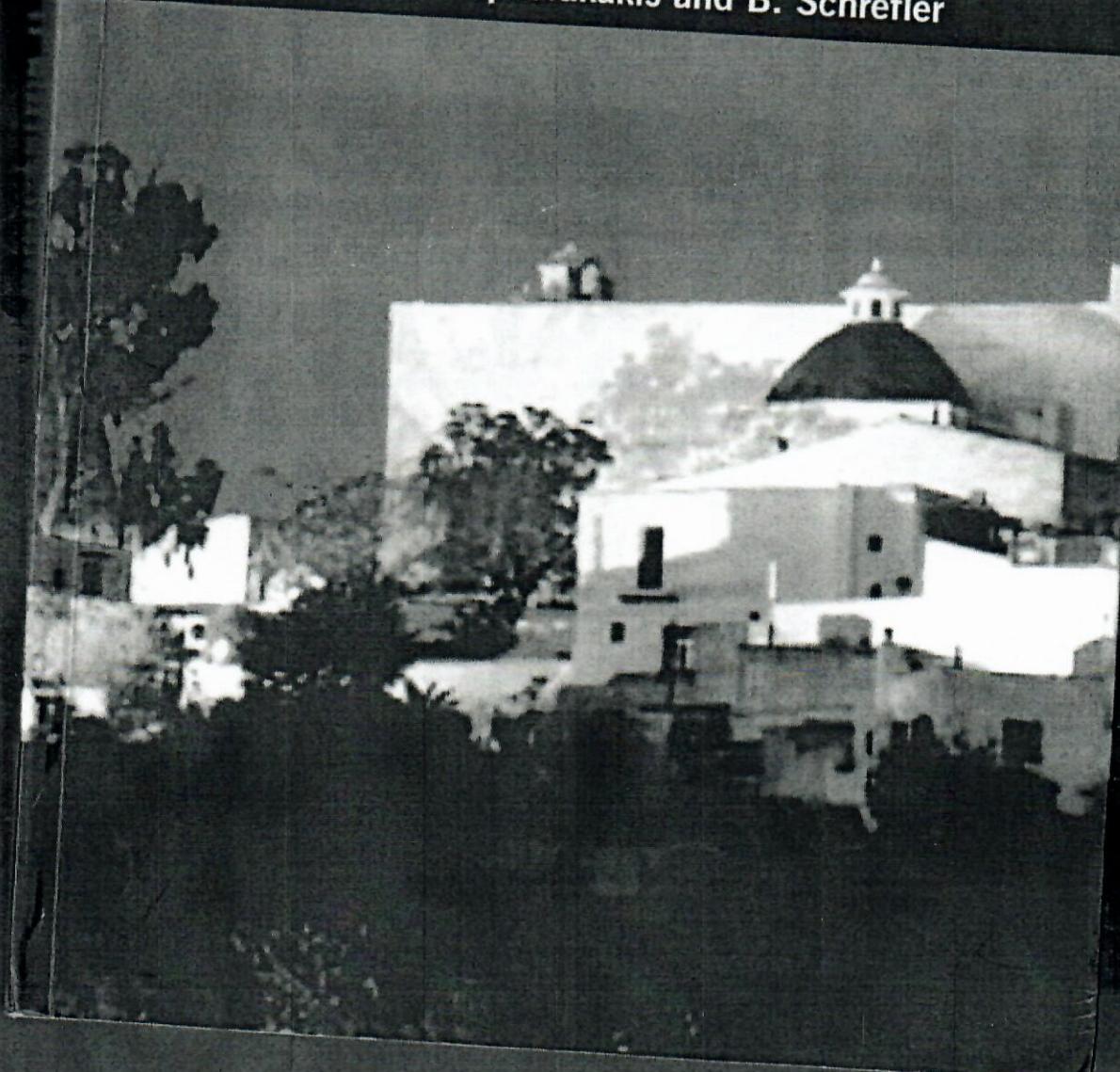


Computational Methods for Coupled Problems in Science and Engineering II

Edited by:

E. Oñate, M. Papadrakakis and B. Schrefler



Computational Methods for Coupled Problems in Science and Engineering II Coupled Problems 2007

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This is the second conference in the framework of the International Conference on Computational Methods in Engineering.

The increasing need for more accurate and reliable numerical methods accounting for all relevant physical phenomena requires the development of new numerical techniques. This conference will provide a new level of interaction between researchers and practitioners, which will lead to a deeper understanding of the problems and to significant improvements in the numerical methods.

The objective of this conference is to bring together leading experts in the state of the art in numerical methods and techniques for solving coupled problems in science and engineering. The conference will also provide a new level of interaction between researchers and practitioners, which will lead to a deeper understanding of the problems and to significant improvements in the numerical methods.

The conference is organized by the International Center for Numerical Methods in Engineering (CIMNE), the Universitat Politècnica de Catalunya (UPC), the National Research Council of Padova (Italy) and the International Association for Computational Mechanics (IACM). The conference is supported by the International Association for Computational Mechanics (IACM) and the International Society for Finite Elements in Engineering (ISFE).

Altogether over 100 papers have been presented, which reflect the latest developments in the field of computational mechanics and its applications in science and engineering.

This volume contains the proceedings of the conference. The editors would like to thank all the authors for their contributions and hope that the volume will be useful for the scientific community.

The editors would like to thank the organizing committee at the International Center for Numerical Methods in Engineering (CIMNE), the Universitat Politècnica de Catalunya (UPC), the National Research Council of Padova (Italy) and the International Association for Computational Mechanics (IACM) for their support and cooperation.

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E. Oñate, M. Papadrakakis and B. Schrefler (Eds.)

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NUMERICAL METHODS FOR COUPLED NONLINEAR PROBLEMS OF DYNAMIC THERMOELASTICITY AND SHAPE MEMORY ALLOYS MODELING

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Key words: Phase transformation, martensite, free energy, microstructure, finite element

Abstract. A crystallographic framework is employed and free energy density is derived for phase transformation in shape memory alloys. Resulting coupled nonlinear dynamic system in strong form and weak form are analyzed followed by numerical implementation and simulation of dynamic phase transformation in a thin film.

1 INTRODUCTION

Initiated by the analysis of thermal stresses due to a thermal shock at the boundary in early 1950s (the Danilovskaya problem), coupled dynamic thermoelasticity has been an important area of applications of tools and methods developed for coupled problems. While initially such application-driven problem relied mainly on linear models, over recent decades the class of nonlinear coupled dynamic problems of thermoelasticity has grown substantially. Some of the most intriguing examples of such problems are brought about by smart materials and structures technologies where materials like Shape Memory Alloys (SMAs) found numerous applications. In this contribution, we start from the general 3D model of dynamic nonlinear thermoelasticity, focusing on models for the dynamics of SMAs and associated phase transformations where nonlinear thermomechanical coupling is essential. First, we describe center-manifold based reduction procedures allowing to construct systematically new simplified models preserving essential features of the SMA dynamics. For some special cases, the reduction procedure can be carried out with the

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Proper Orthogonal Decomposition (POD) methodology and we demonstrate this on an example. In the remainder of this contribution, our main focus is on the development of a new model based on the Landau theory and on exploring its coupling with the microstructural compatibility under the macroscopic continuum deformation framework. Computational methodologies based on finite volume and finite element implementations of the developed models will be discussed with examples.

2 Ginzburg-Landau free energy model

We denote the order variables $\eta_k \in [0, 1]$, where $k = 1, \dots, N$ indicates the number of martensitic variants. $\eta_k = 0 \forall k$ defines the austenite phase (A phase) and $\eta_k = 1, \eta_j = 0, k \neq j$ defines the k th variant of martensite (M_k). According to the point group of crystallographic symmetry, only one type of martensite is allowed to exist at a material point, except when that material point is on the interface between two different phases (i.e., on a diffused interface or on a domain wall). By denoting the vector of the order variables as $\boldsymbol{\eta} = \{\eta_1, \dots, \eta_N\}^T$, the Gibbs free energy density is defined as $G(\boldsymbol{\sigma}, \theta, \boldsymbol{\eta})$. Here $\boldsymbol{\sigma}$ is the stress tensor, θ is the temperature. In addition to the existence of an energy well, a default property of the free energy density to be ensured by scaling and for convenience is that at $\theta = \theta_c$ (the equilibrium temperature of the reference phase or the parent phase), the free energy density under stress-free condition must vanish, that is, $G(0, \theta_c, \boldsymbol{\eta}) = 0$. The total (finite) strain is discontinuous across an interface between A phase and M_k phase (denoted as A- M_k interface) and also across an interface between two different variants of martensite phases (denoted as M_j - M_k interface). The finite strain tensor $\boldsymbol{\varepsilon}$ is decomposed into the elastic part and the transformation-induced part as

$$\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_{ei} + \sum_{k=1}^N \boldsymbol{\varepsilon}'_k \varphi(\eta_k) = -\frac{\partial G}{\partial \boldsymbol{\sigma}}, \quad (1)$$

where $\varphi(\eta_k)$ is a polynomial in η_k and $\boldsymbol{\varepsilon}'_k, k = 1, \dots, N$ are the transformation strain tensors [1] obtained using experiments. The structure of the initially unknown polynomial $\varphi(\eta_k)$ is such that it satisfies the following two conditions: $\varphi(0) = 0$, $\varphi(1) = 1$. The frame-invariance property of the free energy density is imposed by the polynomial structure in η_k such that interchanges between two indices produce identical structure of G . For a compatible microstructure that minimizes $G \in \mathcal{K}$, where \mathcal{K} is the sequence of energy wells, it follows from the Cauchy-Born hypothesis that the new lattice vector $\hat{\mathbf{e}}_k^m$ of the M_k phase can be obtained by proper rotation of lattice vector $\hat{\mathbf{e}}^0$ of A phase, that is,

$$\hat{\mathbf{e}}_k^m = \mathbf{F}^m \mathbf{U}_k^m \mathbf{F}^a \hat{\mathbf{e}}^0, \quad (2)$$

where \mathbf{F}^m and \mathbf{F}^a are the elastic deformation gradients in the M_k phase and the A phase, respectively, and \mathbf{U}_k^m is the stretch tensor (transformation matrix [1]) for A- M_k transformation. In the absence of stress, $\mathbf{F}^m = \mathbf{F}^a = \mathbf{R}$ is a rigid rotation. Therefore, in

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$$\varepsilon = \varepsilon_k^t = \frac{1}{2}(\mathbf{U}_k^{m^T} \mathbf{U}^m - \mathbf{1}), \quad \varphi(\eta_k = 1) = 1, \quad \eta_j = 0, \forall j \neq k. \quad (3)$$

Equation (3) describes the stable M_k phase and gives additional properties regarding the polynomial $\varphi(\eta_k)$. Material symmetry under proper rotation of the lattice vector is preserved due to the decomposition in Eq. (1). The Gibbs free energy density then takes the following form.

$$G(\eta) = -\frac{1}{2}\sigma : \left[\lambda_0 + \sum_{k=1}^N (\lambda_k - \lambda_0)\varphi(\eta_k) \right] : \sigma - \sigma : \sum_{k=1}^N \varepsilon_k^t \varphi(\eta_k) - \sigma : \left[\varepsilon_{\theta 0} + \sum_{k=1}^N (\varepsilon_k^\theta - \varepsilon_0^\theta)\varphi(\eta_k) \right] + \sum_{k=1}^N f(\theta, \eta_k) + \sum_{i=1}^{N-1} \sum_{j=i+1}^N F_{ij}(\eta_i, \eta_j), \quad (4)$$

where λ_k is the second-order forth-rank compliance tensor for the kth martensitic variant (M_k phase), λ_0 is for austenite phase (A phase), $\varepsilon_0^\theta = \alpha_0(\theta - \theta_e)$, $\varepsilon_k^\theta = \alpha_k(\theta - \theta_e)$, θ_e is the temperature at which the stress-free martensite losses stability. α_0 and α_k are the thermal expansion tensors for A and M_k phases, respectively. $f(\theta, \eta_k)$ is the chemical part of the free energy of the M_k phases and assumed in the form of a polynomial which is to be determined. F_{ij} is an interaction potential required to preserve the frame-invariance of G with respect to the point group of symmetry and uniqueness of the multivariant phase transformation at a given material point. The description of the order variables can now be generalized with three sets of order parameters: $\bar{0} = \{0, \eta_k = 0, 0\}$ for A phase, $\bar{1} = \{0, \eta_k = 1, 0\}$ for M_k phase and $\bar{\eta}_k = \{0, \eta_k, 0\}$, $\eta_k \in (0, 1)$ for diffused A - M_k interface. The role of the first-order kinetics in the order variables is to assist in reaching the bottom of the energy well, i.e.,

$$\frac{\partial G}{\partial \eta_k} = 0, \quad \eta = \bar{0}, \bar{1}, \quad (5)$$

$$\frac{\partial^2 G}{\partial \eta_k^2} \leq 0, \quad \eta = \bar{0} \quad (A \rightarrow M_k), \quad \frac{\partial^2 G}{\partial \eta_k^2} \leq 0, \quad \eta = \bar{1} \quad (M_k \rightarrow A). \quad (6)$$

The transformation energy associated with A \leftrightarrow M_k transformation is

$$G(\sigma, \theta, \bar{0}) - G(\sigma, \theta, \bar{1}) = \sigma : \varepsilon_k^t - \Delta G^\theta, \quad (7)$$

where ΔG^θ is the jump in the free energy due to phase transformation. With the help of Eqs. (2)-(7), we determine $\varphi(\eta_k)$ and $f(\theta, \eta_k)$ (see [2] for the details). According to Landau theory, a quadratic polynomial in strain components can be adequate to describe the free energy.

3 Variational framework and finite element discretization

We relate the elastic part of displacements to the elastic strain $\boldsymbol{\varepsilon}_{el}$ via the linear strain-displacement relation, that is, $\boldsymbol{\varepsilon}_{el} = ((\nabla \mathbf{u}) + (\nabla \mathbf{u})^T)/2$. With this assumption of strain and Eq. (1), it is now obvious that the order variables $\eta_k, k = 1, \dots, N$, are to be treated as internal variables in the variational formulation. We want to interpolate the fields $\mathbf{u}(x, y, z, t)$, $\theta(x, y, z, t)$ and $\eta_k(x, y, z, t)$ over the domain $\Omega(x, y, z) \subset R^3$ with Lipschitz continuous boundary $\partial\Omega$, using fixed-order finite elements with h -refinement. We consider the Lagrangian isoparametric interpolation function \mathbf{N}_e , $\{u_1, u_2, u_3\}^T = \mathbf{N}_e \mathbf{v}^e$, $\theta = \mathbf{N}_e \theta^e$, $\eta = \mathbf{N}_e \eta^e$, $\mathbf{v} = \{u_1, u_2, u_3, \theta, \eta_1, \dots, \eta_N\}^T$. Here, the superscript e indicates element nodal quantities. By introducing admissible weights $\{\bar{u}_i, \bar{\theta}, \bar{\eta}_k\}$ chosen from the linear span of \mathbf{v}^e , the variational formulation of the problem can be stated as follows

$$\delta\Pi = \delta\Pi_{PT} + \delta\Pi_\theta + \delta\Pi_u + \delta W = 0, \quad t \in [0, +\infty] \quad (8)$$

where Π_{PT} is the phase transformation energy, Π_θ is the thermal energy, Π_u is the strain energy and W is the external work done over the sample. By integrating Eq. (8) by parts, we obtain the finite element approximation

$$\mathbf{M} \frac{\partial^2 \mathbf{v}}{\partial t^2} + \mathbf{D} \frac{\partial \mathbf{v}}{\partial t} + \mathbf{K} \mathbf{v} = \mathbf{f}, \quad (9)$$

with initial state of microstructure: $\mathbf{v}(t) = \mathbf{v}(0)$, $\frac{\partial}{\partial t} \mathbf{v}(t) = \mathbf{0}$.

4 Deformation, phase kinetics and multiple scales

A smoothed version of the transformation conditions in Eqs. (5)-(6) leads to the time-dependent Ginzburg-Landau phase kinetics, where the fast time scale needs to be controlled depending on the global time stepping (in slow time scale) in the finite element time integration. Choice of the length-scale for defining η_k is arrived at by applying a finite-difference scheme to the phase kinetic equation.

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This book contains the Abstracts of the papers presented at the Second International Conference on Computational Methods for Coupled Problems in Science and Engineering (COUPLED PROBLEMS 2007) held in Santa Eulalia, Ibiza, Spain from May 21-23, 2007.

The objective of the conference was to present and discuss state of the art mathematical models, numerical methods and computational techniques for solving accurately and with affordable computing times

coupled problems of multidisciplinary character in science and engineering. Emphasis was given to showing the potential of new computational methods for solving practical problems of industrial interest.

The papers included in the book provide an overview of the formulation and computational solutions of real life problems with a multidisciplinary vision, accounting for all the complex couplings involved in their physical description.

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