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A variational treatment of material configurations with application to interface motion and microstructural evolution

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ABSTRACT

We present a unified variational treatment of evolving configurations in crystalline solids with microstructure. The crux of our treatment lies in the introduction of a vector configurational field. This field lies in the material, or configurational, manifold, in contrast with the traditional displacement field, which we regard as lying in the spatial manifold. We identify two distinct cases which describe (a) problems in which the configurational field's evolution is localized to a mathematically sharp interface, and (b) those in which the configurational field's evolution can extend throughout the volume. The first case is suitable for describing incoherent phase interfaces in polycrystalline solids, and the latter is useful for describing smooth changes in crystal structure and naturally incorporates coherent (diffuse) phase interfaces. These descriptions also lead to parameterizations of the free energies for the two cases, from which variational treatments can be developed and equilibrium conditions obtained. For sharp interfaces that are out-of-equilibrium, the second law of thermodynamics furnishes restrictions on the kinetic law for the interface velocity. The class of problems in which the material undergoes configurational changes between distinct, stable crystal structures are characterized by free energy density functions that are non-convex with respect to configurational strain. For physically meaningful solutions and mathematical well-posedness, it becomes necessary to incorporate interfacial energy. This we have done by introducing a configurational strain gradient dependence in the free energy density function following ideas laid out by Toupin (1962, Elastic materials with couple-stresses. Arch. Ration. Mech. Anal., 11, 385–414). The variational treatment leads to a system of partial differential equations governing the configuration that is coupled with the traditional equations of nonlinear elasticity. The coupled system of equations governs the configurational change in crystal structure, and elastic deformation driven by elastic, Eshelbian, and configurational stresses. Numerical examples are presented to demonstrate interface motion as well as evolving microstructures of crystal structures.

1. Introduction

We present a variational treatment of evolving configurations in solids. Of interest to us are problems in which a kinematic field can be identified, which describes the essential aspects of the material's configuration, while another distinct field, the displacement, furnishes the kinematics necessary for representing the nonlinear elastic response. Such a separation is possible upon a suitable definition of configurations for the cases at hand. A series of mathematical steps can then follow: The total free energy can then be

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written as a functional of both the configurational and the displacement fields. With it, we can seek equilibrium states that render the free energy stationary with respect to both fields. The corresponding Euler–Lagrange equations governing the configurational and displacement fields can be solved. The motivation from physics comes of asking whether a solid under load can seek to reach equilibrium by varying some configurational degree of freedom that can be identified as being distinct from the displacement field.

The somewhat abstract arguments laid out above have relevance to crystalline solids that undergo phase transformations coupled with elastic deformation: In a classical continuum setting, the elastic deformation is obtained from the displacement, which is the only kinematic field. No phenomena are sought to be modeled, other than the mapping of the reference to current placements. In this setting, the reference and material placements coincide, and most importantly, they are fixed. In contrast stands any phenomenon in which, the material configuration evolves from a *reference material configuration*, and can be represented, on a physical basis, by a configurational field that is distinct from the displacement field. Here, we are concerned with two specific examples: (a) In a multi-phase solid where phase change occurs at interphase interfaces, the configurational field would represent interface migration. The phase, and therefore the crystal structure at a material point will change if the interface migrates through that point. This causes a change in the material configuration of the point. Since the crystal structure (material configuration) changes across the mathematically sharp interface, the latter is incoherent. (b) Alternately, in a multi-phase solid, the crystal structure may change smoothly from one phase to another over an interface that has finite width, rather than being mathematically sharp. In this case also, the material configuration evolves with the crystal structure. Clearly, this would be a case of coherent interphase interfaces. Here too, the configurational field would represent the crystal structure at any point in the solid as a map from some well-defined, reference material configuration.

In each of cases a and b, with the evolved material configuration determined as above, the displacement field can be defined as the point-to-point map from this configuration to the current/deformed placement that lies in the spatial manifold. An elastic deformation can then be identified from this displacement field.

With two distinct kinematic fields thus identified, the response of the solid can be described by parameterizing the free energy functional in terms of these two fields. The imposition of equilibrium as the conditions of stationarity under variations on the configurational and displacement fields reveals two sets of Euler–Lagrange equations. As expected, one set contains the standard partial differential equations of elasticity. The second set is novel, and consists of partial differential equations and accompanying boundary conditions that involve the conventional elastic stress, the Eshelby stress, as well as a distinct configurational stress.

The treatment of a configurational force, distinct from standard, Newtonian, forces acting on imperfections in a crystal lattice was given by Eshelby (1951), building off work from the late nineteenth century (Burton, 1892; Larmor, 1897). The last two decades have seen a resurgence in the literature on configurational forces. Some of the theoretical underpinnings can be found in Gurtin (2000), Maugin (1995), Kienzler and Herrmann (1997), Steinmann (2002), Maugin (2011) and Vu and Steinmann (2012). Applications have also been developed, such as to finite element discretization (Mueller and Maugin, 2002), to the dynamics of defects (Acharya and Fressengeas, 2012), to spatial and material covariant balance laws (Yavari et al., 2006) for modeling elastic inclusions (Yavari and Goriely, 2013), and to fracture mechanics (Denzer and Menzel, 2014). Configurational force equations can be derived in the setting of classical balance laws, or, with appropriate assumptions, within a variational framework. Gurtin (2000) regards configurational forces as fundamental quantities in continuum physics, analogous to standard forces. On that premise, he regards configurational balance laws as the corresponding, fundamental laws that must exist in order to govern these forces. This has led to a debate on whether new physics is posited by the introduction of configurational forces (Maugin, 2011; Podio-Guidugli, 2002). The work we present here lies within a variational setting, and circumvents this debate by relying on the (perhaps) more accepted notion of equilibrium to arrive at balance laws as Euler–Lagrange equations of free energy functionals. The resulting partial differential equation for configurational equilibrium also arises in Gurtin (2000), and in Maugin (2011), where it has been called the fully material equilibrium equation.

We consider first the problem of configurational changes taking place at a sharp, migrating interface between two solid material phases. We show that the variational method produces a partial differential equation of configurational equilibrium in addition to the standard partial differential equation of elasticity. Assuming satisfaction of quasi-static elastic equilibrium, the partial differential equation for configurational equilibrium is identically satisfied everywhere except on the interface itself. There, it takes the form of a jump condition, which also vanishes if equilibrium is satisfied at the interface. However, it is of interest to consider solids that are far from equilibrium, and therefore have migrating interfaces. Then, the second law of thermodynamics provides guidance for choosing a sufficient form for the interface velocity. We adopt the well-known and widely used level set method (Osher and Sethian, 1988) to track the interface's motion based on this velocity. Here, we list just a few of a vast number of level set applications: Barth and Sethian (1998) modeled an isotropic etching process with a constant velocity and a directional etching process with a velocity dependent on the interface orientation. Macklin and Lowengrub (2006) modeled tumor growth with a curvature dependent velocity. The velocity in oxidation problems modeled by Rao et al. (2000), Rao and Hughes (2000), Garikipati and Rao (2001) is based on material composition. Finally, we note that Kalpakides and Arvanitakis (2009) used a velocity based on configurational forces to model ferroelastic materials, although it is arrived at differently than in the present work.

We next turn to the problem of smoothly varying configurational changes in crystal structure that occur over interfaces of finite width. The smoothness implies that the configurational change extends over finite sub-volumes and transforms the crystal structure from the parent to the daughter phases. Therefore, it is in contrast to the case of phase transformation only at a migrating sharp interface. The configurational change of the crystal structure over the volume suggests that there is a contribution to the free energy density function, which is associated with this configurational field. The variational treatment based on stationarity of the free energy functional leads to a partial differential equation for configurational balance that holds throughout the volume of the crystalline solid. There is therefore a fundamental difference in the form of the governing equations from that for phase changes that occur only