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Phase field approach with anisotropic interface energy and interface stresses: Large strain formulation

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ABSTRACT

A thermodynamically consistent, large-strain, multi-phase field approach (with consequent interface stresses) is generalized for the case with anisotropic interface (gradient) energy (e.g. an energy density that depends both on the magnitude and direction of the gradients in the phase fields). Such a generalization, if done in the "usual" manner, yields a theory that can be shown to be manifestly unphysical. These theories consider the gradient energy as anisotropic in the *deformed* configuration, and, due to this supposition, several fundamental contradictions arise. First, the Cauchy stress tensor is non-symmetric and, consequently, violates the moment of momentum principle, in essence the Herring (thermodynamic) torque is imparting an unphysical angular momentum to the system. In addition, this non-symmetric stress implies a violation of the principle of material objectivity. These problems in the formulation can be resolved by insisting that the gradient energy is an isotropic function of the gradient of the order parameters in the *deformed* configuration, but depends on the direction of the gradient of the order parameters (is anisotropic) in the *undeformed* configuration. We find that for a propagating nonequilibrium interface, the structural part of the interfacial Cauchy stress is symmetric and reduces to a biaxial tension with the magnitude equal to the temperature- and orientation-dependent interface energy. Ginzburg–Landau equations for the evolution of the order parameters and temperature evolution equation, as well as the boundary conditions for the order parameters are derived. Small strain simplifications are presented. Remarkably, this anisotropy yields a *first order* correction in the Ginzburg–Landau equation for small strains, which has been neglected in prior works. The next strain-related term is third order. For concreteness, specific orientation dependencies of the gradient energy coefficients are examined, using published molecular dynamics studies of cubic crystals. In order to consider a fully specified system, a typical sixth order polynomial phase field model is considered. Analytical solutions for the propagating interface and critical nucleus are found, accounting for the influence of the anisotropic gradient energy and elucidating the distribution of components of interface stresses. The orientation-dependence of the nonequilibrium interface energy is first suitably defined and explicitly determined analytically, and the associated width is also found. The developed formalism is applicable to melting/solidification and crystal-amorphous transformation and can be generalized for martensitic and diffusive phase transformations, twinning, fracture, and grain growth, for which interface energy depends on interface orientation of crystals from either side.

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1. Introduction

Phase field approach: Ginzburg–Landau, or phase field, approaches are routinely used to simulate various structural changes, including first-order solid–solid phase transformations (PTs) (Artemev et al., 2001; Chen, 2002; Finel et al., 2010; Jin et al., 2001a; Levitas et al., 2004; Levitas and Lee, 2007; Vedantam and Abeyaratne, 2005), melting (Anderson et al., 2001; Slutsker et al., 2006; Wheeler and McFadden, 1997), and also the evolution of multigrain structures (Kobayashi et al., 1998), as well as twinning (Clayton and Knap, 2011a,b; Hildebrand and Miehe, 2012; Levitas et al., 2009, 2013; Levitas and Roy, 2015). There are a number of books on the phase field approach (Provatas and Elder, 2010; Salje, 1991; Toledano and Dmitriev, 1996; Toledano and Toledano, 1998; Umantsev, 2012), but these, however, do not include any substantial treatment of mechanics. In phase field modeling, the central concept is the introduction of order parameters η_i that describe material instabilities during PTs in a continuous way. The energy density of the system depends on the strain tensor, temperature, the order parameters, and their gradients, which provides an energy penalty for the formation of interfaces. For a given strain and temperature, the energy density has as many minima in the order parameter space as there are accessible phases or structural states of system. The time evolution of the order parameters describes the evolution of a multi-connected microstructure. This evolution is obtained by the solution of the Ginzburg–Landau equations, which represent linear relationships between $\dot{\eta}_i$ and the generalized forces X_i thermodynamically conjugated to $\dot{\eta}_i$, and coupled to all equations derived through continuum thermomechanics. The phase field approach is computationally attractive because the interfaces between phases appear and evolve automatically as a result of the solution to the above-mentioned equations obviating the need to develop special methods for tracking them. The main theoretical advantage of the phase field approach, in comparison with sharp interface approach, is that it contains information about all intermediate states between phases and corresponding energy barriers, as well as including stationary heterogeneous intermediate states such as critical nuclei. Before examining phase field models in detail, however, we now explore the classical ideas that frame the analysis of interface motion in systems under stress.

Interface energy and generalized forces: Classically, a sharp interface between two phases has a total interface energy $\Gamma = \int \gamma \, dA$ or, for a homogeneous γ, $\Gamma = \gamma A$, where A is the interface area in the deformed state at a point in time and γ is the interface energy per unit area. For liquid–liquid and liquid–gas interfaces, γ is independent of the change in interface area and consequently interface strain. For interfaces that involve solid phases, γ may dependent on the change in interface area due to interface strain. For an anisotropic interface energy we write $\gamma = \gamma(\boldsymbol{k})$, where $\boldsymbol{k}$ is the unit normal to the interface. An interface is subjected to the following generalized forces related to three different processes of its evolution.

(a) Generalized forces preventing interface contraction called interface stresses (Gibbs, 1948), which represent the biaxial tension within interface (Fig. 1a). In the simplest case of small strain and isotropic stresses within interface, the magnitude $\bar{\sigma}^S$ of the interface stress is defined by the following equation:

$$\bar{\sigma}^S dA = d\Gamma = d(\gamma A) = (\gamma + A\partial\gamma/\partial A)\, dA \Rightarrow \bar{\sigma}^S = \gamma + A\partial\gamma/\partial A = \gamma + \partial\gamma/\partial\varepsilon_s = \bar{\sigma}_{st} + \bar{\sigma}_e^S, \tag{1}$$

where $d\varepsilon_s = dA/A$ is the increment of the interface strain and subscript st indicates the structural part of the interface stresses. This is the Shuttleworth equation (Shuttleworth, 1950), see also review by Fischer et al. (2008). The interface stress consists of two parts, one, $\bar{\sigma}_{st} = \gamma$, is the same as for a liquid–liquid interface, and another, $\bar{\sigma}_e^S$, is due to elastic deformation of an interface. The later can be anisotropic, i.e., tensorial, in more general case. Note that the expressions with a "bar" above them, such as $\bar{\sigma}^S$, have units of force per unit length, and the notation is used to distinguish these quantities from actual stresses (i.e., force per area), which can be singular at the interface in the sharp interface limit.

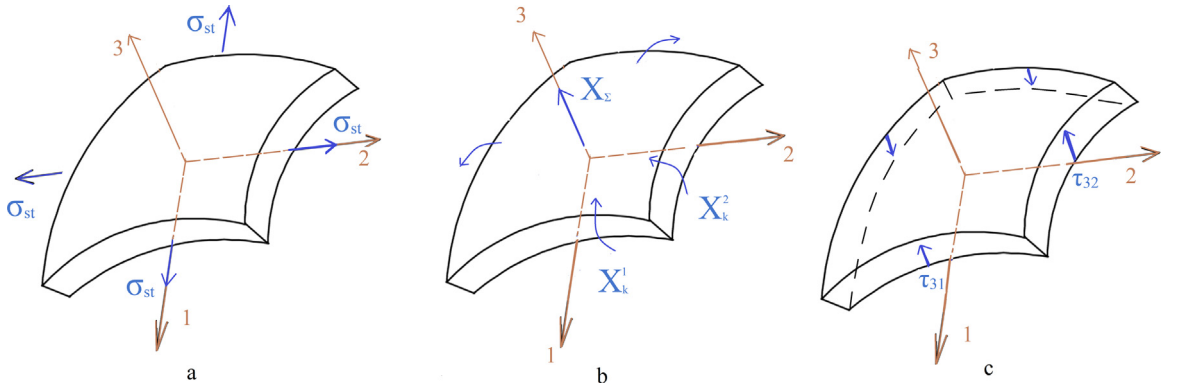

Fig. 1. A representation of the generalized forces acting at an interface. (a) Interface stresses, which represent biaxial tension and contribute directly to mechanics, i.e., to the momentum equation; (b) the driving force for the translational interface propagation X_Σ (the Eshelby driving force, shown conditionally as a vector) and for the interface reorientation $\boldsymbol{X}_k$ (Herring torque). Both X_Σ and $\boldsymbol{X}_k$ are thermodynamic (configurational) forces, which do not contribute directly to the mechanics of the system, namely, momentum balance and the moment of momentum principle. (c) Artificial nonsymmetric interface shear stresses, which appear in the previous theories and are eliminated in the current paper. They produce torque, which violates the moment of momentum principle.