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Asymptotic analysis of hierarchical martensitic microstructure

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ABSTRACT

We consider a hierarchical nested microstructure, which also contains a point of singularity (disclination) at the origin, observed in lead orthovanadate. We show how to exactly compute the energy cost and associated displacement field within linearized elasticity by enforcing geometric compatibility of strains across interfaces of the three-phase mixture of distortions (variants) in the microstructure. We prove that the mechanical deformation is purely elastic and discuss the behavior of the system close to the origin.

1. Introduction

Solid-to-solid phase transformations are often accompanied by the formation of unusual and intriguing mixtures of phases at the mesoscale spanning nanometers to microns in length scales (Khachaturyan, 1983). In the case of metallic alloys, below the transition temperature it is common to observe the coexistence of fine layers of martensitic or product twins (or "variants") with the parent austenite phase of higher symmetry. Martensitic transformations are displacive, are driven by shear strain and/or shuffles (intracell atomic displacements), and are invariably first-order in nature that leads to hysteresis and metastability (Bhattacharya, 2003). The rich microstructure seen in high resolution electron microscopy (HREM) is often a manifestation of this metastability (Manolikas and Amelinckx, 1980; Kitano and Kifune, 1991). Various approaches have been utilized over the last several decades to model the emergence of microstructure in martensites. They are largely variational using a free energy potential, and either use finite deformation, sharp interfaces and iteratively minimize a free energy, or start with random initial conditions and evolve a free energy potential according to some dynamics (Porta and Lookman, 2013). The traditional phase field approach is often used in the limit of small strains, and methods based on Ginzburg–Landau theory can be applied for small strains as well as finite deformation.

The study of mixtures in the framework of a variational setting traces back to the work of Ball and James (1987). Their technique consists of matching different crystal phases, possibly at different scales, through geometric compatibility. In the literature, this idea has been widely applied in the analysis of periodic mixtures, the situation in which the physical and geometrical properties of these mixtures are repeated periodically in an elastic body.

Even though the case of periodic microstructure is of central importance in the modeling of composite materials, and it has become a classic subject of study, the situation related to more general microstructure, and specifically the case of self-similar fine hierarchies, remains to be fully explored. In fact, there are a number of fascinating open problems and questions, among which is the study of a large family of fine hierarchical structures observed in artificial polymers and biological

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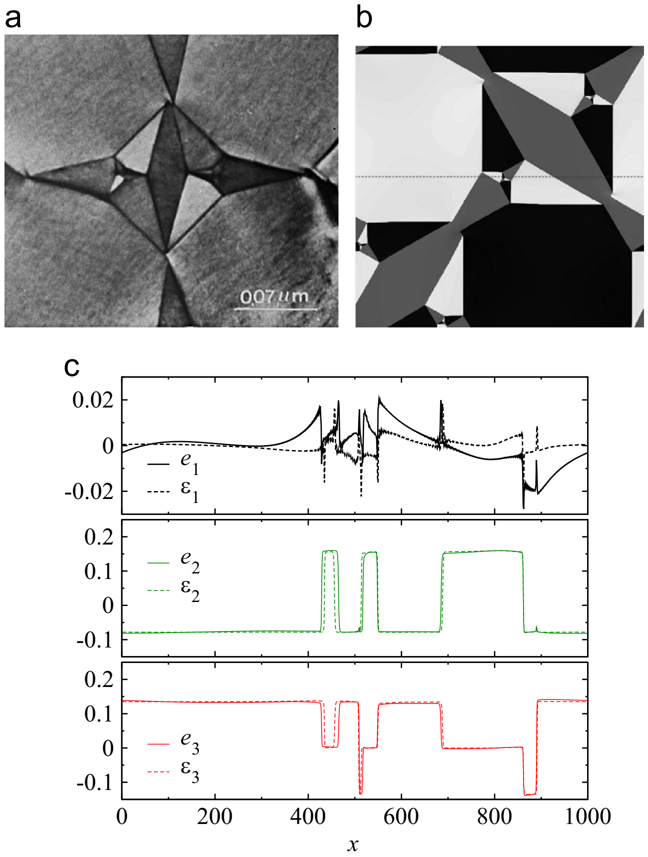

Fig. 1. (a) Experimental observation of the tripole-star microstructure in lead orthovanadate (Manolikas and Amelinckx, 1980). The two stars are modeled as rank-one three-phase martensitic mixtures, (b) numerical solution of the mechanical equilibrium equations corresponding to the non-linear elastic model defined in Eqs. (2.6) and (2.9) and (c) comparison between the strain fields obtained numerically in the approximation of linear elasticity (dotted lines) and with the full nonlinear model (solid lines) (see also Porta and Lookman, 2013). The graphic shows the strain profiles along a line which crosses the tripole-star microstructure (indicated with a dotted line in (b)). In both cases the choice of the parameters of the model yields $\epsilon \approx 0.156$.

materials (e.g., bones and leaves). Our emphasis will be on the family of heterogeneities in which there is an interaction of topological singularities that leads to fascinating (non-periodic) microstructure.

In this paper we focus on the class of hexagonal-to-orthorhombic transformations where three equivalent stretching directions of the parent austenite phase give rise to three orientations of the product martensite. Examples of compounds undergoing this transformation include the mineral Mg-cordierite, $Mg_2Al_4Si_5O_{18}$, and Mg–Cd alloys (Kitano and Kifune, 1991). Closely related materials include those undergoing a hexagonal-to-monoclinic transformation, such as lead orthovanadate, $Pb_3(VO_4)_2$, and samarium sesquioxide, Sm_2O_3 (Manolikas and Amelinckx, 1980). As the variants need to rotate to match at the domain walls, and the domain walls connecting the variants may intersect, these materials provide us with an excellent opportunity to study disclinations in crystals. Disclinations are formed when the nodes generated by the intersection of the domain walls do not close to an angle of 2π.

We will study the hexagonal-to-orthorhombic transformation in two dimensions (2D) for which the corresponding transformation is triangle-to-centered-rectangle. As the compounds consist of stacking or layering of tetrahedral units, the microstructure is essentially homogeneous perpendicular to the plane of the paper and therefore 2D is justified. One of the most intriguing microstructures observed in this transformation is the self-similarly nested tripole-star pattern (see Fig. 1(a)). These transformations have recently been the object of extensive numerical study. In Ref. Porta and Lookman (2013) the modeling is based on the minimization of a non-convex Ginzburg–Landau potential, both in the scenario of finite and infinitesimal elasticity. It can be observed that in this microstructure the deformation gradient is (nearly) piecewise constant, with three possible strain values that correspond to the three wells of the free energy density. As a first approximation, the sets where the deformation gradient is constant are particular *kyte*-shaped polygons. These polygons are all identical up to a rotation and a rescaling, close to the center of the star, and their measure tends to zero.

A thorough theory that treats microstructure and other phenomena, such as disclinations, dislocations, cavitations or cracks simultaneously, is to the best of our knowledge, still lacking. Such a theory would provide an important tool to study various classes of phenomena in materials science. Focusing on the case of linearized elasticity, the main result of this paper