

On modelling of the one dimensional pseudoelastic effect of shape memory alloys

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Received: 27 August 2024 / Accepted: 31 December 2024

Abstract. Last decades, a qualitative leap in materials engineering was observed, through developing new materials or discovering new properties. The shape memory alloys are a group of materials exhibiting singular behaviour under a coupled thermomechanical loading, and they are widely used in numerous applications because of their properties. To exploit these properties in engineering, several constitutive models of were developed. The aim of this work is to build a constitutive model that could describe the pseudoelastic behaviour of shape memory alloys in a simpler and more accurate way. Based on thermodynamics and mechanics laws and principles, the developed constitutive model was implemented in an algorithm and compared with experimental data in order to assess its accuracy. The obtained results indicated that the agreement between the real and computer-simulated stress-strain curves was good. This reaffirmed the model's ability to predict the pseudoelastic behaviour of the shape memory materials under various loading states. These results thus validate especially the temperature sensitivity of Nitinol alloys, which should be taken into account when designing devices that need to function reliably.

Keywords: Pseudoelasticity / memory / thermomechanical / transformation / fraction

1 Introduction

The basic materials that go into making modern technology are what drive its progress. The advancement of technology can benefit from a wide variety of materials. Among these categories are smart materials, which are recognized for exhibiting a variety of distinct properties in contrast to other kinds of materials [1].

Lightweight and flexible systems are becoming more and more in demand in structural engineering, robotics, and aerospace, where the emergence of smart materials and structures is transforming design ideas [2].

Different smart or responsive materials are utilized in the modern era of technology. These materials can change their structure, size, or mechanical qualities in response to external stimuli, such as a certain level of mechanical stress, pressure, temperature, pH, or UV radiation. As the world's temperatures rise and weather patterns grow more severe and unpredictable [3].

Shape memory alloys, sometimes known as SMAs, are among the greatest kinds of smart materials. They have been the focus of much commercial and scientific attention since their discovery in the early 1930s [4].

Moreover shape memory alloys constitute a unique class of multifunctional materials that can change their behavior in response to mechanical or thermal stimulation are now widely used in a variety of applications [5,7].

The majority of research on shape memory alloys (SMAs) has been done with NiTi SMA. It should be noticed that before the discovery of the shape memory effect (SME) in a nickel-titanium (NiTi), by William Buehler and Frederick Wang in 1962, the importance and the demand of SMAs for most engineering and technical applications was not positively realized, it is the most well-known SMA [8,9].

NiTi shape-memory alloys have found extensive application in industries like electronic equipment, aircraft, and biomedicine military applications, telecommunications, and industrial process control, technical applications because of their exceptional form recovery qualities, including the pseudoelastic effect (PE) and shape memory effect (SME) [10-13].

In addition, shape memory alloy (SMA) offers superior fatigue, corrosion resistance, and high damping in addition to its two distinctive qualities of shape memory and superelasticity. As a result, SMA is frequently utilized for vibration control and reinforcing in the field of civil engineering. It is distinguished by its low modulus of elasticity, moderate density, reasonable impact resistance and ductility, high strength at room temperature and raised temperatures, and biocompatibility that is susceptible to changes in temperature and composition [14,15].

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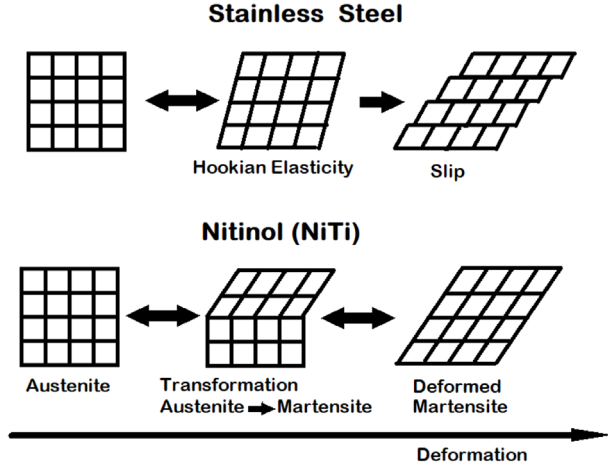


Fig. 1. Schematic presentation of lattice structure changes caused by applied stress in stainless steel or nitinol [18].

Even though having outstanding mechanical properties, NiTi SMAs have limited uses due to their high material cost and challenging metal formation [16].

The widespread use of conventional materials has been made possible by their well-known behavior, but novel uses in the medical and aerospace fields have been made possible by the discovery of new features resulting from the unique behavior of materials known as shape memory alloys. Scientists and academics have paid close attention to this peculiar behavior. As a result, several models were put forth. These models are expanded versions of common materials based on framework theories and the laws of thermodynamics [17].

There are two phases in these materials: the austenite phase and the martensite phase. SMAs undergo phase transitions, going from the austenite to the martensite and back again.

The elastic (reversible) response to an applied stress produced by a phase transition between a SMA's austenite and martensite phases is called superelasticity (SE), sometimes known as pseudoelasticity. Pseudoelasticity, in contrast to the shape memory effect, occurs independently of temperature. SE occurs at a high enough temperature where the alloy is in its parent phase and its original shape and there is a stable austenite phase. An austenite phase may be stimulated to change into a stable, detwinned martensite phase also referred to as "stress-induced martensite" by applying a mechanical strain. This strain is accommodated by the immediate regions related shear.

Compared to conventional elastic deformation, which can only handle strains of up to around 0.5% for most metals, NiTi SMAs allow for relatively significant strains of up to 8% without plastic deformation. However, martensitic phase changes must account for all of the deformation in order for this phenomena to occur. It is possible that some traditional plastic flow (dislocation glide) will occur if an extreme strain is applied, and the process will be irreversible (Fig. 1) [19,20].

Note that these materials have a very basic use: they can be easily deformed by applying an external force, and when heated over a specific temperature either internally or externally they will contract or return to their original shape (For example Joule heating in case of some applications) [21].

The effect of pseudoelasticity, on which we focused in this work, is the ability of SMA to deform in large proportions and to recover their initial configuration upon unloading. This behaviour is observable when an increasing stress is applied to a volume of SMA, in quasi-isothermal conditions, from a totally austenitic state, i.e. when the test temperature $T > A_s^0$ (Figs. 2 and 3).

The application of a stress causes the elastic deformation of the austenite, followed by the martensitic transformation from the martensite start stress σ_{Ms} up to the martensite finish stress σ_{Mf} where all the austenite is transformed into martensite. During unloading, the martensite deforms elastically up to the austenite start stress σ_{As} from which the austenitic transformation begins which ends as soon as the stress $\sigma < \sigma_{Af}$.

In this paper, the work focused on the pseudoelastic effect, a constitutive model was built and the algorithm was developed using MATLAB. The experimental data were supplied by obtained results through the study of Ng et al. [23].

2 Methods and materials

2.1 Constitutive equations

First of all let us consider a representative elementary volume (Fig. 4)

Fraction of martensite is given by:

$$f = \frac{V_M}{V_A + V_M}. \quad (1)$$

The thermodynamic potential used in this work is Gibbs free energy density, which is denoted FED (Free Energy Density) can be written as [22,24]:

$$FED(\sigma, T, f) = -\frac{\sigma^2}{2} \cdot \left[\frac{1-f}{E_A} + \frac{f}{E_M} \right] - \sigma \cdot f \cdot \varepsilon^0 + B \cdot f \cdot (f+1) \cdot (T - T^0) + C \cdot f \cdot (f-1) \quad (2)$$

$\frac{\sigma^2}{2} \cdot \left[\frac{1-f}{E_A} + \frac{f}{E_M} \right]$: Elastic energy of deformation; $\sigma \cdot f \cdot \varepsilon^0$: Mechanical work associated with the transformation of martensite; $B \cdot f \cdot (f+1) \cdot (T - T^0)$: Free energy of phase change; $C \cdot f \cdot (f-1)$: Energy of interaction between martensite and austenite; E_A and E_M : Young modulus respectively of austenite and martensite; ε^0 : Maximum deformation along an axis; T^0 : Reference temperature; B and C: Constants to be determined.

The dissipation occurring during the transformation leads to consider Clausius inequality:

$$-\frac{\partial FED}{\partial f} \cdot \frac{df}{dt} \geq 0. \quad (3)$$

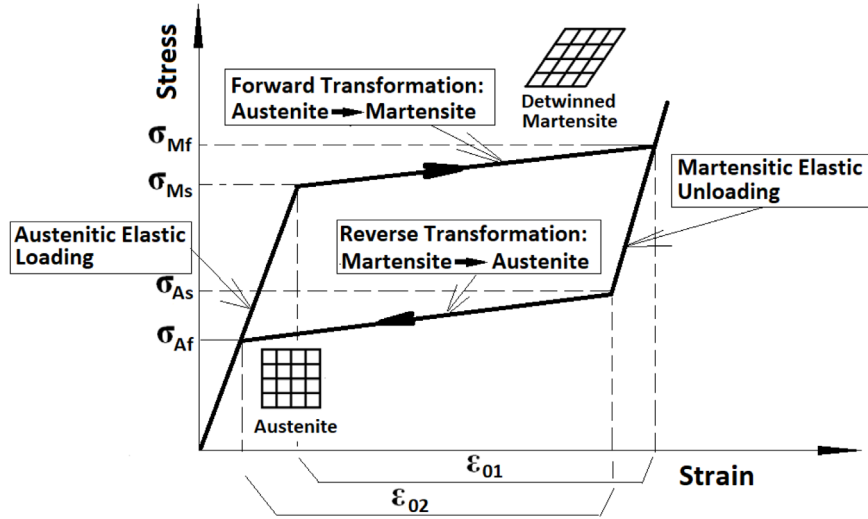


Fig. 2. Diagram illustrating pseudoelasticity effect [22].

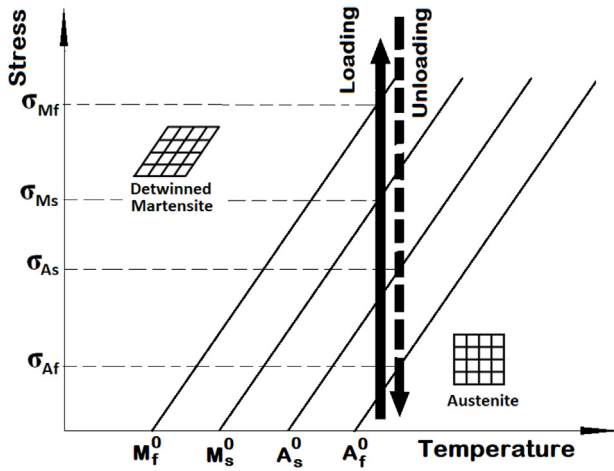


Fig. 3. Path of loading [22]. σ_{MS} : Martensite start stress; σ_{Mf} : Martensite finish stress; σ_{AS} : Austenite start stress; σ_{Af} : Austenite finish stress; M_s^0 : Martensite temperature start (Zero-stress); M_f^0 : Martensite temperature finish (Zero-stress); A_s^0 : Austenite temperature start (Zero-stress); A_f^0 : Austenite temperature finish (Zero-stress); ϵ_{01} : Maximum strain in forward transformation; ϵ_{02} : Maximum strain in reverse transformation.

Driving force, deriving from the thermodynamic potential FED is given by:

$$-\frac{\partial FED}{\partial f} = THD^F. \quad (4)$$

Since there is dissipation during the transformation of martensite into austenite (and austenite to martensite as well), it can be assumed that dissipation pseudo-potential exists, denoted PTH^D , then quantified by the suggested expression:

$$PTH^D = -K \left(\frac{f^3}{3} + \frac{f^2}{2} \right) - Hf \quad (5)$$

K and H are constants to be determined.

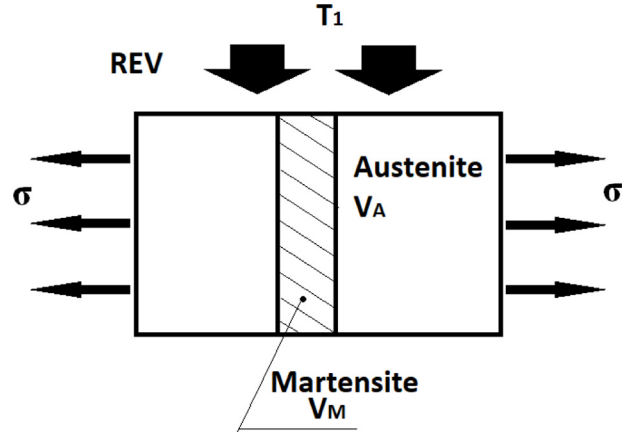


Fig. 4. Representative elementary volume.

Taking into account that dissipative force driving denoted DIS^F is derived from dissipative pseudo-potential PTH^D :

$$-\frac{dPTH^D}{df} = DIS^F. \quad (6)$$

This will give:

$$DIS^F = Kf(f+1) + H. \quad (7)$$

The transformation of austenite into martensite (Forward transformation) occurs when the following condition is satisfied:

$$THD^F = DIS^F. \quad (8)$$

Let us consider the following criteria function denoted Ω^{FOR} :

$$\Omega^{FOR}(\sigma, f, T) = THD^F - DIS^F. \quad (9)$$

Then:

$$\Omega^{FOR}(\sigma, f, T) = \frac{\sigma^2}{2} \cdot \left[\left(\frac{1}{E_M} \right) - \left(\frac{1}{E_A} \right) \right] + \sigma \cdot \varepsilon^0 - B \cdot (2f + 1) \cdot (T - T^0) - C \cdot (2f - 1) - K \cdot f \cdot (f + 1) - H = 0. \quad (10)$$

Since the function $\Omega^{FOR}(\sigma, f, T)$ is zero, it is consistent that its time derivative is also zero:

$$\frac{d\Omega^{FOR}}{dt} = \frac{\partial \Omega^{FOR}}{\partial \sigma} \cdot \frac{d\sigma}{dt} + \frac{\partial \Omega^{FOR}}{\partial T} \cdot \frac{dT}{dt} + \frac{\partial \Omega^{FOR}}{\partial f} \cdot \frac{df}{dt} = 0. \quad (11)$$

Then:

$$\left[\sigma \cdot \left(\frac{1}{E_M} - \frac{1}{E_A} \right) + \varepsilon^0 \right] \cdot \dot{\sigma} - B \cdot (2f + 1) \cdot \dot{T} + [-2B \cdot (T - T^0) - 2C - K \cdot (2f + 1)] \cdot \dot{f} = 0. \quad (12)$$

Equation (11) leads to:

$$\dot{f} = \frac{\left[\sigma \cdot \left(\frac{1}{E_M} - \frac{1}{E_A} \right) + \varepsilon^0 \right] \cdot \dot{\sigma} - B \cdot (2f + 1) \cdot \dot{T}}{-2B \cdot (T - T^0) - 2C - K \cdot (2f + 1)} \quad (13)$$

when it comes into isothermal case, equation (12) will be rewritten as following:

$$\dot{f} = \frac{-\left[\sigma \cdot \left(\frac{1}{E_M} - \frac{1}{E_A} \right) + \varepsilon^0 \right] \cdot \dot{\sigma}}{-2B \cdot (T - T^0) - 2C - K \cdot (2f + 1)}. \quad (14)$$

In case of reverse transformation:

$$THD^F = -DIS^F. \quad (15)$$

The criteria function denoted Ω^{REV} will be written as:

$$\Omega^{REV}(\sigma, f, T) = THD^F + DIS^F. \quad (16)$$

Then

$$\Omega^{REV}(\sigma, T, f) = \frac{\sigma^2}{2} \cdot \left[\left(\frac{1}{E_M} \right) - \left(\frac{1}{E_A} \right) \right] + \sigma \cdot \varepsilon^0 - B \cdot (2f + 1) \cdot (T - T^0) - C \cdot (2f - 1) + K \cdot f \cdot (f + 1) + H. \quad (17)$$

Similarly to equation (12), the expression of fraction rate is written as following:

$$\dot{f} = \frac{\left[\sigma \cdot \left(\frac{1}{E_M} - \frac{1}{E_A} \right) + \varepsilon^0 \right] \cdot \dot{\sigma} - B \cdot (2f + 1) \cdot \dot{T}}{-2B \cdot (T - T^0) - 2C + K \cdot (2f + 1)}. \quad (18)$$

Table 1. Experimental data ($T = 65^\circ\text{C}$).

σ_{MS} (MPa)	268	E_M (Mpa)	18442
σ_{MF} (MPa)	275	M_s^0 (K)	279
σ_{AS} (MPa)	62	ε_{10}	0.06106
σ_{Af} (MPa)	37	ε_{02}	0.05903
E_A (MPa)	25775		

Table 2. Parameters of the model.

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

In isothermal case ($T = \text{cte}$):

$$\dot{f} = -\left[\sigma \cdot \left(\frac{1}{E_M} - \frac{1}{E_A} \right) + \varepsilon^0 \right] \cdot \frac{\dot{\sigma}}{\{-2B \cdot (T - T^0) - 2C + K \cdot (2f + 1)\}}. \quad (19)$$

2.2 Determination of constants B, C, K and H

The experimental data, were supplied by (Ng et al.) work. They carried out a set of experiments in polycrystalline NiTi shape memory alloy tubes by tensile testing at different temperatures: $T = 46^\circ\text{C}$, $T = 56^\circ\text{C}$, $T = 65^\circ\text{C}$ and $T = 70^\circ\text{C}$ [23].

In order to determine constants B, C, K and H, we used experimental results obtained at $T = 65^\circ\text{C}$ and they are illustrated by Table 1.

The reference temperature was fixed:

$$T^0 = M_s^0.$$

At the start of the forward transformation we have the following conditions:

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

$$\begin{aligned} \Omega^{FOR}(\sigma = \sigma_{MS}, T = T_1, f = 0) \\ = \left(\frac{\sigma_{MS}^2}{2} \right) * \left(\frac{1}{E_M} - \frac{1}{E_A} \right) + \sigma_{MS} * \varepsilon_{01} - B \\ * (T_1 - M_s^0) + C - H = 0. \end{aligned} \quad (20)$$

At the end of forward transformation:

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

$$\begin{aligned}
\Omega^{FOR}(\sigma = \sigma_{MF}, T = T_1, f = 1) \\
= \left(\frac{\sigma_{MF}^2}{2} \right) * \left(\frac{1}{E_M} - \frac{1}{E_A} \right) + \sigma_{MF} * \varepsilon_{01} - 3B \\
* (T_1 - M_s^0) - C - H = 0.
\end{aligned} \quad (21)$$

At the start of the reverse transformation:

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

$$\begin{aligned}
\Omega^{REV}(\sigma = \sigma_{AS}, T = T_1, f = 1) \\
= \left(\frac{\sigma_{AS}^2}{2} \right) * \left(\frac{1}{E_M} - \frac{1}{E_A} \right) + \sigma_{AS} * \varepsilon_{02} - 3B \\
* (T_1 - M_s^0) + 2 * K + H = 0.
\end{aligned} \quad (22)$$

At the end of the reverse transformation:

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

$$\begin{aligned}
\Omega^{REV}(\sigma = \sigma_{AF}, T = T_1, f = 0) \\
= \left(\frac{\sigma_{AF}^2}{2} \right) * \left(\frac{1}{E_M} - \frac{1}{E_A} \right) + \sigma_{AF} * \varepsilon_{02} - B \\
* (T_1 - M_s^0) + C + H.
\end{aligned} \quad (23)$$

The constants B, C, K and H were computed and put in [Table 2](#).

3 Results and discussion

The algorithm is based on the calculation of criteria function Ω^{FOR} when it is zero the transformation occurs then an updating of both stress and martensite fraction is achieved, else stress is only updated. The same approach is followed regarding the reverse transformation.

The results obtained, after having performed the simulation, are illustrated by figures ([Figs. 3–7](#)).

First of all Figures 5a, 6a, 7a and 8a show the history of the mechanical load for each case of numerical simulation. Figure 5b at $T=46^\circ\text{C}$ shows only a gap, because of imperfect austenite elastic behavior of NiTi (Seeming to be related to the existence of the R phase), at the end of austenite elastic loading. The results illustrated by Figures 6b, 7b and 8b are in a good agreement with experimental curves, especially at $T=65^\circ\text{C}$ and above. The evolution of martensite fraction computed and shown in Figures 5c, 6c, 7c and 8c, in addition to being the main indicator of occurring transformation, fits the constitutive model well.

Finally Figure 9 illustrates the ability of the model to respond at any temperature.

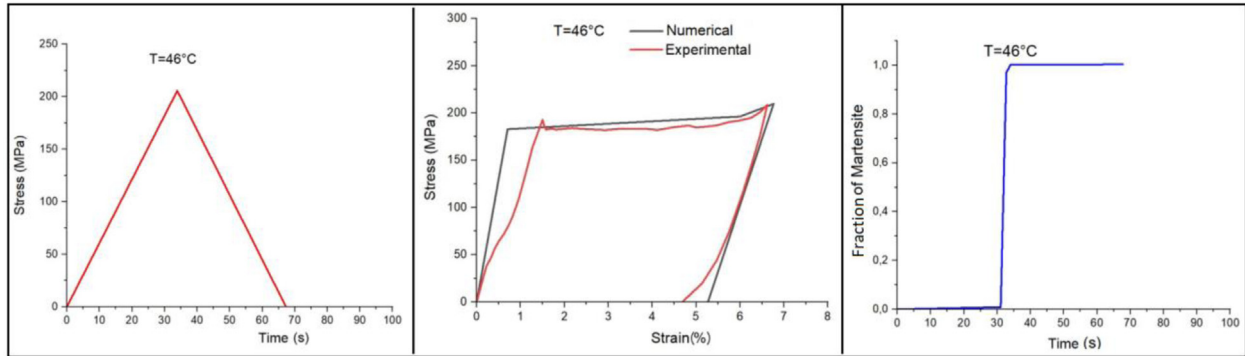


Fig. 5. At $T = 46^\circ\text{C}$: (a) History of mechanical loading, (b) stress vs strain, (c) evolution of martensite fraction.

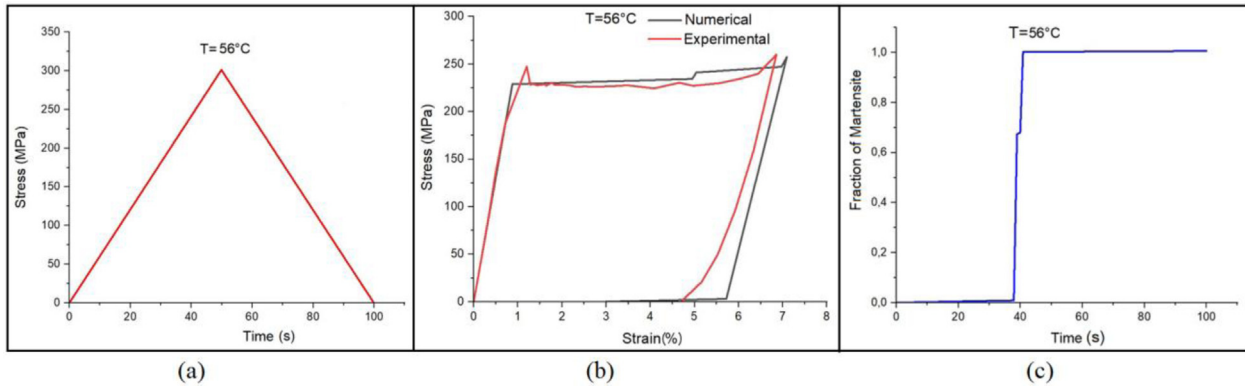


Fig. 6. At $T = 56^\circ\text{C}$: (a) History of mechanical loading, (b) stress vs strain, (c) evolution of martensite fraction.

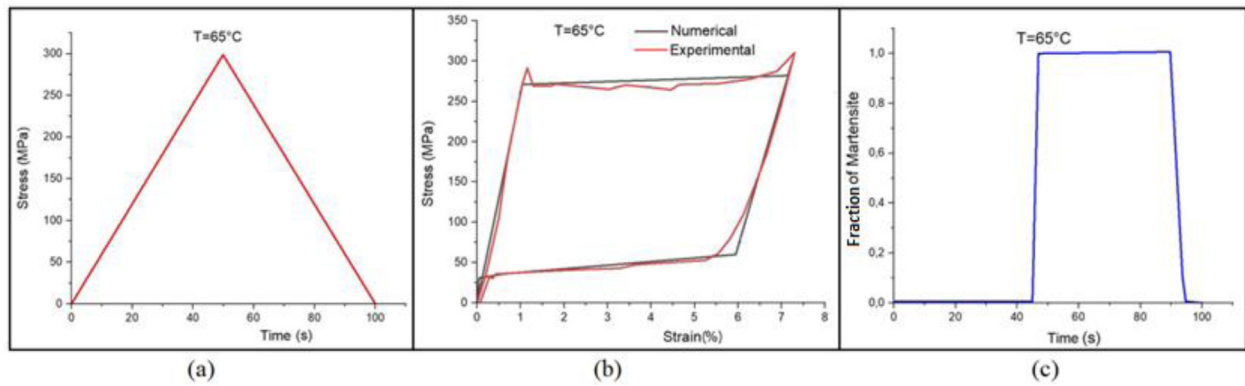


Fig. 7. At $T = 65^\circ\text{C}$: (a) History of mechanical loading, (b) stress vs strain, (c) evolution of martensite fraction.

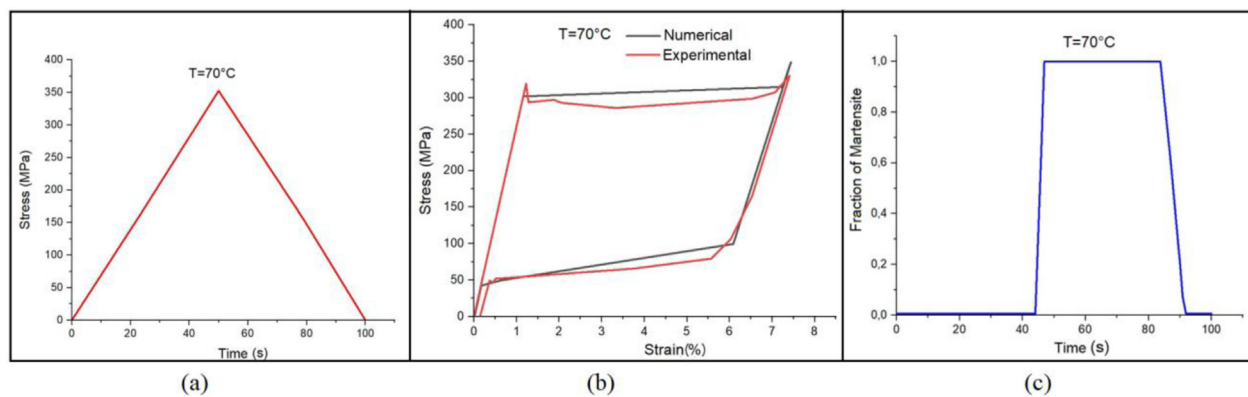


Fig. 8. At $T = 70^\circ\text{C}$: (a) History of mechanical loading, (b) stress vs strain, (c) evolution of martensite fraction.

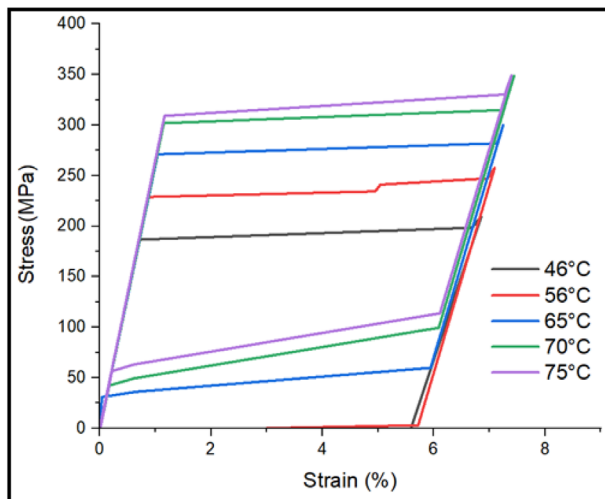


Fig. 9. Response of the model at different temperatures.

4 Conclusion

In this paper, it was focused on the pseudoelasticity effect of shape memory alloys. The constitutive equations were written following mechanics and thermodynamics laws. An algorithm was built and allowed implementing

necessary experimental data, the results showed that the model, accurately describes the material's behavior at various temperatures and matches experimental data well.

The model's ability to forecast the pseudoelastic effect in NiTi alloys is strengthened by experimental data, which is important for applications that need precise control over mechanical properties through temperature manipulation.

Funding

None stated.

Conflicts of interest

The authors state no conflict of interest.

Data availability statement

No new data/codes were created or analyzed in this study.

Author contribution statement

The work was distributed between all the authors on this article.

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Cite this article as: I. Zidane, M. Belkacem, On modelling of the one dimensional pseudoelastic effect of shape memory alloys, *Mechanics & Industry* 26, 6 (2025), <https://doi.org/10.1051/meca/2024040>

Stress-dependent calibration of a thermoelastic constitutive model for Cu-Zn-Al shape memory alloys

J Strain Analysis
1–10
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DOI: 10.1177/03093247261422816
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Abstract

Shape memory alloys (SMAs) have gained significant attention for their unique thermomechanical properties. This paper presents a phenomenological model for the thermoelastic strain–temperature response of Cu-Zn-Al SMAs. The constitutive equations are derived from thermodynamics, and parameters are calibrated at two constant stresses (65 and 100 MPa) using data for the same alloy from the literature. The simulations reproduce, after calibration, the transformation-strain amplitude and the hysteresis width at each stress. A key observation is that fitted parameters vary with the applied stress, which highlights the model's descriptive capability under specified loading and its limitations as a predictive tool without additional functionalization and data.

Keywords

shape memory alloys, constitutive modeling, thermomechanical behavior, computational materials science, intermetallic alloys, strain–temperature response

Date received: 1 August 2025; accepted: 24 January 2026

Introduction

The defining feature of Shape Memory Alloys (SMAs) lies in their capacity to revert to a predefined shape following substantial deformation, a behavior governed by a solid-state transformation between austenitic and martensitic phases that occurs in the two directions. This mechanism results in two principal functional effects: the thermally driven shape memory effect (SME), and super elasticity (SE), which enables recoverable large strain under applied stress. Owing to these properties, alloys such as NiTi and Cu-Zn-Al have been employed in aerospace, biomedical, and robotic systems that require compact, fatigue-resistant, and thermally responsive components.^{1,2}

Due to their ability to sustain significant, reversible deformations while maintaining structural integrity, SMAs have become key functional materials across multiple engineering disciplines. Their durability, adaptability, and responsiveness under thermal and mechanical stimuli make them particularly suitable for environments requiring compact and intelligent components. In the biomedical field, NiTi-based SMAs are widely used in self-expanding stents, orthodontic appliances, and orthopedic implants, where controlled shape recovery is essential. Aerospace applications capitalize

on these alloys in morphing structures, thermally actuated flight control elements, and vibration damping systems. Similarly, robotics and automotive systems utilize SMAs for the development of lightweight actuators and sensors, offering energy-efficient alternatives to conventional electromechanical designs. The broad adoption of SMAs is thus driven by both their material behavior and the functional advantages they bring to high-performance, reliability-critical systems.^{2–4}

Recent advances in SMAs research have centered on three complementary goals: enhancing material performance, enabling smarter applications, and refining predictive modeling. On the materials front, high-temperature SMAs (HT-SMAs) have expanded the thermal operating window for aerospace and automotive systems, while nanostructured and additively manufactured variants offer improved mechanical strength

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and geometric flexibility. These innovations have supported the development of next-generation components, such as fast-response, low-power actuators used in robotics and biomedical technologies. In parallel, computational modeling is progressing through more accurate phase transformation frameworks and the integration of machine learning algorithms, which are markedly improving the ability to simulate and control SMAs behavior across diverse loading conditions.^{5–7}

Indeed, refining predictive modeling, as mentioned previously, involves creating frameworks capable of capturing more complex material responses beyond simple transformations. For example, to improve accuracy, recent phenomenological models have been modified to account for the distinct material behavior under different loading modes, such as the tension-compression asymmetry inherent in many SMAs.⁸ Furthermore, advanced constitutive models are being developed to predict long-term performance, incorporating temperature-dependent degradation functions to simulate phenomena like functional fatigue under thermomechanical cycling.⁹ These focused efforts highlight the field's progression toward more specialized and reliable models for real-world engineering challenges.

The development of phenomenological models for SMAs has progressed through a series of increasingly sophisticated frameworks aimed at capturing their complex thermomechanical response. A foundational contribution came from Tanaka,¹⁰ who introduced a transformation function to describe the evolution of the martensitic phase fraction under combined thermal and mechanical loads. Building on this foundation Liang and Rogers,¹¹ incorporated thermodynamic principles into the modeling structure, thereby improving its physical consistency and practical relevance Brinson.¹² further advanced the approach by differentiating between twinned and detwinned martensite, enabling a more accurate representation of the material's hysteresis and transformation path dependencies.

Building upon phenomenological foundations, recent SMA modeling efforts have expanded across multiple scales to improve both physical accuracy and numerical implementation.

At the macroscopic level, Lagoudas et al.² introduced a comprehensive thermodynamic framework based on internal variables, enabling reliable simulation of SMAs under complex, path-dependent loading conditions. At the microstructural scale, Peultier et al.¹³ developed crystallographic-based models to capture grain-level phase transformations with greater fidelity. Volkov and Sakharov¹⁴ addressed numerical challenges by improving the stability and efficiency of simulation procedures, while Auricchio et al., in addition to their developed model contributed finite element implementations that made SMAs models applicable to real-world structural systems.¹⁵ Finally, the multi-scale approaches advanced by Chemisky et al.¹⁶ provided an integrative framework linking

microscopic transformation mechanisms with macroscopic mechanical behavior, enhancing predictive capabilities across disciplines.

The field of SMAs continues to evolve, with significant advancements in several areas. This include the development of advanced phenomenological models capable of capturing the non-linear thermomechanical behavior of SMAs more accurately under complex loading conditions, such as in the presence of stress concentrations,¹⁷ as well as in-depth investigations into the fundamental elastic behavior of common alloy systems.¹⁸ Concurrently, innovative fabrication methods are being intensely investigated.¹⁹ The present work contributes by focusing specifically on the thermoelastic effect, where the phase transformation is primarily thermally-induced. This is distinct from pseudo elasticity, where the transformation is stress-induced, allowing for large, reversible strains at a near-constant temperature. Understanding this distinction is critical for engineering design; the thermally-induced thermoelastic effect is ideal for temperature-triggered actuators used in aerospace and robotics, while the stress-induced pseudo elasticity is crucial for applications requiring passive energy dissipation or super-stretching capabilities, such as seismic dampers or resilient medical stents. This work focuses only on the thermoelastic effect, which has been modeled separately from pseudo elasticity by the authors in prior research.²⁰

This study addresses the strain–temperature coupling observed during phase transformation in Shape Memory Alloys by developing a dedicated phenomenological model. The constitutive structure of the model is derived from the fundamental principles of thermodynamics and continuum mechanics, and is formulated to capture transformation strain evolution under thermomechanical loading Figure 1. The numerical implementation in MATLAB enables parametric simulations to analyze the influence of key material parameters and loading conditions on the alloy's macroscopic behavior.

Under constant stress σ_0 , Shape Memory Alloys exhibit a characteristic strain–temperature response as they undergo a thermal cycle, as illustrated in Figure 2. Initially in the austenitic phase, the material is cooled, initiating a forward phase transformation to martensite at the martensite start temperature M_s^σ , which completes at M_f^σ . Upon subsequent heating, the reverse transformation begins at the austenite start temperature A_s^σ , concluding with full shape recovery when the temperature reaches A_f^σ . This reverse transformation sequence reflects the core behavior underlying the shape memory effect in SMAs.

In this study we developed a phenomenological model able to describe the Cu-Zn-Al SMAs thermomechanical behavior based on thermodynamics laws. The model was implemented in a built algorithm using MATLAB. To judge the efficiency, we used experimental results to calibrate this model and the results were satisfactory.

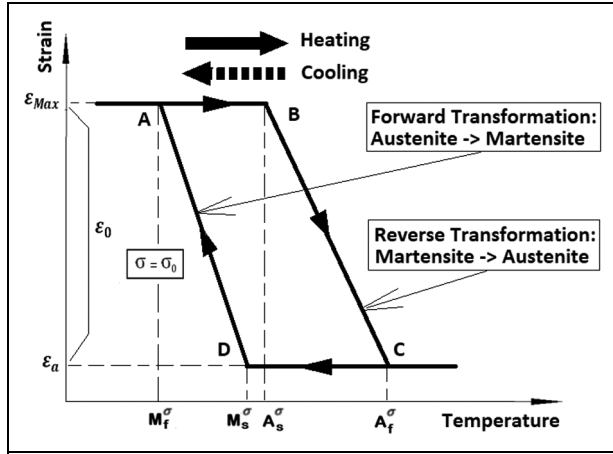


Figure 1. Diagram showing the strain-temperature hysteresis effect.

M_s^σ : martensite start temperature; M_f^σ : martensite finish temperature; A_s^σ : austenite start temperature; A_f^σ : austenite finish temperature; ε_0 : overall transformation strain amplitude; ε_d : strain before transformation.

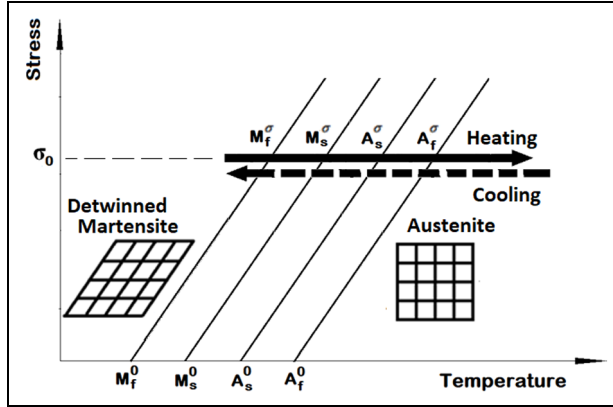


Figure 2. The path of strain-temperature.

Methods and materials

Constitutive equations

To develop the constitutive model, a representative volume element (RVE) is considered, containing coexisting austenite and martensite phases. This volume serves as the basis for analyzing the local transformation mechanisms under thermomechanical loading, as illustrated in (Figure 3):

The martensite volume fraction, denoted by f , is defined as the ratio of the martensite volume V_M to the total volume:

$$f = \frac{V_M}{V_M + V_A} \quad (1)$$

The thermodynamic behavior is governed by the free energy density function:

$$E_f^d(\sigma, T, f) = E_e^d + E_{tr}^d + E_{ph}^d + E_{int}^d \quad (2)$$

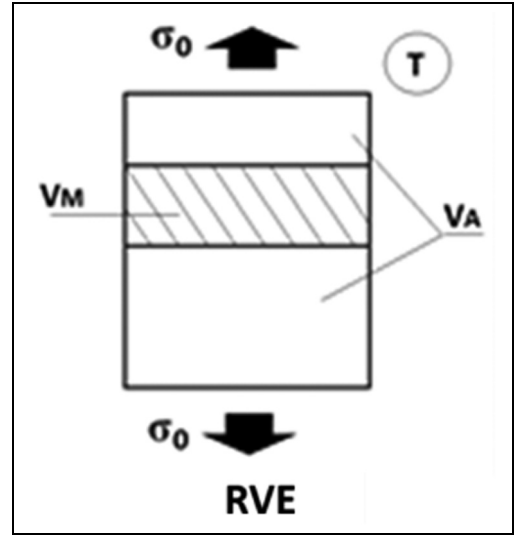


Figure 3. A representative volume element (RVE), under thermomechanical loading, illustrating the coexisting of austenite (V_A) and martensite (V_M) phases.

Where:

σ , T and f are respectively applied stress, temperature and martensite fraction. σ and T are control variables, f is an internal variable.

E_{el}^d : Elastic energy density

The elastic energy density E_{el}^d is:

$$E_{el}^d = -\frac{\sigma^2}{2} \cdot \left[\frac{1-f}{E_A} + \frac{f}{E_M} \right] \quad (3)$$

E_{tr}^d : Density of mechanical work associated with the phase transformation

The density of mechanical work associated with the phase transformation E_{tr}^d is:

$$E_{tr}^d = -\sigma f \varepsilon_0 \quad (4)$$

E_{ph}^d : Density of energy associated with phase change

The density of energy associated with phase change E_{ph}^d is:

$$E_{ph}^d = f(f+1)B(T-T_0) \quad (5)$$

E_{int}^d : Interaction energy density between martensite and austenite

The Interaction energy density between martensite and austenite E_{int}^d is:

$$E_{int}^d = Cf(f-1) \quad (6)$$

Combining these components, the total free energy density function is:

$$E_d^f(\sigma, T, f) = -\frac{\sigma^2}{2} \cdot \left[\frac{1-f}{E_A} + \frac{f}{E_M} \right] - \sigma f \varepsilon_0 + f(f+1)B(T-T_0) + Cf(f-1) \quad (7)$$

In this expression, E_A and E_M are the Young's moduli of the austenite and martensite phases, respectively. The term ε_0 represents the maximum transformation strain, (Cooling makes the cubic austenite lattice unstable and it transforms into the monoclinic martensite lattice, producing strain), while T_0 is the reference temperature, set as the martensite start temperature at zero stress M_n^0 . The coefficients B and C are material parameters that must be determined experimentally through calibration.

The thermodynamics potential $E_d^f(\sigma, T, f)$ depends on control variables σ , T and the internal variable f .

Because the dissipation is occurring during the phase transformation, it is assumed that only the deriving force of the thermodynamics potential $\frac{\partial E_d^f}{\partial f}$ for the martensite fraction is the driving force which can be denoted F_d^{dr} and expressed as follows:

$$-\frac{\partial E_d^f}{\partial f} = F_d^{dr} \quad (8)$$

The second law of thermodynamics is expressed by Clausius inequality^{2,3}:

$$-\frac{\partial E_d^f}{\partial f} \cdot \frac{df}{dt} \geq 0 \quad (9)$$

The existing dissipation occurring during the transformation, leads us to assume that there is a pseudo potential, denoted by P^d

The pseudo potential P^d is:

$$P^d = -K \left(\frac{f^3}{3} + \frac{f^2}{2} \right) - Hf \quad (10)$$

Analogously to the thermodynamic potential, a dissipative force which derives of the dissipation pseudo potential denoted F_d^{dis}

The dissipative force is:

$$-\frac{dP^d}{df} = F_d^{dis} \quad (11)$$

Equation (8) leads to:

$$F_d^{dr} = -\frac{\partial E_d^f}{\partial f} = \frac{\sigma^2}{2} \left[\left(\frac{1}{E_M} \right) - \left(\frac{1}{E_A} \right) \right] + \sigma \varepsilon_0 - B(2f+1)(T-T_0) - C(2f-1) \quad (12)$$

Equation (10) gives the expression of the dissipative force:

$$F_d^{dis} = Kf(f+1) + H \quad (13)$$

The transformation occurs when an necessary condition is satisfied, let us introduce a criteria function ϕ^{For} for forward transformation case:

The criteria function ϕ^{For} is:

$$F_d^{dr} - F_d^{dis} = \phi^{For} \quad (14)$$

Similarly, for reverse transformation:

$$F_d^{dr} + F_d^{dis} = \phi^{Rev} \quad (15)$$

The forward transformation occurs if the following condition is satisfied:

$$\phi^{For}(\sigma, T, f) = 0 \quad (16)$$

This leads to equation (17):

$$\frac{\sigma^2}{2} \left[\left(\frac{1}{E_M} \right) - \left(\frac{1}{E_A} \right) \right] + \sigma \varepsilon_0 - B(2f+1)(T-T_0) - C(2f-1) - Kf(f+1) - H = 0 \quad (17)$$

Beside the condition equation (16), the consistency of the transformation should be taken into account equation (18):

$$\frac{d\phi^{For}(\sigma, T, f)}{dt} = \left(\frac{\partial \phi^{For}}{\partial \sigma} \right) \cdot \left(\frac{d\sigma}{dt} \right) + \left(\frac{\partial \phi^{For}}{\partial T} \right) \cdot \left(\frac{dT}{dt} \right) + \left(\frac{\partial \phi^{For}}{\partial f} \right) \cdot \left(\frac{df}{dt} \right) = 0 \quad (18)$$

Then we obtain (equation (19)):

$$\left[\sigma \left(\frac{1}{E_M} - \frac{1}{E_A} \right) + \varepsilon_0 \right] \dot{\sigma} - B(2f+1) \dot{T} + [-2B(T-T_0) - 2C - K(2f+1)] \dot{f} = 0 \quad (19)$$

Taking into account that the transformation occurs isobarically ($\sigma = \sigma_0$), this allows obtaining the evolution of the martensite fraction (20):

$$\dot{f} = \frac{B(2f+1) \dot{T}}{-2B(T-M_s^0) - 2C - K(2f+1)} \quad (20)$$

The reverse transformation occurs when (21):

$$\phi^{Rev}(\sigma, T, f) = 0 \quad (21)$$

Table 1. Experimental data for Cu-Zn-Al at 65 MPa.²¹

M_s^σ (K)	324	A_s^σ (K)	330
M_f^σ (K)	311	A_f^σ (K)	340
E_A (MPa)	72,000	ε_0	0.0255
E_M (MPa)	70,000	ε_a	0.001063

Table 2. Experimental data for Cu-Zn-Al at 100 MPa.²¹

M_s^σ (K)	323	A_s^σ (K)	330
M_f^σ (K)	317	A_f^σ (K)	338
E_A (MPa)	72,000	ε_0	0.0341
E_M (MPa)	70,000	ε_a	0.00139

This will give equation (22):

$$\frac{\sigma^2}{2} \left[\left(\frac{1}{E_M} \right) - \left(\frac{1}{E_A} \right) \right] + \sigma \varepsilon_0 - B(2f + 1)(T - T_0) - C(2f - 1) + Kf(f + 1) + H = 0 \quad (22)$$

The evolution of the martensite fraction is given by equation (23):

$$\dot{f} = \frac{B(2f + 1)\dot{T}}{-2B(T - M_s^0) - 2C + K(2f + 1)} \quad (23)$$

Model calibration and parameter identification

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 (24)–(27) using the characteristic transformation temperatures (M_n^σ , M_f^σ , A_s^σ , A_f^σ) for each case.

Calibration at 65 MPa. For the 65 MPa stress level, the required experimental values were sourced from the study conducted by Bourbon et al.²¹ On a Cu-Zn-Al alloy (Cu –25.57% Zn – 4.09% Al). The characteristic values used for the calibration are presented in Table 1.

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.²¹ The characteristic transformation temperatures extracted from this data are listed in Table 2. These values were subsequently used to solve the system of equations and determine the model parameters specific to this stress level.

Table 3. Calibrated model parameters for Cu-Zn-Al at $\sigma = 65$ MPa.

$B(\text{MPa} \cdot \text{K}^{-1})$	0.027128
$C(\text{MPa})$	–0.047474
$K(\text{MPa})$	0.27806
$H(\text{MPa})$	–0.297643

To find the constants B , C , H and K , we have to use equation (19) and (22) and define the boundary conditions for both forward and reverse transformations.

- At the start of the direct transformation, we have the following conditions:

$$\begin{aligned} \sigma &= \sigma_0; T = M_s^\sigma; f = 0 \\ \left(\frac{\sigma^2}{2} \right) \left(\frac{1}{E_M} - \frac{1}{E_A} \right) + \sigma \varepsilon_0 - B(M_s^\sigma - M_s^0) + C - H &= 0 \end{aligned} \quad (24)$$

- At the end of direct processing:

$$\begin{aligned} \sigma &= \sigma_0; T = M_F^\sigma; f = 1 \\ \left(\frac{\sigma^2}{2} \right) \left(\frac{1}{E_M} - \frac{1}{E_A} \right) + \sigma \varepsilon_0 - 3B(M_F^\sigma - M_s^0) - C - 2K - H &= 0 \end{aligned} \quad (25)$$

- At the start of the reverse transformation:

$$\begin{aligned} \sigma &= \sigma_0; T = A_s^\sigma; f = 1 \\ \left(\frac{\sigma^2}{2} \right) \left(\frac{1}{E_M} - \frac{1}{E_A} \right) + \sigma \varepsilon_0 - 3B(A_s^\sigma - M_s^0) - C + 2K + H &= 0 \end{aligned} \quad (26)$$

- At the end of the reverse transformation:

$$\begin{aligned} \sigma &= \sigma_0; T = A_F^\sigma; f = 0 \\ \left(\frac{\sigma^2}{2} \right) \left(\frac{1}{E_M} - \frac{1}{E_A} \right) + \sigma \varepsilon_0 - B(A_F^\sigma - M_s^0) + C + H &= 0 \end{aligned} \quad (27)$$

Resolving the system of equations (24)–(27) allowed to obtain values of constants B , C , H and K (Tables 3 and 4)

Results and discussions

This section presents the results of the numerical model and discusses its performance by comparing simulations against experimental data at multiple stress levels. The model's parameters are calibrated, its predictive

Table 4. Calibrated model parameters for Cu-Zn-Al at $\sigma = 100$ MPa.

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

capabilities are tested, and its inherent limitations are analyzed.

Numerical simulation and calibration

The developed model was used to simulate the thermoelastic response of a Cu-Zn-Al alloy under two distinct, constant tensile stress levels: 65 and 100 MPa. For each case, a thermal cycle was applied, starting from a high temperature (austenitic phase), cooling to induce the forward martensitic transformation, and subsequently heating to induce the reverse transformation. Constants B , C , H and K were calculated for each case and put in Tables 3 and 4.

The results of numerical simulation are shown by Figures 4 to 7.

Figure 4 illustrates the complete simulation process for the 65 MPa case. It shows the applied thermal load history (Figure 4(a)), the corresponding evolution of the martensite volume fraction, f which acts as the model's internal state variable (Figure 4(b)). Similarly, Figure 5 displays the simulation results for the 100 MPa case, showing the same set of relationships. These figures demonstrate the model's ability to translate a thermal input into a mechanical strain output via the internal phase transformation mechanism.

Figures 6 and 7 illustrate the calibration of the model and its comparison to experimental data from the literature. For both 65 and 100 MPa cases, the model was calibrated using experimental data from (Bourbon et al.).²¹ The two figures compare the simulated hysteresis loops directly with their corresponding experimental data sets. In both cases, the model demonstrates good agreement with the experiments in terms of the overall transformation strain amplitude (ϵ_0) and the general width of the hysteresis. However, a notable discrepancy exists in the transformation kinetics. The model predicts an abrupt, linear transformation, whereas the experimental data shows a more gradual, curved transition. This is a typical characteristic of the employed modeling framework, which simplifies the complex, non-linear nature of the austenite-martensite phase transformation.

Comparative analysis and discussion

Figure 8 presents the final simulated hysteresis loops for both stress levels on a single plot for comparative analysis. The model correctly captures the well-known Clausius-Clapeyron relationship, showing a shift of the hysteresis loop to higher temperatures as the applied stress increases from 65 to 100 MPa. This demonstrates that the model is physically consistent in its response to varying stress.

The central finding of this comparative analysis is that the model's parameters (B , C , K , H) are **stress-dependent**. The necessity of calculating two distinct parameter sets (Tables 3 and 4) to match the experimental data indicates that these are not true material constants, but rather fitting parameters specific to the calibration conditions.

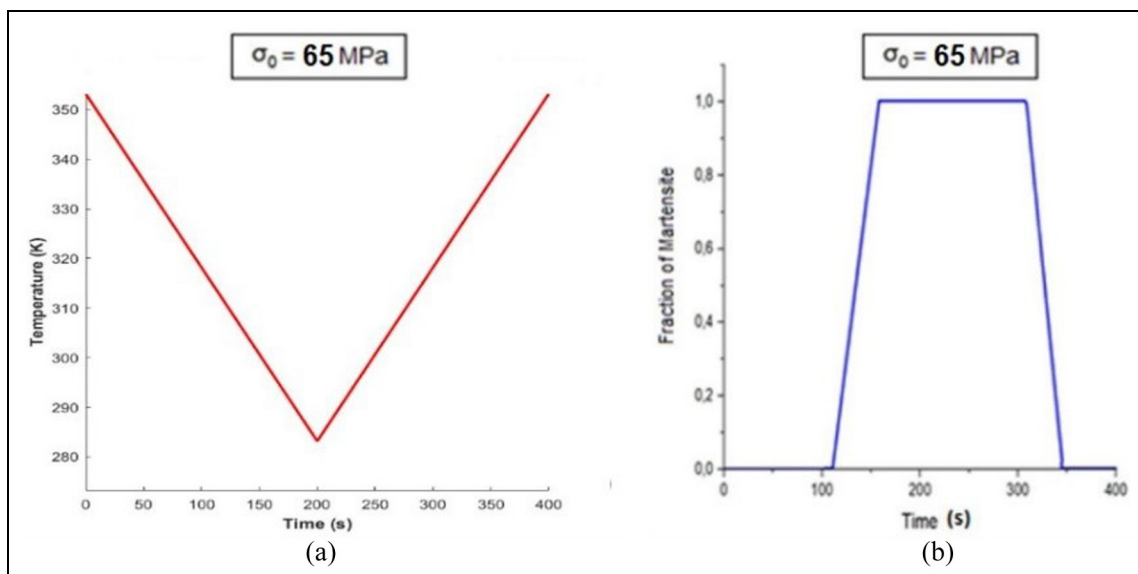


Figure 4. Simulation results for a thermoelastic cycle at $\sigma = 65$ MPa: (a) history of the applied thermal load and (b) evolution of the martensite volume fraction over time.

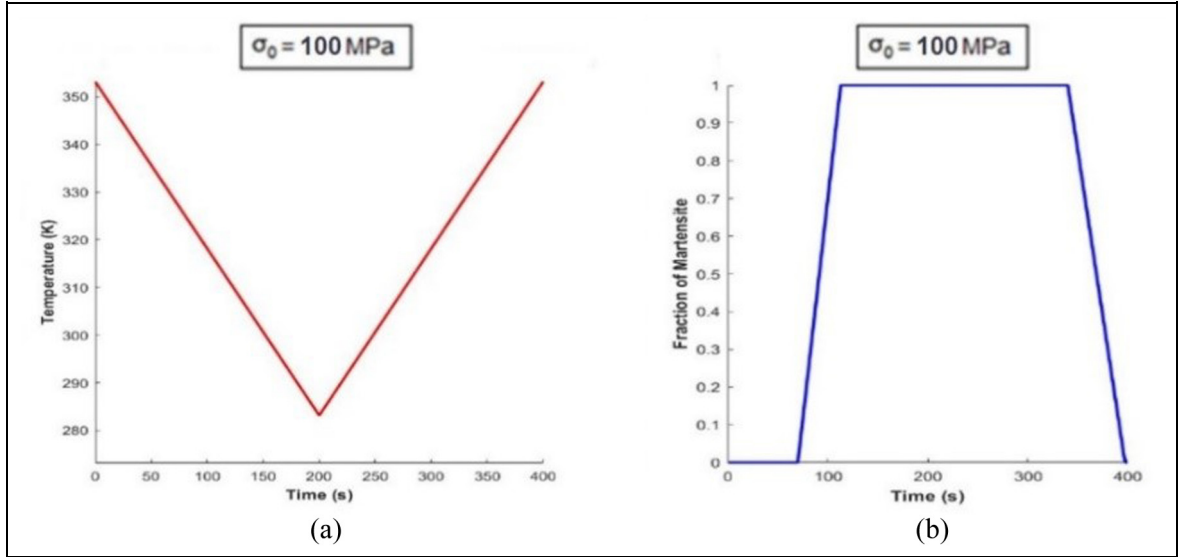


Figure 5. Simulation results for a thermoelastic cycle at $\sigma = 100$ MPa: (a) history of the applied thermal load and (b) evolution of the martensite volume fraction over time.

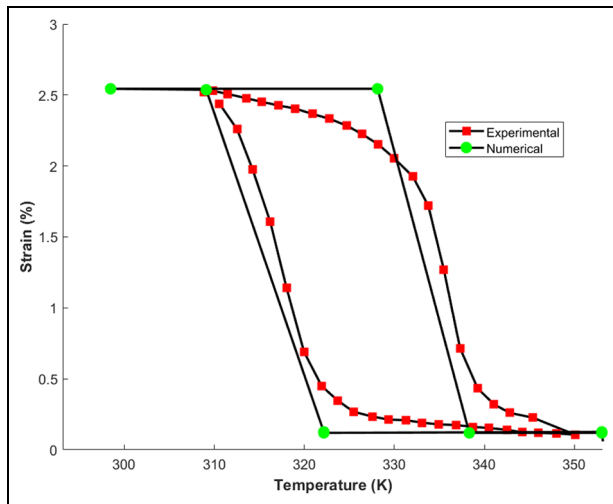


Figure 6. Calibration of the model at 65 MPa. The experimental data (red squares) are compared with the numerical simulation (green dots/black line) from Bourbon et al.²¹

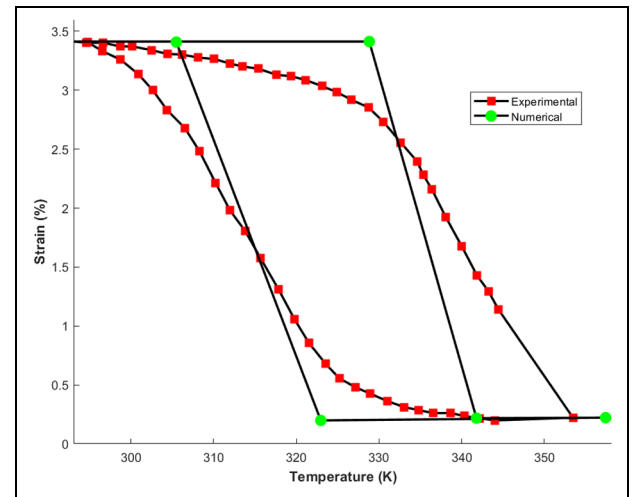


Figure 7. Calibration of the model at 100 MPa. The experimental data (red squares) are compared with the Numerical simulation (green dots/black line) from Bourbon et al.²¹

This observation highlights a key characteristic and limitation of the employed phenomenological model. While the model is highly effective at *describing* the material's behavior for a specific, known loading condition, its ability to *predict* the behavior at a different stress level without prior experimental data is limited. This finding is critical for engineering applications, as it implies that for accurate design, the model must be calibrated for the specific stress range of interest.

This study demonstrates the model's utility as a descriptive tool and simultaneously reveals an important avenue for future research. To develop a truly

predictive model, future work could focus on establishing a functional relationship between the model parameters and the applied stress (e.g. defining $B(\sigma)$, $C(\sigma)$, etc.). Such an enhancement would significantly broaden the model's applicability and reduce the reliance on extensive experimental calibration for each new loading scenario.

Preliminary investigation of the parameter-stress relationship

Building upon the key finding that the model parameters are stress-dependent, we conducted a

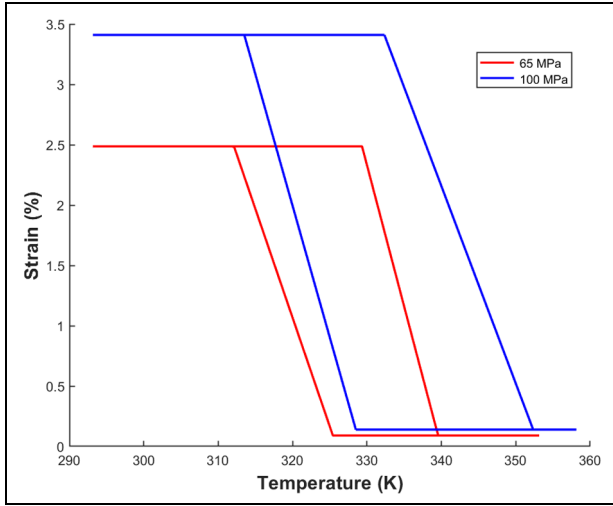


Figure 8. Numerically simulated $\varepsilon - T$ loops for the same Cu-Zn-Al alloy at 65 and 100 MPa, showing that higher stress shifts transformation temperatures to higher values (Clausius–Clapeyron consistency).

preliminary investigation to quantify this relationship. As a first-order approximation, a linear relationship was assumed given the two available data points (at 65

and 100 MPa). This allowed for the derivation of a functional form for each parameter in relation to the applied stress (σ).

This derivation yielded the following set of linear equations, describing the behavior of each parameter within the studied stress range:

- $B(\sigma) = -0.004227 \cdot \sigma - 0.247646$
- $C(\sigma) = 0.045127 \cdot \sigma - 2.980751$
- $K(\sigma) = -0.020451 \cdot \sigma + 1.607345$
- $H(\sigma) = 0.071034 \cdot \sigma - 4.914853$

Figure 9 graphically illustrates these relationships, showing a good fit between the derived linear functions and the calculated data points, but we should notice that with only two calibrated stress levels, a straight line necessarily passes through the two points; this interpolation is illustrative and does not validate a functional form. It is crucial to emphasize that these functions represent a preliminary and illustrative analysis. Nevertheless, this result provides valuable insight by demonstrating a feasible pathway toward a truly predictive model where the parameters are not material constants but rather functions of the loading

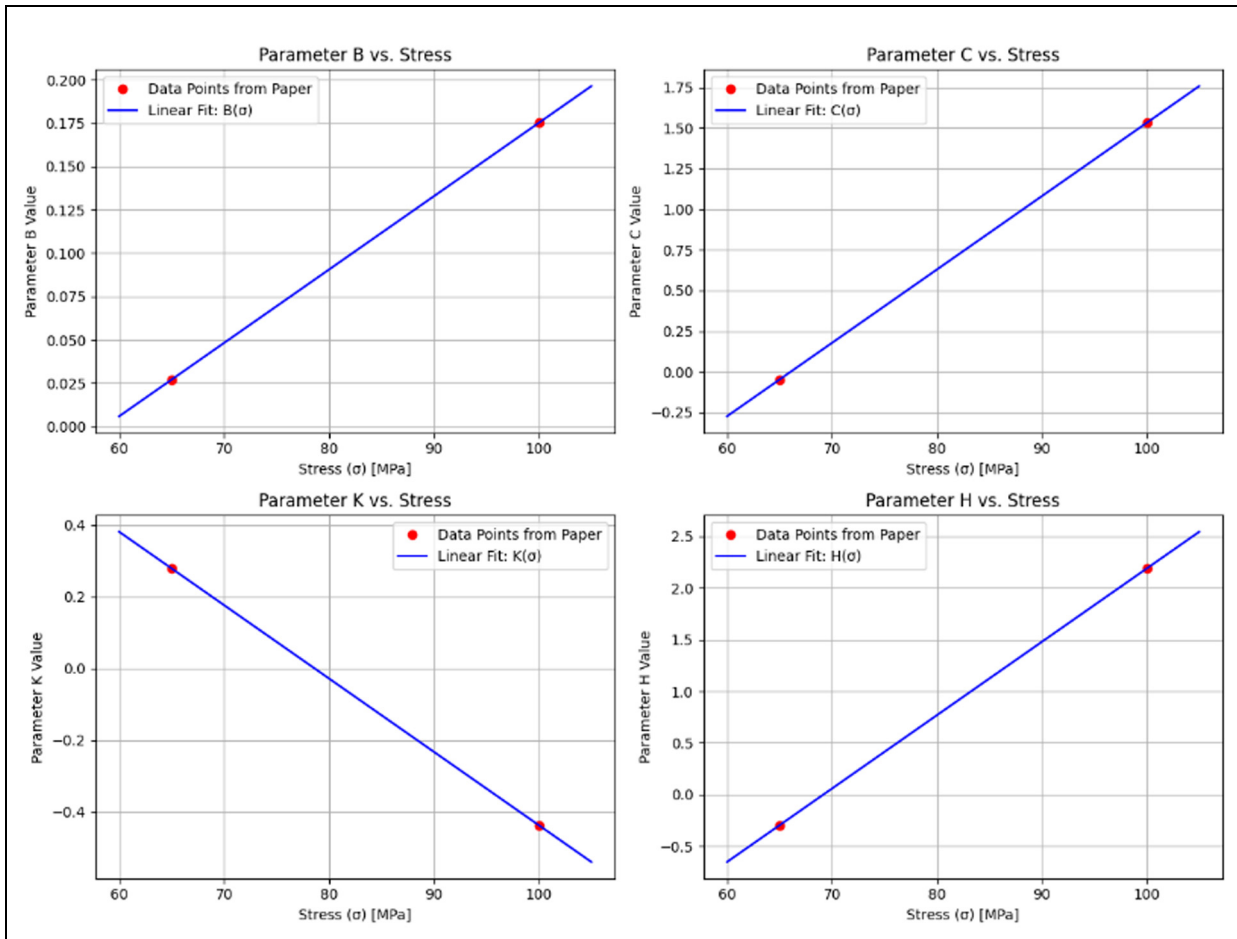


Figure 9. Preliminary linear approximation of the stress-dependence of model parameters (B, C, K, and H). The discrete points represent the calibrated parameter values at 100 and 65 MPa, while the solid lines depict the derived linear functions.

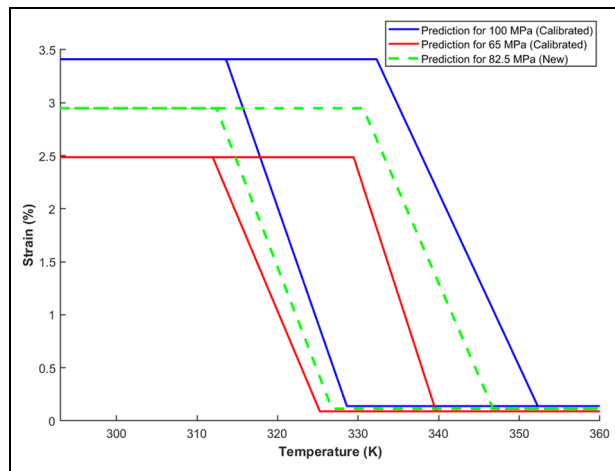


Figure 10. Interpolation at an intermediate stress (82.5 MPa). Dashed green curve: $\varepsilon - T$ loop obtained by interpolating $B(\sigma)$, $C(\sigma)$, $K(\sigma)$, $H(\sigma)$ from the two calibrated stresses (65 and 100 MPa).

Illustration only; no experimental data are available at 82.5 MPa.

conditions. This analysis paves the way for moving beyond the purely descriptive nature of the model.

The validity of these linear relationships is currently confined to the interpolated range of the available data. Further experimental work at multiple stress levels is essential to validate this linear hypothesis or to establish a more accurate, potentially non-linear, relationship. Such future work would enable the construction of a more robust and comprehensive constitutive model.

Interpolation at an intermediate stress (illustration)

To illustrate interpolation at an intermediate stress, we built a simple simulation workflow where the applied stress (σ) is the input. For any given σ , the parameter set $B(\sigma)$, $C(\sigma)$, $K(\sigma)$, $H(\sigma)$ is obtained by linear interpolation between the two calibrated stresses (65 and 100 MPa), and the resulting $\varepsilon - T$ loop is plotted for illustration only.

The workflow was first checked at the two calibrated stresses (65 and 100 MPa) and then used to draw an intermediate loop at 82.5 MPa, for which no experimental data are available; this is an interpolation only.

The dashed green loop in Figure 10 is obtained by linearly interpolating $B(\sigma)$, $C(\sigma)$, $K(\sigma)$, and $H(\sigma)$ between 65 and 100 MPa. This figure is illustrative only and does not constitute prediction or validation. Without independent data at 82.5 MPa, no quantitative assessment can be made; the example simply shows how stress-dependent parameters could be interpolated between calibrated points.

Conclusion

In this study, a phenomenological model for the thermoelastic effect in Cu-Zn-Al (SMAs) was developed and critically analyzed. The model was calibrated against

experimental data at two distinct stress levels (100 and 65 MPa), successfully capturing key material behaviors, including the Clausius-Clapeyron relationship.

The most significant finding of this investigation is that the model's parameters are not material constants but exhibit a clear dependence on the applied stress. This highlights the model's nature as a strong descriptive tool but reveals its inherent limitations as a predictive instrument without re-calibration.

Within the calibrated stresses, the model describes the hysteresis width and the transformation-strain amplitude. The analysis also shows that the fitted parameters vary with stress, which limits predictive use without additional functionalization. We therefore refrain from claims of validation or high-fidelity prediction and instead outline a pathway to parameter functionalization contingent on multi-stress data for the same alloy.

In conclusion, this work not only provides a valuable analysis of the capabilities and limitations of a common modeling framework but also presents and outlines a clear strategy for parameter functionalization, without claiming validation. The findings lay the groundwork for future research focused on validating and refining these parameter functions with more extensive experimental data, which would enable the development of a truly robust and versatile tool for engineering design.

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Author contributions

Imade Zidane: Conceptualization, Software, Validation, Formal analysis, Investigation, Writing – Original Draft.
Belkacem Meddour: Methodology, Supervision, Writing – Review & Editing.

Funding

The authors received no financial support for the research, authorship, and/or publication of this article.

Declaration of conflicting interests

The authors declared no potential conflicts of interest with respect to the research, authorship, and/or publication of this article.

Data availability statement

The experimental data used for model validation in this study are sourced from previously published works as cited in the manuscript. The simulation data generated during the current study are available from the corresponding author on reasonable request.

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