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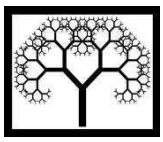

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Numerical Analysis of Complex Systems Evolution with Phase Transformations at Different Spatial Scales

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Abstract

This paper shows the existence of a critical dimension for finite length nanowires exhibiting shape memory effects. We give a brief survey of phase transformations, their classifications, and provide the basis of mathematical models for the phenomena involving such transformations, focusing on shape memory effects at the nanoscale. Main results are given for the dynamic of square-to-rectangular transformations modelled on the basis of the modified Ginzburg-Landau theory. The results were obtained by solving a fully coupled system of partial differential equations, accounting for the thermal field, a feature typically neglected in recent publications on the subject when microstructures of nanowires were modelled with phase-field approximations. Representative examples are shown for nanowires of length 2000nm and widths ranging from 200nm to 50nm. The observed microstructure patterns are different from the bulk situation due to the fact that interfacial energy becomes comparable at the nanoscale with the bulk energy.

Keywords: phase transformations, nanoscale, shape memory effects, Ginzburg-Landau theory, nonlinear thermoelasticity.

1 Introduction

Phase transformations are ubiquitous in many problems of science and engineering where we have to analyze the evolution of complex nonlinear systems. A complex system usually has interconnected parts such that one or more properties (or the behavior) of the system is not obvious from the properties (or the behaviors) of the individual parts. Alternatively, a complex system may operate under the combined influence of

several different physical fields that can bring new properties and/or behavior of the system compared to the situation where each such field acts separately. Complex systems may include human factors as it is known that with the increasing complexity of technological systems that operate in dynamically changing environments and require human supervision or a human operator, the relative share of human errors is increasing across all modern applications [17]. In some cases, the associated models can be constructed on the basis of the Markov Chain approximation methodology linking deterministic and stochastic situations [11]. Furthermore, many complex systems, including those exhibiting phase transformations, often require some phenomenological paradigms for atomistic matter interactions and/or incorporating stochastic elements into mathematical models which is often done with the concept of relativistic Brownian motion. We do not consider such models in the present paper, but we refer the interested reader to a recent survey [4] as well as to applications of some of these models [29, 17]. In what follows, we focus on those complex systems which are coupled via interacting components and/or fields, and which are usually well described by problems of thermolasticity [12, 26], including hyperbolic [24], electroelasticity [18, 21], flexoelectricity [22], thermo-piezoelectricity [13, 23] and other problems of coupled field theory [14, 28].

In this contribution, we consider one class of such problems that are brought about by smart materials and structures technologies where materials with shape memory effect found numerous applications at different spatial scales. In particular, we start from the general 3D model of dynamic nonlinear thermoelasticity, based on a coupled system of partial differential equations (PDEs), which we first apply for the description of shape memory alloys (SMA) dynamics and associated phase transformations. With the center-manifold-based procedures this general model can be reduced systematically to new simplified models preserving essential features of the SMA dynamics [15]. For some special cases, the reduction procedures can be carried out very efficiently with the Proper Orthogonal Decomposition (POD) methodology, while for other cases techniques such as finite volume [27] and finite element methods can be used. For practical numerical simulations of SMA samples, the constructed mathematical model of coupled nonlinear system of PDEs can also be reduced to a system of differential-algebraic equations, where the Chebyshev collocation method can be employed for the spatial discretization, while the backward differentiation can be used for the integration in time [26]. We briefly survey these numerical methodologies. From a mathematical point of view, the system we are dealing with is a system of coupled nonlinear time-dependent PDEs, known as the Ginzburg-Landau-Devonshire system. The effect of internal friction on wave propagation patterns under shock loadings can be analyzed in such systems via implementing stress boundary conditions. In the last part of this contribution, we discuss a relatively simple and computationally inexpensive model to study phase transformations in finite nanostructures with our major focus given here to nanowires of finite length. We show that in the latter case, the models describing shape memory effects at the mesoscopic level can be reduced to a 2D case and we demonstrate our results on the example of the cubic-to-tetragonal transformations.

2 Phase Transformations and Their Applications

Phase transformations have been firmly in the realm of science and engineering at least from 1876 due to works of J.W. Gibbs. In engineering, physical, chemical, geological, climate sciences phase transformations are indispensable in studying complex phenomena, systems, and processes. There is a growing interest to phase transformation phenomena in biological sciences, in particular when we have to deal with biomolecular structures, cell biology problems, and in many other areas (e.g., [9, 19]). Space science and astrophysics are also the areas were phase transformations found numerous applications. They are also becoming more frequent in less traditional areas of social sciences, finance and other fields (e.g. [29] and references therein).

Although, in the mathematics community the original studies of phase transformations are often associated with the name of J. Stefan (1889), the earlier contributions of J. W. Gibbs played a substantial role in the development of theory of phase transformations. His work "On the Equilibrium of Heterogeneous Substances" finalized in 1900 represented an important milestone in this theory. Other important contributions include works of E. Ising on one-dimensional mathematical models for ordering of spins(1925), and later of L. Onsager (1930) 2D models. The works of L. Onsager (1968) and I. Prigogine (1977) were honored with Nobel prize. The theoretical framework of critical phenomena and phase transitions that is used in this paper is due to L. Landau (1937), E. Lifshitz (1941), V. Ginzburg and L. Landau (1950) and many others, including M.E. Fisher (1959), M.E. Fisher, A.I. Levanyuk (1959), V.L. Ginsburg (1960). This followed by the works of K.G. Wilson on the general problem of fluctuation-driven phase transitions (1972), F. Falk on one-dimensional Landau theory models for materials with memory (1980), and F. Falk and P. Konopka on 3D Landau theory for materials with memory (1990). In its essence, the theory asks the question on how to describe order in terms of irreducible representations of the symmetry group, and introduces the notion of spontaneous symmetry violation, as well the order parameter as a measure of this violation.

Mathematically appealing classification of phase transformations was given by P. Ehrenfest (1933) based on the degree of non-analyticity involved (discontinuity in the corresponding derivatives of the free energy function). In practice, however, we still use a classification that stems from J.W. Gibbs:

- First-order phase transitions are associated with "mixed-phase regimes" where some parts of the system have completed the transition and others have not (examples include the solid/liquid/gas transitions as well as Bose-Einstein condensation),

- Second-order phase transitions are continuous phase transitions which are easier to study (examples include ferromagnetic, superfluids, where critical phenomena are phenomena associated with them),

- Infinite-order phase transitions (examples include quantum phase transitions in

2D; superconductors provide a practical area for studies of these transformations).

In what follows we focus on the first order solid-solid phase transformations.

3 Mathematical Models of Phase Transformations with Non-Monotone Free Energy

The basic idea of the Landau theory lies on the premises that when symmetry is broken under the phase transition, we need to introduce one or more extra variables to describe the state of the system. In particular, the order parameter describes the character and strength of the broken symmetry. The implications of phase transitions are such that the formation of topological defects in the structure is expected, so that the order parameter may take on different values in different parts of the system (e.g., due to thermal fluctuations). It is known that a 3D system can be described by its Helmholtz free energy density f as

$$A = \int d^3x f(m, T), \tag{1}$$

where f is a function of the local order parameter m and T:

$$f(m, T) = f_0(T) + \alpha(T)m^2 + \frac{1}{2}\beta(T)m^4 + ...\text{(Ginzburg term)}. \tag{2}$$

This description can include strongly nonlinear phenomena directly related to phase transformations including hysteresis and other memory effects. A mathematically rigorous notion of hysteresis operators and their systematic analysis is of a relatively recent origin (due to Krasnoselsky, Pokrovsky in the 70-ies). We only note here that the original notion was introduced for parabolic type of equations, while a more practically important case of hyperbolic PDEs with hysteresis remains much less studied. One of the important sources of such complex nonlinear behaviour as hysteresis often lies with coupled dynamic problems which are the rule rather than an exception in mathematics and its applications. Recall that the lack of coupling in the Newton's model led to calculation of speed of sounds that was around 15% off its true value (the model was corrected by Laplace at the time of the development of thermodynamics, more than 100 years later).

The starting point of the Landau-Ginzburg-Devonshire model for the free energy function lies with the assumption that any isothermal equilibrium configuration of the lattice corresponds to a minimum (either local or global) of that function. In order to describe shape memory effects in materials such as alloys we have to account for a possibly of simultaneous existence of several phases: (a) a high temperature phase (austenite) and (b) a low temperature phase (martensite). Therefore, the free energy function would contain a coupling term that couples thermal and mechanical fields

as it is important to be able to deal with different equilibrium configurations of the lattice simultaneously. In a most generic setting, the mathematical description of the appropriate measure starts from the approximation of the free energy function by polynomials with temperature-depending coefficients. This approximation with respect to an order parameter characterising the phase transformation has the following form:

$$\Psi(\vec{\epsilon},\theta) = \psi^0(\theta) + \sum_{i=1}^{\infty} \psi^i(\vec{\epsilon},\theta), \tag{3}$$

where independent parameters of the n-th order for $n = 1, 2, \ldots$ are determined through strain invariants, $\mathcal{I}_j^n$ as follows

$$\psi^n = \sum_{j=1}^{j^n} \psi_j^n \mathcal{I}_j^n \quad \text{and} \quad \psi^0(\theta) = \psi_0^0(\theta)\,. \tag{4}$$

In order to make the free energy function invariant with respect to the symmetry group of austenite, the upper limit of the sum, j^n, is chosen as the number of all invariant directions associated with a representation of the 48th order cubic symmetry group of the parent (austenite) phase. Similar to the Falk-Konopka ideas, by using physically justified assumptions, it is possible to reduce the number of required parameters in the 3D case (although they remain in the general case temperature dependent). For instance, the copper-based alloys (e.g., $\mathrm{Cu}_{14}\ \mathrm{Al}_3\ \mathrm{Ni}_{83}$), we have

$$\Psi = \psi^0(\theta) + \sum_{j=1}^{3} \psi_j^2 \mathcal{I}_j^2 + \sum_{j=1}^{5} \psi_j^4 \mathcal{I}_j^4 + \sum_{j=1}^{2} \psi_j^6 \mathcal{I}_j^6, \tag{5}$$

where, for example, strain invariant $\mathcal{I}_2^2$ is determined by

$$\mathcal{I}_2^2 = \frac{1}{12}(2\epsilon_{33} - \epsilon_{11} - \epsilon_{22})^2 + \frac{1}{4}(\epsilon_{11} - \epsilon_{22})^2. \tag{6}$$

This free energy function is used along with the system of nonlinear thermoelasticity which is written in the spirit of the Landau theory of structural phase transitions [16]:

$$\rho \frac{\partial^2 \mathbf{u}}{\partial t^2} = \nabla_{\mathbf{x}} \cdot \mathbf{s} + \mathbf{F} \quad \text{with} \quad \mathbf{F} = \rho(\mathbf{f} + \hat{\mathbf{f}}) - \hat{\rho}\mathbf{v}\,, \tag{7}$$

$$\rho \frac{\partial e}{\partial t} - \mathbf{s}^T : (\nabla \mathbf{v}) + \nabla \cdot \mathbf{q} = g\,, \tag{8}$$

where

$$g = \rho(h + \hat{h}) - \rho \hat{\mathbf{f}} \cdot \mathbf{v} - \hat{\rho}\left(e - \frac{\mathbf{v}^2}{2}\right). \tag{9}$$

This system is supplemented by corresponding initial and boundary conditions.

For one and two dimensions, this system is substantially simplified, For example, within this framework, the governing equations for the dynamics of a SMA rod are [27]:

$$\rho\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial x}\left(k_1\left(\theta-\theta_1\right)\frac{\partial u}{\partial x} - k_2\left(\frac{\partial u}{\partial x}\right)^3 + k_3\left(\frac{\partial u}{\partial x}\right)^5\right) + F, \tag{10}$$

$$C_v\frac{\partial \theta}{\partial t} = k\frac{\partial^2\theta}{\partial x^2} + k_1\theta\frac{\partial u}{\partial x}\frac{\partial v}{\partial x} + G, \tag{11}$$

where k is the thermal conductivity of the material, C_v is the specific heat constant of the material, $\theta_1 > 0$ (characterises a critical temperature of the material), k_1, k_2 and k_3 are material-specific constants that characterise the material free energy.

A similar model, generalized to the 2D case, is used in the next section for modelling nanowires.

4 Numerical Approximations of Mathematical Models with Phase Transformations

As seen from model (10)-(11), this model incorporates a non-monotone stress-strain relationship. Therefore, it is quite natural to treat the stress-strain dependency as a purely algebraic equation by introducing ϵ, v, and θ as differential variables - this idea for dynamic systems describing shape memory effects was first proposed in [16].

The above methodology is not straightforward to generalize to the general 3D case where we proposed to apply the center manifold technique (CMT). Recall (e.g., [15]) that a centre manifold need not be unique, but the differences between the possible centre manifolds are of the same order as the differences we set out to ignore in establishing the low dimensional model. Next, the centre manifold technique allows us to derive not only governing equations for the model, but also initial and boundary conditions. Finally, the CMT does not need to be linked to just the one equilibrium: it is important in the context of phase transformations where we have to deal with several different equilibrium configurations. This theory in the context of SMA was developed in [15].

We also note that recently, the Chebyshev collocation method was employed for the numerical analysis of the PDE model for phase transformations (10)-(11), followed by the application of an extended proper orthogonal decomposition to construct a set of empirical orthogonal eigenmodes of the dynamics, with which system characteristics can be optimally approximated within a range of different temperatures and under various mechanical and thermal loadings [28].

While constructing numerical approximations to models based on differential equations, conservative approximations, where we wish to preserve invariant properties of the original differential model in the numerical approximation, play a very important

role. Such numerical approximations go back to works of Courant (1928) and they have been developed for large classes of non-linear PDE models too (e.g., Abrashin, 1986; Furihata, 2001, and many others), including coupled systems describing a phase separation phenomenon among others (Canh-Hilliard type of models). Our approach to the construction of such conservative schemes in the context of materials with memory was based on the modified integro-interpolational methodology where in addition to the interpolation of the solution with respect to independent variables, we also perform the Steklov averaging of nonlinear terms. Such schemes were constructed for the first time in the context of SMA in [8] where the interested reader can also find both their theoretical analysis and applications.

4.1 Applications to Finite Length Nanowires

The study of low dimensional nanostructures is an important field in applications with many open problems [6]. At the same, the interest to nanostructured martensitic materials continues to grow as there is evidence to suggest that the unique shape-memory properties of martensitic materials can persist even at the nanoscale, in particular in nanowires [25]. Several new models have recently been proposed in the literature to explain phenomena of pseudoelasticity and shape memory in nanowires (e.g., [5]). The major emphasis was given to the elastic part of behaviour which, however, was not coupled to the temperature field. Similarly, typical Molecular Dynamics (MD) runs, that have been recently carried out for nanowires, are for fixed temperature (e.g. [7]). The authors of [5] claimed that elastic responses were only weakly dependent on temperature. However, a complete thermoelastic analysis was not carried out. Although there are several other publications up to date with MD simulations of finite size nanowires, the issue of temperature is far from trivial within the MD framework [1]. At the same, by now it is clear that a number of important characteristics of nanowires are essentially temperature dependent, including their critical size [1]. Many such characteristics can be well studied by using much more tractable models such as those discussed in Section 3 of this paper. In [2] the authors considered a model based on the Landau phase field framework. However, the temperature was not included as a coupled quantity and only the elastic part of behaviour under fixed temperature was analyzed. In what follows, we adapt the theory and numerical approximations discussed above to the situation where mechanical and thermal fields are coupled. In particular, we solve the following system of partial differential equations:

$$\rho \frac{\partial^2 u_i(\mathbf{r},t)}{\partial t^2} = \sum \frac{\partial \sigma_{ij}(\mathbf{r},t)}{\partial r_j} + \eta \nabla^2 v_i(\mathbf{r},t) \tag{12}$$

$$c_v \frac{\partial T}{\partial t} = k\left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right) + a_2 T e_2 \frac{\partial e_2}{\partial t} + g, \tag{13}$$

where ρ is mass density, $\mathbf{v}$ is time derivative of displacement $\mathbf{u}$, η is damping term, c_v is specific heat constant, k is thermal conductivity and g is thermal loading. The

model is considered in a bounded domain Ω with corresponding initial and boundary conditions.

These equations are coupled through the modified Ginzburg-Landau free energy function which we take in the form for square-to-rectangular transformations (although this can be generalized to other cases too, e.g. [3]):

$$G = \int_{\Omega} \left\{ \frac{A_{22}}{2} \frac{T - T_m}{T_m} (e_2)^2 - \frac{A_{24}}{4} (e_2)^4 + \frac{A_{26}}{6} (e_2)^6 + \frac{A_1}{2} \left[e_1 - x_{12} (e_2)^2 \right]^2 + \frac{A_3}{2} (e_3)^2 + \frac{k_g}{2} ||\nabla \cdot e_2||^2 \right\} d\mathbf{r}, \tag{14}$$

where e_1, e_2 and e_3 are hydrostatic, deviatoric and shear strain respectively defined as $e_1 = (\epsilon_{xx} + \epsilon_{yy})/\sqrt{2}$, $e_2 = (\epsilon_{xx} - \epsilon_{yy})/\sqrt{2}$, $e_3 = (\epsilon_{xy} + \epsilon_{yx})/2$, and $\epsilon_{ij} = [(\partial u_i/\partial x_j) + (\partial u_j/\partial x_i)]/2$ is a Cauchy-Lagrangian strain tensor (with the repeated index convention used); u_i, i $= 1, 2$ are displacement along x and y directions respectively, T is material temperature, T_m is the austenite-martensite transformation temperature, x_{12} is the volume fraction and $\overrightarrow{\mathbf{r}}$ is space coordinate vector of domain Ω. The deviatoric strain e_2 is used as an order parameter to characterize the austenite ($e_2 = 0$) and martensite phase ($e_2 \neq 0$) in the microstructure.

The first three terms in Eq. (14) represents the Landau free energy which defines the first-order phase transformation. The Landau free energy is a convex function of e_2. When the temperature is higher than T_m, only austenite is stable. When the temperature is lower than T_m, e_2 becomes non-convex and has two local minima associated with two martensite variants. If the temperature is around T_m, the Landau free energy has three minima, two of which are associated with martensitic phases and the remaining one associated with austenite. The fourth and fifth term in Eq. (14) stabilizes the twin structure for $T < T_m$ [20]. In addition, the fourth term also considers the effect of volume fraction x_{12}. The strain gradient term $||\nabla \cdot e_2||$ does not contribute to the bulk energy, since there is no gradient within austenite and martensite, it plays a role similar to interface energy (both austenite-martensite and martensite-martensite). This gradient prevents the system from creating an infinite number of interfaces [3].

The stresses acting on the domain Ω can be calculated from Eq. (14) as

$$\sigma_{ij}(\mathbf{r}, t) = \frac{\delta G}{\delta \epsilon_{ij}(\mathbf{r}, t)}. \tag{15}$$

From Eq. (15) under sumplifications, we get

$$\begin{aligned}
\sigma_{11} &= \sqrt{2}(Ae_2 - 2Be_2^3 + 3Ce_2^5 + De_1 - 2De_1e_2x_{12} - De_2^2x_{12} + 2De_2^3x_{12}^2) - k_g\nabla_x^2 e_2 \\
\sigma_{12} &= \sigma_{21} = E\epsilon_{xy}, \\
\sigma_{22} &= \sqrt{2}(-Ae_2 + 2Be_2^3 - 3Ce_2^5 + De_1 + 2De_1e_2x_{12} \\
&- De_2^2x_{12} - 2De_2^3x_{12}^2) - k_g\nabla_y^2 e_2
\end{aligned} \tag{16}$$

with coefficients $A = (A_{22}(T - T_m))/(2T_m)$, $B = A_{24}/4$, $C = A_{26}/6$, $D = A_1/2$ and $E = A_3/2$.

We apply the Finite Element Method to solve this problem. All the simulations have been carried out for Fe-Pd nanowires of 2000 nm in length with varying widths. The displacements have been set to zero along the length and periodic boundary conditions applied at the two ends. All the simulations are carried out for 5 ms with k_g value 1×10^{-4}. The static harmonic elastic constants for Fe-Pd [2] have been taken as follows: $A_1 = 140$ GPa, $A_3 = 280$ GPa, $A_{22} = 212$ GPa, $A_{24} = 17 \times 10^3$ GPa, $A_{26} = 30 \times 10^6$ GPa, $T = 250$ K and $T_m = 265$ K. The volume change x_{12} has been varied in the simulations to study the effect on change of microstructure.

In Fig. 1 we demonstrate the results of coupled modelling of nanowires, where thermal effects were accounted for consistently. In all the simulations, the austenite is shown in green and martensite variants in red and blue (color online). It is found that the martensitic twins are formed in wires of larger widths. At smaller widths, the martensitic transformation is completely suppressed. The microstructure changes from twins at larger width to austenite at the smaller width. It can be noted that the martensitic transformation is completely suppressed below a critical width which in this particular case is around 92nm.

Figure 1: Microstructures of different width nanowires (length is 2000, volume fraction $x_{12} = 0$): (a) 200 nm (b) 95 nm (c) 90 nm (d) 80 nm.

Next, the tensile test (constant displacement) has been carried out on the nanowire of width 200 nm for the uncoupled case. Fig. 2 shows the stress-strain curve for low strain rate 0.5 %. Already this case shows that the thermo-mechanical properties of nanowires may differ substantially from the corresponding properties of the bulk. Furthermore, microstructures at the nanoscale can be highly heterogeneous. At the same time, it is expected that the structure of such a heterogeneity can be quite important for nanostructure properties due to the the fact that the interfacial energy at this scale is comparable with the bulk energy.

5 Conclusion

In this paper we demonstrated the existence of a critical dimension for finite length nanowires exhibiting shape memory effects. We gave a brief survey of phase trans-

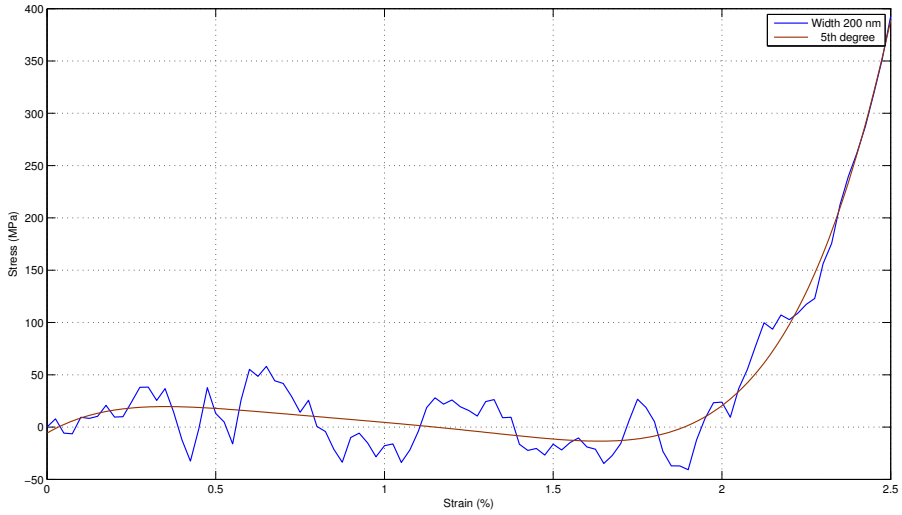

Figure 2: Stress-strain charcteristics of a nanowire with 2000nm width(for strain rate of 0.5 %).

formations, their classifications, and provided the basis of mathematical models for the phenomena involving such transformations, focusing on shape memory effects at the nanoscale. The results of modelling were discussed for the dynamic of square-to-rectangular transformations modelled on the basis of the modified Ginzburg-Landau theory. The results were obtained by solving a fully coupled system of partial differential equations, accounting for the thermal field. This new feature of our model extends recently reported phase-field-based models where thermal field coupling was neglected. Representative examples of modelling were given for nanowires of different widths demonstrating the importance of geometrical constraints in studying properties of nanowires.

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