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Abstract

In the setting of continuum elasticity martensitic phase transformations are characterized by a non-convex free energy density function that possesses multiple wells in strain space and includes higher-order gradient terms for regularization. Metastable martensitic microstructures, defined as solutions that are local minimizers of the total free energy, are of interest and are obtained as steady state solutions to the resulting transient formulation of Toupin's gradient elasticity at finite strain. This type of problem poses several numerical challenges including stiffness, the need for fine discretization to resolve microstructures, and following solution branches. Accurate time-integration schemes are essential to obtain meaningful solutions at reasonable computational cost. In this work we introduce two classes of unconditionally stable second-order time-integration schemes for gradient elasticity, each having relative advantages over the other. Numerical examples are shown highlighting these features.

1 Introduction

Many multi-component materials undergo martensitic phase transformations. Among others, we are interested in transformations from cubic to tetragonal phases observed, e.g., in low-carbon steels [17] and in ferroelectric ceramics $BaTiO_3$ [2], that result in twin formations between martensitic variants. Twinning is a consequence of energy minimization, and is characterized by non-convex free energy density functions that possess three *wells* in strain space corresponding to the three energetically favored tetragonal variants and one local maximum corresponding to the energetically unfavored cubic variant; see Barsch and Krumhansl [6]. The boundary value problems (BVPs) derived for such non-convex density functions give rise to arbitrarily fine phase mixtures, which is a non-physical aspect of the mathematical formulation and results in pathological mesh dependencies in numerical solutions. This is resolved by including the higher-order gradient terms in the energy density functions that represent interface energy, and the resulting BVPs turn into instances of Toupin's theory of gradient elasticity at finite strain [20, 6]. Stable/metastable solutions to these BVPs can provide insight into many physical properties of the materials, such as habit plane normals, volume fractions of martensitic variants, and other homogenized behaviors. While solutions of one-dimensional problems and some restricted linearized two-dimensional problems may be obtained analytically, the complete, nonlinear, finite-strain problems in three dimensions must be treated numerically.

Related problems have been solved numerically in one dimension [22, 23] and in two dimensions for an anti-plane shear model [13], where the solutions to the BVPs were obtained by local and global bifurcation analysis, and metastability of each solution was assessed by evaluating the second variation of the total free energy. In three dimensions the authors reported the first results in [16]; there, similar procedure was adopted, but, due to the quite general boundary conditions, the local bifurcation analysis was not feasible, and solutions were obtained from random initial guesses. In Ref. [16] only coarse microstructures were obtained, and we found it formidable in general three-dimensional problems to have the nonlinear solvers converge to solutions representing microstructures that are fine enough to have practical significance. A possible strategy to overcome this difficulty is *dynamic relaxation*; we recast the original problem of finding metastable solutions of our BVPs as finding steady state solutions of *initial* boundary value problems (IBVPs), adding artificial damping and, possibly, artificial inertia. Crucial to this approach is the use of accurate time-integration schemes that guarantee total energy dissipation. This condition furnishes a notion of stability, *à priori*. In the context of martensitic transformation a dynamic relaxation technique was used by Dondl et al. [8] for a non-convex scalar variational problem in two dimensions, where a convex-splitting method, initially proposed for the Cahn-Hilliard equation [9, 10], was used for unconditional stability. Convex-splitting methods, however, are not feasible for complex non-convex functions such as those we consider here, as identification of convex and concave parts is not obvious.

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