Analysis of Thermoelasticity and First-orderKinetic Coupling in Phase Transforming Solids

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Abstract

A general modeling framework has been developed to analyze the dynamics of multivariant phase transformation in three-dimensional samples of shape memory materials. In this paper we analyze the properties of the coupling between the microscopic phase kinetics due to crystal transformation and the nonlinearity in the continuum thermoelasticity. The model is based on a systematic representation of the Gibbs free energy in stress, temperature and n-dimensional order parameter space. Here n indicates the number of martensitic variants (M). Landau theory has earlier been successfully applied to solve the problem of phase-field evolution in phase transforming solids (see e.g. the works by Artemev et al. [1] and Ichitsubo et al. [2] and the references therein). In the context of diffusion-less transformation in solid described by the Landau theory of first-order kinetics, the order parameters are the scaled ensemble average of the atomic order variables [3]. The diffusion kinetics based on the time-dependent Ginzburg–Landau equation is thus the homogenized form of the spatio-temporal fluctuation due to atomic reordering. Our main objective in this paper is to analyze theorectically as well computationally, how this diffusion kinetics influences the stress-temperature induced dynamics of phase

transformation in microscopic and larger length-scale without attempting to solve a molecular dynamic problem in a coupled manner. Toward this direction we finally arrive at the thermodynamic conservation law whose characteristics is controlled by the phase kinetics. As a starting point we first address the problem of $3D$ free energy representation in context of n-variant martensitic transformation. Our free energy model [4] follows the steps similar to those obtained in the works of Levitas and Preston [5, 6] to arrive at the invariance and uniqueness properties of the free energy. Also the number of order parameters can be reduced with the help of the symmetry properties across the transformation surfaces. In addition to this we relax some of the conditions involving many unknown material constants, which finally leads to a precise description of austenite-martensite transformation energy barrier and variant-variant interaction energy. In our approach the previously observed non-physical minima of the free energy wells are eliminated. We perform detailed analysis of the proposed free energy model in context of austenite-martensite $(A - Mk)$ transformation and variant-variant $(M_i - M_j)$ transformation with sharp interfaces. A link between the evolution of texture using this approach and the classical condition for microstructural compatibility within the framework of continuum deformation theory [7] is discussed. Analytical characterization is then carried out on the existence of diffused interfaces under quasi-static stress-temperature conditions by considering time-independent Ginzburg–Launday equation. Results are compared with those reported by Levitas et al. [8] in context of critical nuclei formation in $NiAl$. Next we turn our attention to the interplay between the diffused states of the variants and the nonlinear thermoelasticity. Relationship between the physical time scale of the atomic reordering process and the time scale at which the hyperbolicity of the thermodynamic conservation is influenced and completely switched to elliptic problem is analyzed. Numerical simulations on the evolution of microstructure are reported.

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