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Multivariant model of martensitic microstructure in thin films

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Abstract

A novel multivariant model of martensite is developed through competing energetics to describe the coarsening, refinement and selection of the microstructure. In contrast with the conventional phase-field methods, a new set of field variables motivated by the hierarchical structure of multirank laminates is employed to represent each variant. As a result, the energy-well structure can be expressed explicitly in an elegant and unified fashion. The framework is applied to the investigation of pattern formation in martensitic thin films with trigonal symmetry. Various intriguing patterns are predicted and are found to be in good agreement with those observed in experiments. In addition, film orientations and patterns necessary to achieve large actuation strains are suggested for dome-shaped and tunnel-shaped microactuators. It is found that the resulting morphologies evolve with coherent interfaces under various loading conditions. This suggests that compatible walls provide a low-energy path during evolution, and the understanding of them leads to novel strategies of large strain actuation.
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Keywords: Martensite; Pattern formation; Thin films

1. Introduction

A martensitic material undergoes a first-order, diffusionless, solid-to-solid phase transformation during which there is a sudden change in the crystal structure at a certain temperature. Crystals going through a thermoelastic martensitic transformation often exhibit the shape-memory effect – a phenomenon where deformation suffered below a critical temperature can be recovered on heating. This property enables these alloys to be used for a variety of applications and makes them attractive candidates for smart materials, since they function as actuators as well as sensors [1–3]. Recently, several proposed designs for creating tiny machines have suggested that the characteristic microstructure patterns can be exploited as device elements [4]. This requires the design of devices that can take full advantage of the inherent microstructure to achieve this goal, which in turn raises many fundamental issues in martensitic materials.

Much work has addressed the formation and description of various aspects of microstructure in bulk crystals but, for a number of reasons, little attention was paid to thin films until recently. A typical film has a characteristic geometry where one dimension is much smaller than the other two with large surfaces. Consequently, a dimensional constraint appears as a new length scale comparable to that of microstructure. Moreover, martensitic crystals are highly anisotropic and nonlinear due to phase transformation. All of these facts have made it difficult to develop suitable theories to describe their behavior in slender structures. Bhattacharya and James [5] employed ideas similar to the notion of Γ-convergence to derive a theory of martensitic single crystal films, and Shu [6] extended it to polycrystalline films. They showed that the microstructure in thin films can be different from that in the bulk, and this enables a novel strategy that directly uses aspects of this microstructure for building new microactuators [7,8]. Bringing these ideas to practical applications requires a thorough understanding and characterization of the

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microstructure and its evolution under stress. This calls for an appropriate model that not only can capture the spirit of the Bhattacharya–James theory but also can serve as a useful tool for evaluating various conditions in the design process. The goal of this paper is to develop such a model and validate it. A strategy exploiting the microstructure and orientation of the film for performance optimization of microactuators is also recommended here.

The key feature of a martensitic phase transformation is the microstructure it generates. The high-temperature austenite phase is cubic, while the low-temperature martensite phase has less symmetry. This gives rise to symmetry-related variants that are identical crystal lattices of martensite with different orientations. The crystal is able to take a specific shape by making a fine-scaled mixture of different variants to accommodate the deformation. However, these variants cannot be arbitrarily mixed; instead, each interface separating different variants has a well-defined crystallographic orientation such that rows of atoms are unbroken across it. As a result, variants of martensite form highly intricate and very characteristic patterns at a length scale much smaller than the size of the sample. To explain these observed patterns, the crystallographic theory of martensite was proposed by Wechsler et al. [9], as well as by Bowles and MacKenzie [10], in the early 1950s. However, this theory is purely kinematic in origin and involves a priori the twinning mode, leading to difficulty in extending it to other circumstances. Ball and James [11] developed a theoretical approach to predict the fine microstructure based on the relaxation of a nonlinear energy function. Khachaturyan [12] and Roitburd [13], on the other hand, used a different theory based on linear elasticity and the Fourier technique for predicting the morphology of crystal microstructures. Both theories are based on energy minimization and can recover the results of the early crystallographic theory. The link between these two was established by Kohn [14], who showed that the latter is the geometrically linear analogue of the former. Bhattacharya and Kohn [15] and Shu and Bhattacharya [16] extended the Ball–James theory to the case of polycrystals.

As analytic solutions obtained from the above-mentioned theories are available only for some simplified problems, this article adopts another perspective by proposing a multivariant framework suitable for simulating patterns of microstructure under a variety of boundary conditions. This problem has been studied by Khachaturyan, Roytburd, Salje, Saxena, Lookman and their collaborators for martensites [17–24], and by Chen and his co-workers for ferroelectrics [25,26]. Other important contributions for microstructure simulation include the works [27–31]. All of them use the conventional time-dependent Ginzburg–Landau (TDGL) model, and choose a suitable set of order parameters and the special polynomial expansions of these parameters at high orders for a particular transformation. Instead, a new set of field variables is introduced to represent each variant here [32]. This approach is motivated by the hierarchical structure of multirank laminates constructed by Bhattacharya [33] for establishing the rule of mixtures. It provides the advantage of expressing the energy-well structure of martensitic variants in a unified fashion, irrespective of the different types of transformation under consideration. Besides, only two parameters are needed in the proposed framework. One is related to the energetic cost due to formation of the interface and the other is the cost due to the deviation from the ground state energy.The extensions of the present framework for simulating domain patterns in ferroelectrics and ferromagnetic shape-memory alloys are currently underway [34,35]. Moreover, this idea of employing laminated domain patterns has been applied to the investigation of ferroelectric switching by Shu et al. [36] and Yen et al. [37].

This article is organized as follows: It starts with the use of energetics to describe the coarsening, refinement and selection of microstructure of martensite in Section 2. This phenomenon has been observed in other physical systems, including self-organized nanoscale patterns in a binary epitaxial monolayer [38] and nanomesa and nanowell formation in a Langmuir–Blodgett ferroelectric polymeric film [39]. The framework is then applied to the investigation of pattern formation in martensitic thin films in Section 3. Ti–Ni in the R-phase state is chosen as the model material. The R-phase transformation is martensitic and thermoelastic, and is characterized by a rhombohedral distortion of the parent B2 structure [40]. While it yields a relatively small shape change, its temperature hysteresis vs. strain is an order of magnitude smaller than that of the monoclinic phase. Thus, it is suitable in transducer applications. Indeed, microactuators exploiting the R-phase transformation of Ti–Ni films have been developed recently with operation frequency around 100 Hz [41]. Various self-accommodation patterns are predicted from simulations. They are satisfied with the interface conditions of the Bhattacharya–James thin film theory [5], and some of them are found to be in good agreement with those observed in experiments. In the last part of Section 3, the model is applied to the design of large strain microactuators by targeting the optimal microstructures and film orientations. Conclusions are drawn in Section 4.

2. Framework and formulation

2.1. Transformation strain

Consider a single crystal of austenite and choose this as the reference configuration. The crystal occupies the region $\Omega \subset \mathbb{R}^3$ in its reference configuration. The displacement and linear strain of the crystal are described by the functions $\mathbf{u}$ and $\boldsymbol{\varepsilon}$. Both are related by

$$\boldsymbol{\varepsilon}[\mathbf{u}] = \frac{1}{2}\left\{\nabla\mathbf{u} + (\nabla\mathbf{u})^{\mathrm{T}}\right\} \tag{1}$$

The austenite has stress-free strain $\boldsymbol{\varepsilon}^{(0)} = \mathbf{0}$. As it is cooled, it transforms to martensite. In shape-memory alloys, the austenite lattice has cubic symmetry, while the martensite

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