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Kinetics of phase transformations in the peridynamic formulation of continuum mechanics

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Abstract

We study the kinetics of phase transformations in solids using the peridynamic formulation of continuum mechanics. The peridynamic theory is a nonlocal formulation that does not involve spatial derivatives, and is a powerful tool to study defects such as cracks and interfaces.

We apply the peridynamic formulation to the motion of phase boundaries in one dimension. We show that unlike the classical continuum theory, the peridynamic formulation does not require any extraneous constitutive laws such as the kinetic relation (the relation between the velocity of the interface and the thermodynamic driving force acting across it) or the nucleation criterion (the criterion that determines whether a new phase arises from a single phase). Instead this information is obtained from inside the theory simply by specifying the inter-particle interaction. We derive a nucleation criterion by examining nucleation as a dynamic instability. We find the induced kinetic relation by analyzing the solutions of impact and release problems, and also directly by viewing phase boundaries as traveling waves.

We also study the interaction of a phase boundary with an elastic non-transforming inclusion in two dimensions. We find that phase boundaries remain essentially planar with little bowing. Further, we find a new mechanism whereby acoustic waves ahead of the phase boundary nucleate new phase boundaries at the edges of the inclusion while the original phase boundary slows down or stops. Transformation proceeds as the freshly nucleated phase boundaries propagate leaving behind some untransformed martensite around the inclusion.

Keywords: Microstructures; Phase transformation; Shape-memory effect; Peridynamics; Stability and bifurcation

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1. Introduction

The shape-memory effect consists of the recovery of apparently plastic deformations of a specimen below a critical temperature, by heating the specimen above this critical temperature. A diffusionless solid-state or martensitic phase transformation is responsible for this effect. The apparently plastic deformation does not come about by lattice slip, but instead is caused by the motion of twin or phase boundaries. It is the kinetics of this motion that is studied here.

In classical continuum theory, these phase transforming materials have been modeled using an energy that has multiple minima, each minimum corresponding to a particular phase or variant of martensite. In a dynamic, or even quasistatic, setting, the usual constitutive information, strain energy density as a function of strain, is insufficient to determine a unique solution. For example, even simple Riemann problems with a single phase or twin boundary in the initial conditions allow a one-parameter family of solutions. Therefore, we require further material information to pick the physically correct solution. Abeyaratne and Knowles (1990, 1991b) have proposed that this extra information may be specified in the form of a nucleation criterion and a kinetic relation.

The nucleation criterion determines whether a new phase will nucleate from a single phase. The kinetic relation determines the kinetics or the rules that govern the evolution of the phase boundary. It relates the velocity to a thermodynamic driving force, these being conjugate variables in the dissipation (or entropy) inequality. The driving force is related to Eshelby's idea of the force acting on a defect (Eshelby, 1956, 1975). The nucleation criterion and the kinetic relation provide uniqueness and well-posedness to initial-boundary value problems. Physically, they can be thought of as a macroscopic remnant of the lattice level atomic motion from one energy well to another that is lost in the continuum theory. However, a systematic derivation from a microscopic theory as well as experimental confirmation remain a topic of active research.

Another approach to overcome the inability of classical continuum mechanics to model the kinetics of phase transformations is to regularize or augment the theory, notably by adding a strain gradient (capillarity) and viscosity to the constitutive relation. This augmented theory leads to a unique solution for the motion of phase boundaries (Abeyaratne and Knowles, 1991a; Truskinovsky, 1993). Further, Abeyaratne and Knowles (1991a) have shown a correspondence between such methods and the kinetic relation. However, nucleation is incompletely explored in this theory, and computational evidence suggests that it is in fact quite difficult. Further, this theory leads to fourth-order equations which are difficult to deal with computationally: they are stiff and one needs smooth elements in the finite element method (see for example, Kloucek and Luskin, 1994; Dondl and Zimmer, 2004).

There is a closely related phase-field approach (see for example, Artemev et al., 2001; Wang et al., 1994) in the infinitesimal strain setting. Here, one uses the transformation strain as an internal variable or order parameter, considers the free energy density as a function of this order parameter and uses linear elasticity to penalize the incompatibility in this internal variable field. This leads to a second-order equation which is computationally attractive. However, the equilibrium and the dynamics can be different from that of the regularized theories described earlier (Bhattacharya, 2003). The connection between this theory and kinetic relations remains unexplored (Killough, 1998 has some discussion on this question), nucleation remains difficult and most studies are quasistatic.