. Material and model parameters for the thermoelastic effect simulation, based on experimental data reported by Bourbon et al. [3]

Parameter	Description	Value	Unit
E_A	Young's Modulus (Austenite)	72000	MPa
E_M	Young's Modulus (Martensite)	70000	MPa
ν	Poisson's Ratio	0.3	-
ϵ^0	Max. Transformation Strain	0.023937	-
M_s^0	Martensite Start Temp. (Zero Stress)	313	K
B	Model Parameter B	0.1149	MPa/K
C	Model Parameter C	-0.675568	MPa
K	Model Parameter K	0.176235	MPa
H	Model Parameter H	0.939082	MPa

IV.3.1 One-Dimensional Uniaxial Simulation

The thermoelastic response of the model is assessed through one-dimensional simulations under non-isothermal conditions. The numerical predictions are compared with experimental results obtained for a Cu–Zn–Al alloy subjected to two constant stress levels, 65 MPa and 100 MPa, as reported by Bourbon et al. [3]. The phenomenological parameters B, C, K, H were calibrated independently for each stress level, based on the characteristic transformation temperatures (M_s^σ , M_f^σ , A_s^σ , A_f^σ) for each case.

The simulation results for the 65 MPa and 100 MPa thermal cycles are presented in Figures IV-11 and IV-12, respectively. These figures illustrate the imposed thermal loading, the associated evolution of the martensite volume fraction, and the resulting strain–temperature response.

IV.3.1.1 Numerical Algorithm for One-Dimensional Thermoelasticity

To simulate the thermoelastic effect, an incremental algorithm is employed where temperature is the control variable and stress is held constant ($\sigma = \sigma_0$). For each temperature increment ΔT , the algorithm computes the increments of martensite fraction Δf and strain $\Delta \epsilon$.

The general evolution law of the martensitic fraction is:

$$\frac{df}{dT} = \frac{B(2f+1)}{[2B(T-T^0) + 2C \pm K(2f+1)]} \quad \text{..... (IV-2)}$$

In finite difference form:

$$\frac{\Delta f}{\Delta T} = \frac{B(2f^k+1)}{[2B(T-T^0) + 2C \pm K(2f^k+1)]} \quad \text{..... (IV-3)}$$

Which leads to:

A. Forward transformation (Cooling, A $\rightarrow$ M)

1- **Initialization:** $T^k, f^k, \sigma = \sigma_0$ (constant)

2. **Compute $\Omega^{FOR}(\sigma, T = T_1, f)$:**

$$\Omega^{FOR} = 0.5 * \sigma * (SA - SM); \sigma + \varepsilon^0 * \sigma * R - B * (2f^k + 1) * (T_1 - T^0) - C * (2f^k - 1) - K * f^k * (f^k + 1) - H$$

3- If $\Omega \leq 0$: no transformation

$$\Delta \varepsilon = 0 \text{ and } \Delta f = 0$$

4- If $\Omega > 0$: martensitic transformation

$$\Delta f = \left[\frac{B(2f^k+1)}{(2B(T^k-T^0) + 2C + K(2f^k+1))} \right] \Delta T$$

$$(\Delta T < 0, \Delta f > 0)$$

$$\Delta \varepsilon = \Delta f * \varepsilon_{01}$$

5- **Update state variable:**

$$T^{k+1} = T^k + \Delta T, f^{k+1} = f^k + \Delta f, \varepsilon^{k+1} = \varepsilon^k + \Delta \varepsilon$$

B. Reverse Transformation (Heating, M $\rightarrow$ A)

1- **Initialization:** $T^k, f^k, \sigma = \sigma_0$ (constant)

2- **Compute $\Omega^{REV}(\sigma, T = T_1, f)$:**

$$\Omega^{REV} = 0.5 * \sigma : (SA - SM) : \sigma + \varepsilon^0 * \sigma : R - B * (2f^k + 1) * (T^1 - T^0) - C * (2f^k - 1) - K * f^k * (f^k + 1) - H$$

3- If $\Omega \geq 0$: no transformation

$$\Delta\varepsilon = 0 \text{ and } \Delta f = 0$$

4- If $\Omega < 0$: reverse transformation

$$\Delta f = \left[\frac{B(2f^k+1)}{(2B(T^k-T^0)+2C-K(2f^k+1))} \right] \Delta T$$

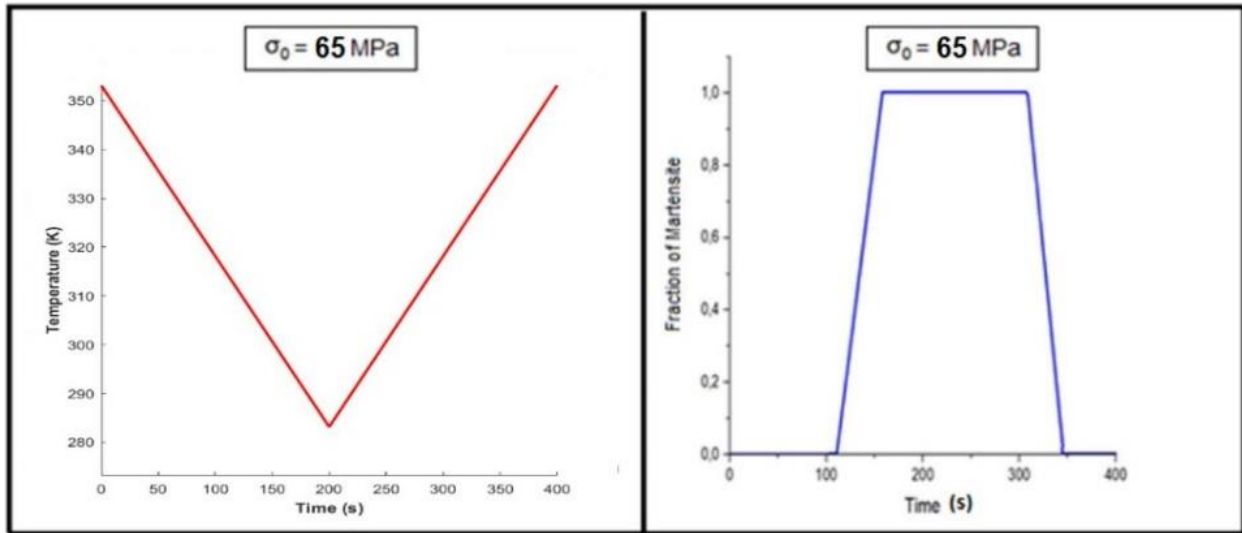
$$(\Delta T > 0, \Delta f < 0)$$

$$\Delta\varepsilon = \Delta f * \varepsilon_{01}$$

5- Update state variable:

$$T^{k+1} = T^k + \Delta T, f^{k+1} = f^k + \Delta f, \varepsilon^{k+1} = \varepsilon^k + \Delta\varepsilon$$

This algorithm is repeated over the entire cooling–heating cycle to generate the complete thermoelastic hysteresis loop.



(a)

(b)

Figure IV.9. Simulation results for a thermoelastic cycle at $\sigma = 65 \text{ MPa}$:

(a) History of the applied thermal load, (b) Evolution of the martensite volume fraction over time.

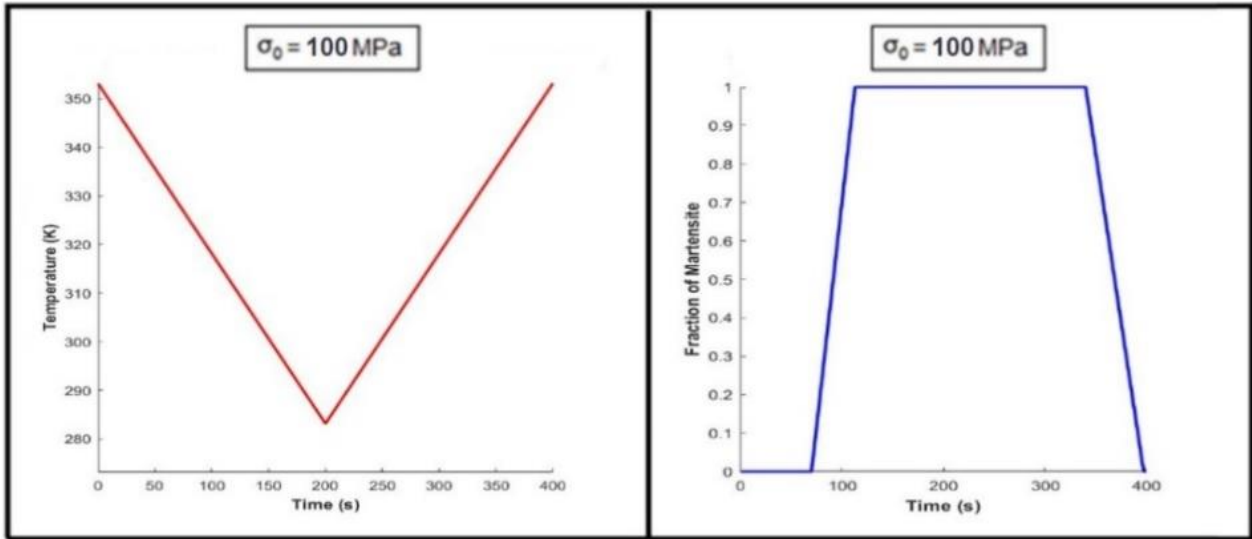


Figure IV.10. Simulation results for a thermoelastic cycle at $\sigma = 100 \text{ MPa}$:

(a) History of the applied thermal load, (b) Evolution of the martensite volume fraction over time.

A direct comparison between the numerical predictions and the experimental data is presented in Figure IV.11 (for 65 MPa) and Figure IV-12 (for 100 MPa). The results show a satisfactory agreement for both stress levels, with the simulations capturing the main characteristics of the thermoelastic response, including the transformation temperatures and the overall shape of the hysteresis loops.

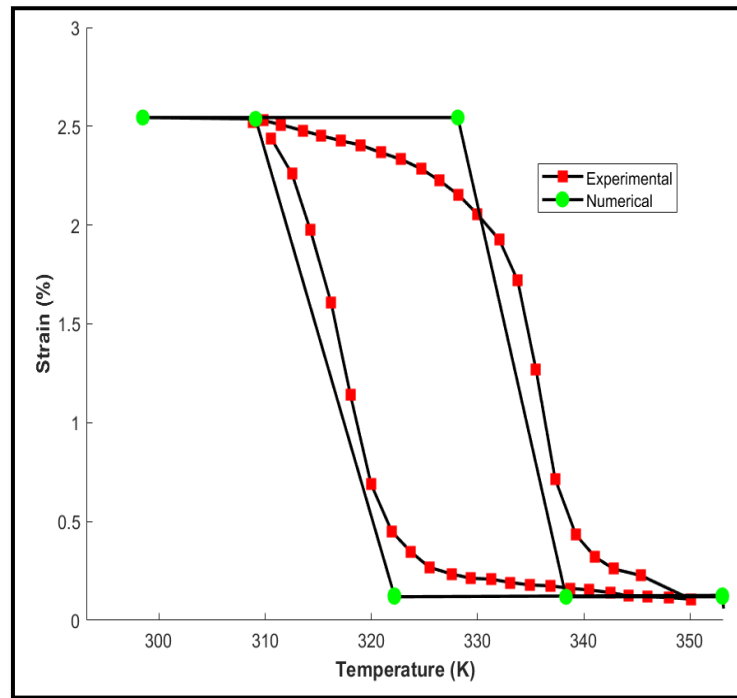


Figure IV.11. Calibration of the model at 65 MPa. The Experimental data (red squares) are compared with the Numerical simulation (green dots/black line) from Bourbon et al.

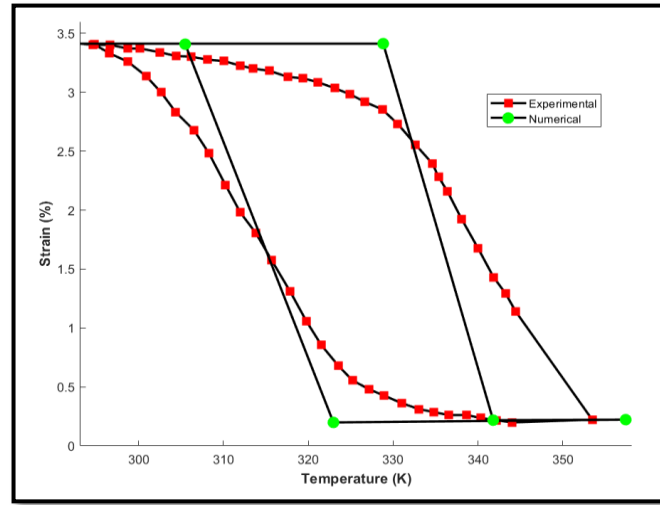


Figure IV.12. Calibration of the model at 100 MPa. The Experimental data (red squares) are compared with the Numerical simulation (green dots/black line) from Bourbon et al.

Finally, Figure IV.13 presents the numerically simulated hysteresis loops corresponding to both stress levels on a single plot, highlighting the stress-induced shift in transformation temperatures, commonly referred to as the material constant effect associated with phase transformation. The comparison between the two stress conditions illustrates the capability of the proposed formulation to represent this effect in a consistent manner, supporting the numerical stability of the model under varying thermo-mechanical loading levels.

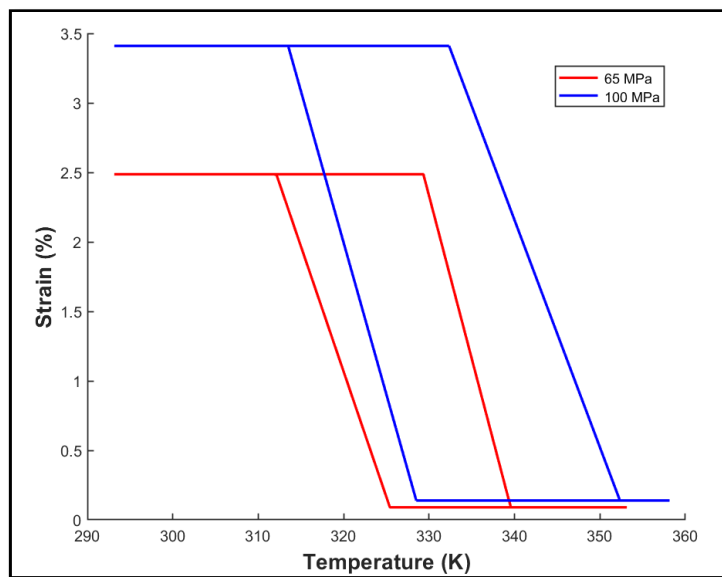


Figure IV.13. Comparison of thermoelastic hysteresis loops for $\sigma = 65$ MPa and $\sigma = 100$ MPa

IV.3.2 Two-Dimensional Plane-Stress Thermoelastic Simulation

The thermoelastic response was extended to a two-dimensional plane-stress configuration representative of thin-layer applications. A 10x10 mm Cu–Zn–Al plate was subjected to a constant biaxial tensile stress state, with equal in-plane stress components $\sigma_{11} = \sigma_{22} = 65$ MPa , while a prescribed thermal cycle was applied, as illustrated in the model setup shown in Figure IV.16. The corresponding thermal loading history is presented in Figure IV.17

The main numerical results are reported in Figure IV.18. The strain–temperature response exhibits the characteristic thermoelastic hysteresis loop, while the evolution of the martensite fraction indicates a fully reversible phase transformation driven by the applied thermal cycle. A detailed examination of the strain components shown in Figure IV.19 reveals comparable in-plane strain responses, with the dominant contribution aligned with the principal loading directions. This behavior is consistent with the imposed biaxial stress state and illustrates the expected response of the constitutive model within a two-dimensional plane-stress formulation.

IV.3.2.1 Numerical Algorithm for Multi-axial Thermoelasticity (2D)

The one-dimensional thermoelastic algorithm is extended to two-dimensional multiaxial configurations by replacing scalar quantities with their tensorial counterparts. The structure of the incremental procedure remains unchanged: temperature is treated as the control variable, while the in-plane stress tensor is maintained at a constant value ($\sigma = \sigma_0$). For each increment of temperature ΔT , the algorithm computes the increments of martensite fraction Δf and strain tensor $\Delta \epsilon$.

The algorithm proceeds as follows:

A. Forward Transformation (Cooling, A $\rightarrow$ M)

1-1. **Initialization** : $T^k, f^k, \sigma = \sigma_1$ (constant)

1-2. Ω^{FOR} Calculation

$$\Omega^{\text{FOR}}(\sigma^1, T^k, f^k) = \frac{1}{2} \cdot \sigma^{1T} \cdot (S_A - S_M) \cdot \sigma^1 + \epsilon^0 \cdot \sigma^{1T} \cdot R - B \cdot (2f^k + 1) \cdot (T^k - T^0) - C \cdot (2f^k - 1) - K \cdot f^k \cdot (f^k + 1) - H$$

- If $\Omega \leq 0$ (elastic) :

$$\Delta \varepsilon = S_A : \Delta \sigma \quad \text{and} \quad \Delta f = 0 \quad (\text{Austenite})$$

$$\Delta \varepsilon = S_M : \Delta \sigma \quad \text{and} \quad \Delta f = 0 \quad (\text{Martensite})$$

- **If $\Omega > 0$ (martensitic transformation) :**

$$\Delta f = \left[B \cdot \frac{(2f^k + 1)}{(2B \cdot (T^k - T^0) + 2C + K \cdot (2f^k + 1))} \right] \cdot \Delta T$$

$$(\Delta T < 0, \Delta f > 0)$$

$$\Delta \varepsilon = [(1 - f^k) \cdot S_A + f^k \cdot S_M] : \Delta \sigma + \varepsilon^0 \cdot R \cdot \Delta f$$

1-7. Update state variable:

$$T^{k+1} = T^k + \Delta T$$

$$f^{k+1} = f^k + \Delta f$$

$$\varepsilon^{k+1} = \varepsilon^k + \Delta \varepsilon$$

$$\sigma^{k+1} = \sigma_1 \text{ (Constant)}$$

B. Reverse Transformation (Heating, $M \rightarrow A$)

$$2-1. \text{ Initialization : } T^k, f^k, \sigma = \sigma_1 \text{ (constant)}$$

2-2. Ω^{REV} Calculation

$$\Omega^{REV} = \frac{1}{2} \cdot \sigma^{1T} \cdot (S_A - S_M) \cdot \sigma^1 + \varepsilon^0 \cdot \sigma^{1T} \cdot R - B \cdot (2f^k + 1) \cdot (T^k - T^0) - C \cdot (2f^k - 1) + K \cdot f^k \cdot (f^k + 1) + H$$

- **If $\Omega \geq 0$ (no transformation) :**

$$\Delta \varepsilon = S_{phase} : \Delta \sigma, \quad \Delta f = 0$$

- **If $\Omega < 0$ (reverse transformation) :**

$$\Delta f = \left[B \cdot \frac{(2f^k + 1)}{(2B \cdot (T^k - T^0) + 2C - K \cdot (2f^k + 1))} \right] \cdot \Delta T$$

$$(\Delta T > 0, \Delta f < 0)$$

$$\Delta \varepsilon = [(1 - f^k) \cdot S_A + f^k \cdot S_M] : \Delta \sigma + \varepsilon^0 \cdot R \cdot \Delta f$$

2-7. Update state variable:

$$T^{k+1} = T^k + \Delta T$$

$$f^{k+1} = f^k + \Delta f$$

$$\varepsilon^{k+1} = \varepsilon^k + \Delta \varepsilon$$

$$\sigma^{k+1} = \sigma_1$$

This multi-axial algorithm provides the foundation for the 2D simulation results presented in the following sections.

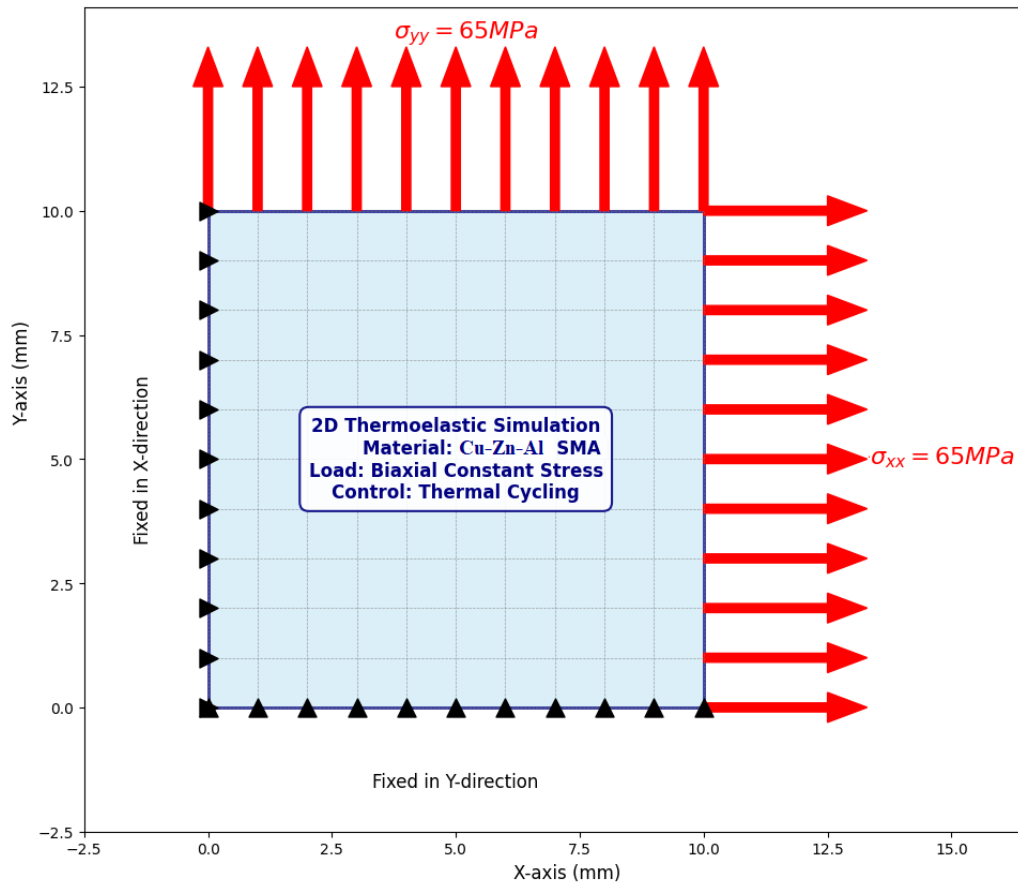


Figure IV.14. Schematic of the 2D model setup for the thermoelastic simulation, showing the mesh, boundary conditions, and the applied thermomechanical loads.

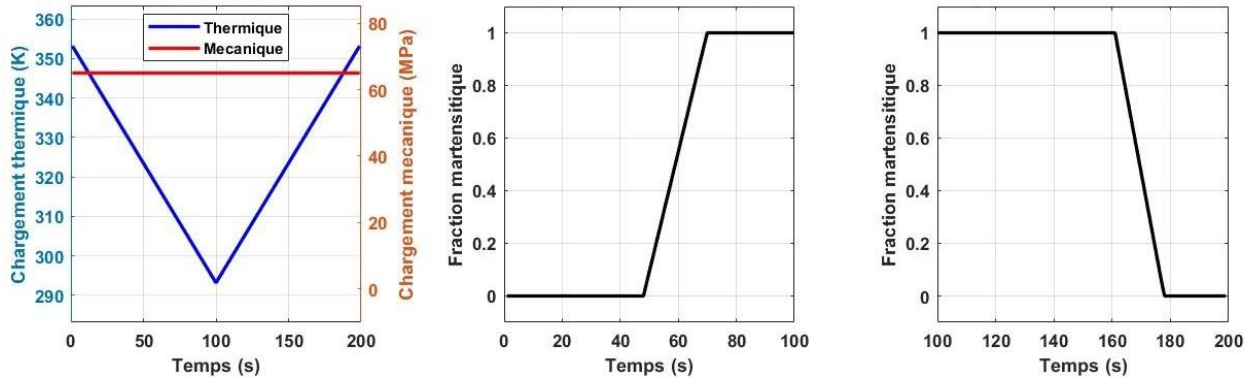


Figure IV.15. Thermomechanical loading history for the 2D simulation and the corresponding evolution of martensite fraction over time.

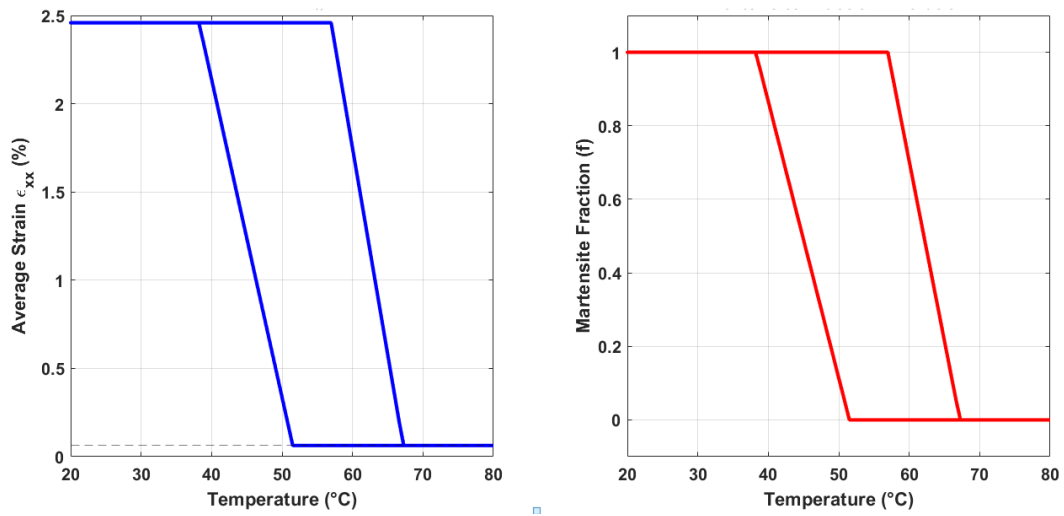


Figure IV.16. Primary results for the 2D simulation, showing the strain-temperature hysteresis loop and the corresponding martensite fraction evolution versus temperature.

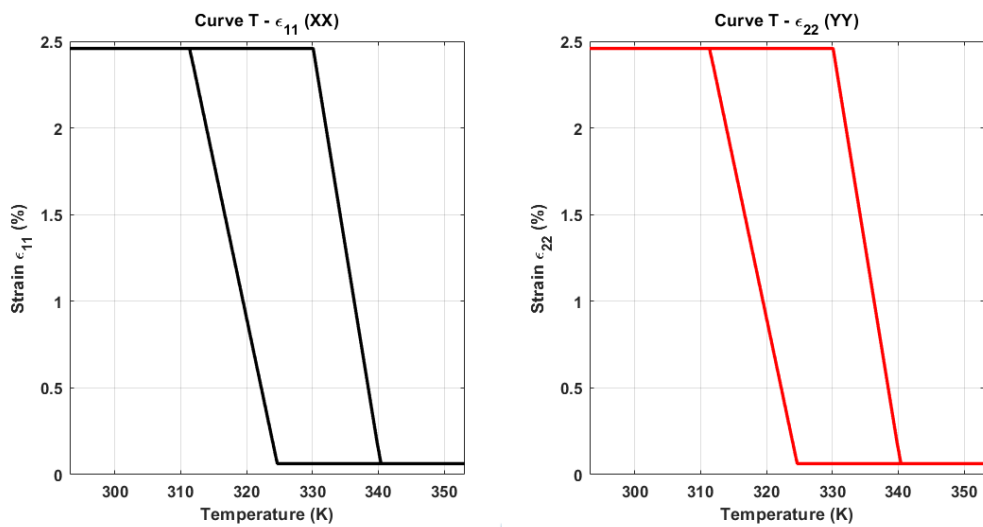


Figure IV.17. Comparison of longitudinal (ϵ_{11}) and transverse (ϵ_{22}) strain components during the thermal cycle.

IV.4 Simulation of the Simple Shape Memory Effect Model

This section examines the capability of the proposed constitutive framework to reproduce the complete thermomechanical cycle associated with the Simple Shape Memory Effect (SME). Particular attention is given to the model's ability to handle successive mechanical and thermal loading stages while consistently accounting for the history-dependent retained strain. The material and model parameters used for these numerical simulations are summarized in Table IV-3.

Table IV.3. Parameters of the phase-based SME model, calibrated from experimental data reported by Ng and Sun. [2]

Parameter	Description	Value	Unit
E_A	Young's Modulus (Austenite)	25775	MPa
E_M	Young's Modulus (Martensite)	18442	MPa
ν	Poisson's Ratio	0.3	-
ϵ^0	Max. Transformation Strain	0.04064	-
σ_s	Martensite Orientation Start Stress	70	MPa
σ_f	Martensite Orientation Finish Stress	120	MPa
M_s	Martensite Start Temperature	279	K
M_f	Martensite Finish Temperature	240	K
A_s	Austenite Start Temperature	296	K
A_f	Austenite Finish Temperature	330	K

IV.4.1 One-Dimensional Uniaxial Simulation

The one-dimensional response of the model is assessed by comparison with experimental data reported by Ng and Sun. for a complete SME thermomechanical cycle. Figure IV-16 presents the comparison between numerical predictions and experimental results for the initial mechanical loading stage at 23 °C, showing a satisfactory agreement in terms of stress–strain response and residual strain.

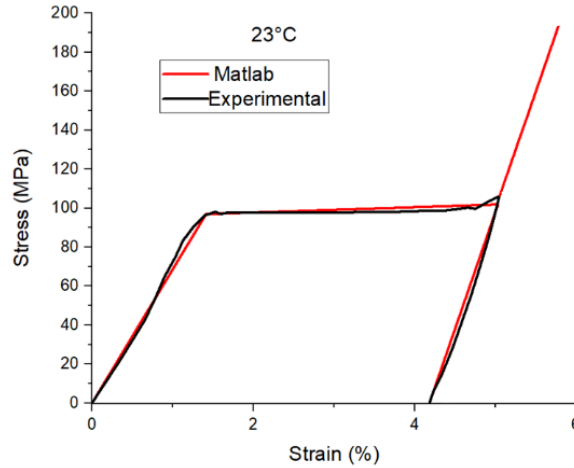


Figure IV.18. Comparison of numerical results (red line) with experimental data (blue line) during the martensitic loading stage at 23°C.

The numerical simulations reproduce the sequence of the four characteristic stages of the SME: martensite orientation during mechanical loading, unloading with retained strain, thermally induced strain recovery under zero stress, and final cooling. The results indicate:

- A loading plateau at approximately 100 MPa with a maximum strain of about 4.5%;
- Retention of a residual strain close to 4% after unloading;
- Complete strain recovery during heating under stress-free conditions;
- Absence of macroscopic strain evolution during the final cooling stage.

The corresponding numerical results are presented sequentially in Figures IV-25 through IV-29, illustrating the consistency of the model response throughout the full thermomechanical cycle.

IV.4.1.1 Numerical Algorithm for the One-Dimensional SME

The simulation of the SME is performed sequentially, with a specific algorithm applied for each of the three distinct stages of the process.

* SME Algorithm (1D)

The study of the simple shape memory effect is divided into three parts:

1- Mechanical Loading (Orientation, $T = T_1$ constant) :

The evolution of the martensite volume fraction f is governed by the following equation:

$$\frac{df}{d\sigma} = \frac{\varepsilon_{01}}{[2B(T-T^0) + 2C + K(2f+1)]} \dots\dots\dots (IV-4)$$

This allows us to compute the increments for f and :

$$\Delta f = \left[\frac{\varepsilon_{01}}{(2B(T^1-T^0) + 2C + K(2f^k+1))} \right] \Delta \sigma \dots\dots\dots (IV-5)$$

$$(f > 0) ; (\sigma > 0)$$

2- Heating ($\sigma = 0$, $M \rightarrow A$):

The evolution of the martensite fraction f is given by:

$$\frac{df}{dT} = - \frac{B(2f+1)}{[2B(T-T^0) + 2C - K(2f+1)]} \dots\dots\dots (IV-6)$$

$$(f < 0) ; (T > 0)$$

This leads to :

$$\Delta f = - \left[\frac{B(2f^k+1)}{(2B(T-T^0) + 2C - K(2f^k+1))} \right] \Delta T \dots\dots\dots (IV-7)$$

$$(T > 0)$$

3- Cooling ($\sigma = 0$):

The evolution of the martensite fraction f is given by:

$$\frac{df}{dT} = - \frac{B(2f+1)}{[2B(T-T^0) + 2C + K(2f+1)]} \dots\dots\dots (IV-8)$$

$$(f > 0)(T < 0)$$

This leads to:

$$\Delta f = - \left[\frac{B(2f^k+1)}{(2B(T-T^0) + 2C + K(2f^k+1))} \right] \Delta T \dots\dots\dots (IV-9)$$

$$(f > 0) ; (T < 0)$$

The algorithm proceeds as follows for each stage of the process:

A. Mechanical Loading (Orientation)

1- **Initialization:** $\sigma^k, f^k, T = T_1$ (constant, low temperature)

2- **Elastic Austenite Case (if purely austenitic) :**

$$\Delta \varepsilon = \frac{\Delta \sigma}{E_A} \text{ and } \Delta f = 0$$

3- **Elastic Martensite Case (if purely martensitic):**

$$\Delta \varepsilon = \frac{\Delta \sigma}{E_M} \text{ and } \Delta f = 0$$

4- **Martensitic Transformation (Orientation):**

$$\Delta f = \left[\frac{\varepsilon_{01}}{(2B(T_1 - T^0) + 2C + K(2f^{k+1}))} \right] \Delta \sigma$$

$$(\Delta f > 0) ; (\Delta \sigma > 0)$$

$$\Delta \varepsilon = \frac{\Delta \sigma}{E_{eq}^k} + \varepsilon_{01} * \Delta f$$

5- **Update State Variables:**

$$\sigma^{k+1} = \sigma^k + \Delta \sigma, f^{k+1} = f^k + \Delta f, \varepsilon^{k+1} = \varepsilon^k + \Delta \varepsilon$$

B- Heating (Thermal Recovery)

1- **Initialization:** $T^k, f^k, \sigma = 0$

2- **No Transformation:**

$$\Delta \varepsilon = 0 \text{ and } \Delta f = 0$$

3- **Reverse Transformation (Recovery):**

$$\Delta f = - \left[\frac{B(2f^{k+1})}{(2B(T^k - T^0) + 2C - K(2f^{k+1}))} \right] \Delta T$$

$$(\Delta f < 0) ; (\Delta T > 0)$$

$$\Delta \varepsilon = \varepsilon_{01} * \Delta f$$

4- **Update State Variables:**

$$T^{k+1} = T^k + \Delta T, f^{k+1} = f^k + \Delta f, \varepsilon^{k+1} = \varepsilon^k + \Delta \varepsilon$$

C- Cooling (Self-Accommodated Martensite Formation)

1- **Initialization:** $T^k, f^k, \sigma = 0$

2- **No Transformation:**

$$\Delta \varepsilon = 0 \text{ and } \Delta f = 0$$

3- **Self-Accommodated Martensite Formation:**

$$\Delta f = - \left[\frac{B(2f^{k+1})}{(2B(T^k - T^0) + 2C + K(2f^{k+1}))} \right] \Delta T$$

$$(\Delta f > 0); (\Delta T < 0)$$

$$\Delta \varepsilon = 0 \text{ (since the strain is self-accommodated)}$$

4- **Update State Variables:**

$$T^{k+1} = T^k + \Delta T, f^{k+1} = f^k + \Delta f, \varepsilon^{k+1} = \varepsilon^k + \Delta \varepsilon$$

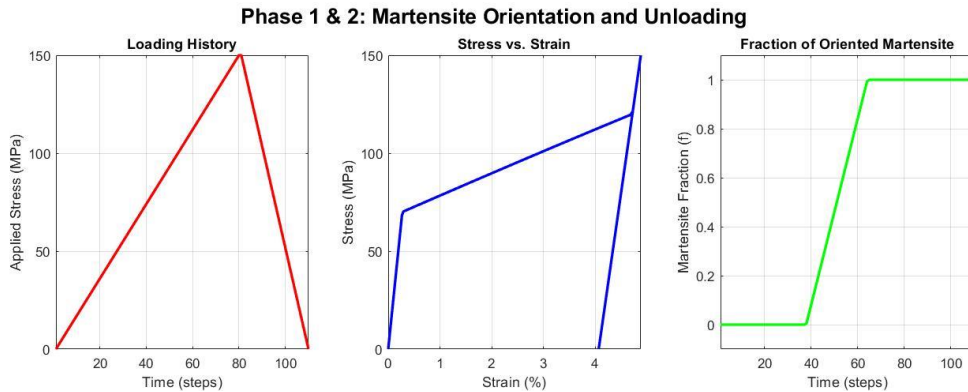


Figure IV.19. Phase 1 & 2: Mechanical loading at low temperature showing martensite orientation and the resulting retained strain upon unloading.

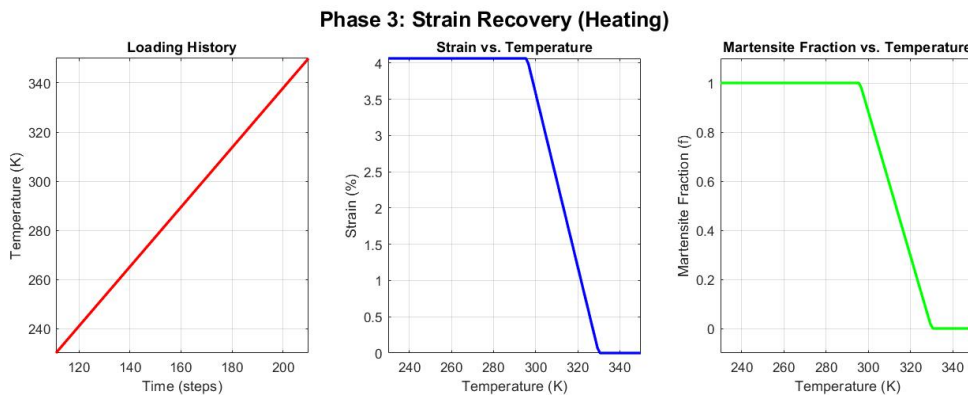


Figure IV.20. Phase 3: Strain recovery during heating under zero stress, showing the reverse transformation from martensite to austenite.

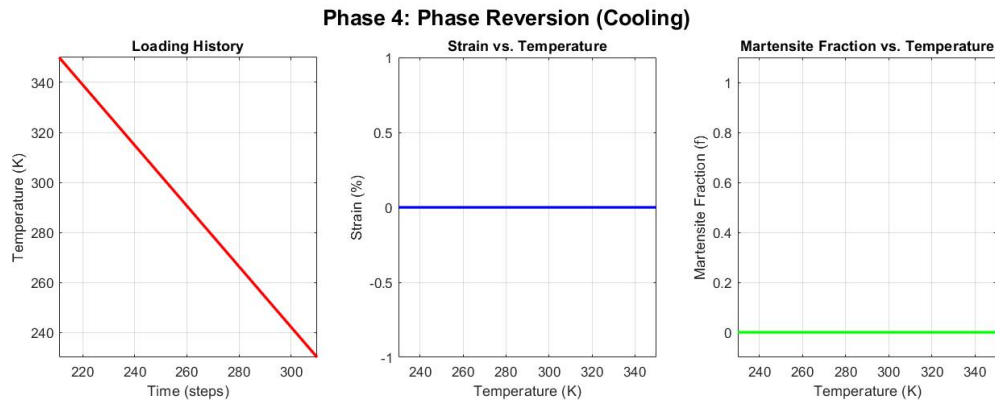


Figure IV.21. Phase 4: Cooling under zero stress, showing zero strain change due to the formation of self-accommodated martensite.

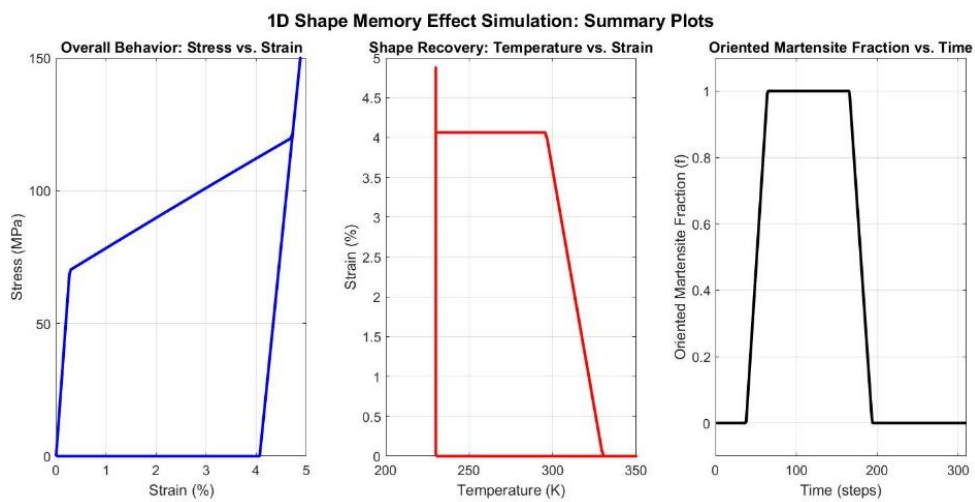


Figure IV.22. Summary plots for the 1D Shape Memory Effect simulation, showing the key behavioral curves for the complete cycle.

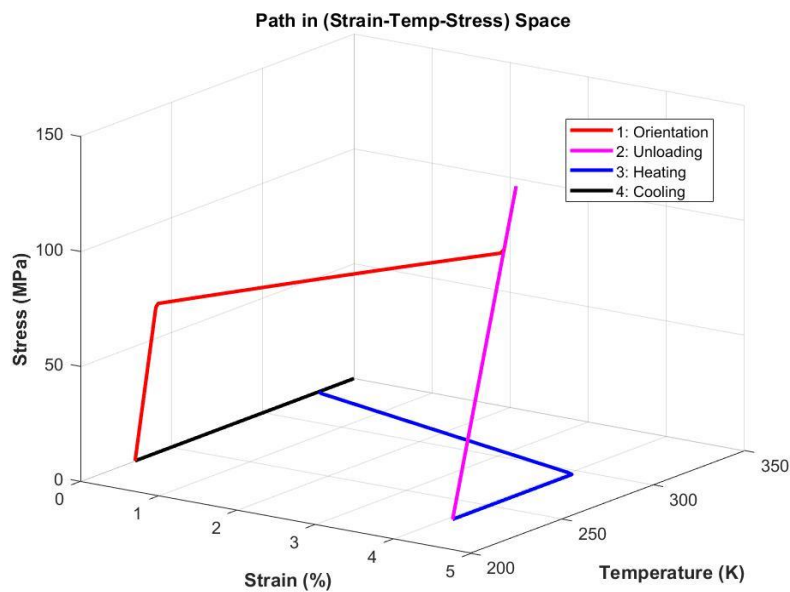


Figure IV.23. Visualization of the complete thermomechanical path in Strain-Temperature-Stress space for the 1D SME cycle.

IV.4.2 Two-Dimensional Uniaxial Simulation

The SME simulation is extended to a two-dimensional plane-stress configuration using a dedicated Python-based implementation. The model setup is illustrated in Figure IV-30. The numerical results, presented phase-by-phase in Figures IV-31, IV-32, and IV-33, illustrate the mechanical orientation stage, the thermally driven strain recovery, and the strain-free cooling phase. A global view of the complete two-dimensional SME cycle is provided in Figure IV-34, highlighting the consistency of the model response under planar loading conditions.

IV.4.2.1 Numerical Algorithm for Multiaxial SME (2D)

The one-dimensional SME algorithm is extended to two-dimensional multiaxial configurations by replacing scalar quantities with their corresponding tensorial forms. The simulation is conducted sequentially, applying a specific numerical procedure to each stage of the SME cycle within a plane-stress framework.

* SME Algorithm (2D)

The study of the simple shape memory effect in a **plane-stress state** (2D) is broken down into three parts:

1. Mechanical Loading (Orientation, $A \rightarrow M$)

1-1. Initialization :

$$\sigma^k \text{ (3}\times\text{1 vector)}, f^k, T = T_1 \text{ (constant)}$$

1-2. Compute Ω^{FOR} :

$$\Omega^{\text{FOR}}(\sigma^k, T^1, f^k) = \frac{1}{2} \cdot \sigma^{kT} \cdot (S_A - S_M) \cdot \sigma^k + \varepsilon^0 \cdot \sigma^{kT} \cdot R - B \cdot (2f^k + 1) \cdot (T_1 - T^0) - C \cdot (2f^k - 1) - K \cdot f^k \cdot (f^k + 1) - H$$

- **If $\Omega \leq 0$ (Elastic) :**

$$\Delta \varepsilon = S_A : \Delta \sigma \quad \text{and} \quad \Delta f = 0 \quad (\text{Austenite})$$

$$\Delta \varepsilon = S_M : \Delta \sigma \quad \text{and} \quad \Delta f = 0 \quad (\text{Martensite})$$

- **If $\Omega > 0$ (forward transformation) :**

$$\Delta f = \frac{[\varepsilon^0 \cdot (R \cdot \Delta \sigma)]}{[2B \cdot (T^1 - T^0) + 2C + K \cdot (2f^k + 1)]}$$

$$(\Delta \sigma > 0, \Delta f > 0)$$

$$\Delta \varepsilon = [(1 - f^k) \cdot S_A + f^k \cdot S_M] \cdot \Delta \sigma + \varepsilon^0 \cdot R \cdot \Delta f$$

1-7. Update State Variables:

$$\sigma^{k+1} = \sigma^k + \Delta \sigma$$

$$f^{k+1} = f^k + \Delta f$$

$$\varepsilon^{k+1} = \varepsilon^k + \Delta \varepsilon$$

2. Heating (Thermal Recovery, $M \rightarrow A$)

2-1. Initialization:

$$\sigma = 0, f^k, T^k$$

2-2. Compute Ω^{REV} :

$$\Omega^{REV}(0, T^k, f^k) = \frac{1}{2} \cdot 0^T \cdot (S_A - S_M) \cdot 0 + \varepsilon_0 \cdot 0^T \cdot R - B \cdot (2f^k + 1) \cdot (T^k - T_0) - C \cdot (2f^k - 1) + K \cdot f^k \cdot (f^k + 1) + H$$

- If $\Omega \geq 0$ (No Transformation) :

$$\Delta \varepsilon = 0 \quad \text{and} \quad \Delta f = 0$$

- If $\Omega < 0$ (Reverse Transformation) :

$$\Delta f = \frac{[B \cdot (2f^k + 1)]}{[2B \cdot (T^k - T^0) + 2C - K \cdot (2f^k + 1)]} \cdot \Delta T$$

$$(\Delta T > 0, \Delta f < 0)$$

$$\Delta \varepsilon = \varepsilon^0 \cdot R \cdot \Delta f$$

2-7. Update State Variables:

$$T^{k+1} = T^k + \Delta T$$

$$f^{k+1} = f^k + \Delta f$$

$$\varepsilon^{k+1} = \varepsilon^k + \Delta\varepsilon$$

3. cooling (Self-Accommodated Martensite)

3-1. Initialization :

$$\sigma = 0, f^k, T^k$$

3-2. Compute Ω^{cool} :

$$\Omega^{cool}(0, T^k, f^k) = -B \cdot (2f^k + 1) \cdot (T^k - T^0) - C \cdot (2f^k - 1) - K \cdot f^k \cdot (f^k + 1) - H$$

- **If $\Omega \leq 0$ (No Transformation):**

$$\Delta\varepsilon = 0 \quad \text{and} \quad \Delta f = 0$$

- **If $\Omega > 0$ (Self-Accommodated Martensite Formation) :**

$$\Delta f = \frac{[B \cdot (2f^k + 1)]}{[2B \cdot (T^k - T^0) + 2C + K \cdot (2f^k + 1)]} \cdot \Delta T$$

$$(\Delta T < 0)$$

$$\Delta\varepsilon = 0$$

3-7. Update State Variables:

$$T^{k+1} = T^k + \Delta T$$

$$f^{k+1} = f^k + \Delta f$$

$$\varepsilon^{k+1} = \varepsilon^k$$

This three-stage algorithm allows for the complete simulation of the one-way shape memory effect in 2D.

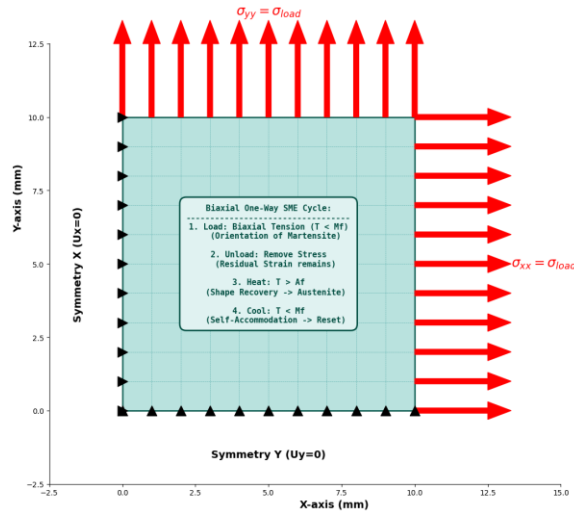


Figure IV.24. 2D Model Setup for SME Simulation

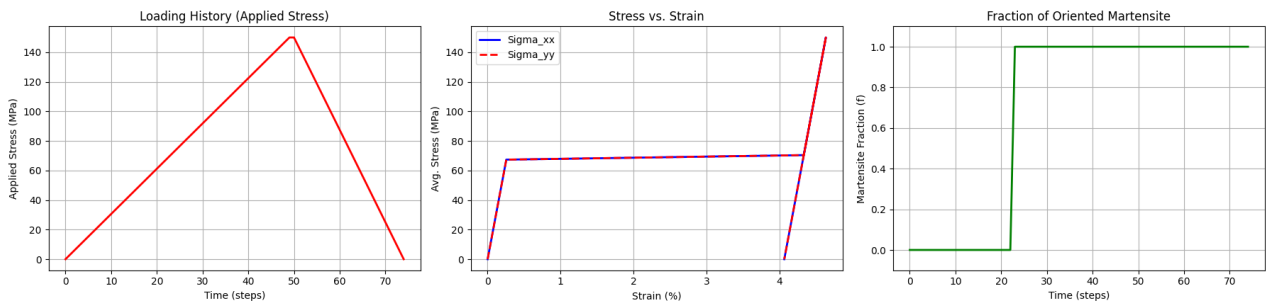


Figure IV.25. Phase 1 & 2: Mechanical Loading and Unloading Response

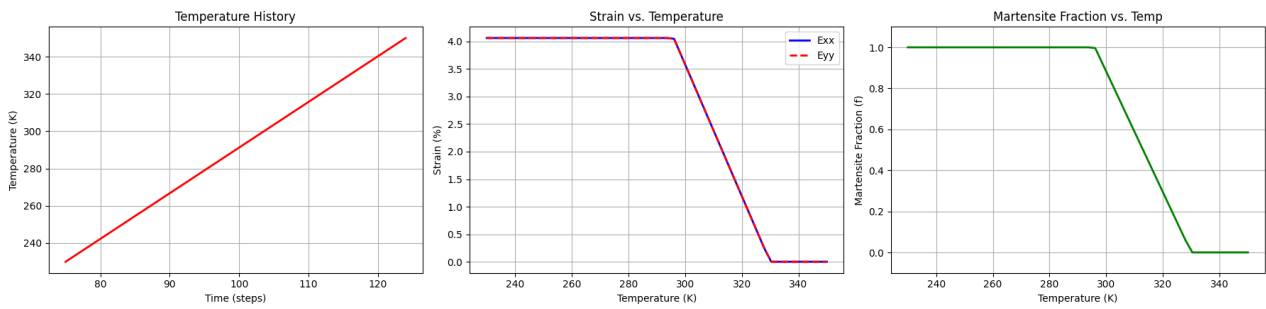


Figure IV.26. Phase 3: Thermal Recovery (Heating) Response

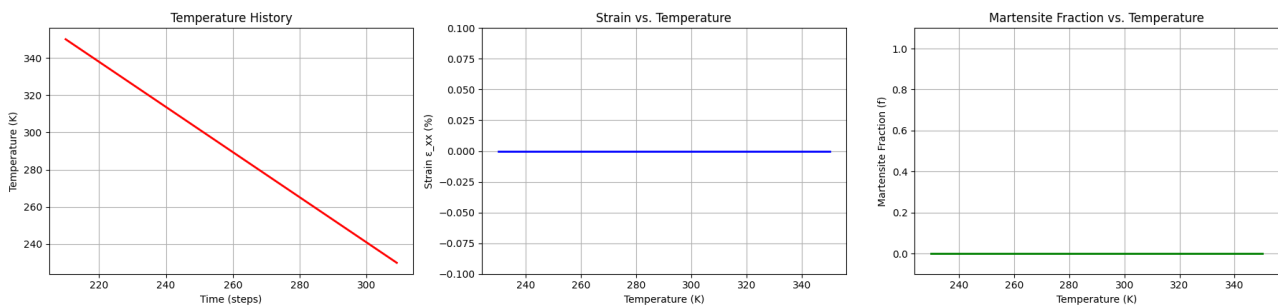


Figure IV.27. Phase 4: Strain-Free Cooling Response.

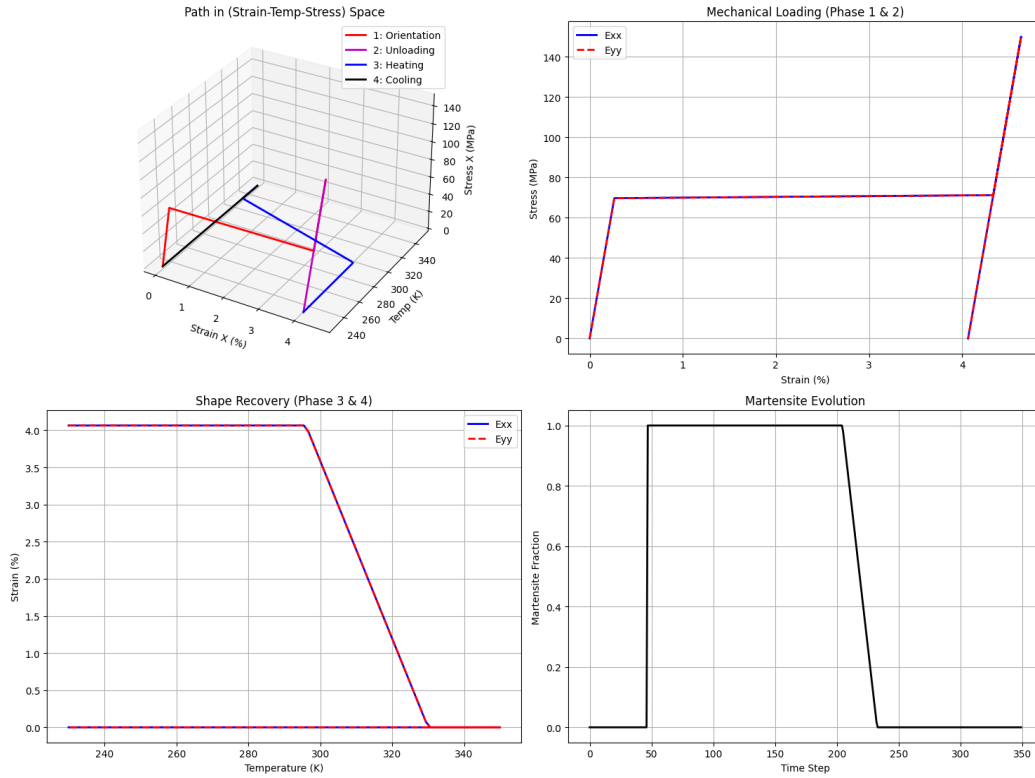


Figure IV.28. Complete 2D SME cycle visualization showing stress-strain response and temperature-strain relationship.

IV.5 Conclusion

This chapter has presented a systematic numerical verification of the constitutive model developed for Shape Memory Alloys. A hierarchical simulation strategy was adopted, progressing from one-dimensional material-point analyses to two-dimensional planar configurations, in order to assess the consistency and stability of the numerical implementation under increasing levels of complexity.

The proposed framework was examined for the principal thermomechanical responses of SMAs, including pseudoelasticity, thermoelastic behavior, and the one-way Shape Memory Effect. The simulations successfully reproduced the characteristic features associated with these phenomena, such as stress- and temperature-driven phase transformations, hysteresis behavior, and the evolution of history-dependent internal variables. These results demonstrate the internal consistency of the model and the correctness of its numerical implementation across different loading paths.

Overall, this chapter establishes a reliable numerical basis for the constitutive framework, providing confidence in its readiness for integration into finite element environments. The verified

model is subsequently employed in the next chapter to investigate the behavior of SMA thin layers under more complex boundary conditions using a full finite element implementation.

IV.6 References

- [1] M. L. Ribeiro, D. Vandepitte, and V. Tita, "Damage model and progressive failure analyses for filament wound composite laminates," *Appl. Compos. Mater.*, vol. 20, pp. 975–992, 2013. doi: 10.1007/s10443-013-9315-x.
- [2] K.L. Ng, Q.P. Sun, "Stress-induced phase transformation and detwinning in NiTi polycrystalline shape memory alloy tubes," *Mechanics of Materials*, vol. 38, pp. 41–56, 2006. doi:10.1016/j.mechmat.2005.05.008
- [3] G. Bourbon, "Contribution à l'étude isotherme et anisotherme du comportement cyclique des AMF," PhD dissertation, Université de Franche-Comté, 1994.
- [4] Zienkiewicz, O. C., Taylor, R. L., & Zhu, J. Z. (2013). *The Finite Element Method: Its Basis and Fundamentals* (7th ed.). Butterworth-Heinemann.
- [5] Dassault Systèmes Simulia Corp. (2022). *Abaqus 2023 Documentation: Abaqus User Subroutines Reference Manual*. Providence, RI, USA.
- [6] I. Zidane, B. Meddour, "On modelling of the one dimensional pseudoelastic effect of shape memory alloys," *Mechanics & Industry*, vol. 26, 2025. doi:10.1051/meca/2024040
- [7] D.C. Lagoudas, *Shape Memory Alloys: Modeling and Engineering Applications*, Springer, 2008.
- [8] L.C. Brinson, "One-dimensional constitutive behavior of shape memory alloys," *Journal of Intelligent Material Systems and Structures*, vol. 4, pp. 229-242, 1993.

CHAPTER V
FINITE ELEMENT
IMPLEMENTATION USING UMAT

V.1 Introduction

This chapter presents the numerical results obtained using Abaqus for shape memory alloy thin plates modeled with a user material subroutine (UMAT). Two numerical simulation cases are considered. The first simulation case focuses on pseudoelastic behavior under a mechanical loading–unloading cycle. The second simulation case examines thermoelastic behavior, corresponding to the shape memory effect under a constant bias stress and a prescribed thermal cycle. The results are presented in terms of field distributions and local response curves in order to assess the mechanical and thermomechanical response of the model.

V.2 Simulation of Pseudoelastic Behavior

V.2.1. Simulation data

The numerical configuration used in this section was chosen to represent a simple SMA thin layer subjected to controlled biaxial mechanical loading. Since the layer thickness is small compared with its in-plane dimensions, a plane-stress assumption was adopted. This simplified configuration makes it possible to verify the UMAT implementation and to analyze the pseudoelastic response under well-defined boundary and loading conditions.

A) Thin layer structure: The geometry considered in this study consists of a square thin layer plate with dimensions 40×40 mm. The geometry is modeled in a two-dimensional (2D) plane stress configuration to represent the thin film behavior efficiently. The geometric representation is shown in Figure V.1.

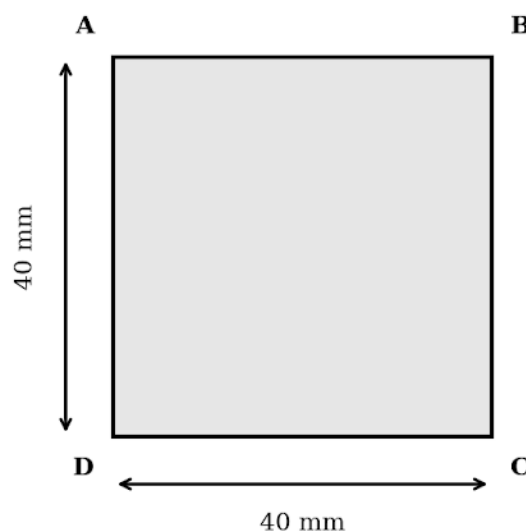


Figure V.1. Geometry of the SMA thin layer.

B) Material : The material used for this simulation is a Nickel-Titanium (NiTi) shape memory alloy. The constitutive behavior is modeled using a UMAT subroutine. The key material parameters are summarized in **Table IV.1**.

C) Mesh : The plate was discretized using standard plane stress elements in Abaqus. A structured mesh was used to ensure numerical accuracy. The mesh statistics are provided in Table V.1.

Table V.1 Mesh characteristics of the finite element model.

Parameter	Value
Global element size	4 mm
Number of elements	100
Number of nodes	121

D) Boundary conditions: The boundary conditions applied to the plate are shown in Figure V.2. The left edge (AD) is fixed in the X-direction ($U_1 = 0$), and the bottom edge (DC) is fixed in the Y-direction ($U_2 = 0$).

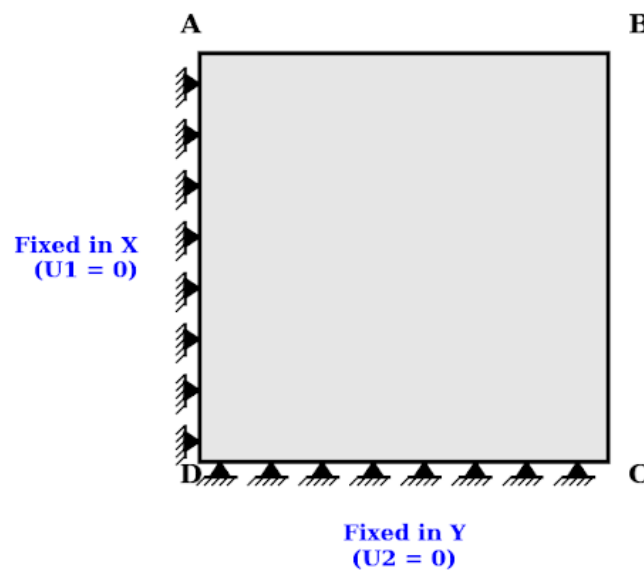


Figure V.2. Boundary conditions applied to the SMA thin layer.

E) Loading: The applied mechanical loading is illustrated in Figure V.3. A biaxial tensile stress of 400 MPa is applied along the top edge (AB) and the right edge (BC).

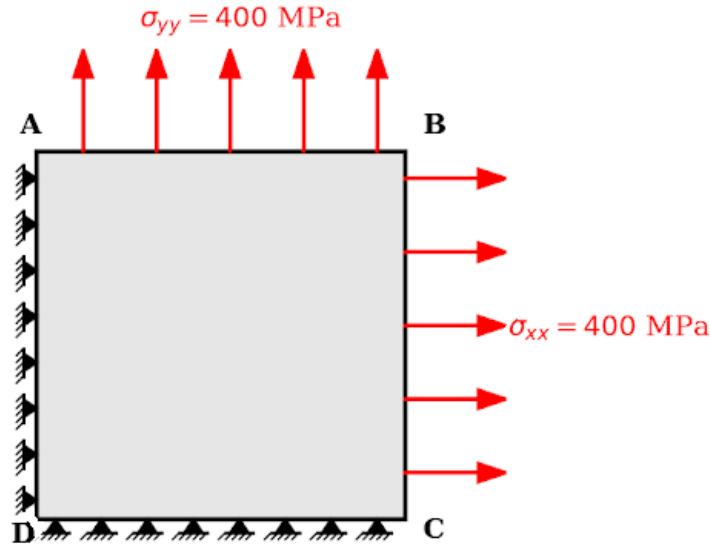
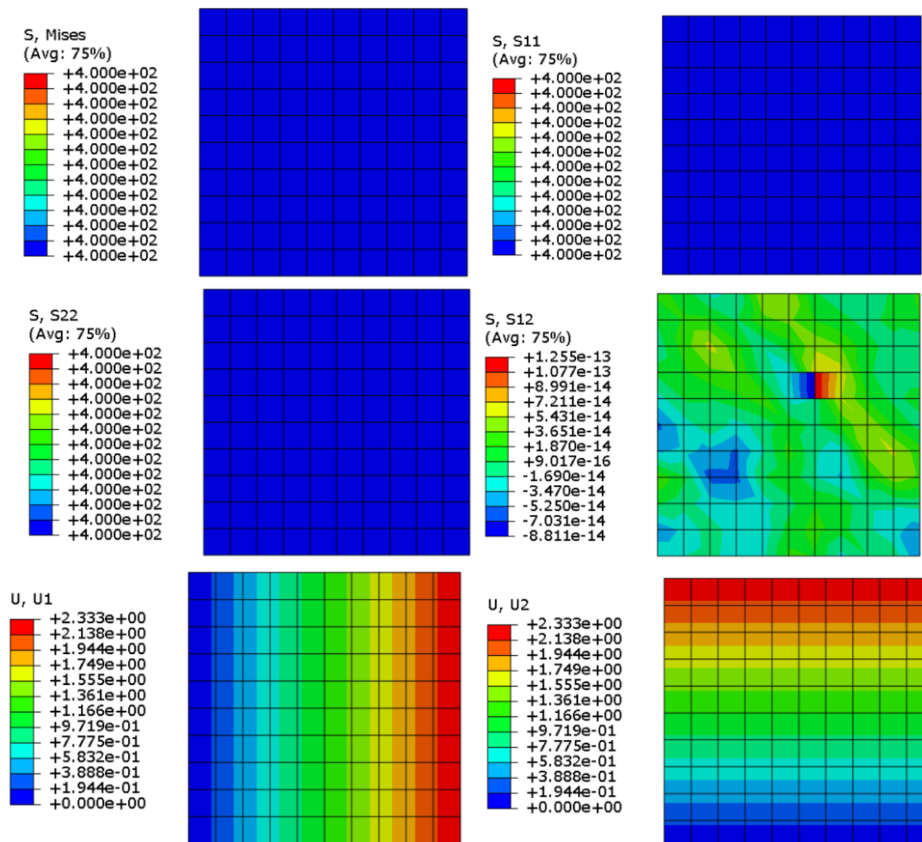


Figure V.3. Biaxial tensile loading applied to the SMA thin layer ($\sigma_{xx} = \sigma_{yy} = 400$ MPa).

V.2.2 Pseudoelastic Numerical Results

V.2.2.1 Step 1: Mechanical Loading (maximum stress, strain, and displacement state)



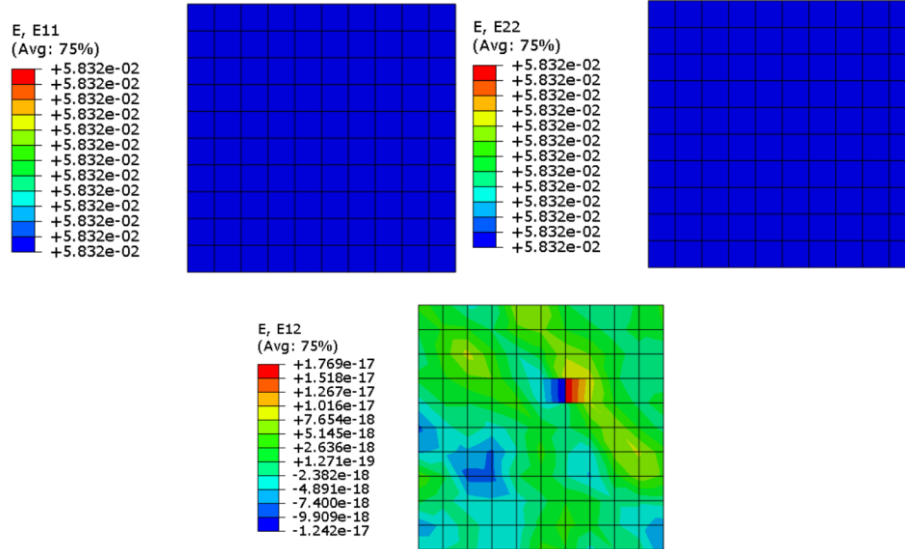


Figure V.4. Pseudoelastic response at the end of tensile loading: contour maps of von Mises stress, S11, S22, S12, U1, U2, E11, E22, and E12.

At the end of the loading step, the stress field reaches a uniform high level across the plate. The von Mises stress is approximately 400 MPa, and both S11 and S22 are also approximately 400 MPa. This equality of S11 and S22 indicates that the loading condition is not a simple uniaxial tension case; rather, it produces a nearly symmetric in-plane normal stress state. From a constitutive perspective, such a loading condition is useful because it activates the pseudoelastic response under a multiaxial stress environment, which is typically more demanding than purely uniaxial loading.

The shear stress component S12 is negligible compared with the normal stresses. Practically, this means that the deformation mode is dominated by normal straining without meaningful shear coupling. The small nonzero values visible in the S12 contour should be interpreted as numerical-level fluctuations, not as a physical shear-driven response.

The displacement contours show smooth, nearly linear gradients across the mesh. The maximum U1 is about 2.333 mm and the maximum U2 is also about 2.333 mm, consistent with the symmetry of the imposed loading. The strain field follows the same trend: E11 is approximately 5.83% and E22 is approximately 5.83%, while E12 remains essentially zero. In other words, the deformation at peak loading is almost entirely normal and spatially homogeneous. This homogeneity is important: it indicates that the computed response is not dominated by local artifacts (such as corner locking or spurious localization) and is therefore well suited for interpreting the material behavior itself.

V.2.2.2 Step 2: Mechanical Unloading (recovery and residual values)

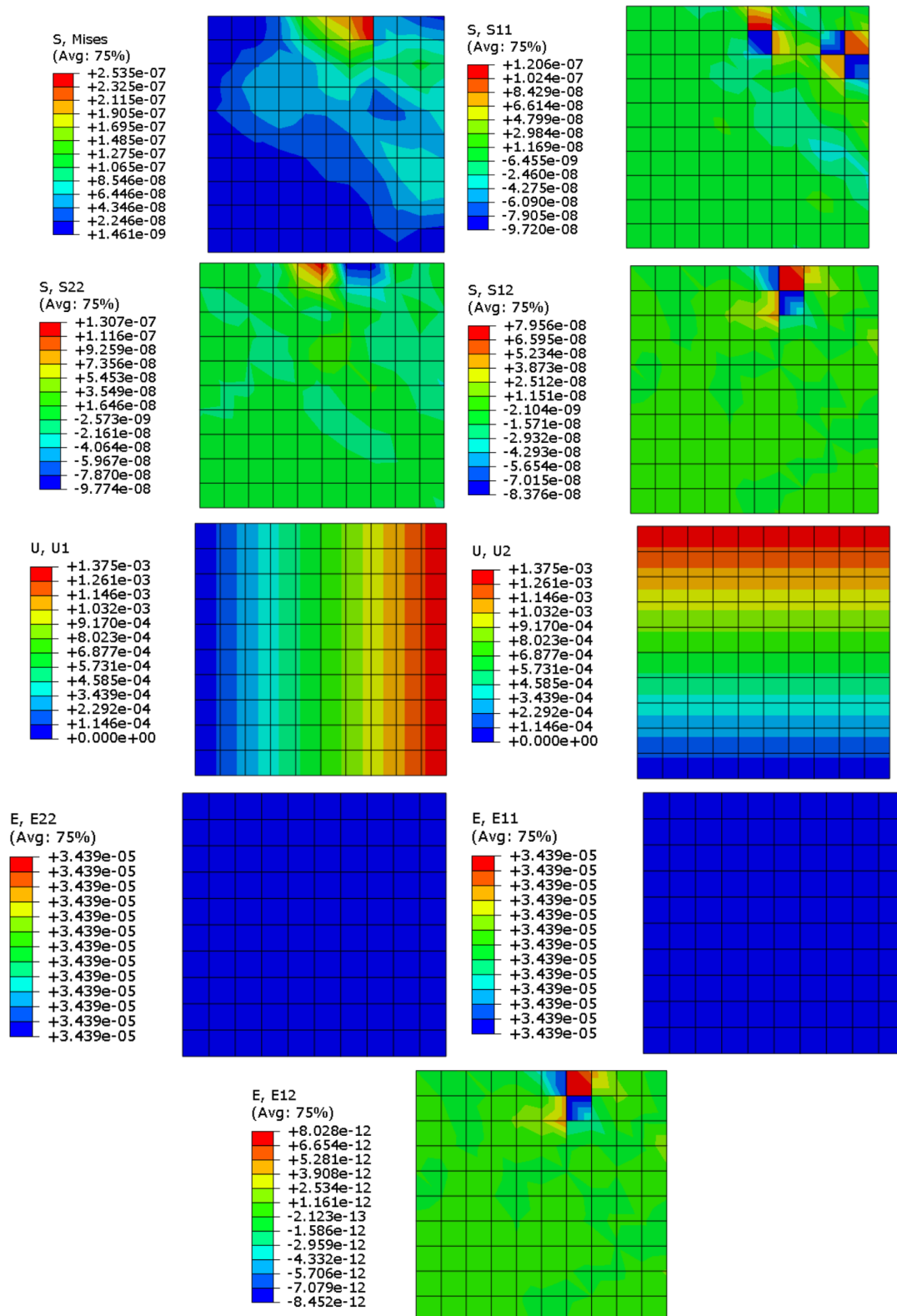


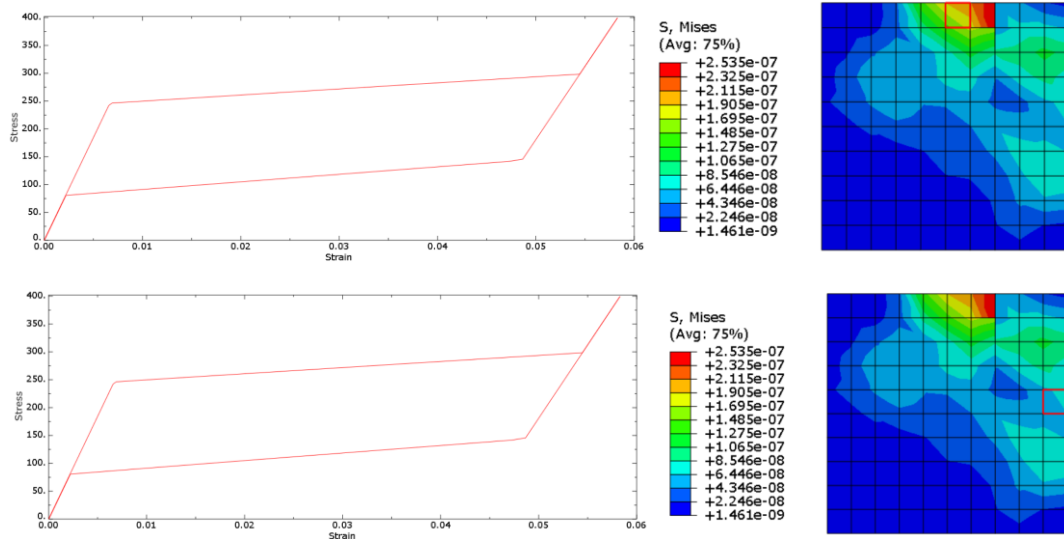
Figure V.5. Pseudoelastic response after unloading: contour maps of stress, displacement, and strain.

After unloading, the stress field returns to negligible values. The maximum von Mises stress is below 0.000001 MPa, and S11 and S22 are of the same negligible order. In mechanical terms, this means the plate is effectively stress-free at the end of the unloading step. This is the expected outcome for a pseudoelastic cycle when the material returns to the initial configuration after reverse transformation.

The displacement and strain fields confirm the recovery. The maximum residual displacement is about 0.0014 mm for both U1 and U2, which is extremely small relative to the peak displacement of 2.333 mm. The residual strains E11 and E22 are about 0.0034%, compared to the peak strain of 5.83%. Expressed differently, the residual strain is roughly 0.06% of the peak strain, which corresponds to about 99.94% recovery. The remaining residual values are sufficiently small to be attributed to numerical tolerances and equilibrium convergence rather than to any meaningful permanent deformation.

Overall, Step 2 provides a clear numerical signature of unloading and recovery: stresses vanish and the plate returns very close to its original shape, consistent with strongly reversible pseudoelastic behavior.

V.2.2.3 Local Stress-Strain Analysis (hysteresis and spatial homogeneity)



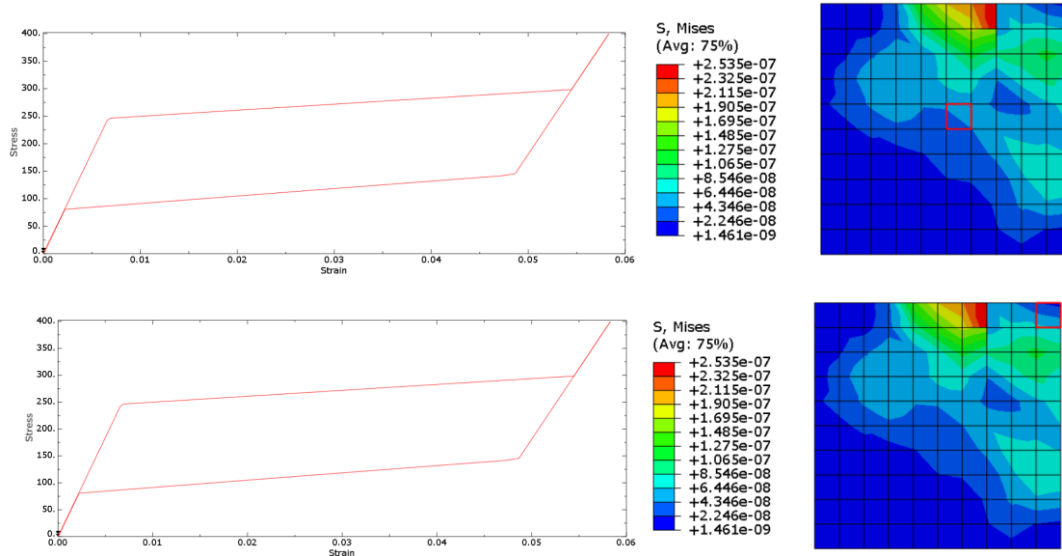


Figure V.6. Pseudoelastic local stress–strain response extracted at the upper-edge corner.

The local stress-strain curves exhibit the characteristic hysteresis loop associated with pseudoelastic cycling in NiTi. During loading, the response shows a change in slope consistent with stress-induced transformation, followed by re-stiffening as the transformation saturates. During unloading, the recovery branch occurs at lower stress levels than the loading branch, producing a closed loop that reflects the energy dissipated during forward and reverse transformation.

Two observations are particularly important. First, the peak levels from the curves are consistent with the field maps: the response reaches about 400 MPa and about 6% strain, matching the contour maxima reported in Step 1. Second, the curves from the centre, mid-edge, and corners are very similar in shape and amplitude. This similarity is consistent with the homogeneous stress and strain contours and indicates that the transformation process develops coherently across the domain without meaningful localization. Minor differences at corners are expected in finite element models due to boundary constraints, but they do not alter the overall conclusion that the simulated response is spatially uniform.

V.3 Simulation of Thermoelastic Behavior

V.3.1 Simulation data

The thermoelastic response is simulated using the same finite element model as in the pseudoelastic case. The SMA thin layer is modeled as a 40×40 mm square plate under plane stress conditions.

B) Material: The material considered is a Cu–Zn–Al shape memory alloy, with its constitutive behavior defined through the UMAT. The material parameters are given in Table IV.2.

C) Mesh: The mesh discretization is identical to that used in the pseudoelastic simulations (Table V.2).

D) Boundary conditions: The applied boundary conditions are shown in Figure V.2. The left edge (AD) is fixed in the X-direction ($U_1 = 0$), and the bottom edge (DC) is fixed in the Y-direction ($U_2 = 0$).

E) Thermoelastic loading: The thermoelastic loading is illustrated in Figure V.7. A constant biaxial tensile stress of 65 MPa is applied along edges AB and BC, while a prescribed thermal cycle is imposed to induce the shape memory effect.

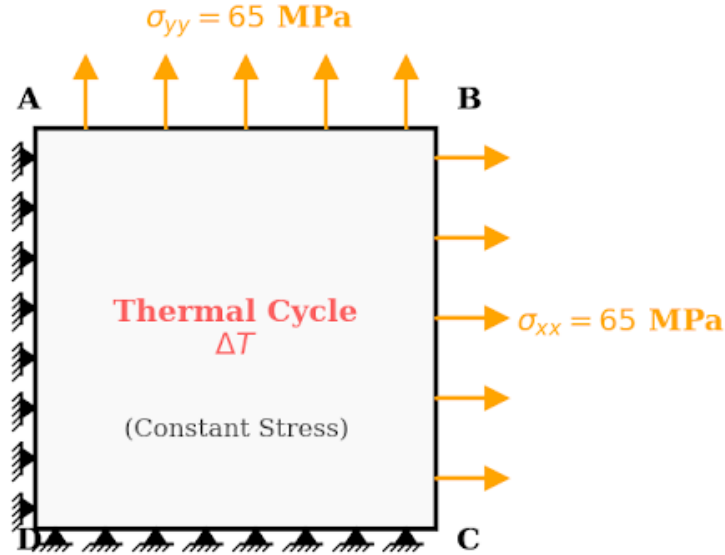
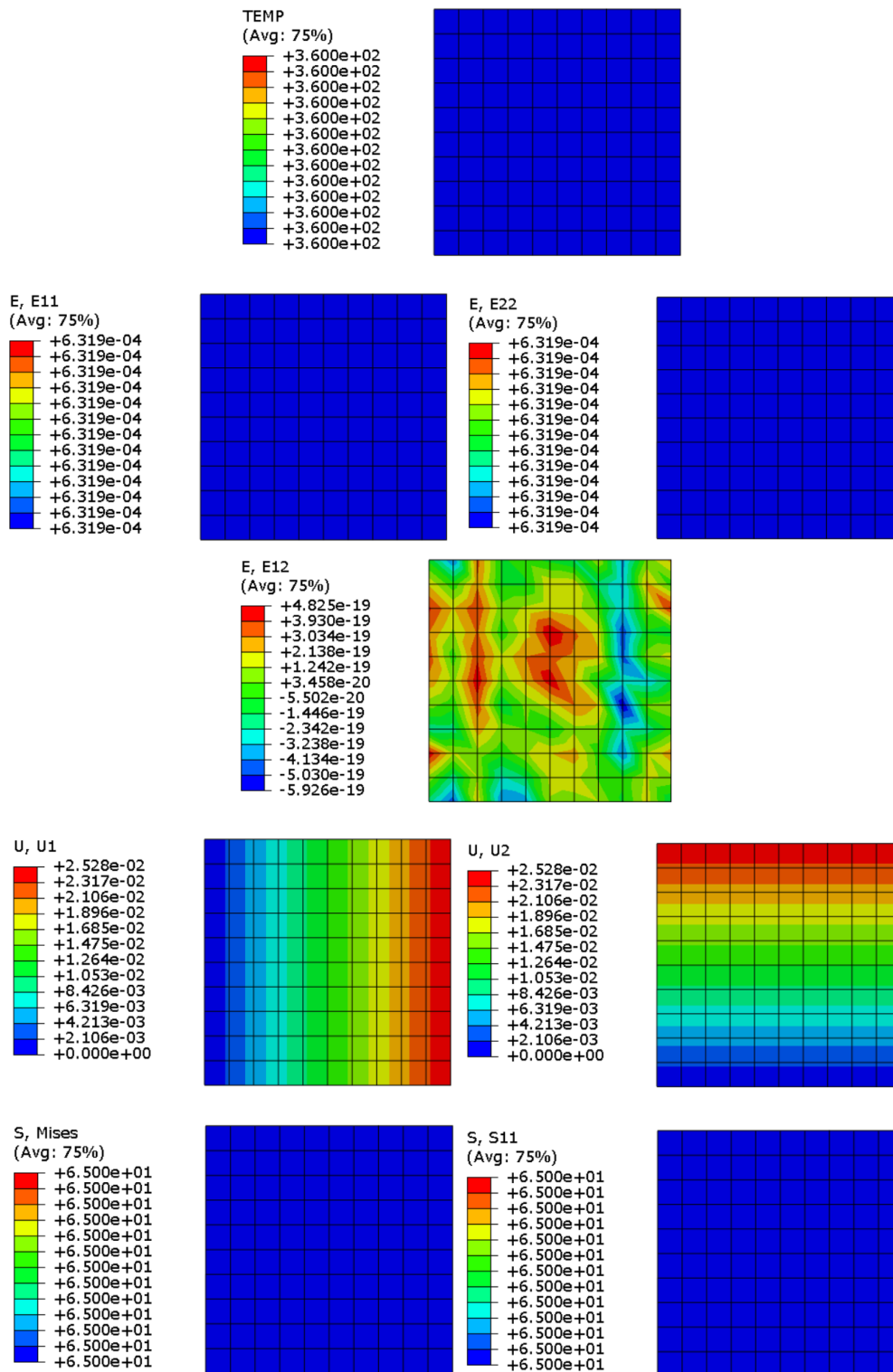


Figure V.7. Thermoelastic loading under constant biaxial tensile stress ($\sigma_{xx} = \sigma_{yy} = 65 \text{ MPa}$) and prescribed thermal cycle.

V.3.2 Thermoelastic Numerical Results (Shape Memory Effect)

V.3.2.1 Step 1: High Temperature State (austenite stability under bias stress)



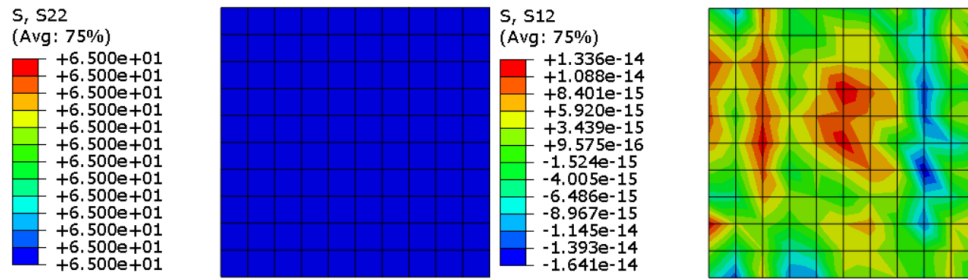
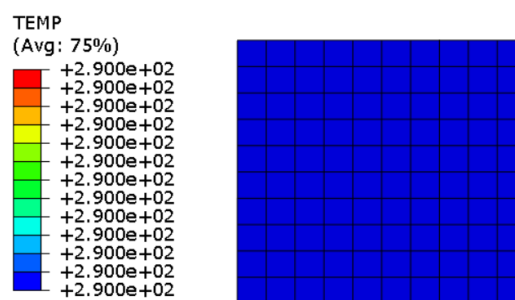


Figure V.8. Thermoelastic response at high temperature: temperature field and contour maps.

In the first thermal step, the temperature is uniform at 360 K across the plate. Under this high-temperature condition, the computed stress field is also uniform, with von Mises stress close to 65 MPa and normal components S11 and S22 close to 65 MPa. The shear component S12 remains negligible. This confirms that the model is in a stable, uniformly loaded bias-stress condition without shear distortion.

The strains are small: E11 and E22 are approximately 0.063%, and the displacements U1 and U2 reach only about 0.0253 mm. The small magnitude of strain at 360 K indicates that the response is dominated by elastic deformation (and any minor thermal expansion embedded in the formulation) rather than by transformation strain. In physical terms, the high temperature favors the austenitic phase, and under the chosen Constant stress level the plate remains in a low-strain state.

V.3.2.2 Step 2: Low Temperature State (cooling and transformation strain under constant bias stress)



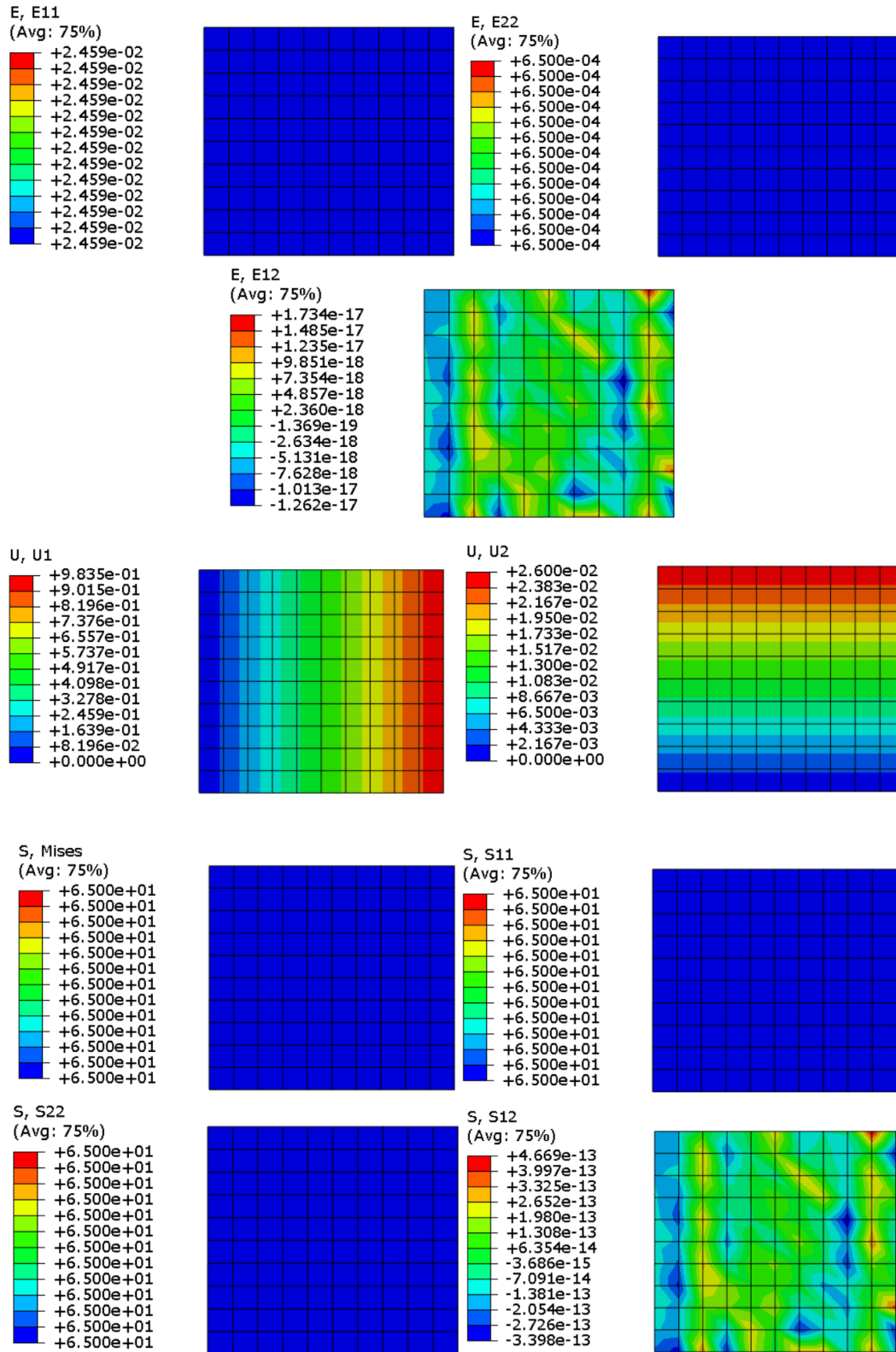


Figure V.9. Thermoelastic response at low temperature: temperature field and contour maps.

In the second thermal step, the temperature is uniformly reduced to 290 K. importantly; the stress state remains essentially unchanged: von Mises stress stays close to 65 MPa, and S11 and S22 remain close to 65 MPa, while S12 remains negligible. This confirms that the simulation

represents cooling under an approximately constant bias stress condition, rather than a mechanically intensified loading step.

The central outcome of Step 2 is the large increase in strain along direction 1. E11 rises to about 2.46%, while E22 remains near 0.065%, close to its Step 1 level. The displacement field reflects the same directional actuation: U1 increases to about 0.9835 mm, whereas U2 remains small at about 0.026 mm. Because the applied stress level is maintained while the temperature changes, this additional deformation cannot be attributed to mechanical loading. Instead, it is a temperature-driven transformation strain developing under Constant load, consistent with martensite formation during cooling and with the classical shape memory effect under load.

The difference in E11 between Step 1 and Step 2 is approximately 2.40% (2.46% minus 0.063%). This value represents the effective actuation strain generated by the thermally induced transformation in the loading direction for this simulation case.

V.3.2.3 Temperature-Strain Analysis (thermal hysteresis and coherence across the mesh)

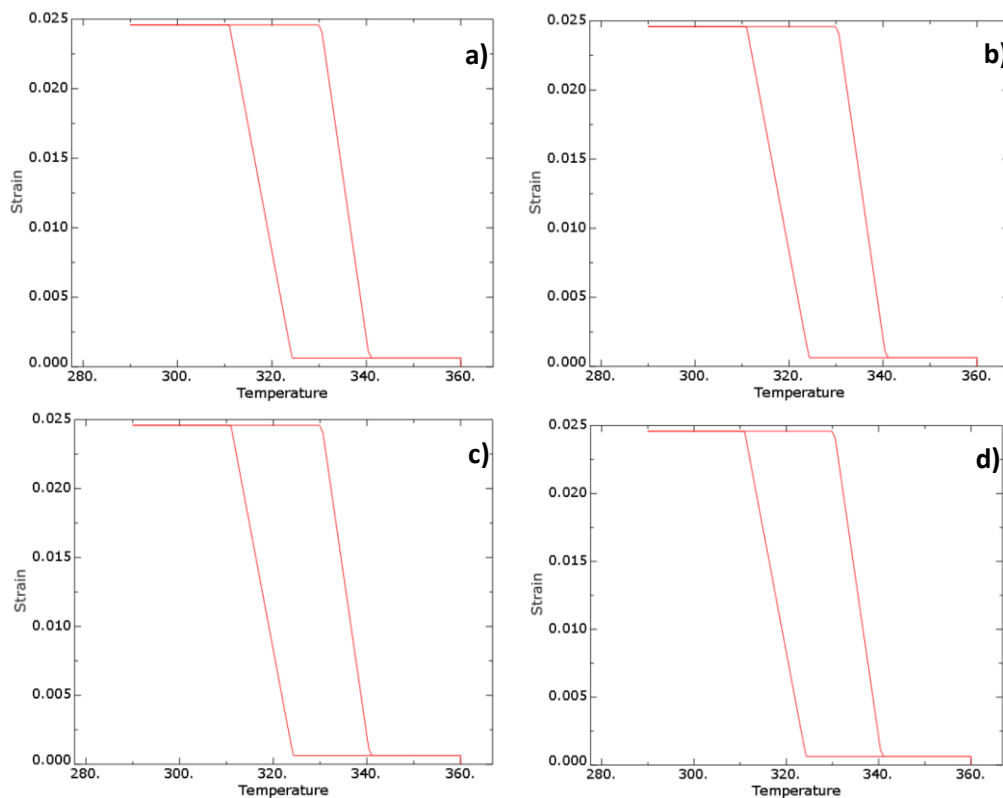


Figure V.10. Thermoelastic temperature–strain response extracted at different locations of the SMA thin layer: (a) center, (b) mid-edge, (c) first corner, and (d) second corner.

The temperature-strain curves show a clear thermal hysteresis loop. The strain alternates between a low level near zero and a high level near 2.4% to 2.5%, which corresponds to the transformation strain developed during cooling and recovered during heating. The transitions occur over narrow temperature intervals, with the strain increase during cooling occurring around the low 300 K range (approximately 310 K to 325 K) and the strain recovery during heating occurring at higher temperatures (approximately 335 K to 345 K). This separation between the cooling and heating transition ranges is the thermal hysteresis that is characteristic of thermoelastic transformation in NiTi.

A key numerical observation is that the curves from the centre, mid-edge, and corners overlap closely. This agrees with the temperature and strain contour maps, which are essentially uniform across the plate. The thermo-mechanical response therefore develops coherently throughout the mesh, indicating a structurally uniform actuation response for the chosen boundary conditions and thermal loading.

V.4 Conclusion

The Abaqus simulations provide a coherent numerical description of two fundamental behaviors of Shape Memory Alloys within a controlled numerical framework.

In the pseudoelastic case, the thin plate reaches a high and spatially uniform stress level of approximately 400 MPa and a peak strain close to 5.83% at the end of the loading stage. Upon unloading, the stress field returns to negligible values, and the residual strain decreases to about 0.0034%, corresponding to an overall strain recovery of approximately 99.94%. The local stress-strain curves exhibit a well-defined pseudoelastic hysteresis loop, and the close similarity of the responses extracted at the centre, mid-edge, and corner locations is consistent with the homogeneous stress and strain distributions observed in the contour fields.

For the thermoelastic case under Constant loading, the high-temperature state at 360 K results in only small elastic strains (on the order of 0.063%) under a nearly constant stress level of approximately 65 MPa. Cooling to 290 K at essentially the same stress level induces a significant transformation strain in the primary loading direction, reaching about 2.46%, while the transverse strain remains close to its initial low value. The temperature-strain curves display a stable thermal hysteresis loop, with similar responses obtained at all monitored locations. This

behavior reflects a spatially coherent, temperature-driven transformation strain developing under constant stress.

GENERAL CONCLUSION

GENERAL CONCLUSION

This thesis addressed the numerical modeling and analysis of the thermomechanical behavior of shape memory alloy (SMA) thin layers subjected to mechanical and thermal loading. The work was motivated by the growing integration of SMA thin layers in compact and functional systems, where their performance is strongly influenced by geometric constraints, boundary conditions, and loading paths.

To meet this objective, a consistent constitutive framework was developed to describe the key mechanisms governing SMA behavior, including stress-induced pseudoelasticity and thermally driven shape memory effects. The formulation was implemented through a user material subroutine (UMAT) and integrated into a finite element environment. Particular emphasis was placed on two-dimensional plane stress configurations, which provide an efficient and physically relevant representation of thin layer behavior.

Beyond the implementation aspect, this work provided a detailed numerical investigation of SMA thin layers under representative loading scenarios. The results highlighted the central role of mechanical constraints in shaping stress distributions, phase transformation paths, and recoverable deformation. In particular, biaxial mechanical loading was shown to significantly limit the pseudoelastic response, whereas thermally driven actuation under Constant load offered more controlled and stable operational conditions.

Several important conclusions emerged from the numerical simulations. The analyses provided clear insight into the interaction between SMA thin layers and their mechanical environment, demonstrating how constraints directly affect functional performance. They also revealed critical stress levels that may arise under purely mechanical loading, identifying potential limitations—such as substrate yielding—for designs relying exclusively on pseudoelastic behavior. In contrast, thermoelastic loading scenarios were found to enable effective actuation while maintaining acceptable stress levels, suggesting safer and more reliable operating modes for SMA-based thin layer devices.

Overall, this work resulted in a numerically verified computational framework that can serve as a predictive tool for the analysis and design of SMA thin layer systems. The proposed approach allows the investigation of different loading paths, boundary conditions, and material

configurations, and provides a solid basis for the development of reliable and efficient smart devices.

Perspectives for future work include extended parametric studies on geometric and material parameters, investigations of thickness scaling toward micro-scale layers, and experimental verification of the numerical predictions. Further developments may also incorporate additional phenomena such as cyclic loading effects, functional fatigue, and damage evolution, in order to enhance the predictive capabilities of the proposed framework.