Mesoscopic description of martensitic phase transformations mediated by dislocations using the Landau-Ginzburg theory

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ABSTRACT

Dislocations in crystals induce incompatibility between elastic strains. We show how this can be related to the densities of crystal dislocations in individual slip systems and how the incompatibility causes nonlocal coupling with elastic strains in the evolving microstructure. The order parameter and thus the corresponding stress fields develop long-range tails that correspond to the superposition of elastic stress fields of individual dislocations. Hence, the stress field of any distribution of dislocations in an arbitrarily anisotropic medium can be calculated just by minimizing the free energy. The corresponding continuous field of Peach-Koehler forces is then employed in a Fokker-Planck equation for the dynamics of the dislocation density. This approach represents a simple self-consistent scheme that yields the evolutions of both the order parameter field and the continuous dislocation density.

1 Introduction

A mesoscopic description (nano to micrometer) of physical processes in solids, where atomic length scales merge with those of the continuum, represents a crucial and perhaps most challenging aspect of understanding material behavior. This arises, for example, during displacive (martensitic) phase transformations where the distortions associated with the strains in unit cells and intra-unit cell displacements (or shuffles) propagate over larger distances so that competing long-range effects lead to the formation of inhomogeneities such as interfaces, spatially correlated domains and complex microstructure. The currently available mesoscopic models for studies of defects focus mainly on the self-organization of dislocations in spatially homogeneous microstructures. The statistical models based on the Fokker-Planck equation have been pioneered by Bakó and Groma [1] and Zaiser [2]. A closer connection with the well-established Kröner's continuum theory of dislocations [3] was developed by El-Azab [4] and the formation of sharp dislocation walls in isotropic media was observed by Limkumnerd and Sethna [5]. Phase field models of dislocation patterning are usually based on the theory of Khachaturyan [6] where the dislocation loops are viewed as coherent platelet inclusions.

Our objective in this paper is to incorporate dislocations into the Landau theory to study martensitic phase transformations in materials containing defects. We consider an anisotropic medium that is described by the elastic constants corresponding to the high-temperature cubic phase. Utilizing Kröner's continuum theory of dislocations [3], we develop a self-consistent scheme that allows simultaneous calculation of the microstructure and the evolution of the dislocation density.

2 Free energy for materials with dislocations

In the following we will consider a square to rectangle phase transformation, where the square corresponds to the austenite phase stable above T_c and the two variants of the rectangle to the martensite that is stable below T_c. We identify three order parameters e_1, e_2 and e_3 that correspond to the three modes of in-plane deformation of the reference square lattice. In particular, $e_1 = (\varepsilon_{11} + \varepsilon_{22})/\sqrt{2}$ measures isotropic dilation, $e_2 = (\varepsilon_{11} - \varepsilon_{22})/\sqrt{2}$ the change of shape and $e_3 = \varepsilon_{12}$ the change of right angles caused by the shear. For the square to rectangle transformation, e_2 is the primary order parameter and e_1, e_3 are secondary order parameters.

The nonzero plastic strains induced by the dislocations cause discontinuities in the displacement field and these are removed by elastic relaxation. The elastic components of the strain tensor are then incompatible with each other and are constrained by $\nabla\times\nabla\times\boldsymbol{\varepsilon} = \boldsymbol{\eta}$, where $\boldsymbol{\eta}$ is the so-called incompatibility tensor. In the two-dimensional case, the only scalar equation that is not satisfied identically reads $\partial_{22}\varepsilon_{11} - 2\partial_{12}\varepsilon_{12} + \partial_{11}\varepsilon_{22} = \eta_{33}$, where $\partial_{ij} \equiv \partial^2/\partial x_i \partial x_j$. Writing the strains in terms of the order parameter fields then yields the incompatibility constraint for the order parameters:

$$\nabla^2 e_1 - (\partial_{11} - \partial_{22})e_2 - \sqrt{8}\partial_{12}e_3 = \eta_{33}\sqrt{2} \quad . \tag{1}$$

The Landau free energy for the martensitic phase transformations is typically constructed using the harmonic term that follows from the elastic strain energy (terms with e_1^2, e_2^2, e_3^2) augmented by even higher-order terms of e_2 that are allowed by symmetry, and by a gradient term proportional to $|\nabla e_2|^2$ which accounts for the energy cost for spatial variation of the order parameter [7]. Writing (1) as $G = 0$ we include the incompatibility constraint using the Lagrange multiplier λ as

$$F = \int_S \Big[\underbrace{\frac{A_2}{2}e_2^2 + \frac{B}{4}e_2^4 + \frac{C}{6}e_2^6}_{f_{loc}} + \underbrace{\frac{A_1}{2}e_1^2 + \frac{A_3}{2}e_3^2}_{f_{nonloc}} + \underbrace{\frac{K_2}{2}|\nabla e_2|^2}_{f_{grad}} + \lambda G \Big] \mathrm{d}\mathbf{r} \quad . \tag{2}$$

The problem is to calculate the primary order parameter e_2 and the incompatibility field η_{33} (i.e. the dislocation density) that minimize the free energy (2). Firstly, we look for the minimum of F with respect to the secondary order parameters e_1, e_3 and the Lagrange multiplier λ. The stationarity conditions $\delta F/\delta e_1 = \delta F/\delta e_3 = \delta F/\delta\lambda = 0$ yield e_1 and e_3 as functionals of e_2 and η_{33}. By substituting these back into (2) the free energy only depends on e_2 and η_{33}.

In the Kröner's continuum theory of dislocations [3], the incompatibility tensor is defined as $\boldsymbol{\eta} = \mathrm{sym}\,(\nabla\times\boldsymbol{\alpha})$, where $\boldsymbol{\alpha}$ is the Nye tensor with components $\alpha_{ij} = B_j/S_i$. Here, $\mathbf{B}$ is the so-called net Burgers vector that is obtained as a vector sum of the Burgers vectors of all crystal dislocations that comprise the mesoscopic cell perpendicular to x_i with area S_i. In our two-dimensional case,

$$\eta_{33} = \alpha_{32,1} - \alpha_{31,2} \tag{3}$$

and, therefore, only edge dislocations with their line directions parallel to x_3 and the Burgers vector components along x_1 and x_2 contribute to this incompatibility. Although the incompatibility (3) is completely determined by the distribution of the net Burgers vectors $\mathbf{B}$, a connection still needs to be made between $\mathbf{B}$ and the density of crystal dislocations that populate individual slip systems. Due to the mesoscopic nature of this model, we cannot invoke individual crystal dislocations but will merely consider their densities in each slip system. This is accomplished by writing

$$\alpha_{3i} = B_i/S_{cell} = \sum_s (n^{s+} - n^{s-})b_i^s \quad , \tag{4}$$

where S_{cell} is the area of one mesoscopic cell, the sum is over all the slip systems s, and n^{s+} and n^{s-} are non-negative densities of crystal dislocations with the Burgers vectors $\mathbf{b}^s$ and $-\mathbf{b}^s$, respectively. Substituting (4) into (3) yields the sought after connection between the densities of crystal dislocations and the mesoscopic incompatibility field:

$$\eta_{33} = \epsilon_{ij} \sum_s \frac{\partial (n^{s+} - n^{s-})}{\partial x_i} b_j^s \quad , \tag{5}$$

where ϵ_{ij} is the antisymmetric Levi-Civita tensor.

We can now proceed to construct a numerical scheme that will minimize the free energy (2) subject to finite dislocation densities n^{s+} and (or) n^{s-}. We will assume that the time scale of relaxation of the order parameter is much shorter than that of the dislocation density. The relaxation of the order parameter field will then be accomplished by the relaxational dynamics

$$\frac{\partial e_2}{\partial t} = -\Gamma \frac{\delta F}{\delta e_2} \quad , \tag{6}$$

where Γ is the mobility coefficient, and during this relaxation we keep the dislocation density fixed. From the relaxed order parameter field we can calculate the strain field and, using the Hooke's law, also the internal stress field. Hence, the components of the Peach-Koehler forces on the dislocations in each mesoscopic cell can be calculated as $F_k^{s\pm} = \mp \epsilon_{jk} \sigma_{jl} b_l^s$ and the corresponding glide component, $\mathbf{F}_{glide}^{s\pm}$, by projecting the former into the individual slip systems s. In order to conserve the total Burgers vector in the simulated domain, the dislocation densities are evolved using the Fokker-Planck equations

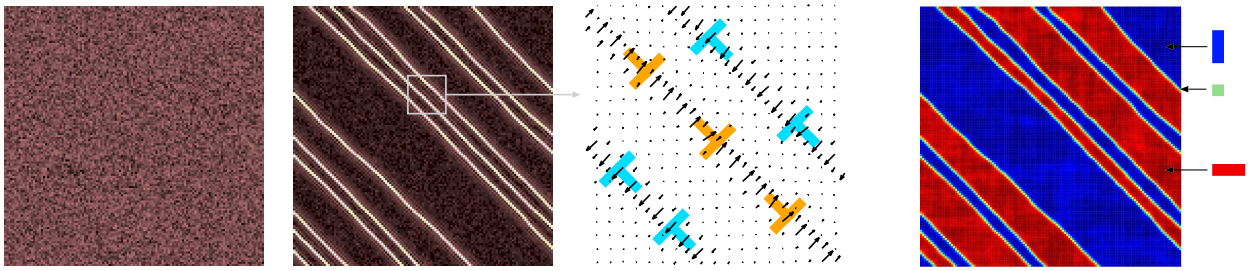
$$\frac{\partial n^{s\pm}}{\partial t} = -D \nabla \cdot [\mathbf{F}_{glide}^{s\pm} n^{s\pm}] \quad . \tag{7}$$

The individual dislocation densities are propagated through the time step Δt and the corresponding new incompatibility field is obtained from (5). In the next step we utilize (6) to calculate the order parameter field e_2 that minimizes the free energy subject to this new incompatibility field. This recursive procedure represents a simple self-consistent scheme for a simultaneous calculation of the microstructure and the dislocation density.

3 Simulations

We will now utilize the procedure outlined above to study the self-organization of dislocations in a single crystal of Fe-30at.%Pd below T_c. The simulated domain consists of 128×128 mesoscopic unit cells, each containing 1000×1000 crystallographic unit cells with the lattice parameter 3.8 Å. Hence, the width of the simulated domain is 48.64 μm. In this material the crystal dislocations responsible for accommodating plastic strain are those with the Burgers vectors $1/2\langle 110 \rangle$, i.e. in our two-dimensional case we consider two slip systems, with the Burgers vectors of the dislocations $\pm 1/2[110]$ and $\pm 1/2[\bar{1}10]$. To each mesoscopic cell we initially assign a dislocation density that is drawn at random from a uniform distribution; this yields the density $\rho = 2 \times 10^{14}$ m^{-2}.

During the minimization the initially spatially uniform dislocation density (Fig. 1a) rapidly develops alternating dislocation walls that decorate the twin boundaries between different variants of the martensite (Fig. 1b). This is shown more clearly in the field of the net Burgers vectors



(a) (b) (c) (d)

Figure 1: Initial (a) and final (b) density of dislocations, where dark regions correspond to low and bright regions to high $|\mathbf{B}|$, respectively. The final field of net Burgers vectors $\mathbf{B}$ is shown in (c). The final field e_2 is shown in (d), where blue and red correspond to the two variants of the martensite and the twin boundaries to the metastable austenitic phase.

in Fig. 1c. The microstructure (i.e. the order parameter field) corresponding to the dislocation density in Fig. 1b,c exhibits well-defined twins corresponding to the two variants of the martensite (Fig. 1d) separated by twin boundaries.

4 Conclusions

The Landau theory outlined in this paper represents the first step in the formulation of a mesoscopic theory for studying martensitic phase transformations mediated by defects. In the framework of Kröner's theory [3] utilized here, the dislocations induce incompatibility between the components of the elastic strain tensor. The "strength" of this incompatibility is related to the densities of crystal dislocations in individual discrete slip systems. The coupling between the order parameter field and the dislocation density introduces competition and frustration in the evolving microstructure and, therefore, the minimization of the free energy is accomplished simultaneously by the order parameter field and the dislocation density. This results in formation of correlated dislocation walls at the twin boundaries. The detailed explanation of this model can be found at `arXiv:0806.4564`.

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