

**Numerical Aspects of Modelling Thermo-Mechanical Wave
Propagation with Phase Transformations**

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NUMERICAL MODEL FOR THERMO-MECHANICAL WAVE PROPAGATION WITH PHASE TRANSFORMATION

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Abstract. *For application developments of ferroelastic material, it is important to understand the interaction between wave propagations and phase transformations. In the current study, a mathematical model and its numerical discretization are constructed to analyze the wave propagation in shape memory alloy rods. The first order martensitic transformations and the associated effects of thermo-mechanical coupling are accounted for by employing the modified Ginzburg-Landau-Devonshire theory. The Landau-type free energy function characterizes different phases, while a Ginzburg term is introduced to account for the domain wall energy during phase transformations. The effect of internal friction on wave propagation patterns is analyzed under shock loadings implemented via stress boundary conditions. For practical numerical simulations of SMA samples, the constructed model of coupled nonlinear system of PDEs is reduced to a system of differential-algebraic equations, where the Chebyshev collocation method is employed for the spatial discretization, while the backward differentiation is used for the integration in time. A series of numerical experiments are carried out on copper-based SMA samples. Propagation of stress waves induced by shock loadings is analyzed for different initial temperature. It is demonstrated that the patterns of wave propagation is complicated at low temperatures by phase transformations, while more regular patterns are observed for high temperature distributions. These observations are in agreement with experiments. Finally, the influence of viscosity effects(due to internal friction) on the overall thermo-mechanical behaviour of rods is analyzed numerically.*

1 Introduction

Shape Memory Alloys (SMA) have been investigated from various aspects by mathematicians, physicists, and engineers in the past decades, due to their unique properties of being able to convert energy between thermal and mechanical fields, which are promising for many application branches such as mechanical and control engineering, biomedicine, communication, robotics and so on [6]. Motivated by application developments, nonlinear wave propagations in the material have been investigated since it is an elementary aspect for the prediction and understanding of dynamical response of the SMAs under dynamical loadings [1, 4, 11].

Compared with conventional wave propagations in solid materials, the impact induced wave propagations in the ferroelastic materials requires deliberate treatments and extra measures to cope with difficulties caused by phase transformations [1, 4, 11]. In general, impact loadings on the ferroelastic materials will cause nonlinear thermo-mechanical waves which are similar to those of other thermo-elastic materials under impact loadings. The differentiation of waves in ferroelastic materials is that the first order martensitic transformation might be induced by the waves. The transformation is reversible, and its native nonlinearity and hysteresis will have a heavy influence on the wave propagation and make the wave propagation pattern more complicated [1, 4, 11].

For the modelling of impact induced wave propagations and phase transformations, a sound constitutive theory is in the heart of the whole model [1, 11]. Various constitutive models have been proposed on mesoscale or microscale to capture the phase boundary movement induced by the dynamical loadings [2, 10]. In Ref. [1, 2], a one-dimensional model for modelling the shock wave propagations with phase transformation was constructed on the basis of a non-convex Helmholtz free energy function, and the whole structure was classified into different domains due to the phase transformation, while the movement of boundaries among domains is modelled using the so called “jumping conditions”. This approach is suitable for microscopic problems, but for engineering applications, the model normally is required at macroscale, and the continuity of the governing equation is essential in many cases. In Ref. [8, 14], the dynamical behaviour of phase boundaries was modelled using a thermo-mechanical coupling approach, but based on a linearized constitutive theory, whose application potential is obviously limited.

For real engineering applications, dynamical response of SMA materials caused by impact loadings need to be understood for design or control purpose at macroscale. For this purpose, displacement and temperature evolution in the material are normally sought. Models on mesoscale is not suitable for the purpose, because another model need to be constructed to bridge macroscale properties and mesoscale domain structures. Another aspect of modelling the dynamics of ferroelastic material under impact loadings is the thermo-mechanical coupling effects. In most of existing investigations, the thermal dynamics are either ignored [1, 4, 10], or modelled separately from the mechanical dynamics [8, 14], which is an obvious deviation from the physics of SMAs, since the thermal and mechanical fields are intrinsically coupled in SMA. When the SMAs are used for damping purpose or other cases where the conversion of energy between the thermal and mechanical field are important, the coupling effects are expected to be particularly important, and the constitutive theory should be constructed by taking into account both fields simultaneously.

In this paper, the nonlinear thermo-mechanical wave propagations in SMA rods induced by impact loadings were investigated at macroscale. To capture the thermo-mechanical coupling and nonlinear nature of the phase transformations, the Ginzburg - Landau theory is applied to model the phase transformations in the SMA rod [11], the governing equation for the mechan-

ical field is obtained using minimization of mechanical energy, while that for the thermal field is obtained using the conservation law of internal energy. By this approach, the mechanical and thermal fields can be intrinsically coupled in the model. Impact loadings at the end of the SMA rod is implemented in terms of stress. Nonlinear wave propagations are simulated with various initial temperatures.

2 The Boundary - Initial Value Problem

We restrict our investigation in one-dimensional cases, as sketched in Figure (1). The SMA rod under consideration occupies an interval $[0, L]$, and is subjected to an impact loading from the right end $x = L$, while another end $x = 0$ is fixed. The rod is thermally insulated at both ends so there is no heat loss (gain) to (from) the ambient environment. Under external loadings, a point (particle) in the SMA rod at x will be carried to a new position $x + u(x, t)$ due to deformation, where $u(x, t)$ is the longitudinal displacement at time t . Obviously, $u(x, t)$ should be continuous at any time and position because the rod is assumed not to be broken. The stress is related to the deformation by $\sigma(x, t) = f(\varepsilon(x, t))$ where $\varepsilon(x, t) = \partial u(x, t) / \partial x$ is the strain.

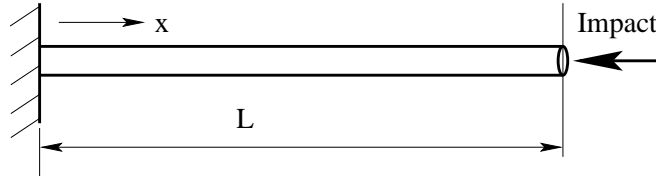


Figure 1: Shape memory alloy rod under impact loadings

For the dynamics of the mechanical field, the Lagrangian function \mathcal{L} is introduced:

$$\mathcal{L} = \int_0^T \int_0^L \left(\frac{\rho}{2} (\dot{u})^2 - \mathcal{F} \right) dt dx, \quad (1)$$

where ρ is the density of the material and \mathcal{F} potential energy density of the material. The differentiating feature of the Ginzburg - Landau theory is that the potential energy density is constructed as a non-convex function of the chosen *order parameters* and temperature θ , as a sum of local energy density (\mathcal{F}_l) and non-local energy density (\mathcal{F}_g). For the current one-dimensional problem, the strain $\varepsilon(x, t)$ is chosen the order parameter, and the local free energy density can be constructed as the Landau free energy density $\mathcal{F}_l(\theta, \varepsilon)$ [3, 7, 11]:

$$\mathcal{F}_l(\theta, \varepsilon) = \frac{k_1(\theta - \theta_1)}{2} \varepsilon^2 + \frac{k_2}{4} \varepsilon^4 + \frac{k_3}{6} \varepsilon^6, \quad (2)$$

where k_1 , k_2 , and k_3 are material-specific constants, θ_1 is the reference transformation temperature.

The non-local free energy density is usually constructed as [3, 7]:

$$\mathcal{F}_g(\nabla \varepsilon) = k_g \left(\frac{\partial \varepsilon}{\partial x} \right)^2, \quad (3)$$

where k_g is also a material-specific constant. The non-local term above accounts for inhomogeneous strain field. It represents energy contributions from domain walls among different phases, which is an analog of the Ginzburg term in semiconductors. In order to account for dissipation

effects accompanying with phase transformations, a Rayleigh dissipation term is introduced here as follows [3]:

$$\mathcal{F}_R = \frac{1}{2}\nu\left(\frac{\partial\varepsilon}{\partial t}\right)^2, \quad (4)$$

where ν is the material-specific constant. The above dissipation term accounts for the internal friction accompanying with the movement of the interfaces between different phases. At macroscale, it stands for the viscous effect of the phase transformation [2].

By substituting the potential energy density into the Lagrangian function given in Eq.(1), and minimizing \mathcal{L} with respect to the displacement field $u(x, t)$, the governing equation for the dynamics of mechanical field can be easily obtained as follows, if the dissipation effects are also taken into account:

$$\rho\ddot{u} = \frac{\partial}{\partial x} (k_1(\theta - \theta_1)\varepsilon + k_2\varepsilon^3 + k_3\varepsilon^5) + \nu\frac{\partial}{\partial t}\frac{\partial^2 u}{\partial x^2} - k_g\frac{\partial^4 u}{\partial x^4}. \quad (5)$$

The dependency of the dynamics of the mechanical field on the temperature is obvious from the above wave equation. For the dynamics of the thermal field, its governing equation can be obtained by using the conservation law for the internal energy e , and obey the thermodynamical laws:

$$\rho\frac{\partial e}{\partial t} + \frac{\partial q}{\partial x} - \sigma\frac{\partial \varepsilon}{\partial t} = 0, \quad (6)$$

where $q = -k\partial\theta/\partial x$ is the heat flux according to the Fourier law for heat conduction, and k is the heat conductance for the material. It is easy to connect the internal energy to the Helmholtz free energy density $\mathcal{H}(\theta, \varepsilon) = \mathcal{F} - c_v\theta \ln \theta$ using the thermodynamical equilibrium condition:

$$e = \mathcal{H} - \frac{\partial \mathcal{H}}{\partial \theta}, \quad \sigma = \frac{\partial \mathcal{H}}{\partial \varepsilon}, \quad (7)$$

where c_v is the specific heat capacitance. By substituting the above relationship into the Eq.(6), the governing equation for the thermal field can be formulated as:

$$c_v\frac{\partial \theta}{\partial t} = k\frac{\partial^2 \theta}{\partial x^2} + k_1\theta\varepsilon\frac{\partial \varepsilon}{\partial t}, \quad (8)$$

The above constructed governing equations for the mechanical and thermal fields are actually based on the same potential energy density $\mathcal{F}(\theta, \varepsilon)$, which is constructed as the Landau free energy density here. It has been shown clearly in Ref.([3, 11, 15]) that the mathematical modelling given by Eq.(5) and Eq.(8) is capable to capture the first order phase transformations in ferroelastic materials, and the intrinsic thermo-mechanical coupling is also captured by introducing such a temperature dependent free energy density. But the numerical simulation has to be deliberately tuned because the very strong nonlinearity and nonlinear coupling between the mechanical and thermal fields.

Considering the fact that, in the current paper, the mechanical loading is implemented in terms of impact stress, it is more convenient if the stress-strain relation is kept as an extra equation for the model and the stress is solved as a dependent variable. This treatment will make the treatment of boundary conditions much easier. For this purpose, the so called ‘‘Differential

Algebraic Equation” (DAE) approach is employed here and the mathematical model can be re-formulated as the following:

$$\begin{aligned} \frac{\partial u}{\partial t} &= v, \quad \rho \frac{\partial v}{\partial t} = \frac{\partial \sigma}{\partial x}, \\ c_v \frac{\partial \theta}{\partial t} &= k \frac{\partial^2 \theta}{\partial x^2} + k_1 \theta \varepsilon \frac{\partial \varepsilon}{\partial t}, \\ \sigma &= k_1(\theta - \theta_1)\varepsilon + k_2\varepsilon^3 + k_3\varepsilon^5 + \nu \frac{\partial v}{\partial x} - k_g \frac{\partial^2 \varepsilon}{\partial x^2}, \end{aligned} \quad (9)$$

where v is particle velocity in the SMA rod.

In the above model, there is no distributed mechanical and thermal loadings included. To complete the model the following boundary conditions are employed for the mechanical and thermal fields;

$$\begin{aligned} \left. \frac{\partial \theta}{\partial x} \right|_{x=0} &= 0, \quad \left. \frac{\partial \theta}{\partial x} \right|_{x=L} = 0, \\ u(0) &= 0, \quad \left. \frac{\partial^2 u}{\partial x^2} \right|_{x=L} = 0, \quad \sigma(L) = g(t) \end{aligned} \quad (10)$$

where $g(t)$ is a given function describing the stress impact profile.

3 Numerical Methodology

As mentioned in the above section, numerical analysis for the wave propagations given by the mathematical model has to be deliberately tuned due to the difficulties caused by the non-linearity and phase transformations. Considering the fact that both dispersion and dissipation of wave propagations will presents in the physics of the current problem, the numerical algorithm for the problem has to tuned to take care of both numerical dissipation and dispersion. At the same time, the accuracy of the algorithm should also be equally concerned. Being aware of these aspects, here a multi-domain decomposition method together with the Chebyshev collocation methods is employed for the purpose, which is a compromise among various aspects of the concern.

3.1 Chebyshev Collocation Methods

For the Chebyshev pseudo-spectral approximation, a set of Chebyshev points $\{x_i\}$ are chosen along the length direction as follows:

$$x_i = L \left(1 - \cos\left(\frac{\pi i}{N}\right) \right) / 2, \quad i = 0, 1, \dots, N. \quad (11)$$

Using these nodes, u, v, θ , and σ distributions in the rod can be expressed in terms of the following linear approximation:

$$f(x) = \sum_{i=0}^N f_i \phi_i(x), \quad (12)$$

where $f(x)$ stands for any of u, v, θ , or σ , and f_i is the function value at x_i . $\phi_i(x)$ is the i^{th} interpolating polynomial which has the following property:

$$\phi_i(x_j) = \begin{cases} 1, & i = j, \\ 0, & i \neq j. \end{cases} \quad (13)$$

It is easy to see that the well known Lagrange interpolants satisfy the interpolating requirements. Having obtained $f(x)$ approximately, the derivative $\partial f(x)/\partial x$ can be easily obtained by taking the derivative of the basis functions $\phi_i(x)$ with respect to x :

$$\frac{\partial f}{\partial x} = \sum_{i=1}^N f_i \frac{\partial \phi_i(x)}{\partial x}. \quad (14)$$

and similarly for the higher order derivatives. All these approximation can be formulated in matrix form, for the convenience of programming.

3.2 Multi-Domain Decomposition

It is well known that the spectral methods are able to give a relative higher accuracy with the same number of nodes for discretization, compared to either finite difference methods or finite element methods. On the other side, when the solution to the problem is not higher-order differentiable, the spectral methods might introduce artificial oscillation due to the Gibbs phenomenon. In the current problem, the impact induced wave propagation might be such a case. To avoid this, a multi-domain decomposition method is employed here.

For this problem, the whole computational domain $\mathcal{D} = [0, L]$ is evenly decomposed into P intervals (subdomains), with an overlap region between each pair of consecutive intervals, as sketched in Figure (2):

$$\mathcal{D} = \bigcup_{p=1}^{p=P} D_p, \quad (15)$$

where the number of subdomains P is chosen according to the specific problem under consideration. In each interval, the Chebyshev collocation methods discussed above is employed to approximate the solution and its derivatives.

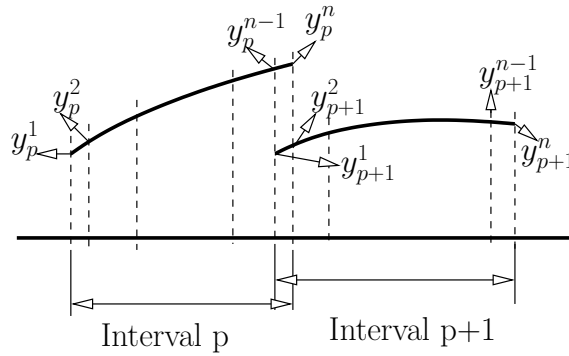


Figure 2: Sketch of domain decomposition and discretization

The coupling between each pair of consecutive intervals can be implemented by setting the following requirements:

$$y_p^n = y_{p+1}^2, \quad y_p^{n-1} = y_{p+1}^1, \quad (16)$$

where the subscript p stands for the interval number, while the superscript n stands for the node number in each interval. Variable y_p^n is the function value at point x_p^n (the n th node in the p th

interval), which could be any of the dependent variables we are solving for. point x_p^n is actually the same node of x_{p+1}^2 , and x_p^{n-1} is the same of x_{p+1}^1 .

The derivatives of functions in the overlapped nodes are approximated by taking the average of their values evaluated from the two intervals involved:

$$\begin{aligned} \left. \frac{\partial y}{\partial x} \right|_{x_p^{n-1}} &= \frac{1}{2} \left(\sum_{i=0}^N y_p^i \left. \frac{\partial \phi_i(x)}{\partial x} \right|_{x_p^{n-1}} + \sum_{i=0}^N y_{p+1}^i \left. \frac{\partial \phi_i(x)}{\partial x} \right|_{x_{p+1}^1} \right), \\ \left. \frac{\partial y}{\partial x} \right|_{x_p^n} &= \frac{1}{2} \left(\sum_{i=0}^N y_p^i \left. \frac{\partial \phi_i(x)}{\partial x} \right|_{x_p^n} + \sum_{i=0}^N y_{p+1}^i \left. \frac{\partial \phi_i(x)}{\partial x} \right|_{x_{p+1}^2} \right), \end{aligned} \quad (17)$$

The approximation to the second order derivatives can be done using the same average for the nodes in overlapped region.

3.3 Backward Differential Formula Methods

By employing the multi-domain decomposition methods combined with the Chebyshev collocation methods, the given set of partial differential equations in Eq. (9) can be converted into a DAE system, which can be sketched as the following form:

$$\mathbf{M} \frac{d\mathbf{X}}{dt} + \mathbf{N}(t, \mathbf{X}, g(t)) = 0, \quad (18)$$

where \mathbf{X} is the vector collecting all the variables we are solving for, \mathbf{M} is a singular matrix, \mathbf{N} is a vector collecting nonlinear functions produced by spatial discretization. The resultant DAE system is a stiff system and has to be solved by an implicit algorithm. Here the second order backward differentiation formula method is employed for the purpose. By discretizing the time derivative using the second order backward approximation, the DAE system can be converted into an algebraic system on each time level, which can be formulated in a form as follows:

$$\mathbf{M} \left(\frac{3}{2} \mathbf{X}^n - 2 \mathbf{X}^{n-1} + \frac{1}{2} \mathbf{X}^{n-2} \right) + \Delta t \mathbf{N}(t_n, \mathbf{X}^n, g(t_n)) = 0, \quad (19)$$

where n denotes the current computational time layer. For each computational time layer, iterations must be carried out using Newton's method for \mathbf{X}^n by use of \mathbf{X}^{n-1} and \mathbf{X}^{n-2} . Starting from the initial value, the vector of unknowns \mathbf{X} can be solved for all specified time instances employing this algorithm.

4 Numerical Experiments

A series of numerical experiments have been carried out to investigate the nonlinear wave propagations in the SMA rod involving phase transformations. All experiments reported here are carried out on a $\text{Au}_{23}\text{Cu}_{30}\text{Zn}_{47}$ rod, with a length of 1 cm. The physical parameters, except ν and k_g , for this specific material are taken the same as those in [15], which are listed as follows for the sake of convenience:

$$\begin{aligned} k_1 &= 480 \text{ g/ms}^2\text{cmK}, & k_2 &= 6 \times 10^6 \text{ g/ms}^2\text{cmK}, & k_3 &= 4.5 \times 10^8 \text{ g/ms}^2\text{cmK}, \\ \theta_1 &= 208 \text{ K}, & \rho &= 11.1 \text{ g/cm}^3, & c_v &= 3.1274 \text{ g/ms}^2\text{cmK}, & k &= 1.9 \times 10^{-2} \text{ cmg/ms}^3\text{K}. \end{aligned}$$

Numerical experiments indicate that there is no remarkable effect from the value of the Ginzburg coefficient k_g in wave propagations and phase transformations under external loadings, as far as its value is relatively small compared to k_1 . So this coefficient is uniformly chosen

as $k_g = 0.05k_1$ for all the numerical experiments here. The internal friction coefficient is not an easily obtainable constant, and is chosen here as a small fraction of k_1 as $0.01k_1$. The whole rod is divided into 7 sub-intervals, in each interval there are 15 nodes for spatial discretization. All the simulations are carried in the time span $[0, 0.2]$ ms, and the time stepsize for the integration is chosen as 2.5×10^{-5} ms.

It has been shown [11, 15] that the Landau free energy density has only one local minimum at high temperature and there is no phase transformation in the material in this case. While at low temperature, the free energy density has two symmetrical local minima, which are associated with two martensite variants (martensite plus and minus) in the Ginzburg - Landau theory. Phase transformations between the two martensite variants might be induced by mechanical loadings. If the temperature is intermediate, there are three local minima, the third one at the center is associated with the austenite. In the last case, there are mesostable phases, and phase transition between austenite and martensite might be induced by mechanical loadings.

To demonstrate the effect of phase transformations on the nonlinear thermo-mechanical wave propagations in the SMA rod, three representative temperatures are chosen for the illustration purpose here. The first experiment is carried out with the initial condition: $u = v = s = 0$, $\theta = 300K$ as a high temperature example, and the impact loading is set as:

$$g(t) = \begin{cases} 4 \times 10^3, & 0 \leq t \leq 0.006 \\ 0, & t > 0.006 \end{cases} \quad (20)$$

which can be regarded as an approximation to a pulse stress impact on the SMA rod.

The strain and temperature evolution in the SMA rod is plotted versus time in the top row of Figure (3). Numerical results show clearly that the impact induced wave propagates along the negative x direction firstly, then hit and bounce back at $x = 0$. The temperature evolution indicates that there is an associated thermal wave induced by the mechanical wave due to the thermo-mechanical coupling effect. The propagation pattern of the thermal wave is similar to that of the mechanical wave. The oscillation in the displacement evolution due to the stress impact is plotted in the left bottom subplot of Figure (3). To show the wave propagation more precisely, the strain distributions at four chosen time instances are plotted together in the right bottom subplot of Figure (3). It is shown that the strain distribution in the rod is relatively smooth and there is no obvious sharp interface between different strain values. The wave propagation speed can be estimated by the location of the wave frontier plotted in the figure. With the current initial temperature, the strain wave is bounced back from $x = 0$ and its frontier is around $x = 0.6$ when $t = 0.025$.

The second example is performed with the same computational conditions and loading, except that the initial temperature now is set $\theta = 250K$, the numerical results for this case is presented in a similar way in Figure (4). By comparing the results with those of the first experiment, it is easy to see that the strain and temperature waves are not that regular as those in the first experiments. This can be explained by the theory that there are phase transformations induced in the rod. The frontier of the waves are more obvious and wave propagation pattern is more complicated. The oscillation in the displacement evolution has only two peaks in this case, while three peaks are found in the first experiment. At the four chosen time instances, the strain distributions are not that smooth as those with higher temperature, oscillations occur in the strain distributions, due to the phase transformations between martensite and austenite. At $t = 0.025$, the wave frontier is around $x = 0.4$ and propagating long the positive x direction. It indicates that the wave speed is a little lower than that in the first experiments. Similarly, there is a thermal wave caused by the mechanical wave due to the coupling.

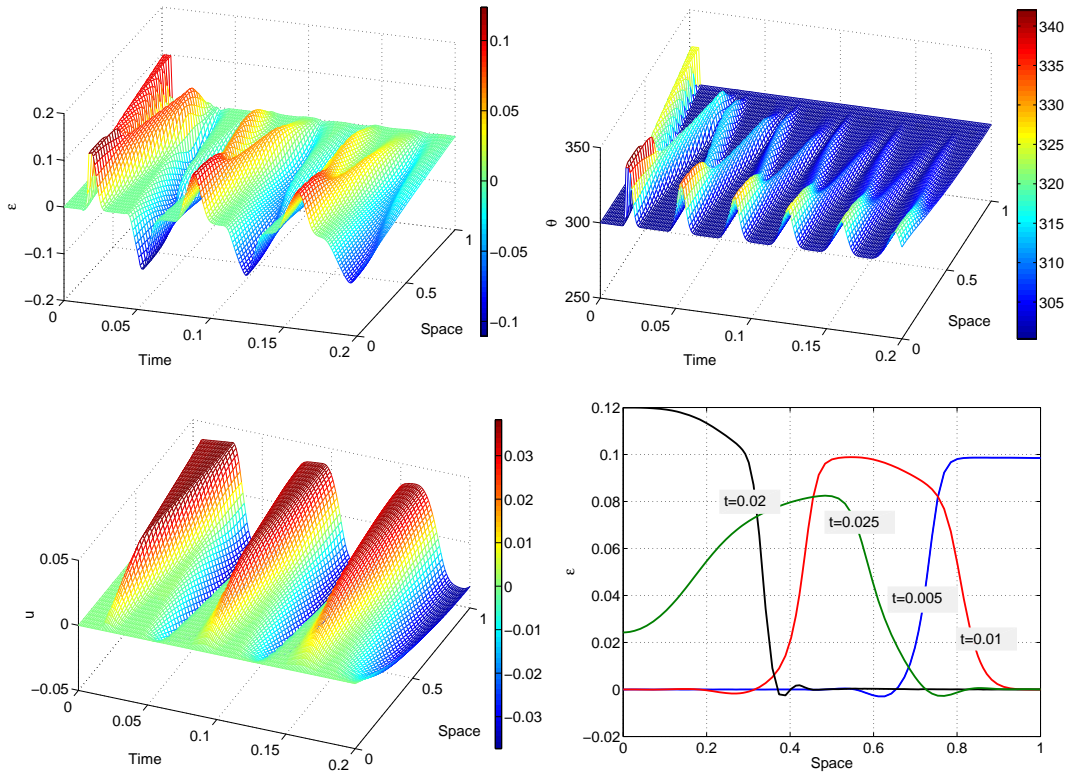


Figure 3: Nonlinear thermo-mechanical wave propagation in shape memory alloy rod caused by a stress impact, initial temperature is $\theta = 300K$

For the third experiment, the initial temperature is set $\theta = 210K$. Because only martensite is stable with this temperature, the initial displacement of the SMA rod is set $u = 0.118x$ (0.118 is the estimated transformation strain with the given temperature using the Landau free energy density). The numerical results for this case are presented in Figure (5). The results indicate that the whole SMA rod is classified into two domain, one consists of martensite plus (with positive strain value) and another one minus (with negative strain values). The interface between the two domain is driven by the impact stress loading, as sketched in the left top subplot in Figure (5). With the current computation conditions, the wave hit the end of the rod at $x = 0$ only once and bounce back. There is only one peak in the displacement oscillation. In both of the martensite plus and minus domain, there are minor waves presented. The wave propagation speed is much lower compared to those of previous experiments, and the wave speed changes more remarkably during the propagation process. At $t = 0.03$, the wave frontier is at $x = 0.2$ and not achieve the end $x = 0$ yet.

To investigate the effect of the internal friction, the final experiment is done with different internal friction coefficients, while all other computation conditions are the same with those in the third experiment. The numerical results are presented in Figure (6). In the top row of Figure (6), the strain evolution and strain distributions at four chosen time instances are presented for $\nu = 20$, while in the bottom, those for $\nu = 30$ are presented. It is shown clearly by the strain distributions at the chosen time instances that the wave propagation speed decreases when the internal friction coefficient increases. When ν is increased to 30, the impact stress loading is not able to convert the whole SMA rod from martensite minus to plus, while the same impact loading can do the job when $\nu = 20$ and less, because less energy is dissipated due to the

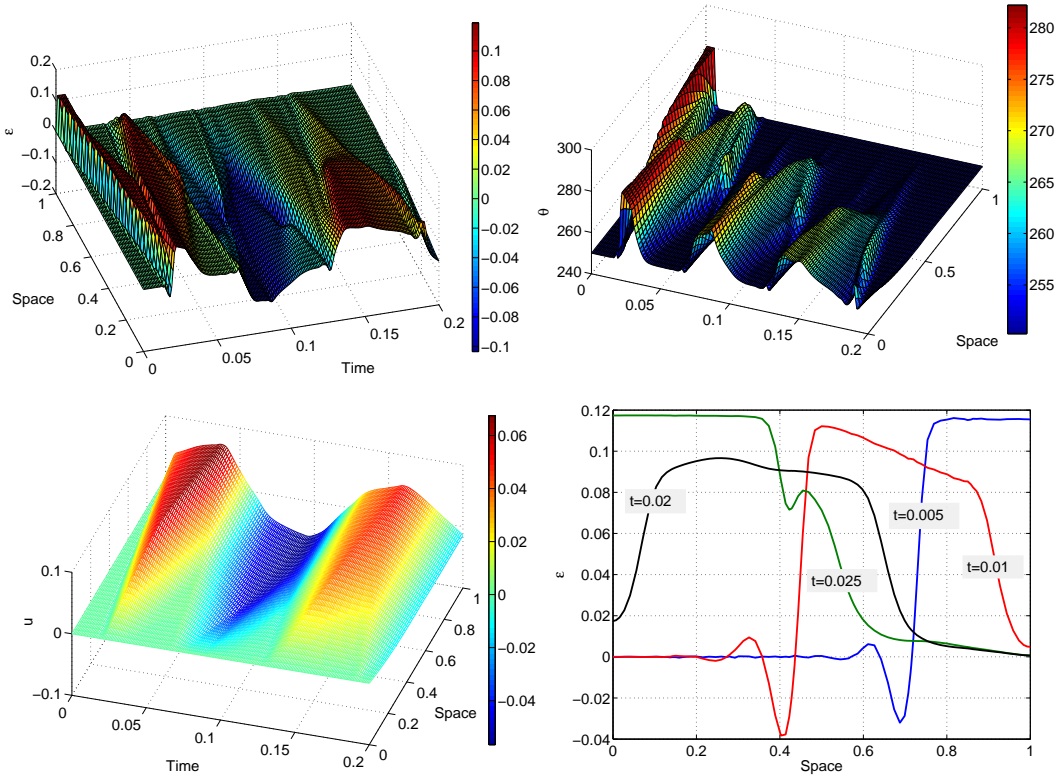


Figure 4: Nonlinear thermo-mechanical wave propagation in shape memory alloy rod caused by a stress impact, initial temperature is $\theta = 250K$.

internal friction ν is smaller.

From the above numerical experiments, it is shown that nonlinear thermo-mechanical wave propagations caused by impact loadings are influenced by the material temperature. Thermal waves could be induced by impact mechanical loadings. Numerical results show that the wave propagation pattern is more complicated when phase transformations are involved, and dynamical response of the material is very different from those with no phase transformations.

5 Conclusions

In this paper, we constructed a mathematical model for wave propagations in a shape memory alloy rod induced by a stress impact. We employed the modified Ginzburg - Landau theory for the mathematical modelling, by which the first order martensite phase transformations are modelled and the thermo - mechanical coupling is captured. Multi-domain decomposition is employed together with Chebyshev collocation methods for spatial discretization, and the backward differentiation formula is used for solving the differential algebraic system. The nonlinear thermo-mechanical wave propagations in the SMA rod are simulated with various initial temperatures. The effect of phase transformations on the wave propagations are investigated.

REFERENCES

- [1] Abeyaratne, R., Knowles, J.K., Dynamics of propagating phase boundaries: thermoelastic solids with heat conduction. *Arch. Rational Mech. Anal.* **126**, (1994) 203- 230.

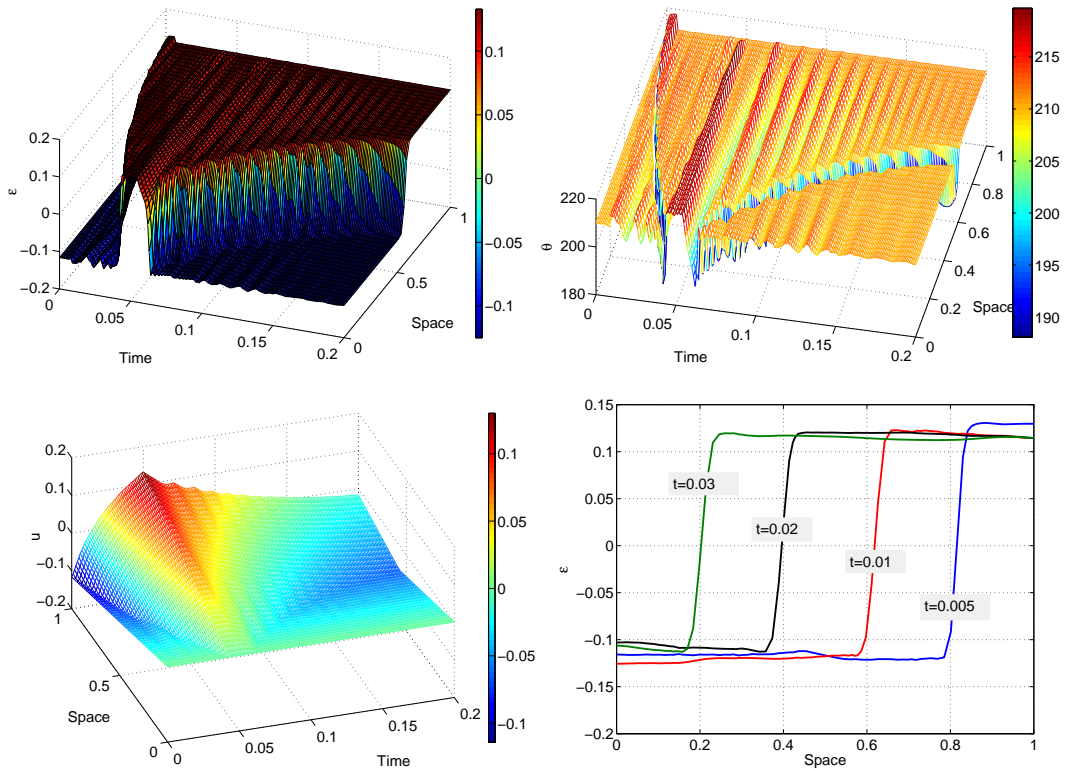


Figure 5: Nonlinear thermo-mechanical wave propagation in shape memory alloy rod caused by a stress impact, initial temperature is $\theta = 210K$

- [2] Abeyaratne, R., and Knowles, J. K., On a shock-induced martensitic phase transition, *J. Appl. Phys.* **87** (2000), 11231134.
- [3] Bales, G.S. and Gooding, R.J., Interfacial dynamics at a 1st-order phase-transition involving strain dynamic twin formation. *Phys. Rev. Lett.*, **67**, (1991) 3412.
- [4] Berezovski, A. and Maugin, G. A., Stress-induced phase transition front propagation in thermoelastic solids *Eur. J. Mech.- A/Solids*, **24** (2005), 1-21
- [5] Bekker, A., Jimenez-Victory, J. C., Popov, P., and Lagoudas, D. C., Impact Induced propagation of phase transformation in a shape memory alloy rod, *Int. Jour. Plasticity*, **18** (2002) 1447-1479.
- [6] Birman, V., Review of mechanics of shape memory alloys structures, *Appl. Mech. Rev.* **50** (1997) 629-645.
- [7] Chaplygin, M. N., Darinskii, B. M., and Sidorkin, A. S., Nonlinear Waves in Ferroelastics, *Ferroelectrics*, **307** (2004) 1-6.
- [8] Chen, Y.C., Lagoudas, D. C., Impact induced phase transformation in shape memory alloys, *Journal of the Mechanics and Physics of Solids*, **48** (2000) 275 - 300.
- [9] Dai, X. Y., Tang, Z. P., Xu, S. L. Guo, Y. B., and Wang, W. Q., Propagation of macroscopic phase boundaries under impact loadings, *Int. Jour. Impact Eng.* **30** (2004) 385-401.

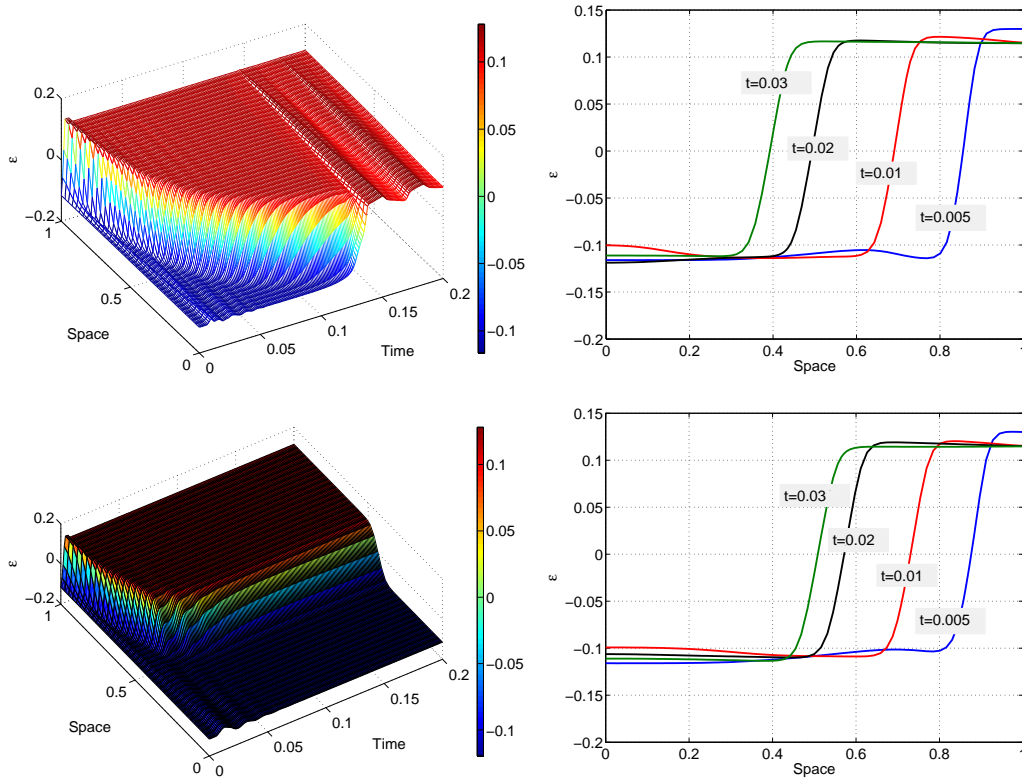


Figure 6: Numerical simulation of thermo-mechanical waves with different internal friction coefficients, with initial temperature $\theta = 210K$.

- [10] Dai, H. H., Kong, D. X., The propagation of impact-induced tensile waves in a kind of phase transformation materials, *Jour. Comput. App. Math.* (2006), in press.
- [11] Falk, F., Ginzburg-Landau theory and solitary wave in shape memory alloys, *Z. Phys. B - Condensed Matter* **54** (1984) 159-167.
- [12] Knowles, J. K., Impact Induced Tensile Waves in a rubberlike material, *SIAM J. Appl. Math.* Vol. 62 (4) (2002) 1153 - 1175.
- [13] Knowles, J. K., On shock waves in a special class of thermoelastic solids, *Int. Jour. Non-linear Mechanics*, **40** (2005) 387-394.
- [14] Lagoudas, D. C. , Ravi-Chandar, K., Sarh, K., and Popov, P., Dynamic loading of polycrystalline shape memory alloy rods, *Mechanics of Materials* **35** (2003) 689 - 716.
- [15] Niezgodka, M., Sprekels, J.: Convergent numerical approximations of the thermomechanical phase transitions in shape memory alloys. *Numerische Mathematik* **58**(1991) 759-778.

Preface

This book contains the edited version of the Abstracts of Plenary and Keynote Lectures and Papers, and a companion CD-ROM with the full-length papers, presented at the III European Conference on Computational Mechanics: Solids, Structures and Coupled Problems in Engineering (ECCM-2006), held in the National Laboratory of Civil Engineering, Lisbon, Portugal 5th - 8th June 2006. The book reflects the state-of-art of Computation Mechanics in Solids, Structures and Coupled Problems in Engineering and it includes contributions by the world most active researchers in this field.

ECCM-2006 is a continuation of the very successful Conferences held in Munich, Germany (1999) and Cracow, Poland (2001) and it is organized by the European Committee of Computational Solid and Structural Mechanics (ECCSM) of the European Community on Computational Methods in Applied Science (ECCOMAS) in collaboration with the Portuguese Association of Theoretical, Applied and Computational Mechanics (APMTAC), the Technical University of Lisbon and the National Laboratory of Civil Engineering. ECCM-2006 is attended by about 1000 participants from 70 countries. More than 1300 Abstracts were submitted to ECCM-2006. Altogether, 6 plenary lectures, 35 keynote lectures and 800 papers are presented in 58 organized symposia. A companion book, containing the edited version of the majority of Plenary and Keynote Lectures, entitled Computational Mechanics: Solids, Structures and Coupled Problems in Engineering is also published by Springer 2006.

The Proceedings of the Conference could not be possible without the sponsorship and financial support of: European Community on Computational Methods in Applied Science (ECCOMAS); European Committee of Computational Solids and Structural Mechanics (ECCSM); International Association of Computational Mechanics (IACM); Portuguese Association of Theoretical, Applied and Computational Mechanics (APMTAC); Foundation of Science and Technology (Portugal); Calouste Gulbenkian Foundation (Portugal); Technical University of Lisbon (Portugal); National Laboratory of Civil Engineering (Portugal); Instituto Superior Técnico (Portugal).

The Editors are grateful to all authors and to the reviewers that helped ensuring the scientific quality, allowing for this book to be published before ECCM-2006. We acknowledge the support of Mr. Pedro Pinto of the Technical University of Lisbon, in the editing of the book. The Editors are also grateful to all Members of Executive, Organizing, Advisory and Scientific Committees and to the organizers of the Symposia, whose work made possible the success of ECCM-2006. We are grateful to Andrea Marques and Ana Catarina Amador for their effort and valuable assistance in the conference and preparation of this book.

Technical University of Lisbon, Portugal, June 2006

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