KINETICS OF PHASE BOUNDARIES IN THE PERIDYNAMIC FORMULATION OF CONTINUUM MECHANICS

KAUSHIK DAYAL* AND KAUSHIK BHATTACHARYA†

* Division of Engineering
California Institute of Technology,
Pasadena, California 91125, USA.
kaushik@ugcs.caltech.edu

† Division of Engineering
California Institute of Technology,
Pasadena, California 91125, USA.

The dynamics of phase boundaries is of great interest for the understanding of hysteresis in active materials. This is a challenging problem as the dynamics of defects including phase and twin boundaries in the classical theory requires material information in the form of a kinetic relation, beyond that present in the usual constitutive relation between stress and strain [1]. Further, computation is difficult as one needs to track these defects. Phase field type models get around this difficulty by involving strain gradient and viscosity, but these add to the computational complexity.

We report on an alternative approach using the peridynamic theory [2,3]. This is a nonlocal formulation of continuum mechanics that involves only the displacement field and not its spatial derivatives, such as strain and strain gradients. This makes it especially attractive to model defects such as phase boundaries and cracks. In a heuristic analogy with molecular dynamics, the peridynamic equation of motion at a point in a body is postulated to be [2]:

$$\rho \partial_{tt} \mathbf{u}(\mathbf{x}, t) = \int_\Omega \mathbf{f}(\mathbf{u}(\mathbf{x}', t) - \mathbf{u}(\mathbf{x}, t), \mathbf{x}' - \mathbf{x}) dV_{\mathbf{x}'} \tag{1}$$

where $\mathbf{x}$ is the reference configuration coordinates, $\mathbf{u}(\mathbf{x}, t)$ is the displacement field, $\mathbf{f}(\delta\mathbf{u}, \delta\mathbf{x})$ is the force between two volume elements with separation in the reference $\delta\mathbf{x} := \mathbf{x}' - \mathbf{x}$ and relative displacement $\delta\mathbf{u} := \mathbf{u}(\mathbf{x}', t) - \mathbf{u}(\mathbf{x}, t)$, and ρ is the density in the reference. As this equation does not involve derivatives of the displacement field, it can be applied at any point in the body, without any requirements on the smoothness of the deformation, and all material information is carried by the function $\mathbf{f}(\delta\mathbf{u}, \delta\mathbf{x})$.

We specify an inter-particle interaction relation appropriate for a phase transforming material, and show that one does not need the extra nucleation criterion and kinetic relation in this theory. Instead, we show through the study of various boundary value problems that the nucleation and propagation of phase boundaries is completely specified from within the peridynamic theory.

We show that phase boundaries may be viewed as traveling waves in this theory, and their propagation induces a kinetic relation. We derive a nucleation criterion by examining the dynamic stability of a nominally single phase displacement field. The results of this analysis show good agreement with the boundary-value calculations. This provides an new perspective on nucleation as a dynamic instability and phase boundaries as traveling waves in microscopic theories.

We then exploit the computational efficiency of this method to attack a two dimensional problem of a phase boundary impinging on a defect. Our numerical simulation reveals an unusual mechanism that allows the phase boundary to bypass the defect without requiring large distortions. As the acoustic waves leading the phase boundary interact with the stress field of the defect, they nucleate a new phase boundary that then propagates, as the original phase boundary comes to rest.

References

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Keywords: peridynamics, phase transformation, kinetic relation