Dislocation formation and plastic flow in binary alloys in three dimensions

Minami, A; Onuki, A

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Dislocations often play decisive roles in various phase transformations in crystalline solids. They are produced when the lattice constants or the crystalline structures of the two phases are not close.\textsuperscript{1} With their appearance the continuity of the lattice planes through the interfaces is lost partially or even completely, resulting in the so-called coherency loss. In particular, coarsening of incoherent microstructures has been studied in fcc Al-Sc alloys.\textsuperscript{2} It is also known that dislocations are proliferated in plastic flow. In two phase states such dislocations grow into the softer regions with their ends pinned at the interfaces.\textsuperscript{3,4} As a result, mechanical properties of two phase solids are very different from those of one phase solids.\textsuperscript{1}

Most theoretical papers on the elastic effects in phase transitions have treated the coherent case without dislocations.\textsuperscript{5-8} Theory in the incoherent case is much more difficult and numerical studies have been performed in two dimensions (2D)\textsuperscript{9-11} and in three dimensions (3D).\textsuperscript{12} In these simulations dislocations have been treated as singular points or lines in the linear elasticity scheme. Though in 2D, we recently presented numerical results of dislocation formation and gliding in two phase solids\textsuperscript{13} on the basis of a simple nonlinear elasticity theory.\textsuperscript{14} In 3D, however, dislocations are mobile curved lines and assume very complex configurations and 3D simulations are needed to understand the real physical processes.\textsuperscript{15,16} In this Rapid Communication we will develop a 3D nonlinear elasticity theory, perform 3D simulations both in one and two phase states, and provide physical pictures of these complex phenomena. A merit of our approach is its extreme simplicity, while it still captures the realistic dislocation dynamics.

We consider an AB alloy without vacancies and interstitials, where the order parameter $\psi$ is the composition difference in the range $-1 \leq \psi \leq 1$. In the free energy $F = \int d\mathbf{r} f$, $\psi$ is coupled to the elastic displacement $\mathbf{u} = (u_x, u_y, u_z)$. The free energy density $f$ is written as

$$f = \frac{k_B}{v_0} \left[ T \frac{1 + \psi}{2} \ln(1 + \psi) + T \frac{1 - \psi}{2} \ln(1 - \psi) - T_0 \frac{\psi^2}{2} \right]$$

$$+ \frac{1}{2} C |\nabla \psi|^2 + \alpha \psi \varepsilon + f_{el}(\mathbf{u}, \psi).$$

The first term is the Bragg-Williams free energy density where $v_0$ is the volume of a unit cell, $T_0$ is the critical temperature in the absence of the elastic coupling. The second term is the gradient term. The third term is the coupling between $\psi$ and the dilatation strain $\varepsilon = \nabla \cdot \mathbf{u}$ arising from the atomic size difference of the two components.\textsuperscript{3} The last term is the elastic free energy,

$$f_{el} = \frac{1}{2} Ke^2 + \Phi(e_2, e_3) + \Psi(e_4, e_5, e_6).$$

Supposing a cubic solid with the principal axes in the $x$, $y$, and $z$ directions, we define the strain components as

$$e_2 = \varepsilon_{xx} - \varepsilon_{yy}, \quad e_3 = (2 \varepsilon_{zz} - \varepsilon_{xx} - \varepsilon_{yy})/\sqrt{2},$$

$$e_4 = \varepsilon_{xy}, \quad e_5 = \varepsilon_{xz}, \quad e_6 = \varepsilon_{yz},$$

where $e_{ij} = (\partial u_i / \partial x_j + \partial u_j / \partial x_i)/2$. The diagonal strains $e_2$ and $e_3$ give rise to a contribution due to stretching,

$$\Phi = \frac{\mu_2}{4\pi^2} \left[ 3 - \cos(2\pi e_{2z}) - \cos(2\pi e_{3z}) - \cos\left(\frac{4\pi}{\sqrt{6}} e_3\right) \right],$$

where $e_{2z} = e_2/\sqrt{2} \pm e_3/\sqrt{6}$. The shear strains $e_4$, $e_5$, and $e_6$ give rise to a shear contribution,

$$\Psi = \frac{\mu_3}{4\pi^2} \left[ 3 - \cos(2\pi e_4) - \cos(2\pi e_5) - \cos(2\pi e_6) \right].$$

Notice that $\Phi$ and $\Psi$ are invariant with respect to a $\pi/2$ rotation around the $x$ axis, which changes the strains as $e_2' = e_2/\sqrt{3} e_{3z}/2$, $e_3' = (\sqrt{3} e_2 - e_3)/2$, $e_4' = e_6$, $e_5' = -e_5$, and $e_6' = -e_4$. Similarly, they are invariant with respect to $\pi/2$ rotations around the $y$ and $z$ axes.\textsuperscript{17} For small strains we obtain the standard forms, $\Phi \equiv \mu_2 e_2^2/2$ and $\Psi \equiv \mu_3 (e_4^2 + e_5^2 + e_6^2)/2$, in the linear elasticity theory.\textsuperscript{18} The crystal is also unchanged with respect to shear deformation $u_z \rightarrow u_z + y$ or $e_4 \rightarrow e_4 + 1$ in the $xy$ plane. Thus $f_{el}$ is required to be a periodic function of $e_4$, $e_5$, and $e_6$ with period 1. The simplest elastic energy satisfying these requirements is given by Eq. (2). The elastic moduli $\mu_2$ and $\mu_3$ depend on $\psi$ as\textsuperscript{8}

$$\mu_2 = \mu_{20} + \mu_{21} \psi, \quad \mu_3 = \mu_{30} + \mu_{31} \psi,$$

while the bulk modulus $K$ is a constant. For positive $\mu_{20}$ and $\mu_{30}$ the regions with larger (smaller) $\psi$ are harder (softer) than those with smaller (larger) $\psi$. It is known that aniso-
tropic elastic deformations tend to be localized in the softer regions in phase separation.\(^8\)

The lattice velocity \(v = \frac{\partial u}{\partial t}\) obeys

\[
\rho \frac{\partial v}{\partial t} = \nabla \cdot \bar{\sigma} + \eta_0 \nabla^2 v,
\]

where \(\rho\) is the mass density and \(\bar{\sigma} = \{\sigma_{ij}\}\) is the elastic stress tensor \((=\frac{\partial f}{\partial \varepsilon_{ij}})\). For example, \(\sigma_{xy} = \frac{\mu_3 \sin(2\pi \varepsilon_{4})}{2\pi}\). The nonlinearity of \(\bar{\sigma}\) is most important in Eq. (7). We introduce the shear viscosity \(\eta_0\), which gives rise to damping of \(u\). The composition is governed by the diffusive equation

\[
\frac{\partial \psi}{\partial t} = \nabla \cdot \lambda(\psi) \nabla \frac{\delta}{\delta \psi} F.
\]

The kinetic coefficient is assumed to be of the form \(\lambda(\psi) = \lambda_0 (1 - \psi^2)\). Then \(\psi\) obeys a simple diffusion equation in the

FIG. 1. Stress vs strain in a one phase state (broken line) and in a two phase state under cyclic shear (solid line). There are no defects initially. Edge dislocations appear in plastic flow.

FIG. 2. (Color online) Shear strain \(\varepsilon_4\) exhibiting slip planes (upper plate) and shear deformation energy \(\Psi\) at \(z=20\) with peaks at dislocation cores (lower plate) in a one phase state at \(\gamma=0.296\). A 1/4 of the total plane is shown in the lower figure. The \(x\), \(y\), and \(z\) axes are in red, blue, and green, respectively.

FIG. 3. (Color online) Time evolution of \(\varepsilon_4\) (upper figures) and \(\Psi\) (lower figures) under shear \(\gamma = \dot{\gamma} t\). They take large values on slip planes and dislocation cores, respectively. Blue regions represent hard domains. Dislocation loops are trapped at the interfaces.
dimensionless kinetic coefficients are

and

The mesh size is equal to the lattice constant \( a \). We applied average shear strain \( \gamma = (\partial u_y / \partial y) = (e_4) \) and imposed the periodic boundary condition on the deviation \( \delta u = (u_x - \gamma y, u_y, u_z) \). We set \( K/\mu_{20} = 4.5, \alpha/\mu_{20} = 1.5, \) and \( k_B T_0/v_0\mu_{20} = 0.05 \) in terms of \( \mu_{20} \) in Eq. (6). Space, time, and temperature will be measured in units of \( a, \tau_0 = a(\rho/\mu_{20})^{1/2}, \) and \( v_0\mu_{20}/k_B \). We assume weak cubic elastic anisotropy with \( \mu_{30}/\mu_{20} = 1.1 \) and moderate elastic inhomogeneity with \( \mu_{21} = 0.6\mu_{20} \). The spinodal temperature, below which one phase states become unstable, is then \( T_s = 0.43 \) at \( (\psi) = 0 \). The dimensionless kinetic coefficients are \( \lambda^* = \lambda_0\tau_0\mu_{20}d^2 = 10^{-4} \) and \( \eta^* = \eta_0/\tau_0\mu_{20} = 0.1 \). The relaxation of \( u \) is faster than that of \( \psi \) by \( \eta^*/\lambda^* = \eta_0/D_0 = 10^3 \), so we integrated Eq. (7) using an implicit Crank-Nicolson method. In Fig. 1 we show the average stress \( \langle \sigma_y \rangle \) in units of \( \mu_{20} \) after application of shear at \( t = 0 \). The shear rate \( \dot{\gamma} = d\gamma/dt \) will be measured in units of \( \tau_0^{-1} \).

In the one phase case we set \( T = 0.5 \) and \( \dot{\gamma} = 10^{-4} \). The initial value of \( u \) is a random Gaussian number with variance 0.01\( a \) at each lattice point. The stress exhibits a sharp overshoot with appearance of edge dislocations. In our case the instability point of homogeneous states is given by \( \partial^2\psi/\partial \gamma^2 = \mu_3 \cos(2\pi e_4) = 0 \) or \( e_4 = 1/4 \). Figure 2 displays a 3D snapshot of the shear strain \( e_4 \) and a 2D cross section of the shear elastic energy \( \psi \) at \( z = 20 \) for \( \gamma = 0.296 \). We can see multiple formation of slip planes (upper plate) and edge dislocations (lower plate). The core regions have higher \( \psi \). As in 2D,14 these dislocations do not disappear even if the shearing is stopped. They can be metastable due to the Peierls potential arising from the discrete lattice structure.22

In the two phase case we prepared a coherent domain structure at \( T = 0.42 \) with \( (\psi) = 0 \), where the cuboidal domains are harder than the percolating matrix.8 We then applied cyclic shear defined by \( \dot{\gamma} = 10^{-3} \) for \( 0 < t - m_0 < t_0 / 2 \) and \( \dot{\gamma} = -10^{-3} \) for \( t_0 / 2 < t - m_0 < t_0 \) (\( n = 0, 1, \cdots \)) with period \( t_0 = 780 \), as shown in Fig. 1. Since \( e_4 \) takes considerably large values (~0.1) near the interfaces, dislocation formation is triggered earlier than in the one phase case. From the second cycle, \( \gamma \sim 0.1 \) and 0.3 even for \( \langle \sigma_y \rangle = 0 \), and \( \langle \sigma_y \rangle \sim -0.13 \) even for \( \gamma = 0 \). Figure 3 shows snapshots of \( e_4 \) and \( \psi \) at the three points marked in Fig. 1. The dislocation loops form the boundaries of the slip planes extending into the soft regions, while their ends are trapped at the interfaces. Figure 4 shows 2D cross sections of \( (u_x, -\gamma y, u_z) \) and \( \psi \).

In plastic flow we define a regular elastic strain \( \gamma_{el} \) by \( \langle \sigma_{y_{el}} \rangle = \mu_3 \sin(2\pi \gamma_{el}) / 2 \pi \) in terms of the average stress. We then define the average defect energy density,

\[
f_D(t) = \langle f_{el} \rangle(t) - \langle f_{el}(0) \rangle - \langle \psi(\gamma_{el}, 0, 0) \rangle,
\]

in the course of cyclic shear. The first term is the average elastic energy density at time \( t \), the second term is that at \( t \)}
ever, \( f_\text{D}(\ell) \) is around \( 10^{-3} \mu_\text{D} \) for \( \gamma \approx 0.3 \) from the second cycle. For larger \( \gamma \), however, \( f_\text{D}(\ell) \) increases abruptly with increasing \( \gamma \), where the Peierls potential is broken and the dislocation loops begin to expand. If dislocations give rise to an elastic energy density of order \( 10^{-3} \mu_\text{D} \), the dislocation line density becomes of order \( 2 \times 10^{-3} / a^2 \). The same order of magnitude can also be obtained directly if the total length of high-value regions of \( \Psi \) is divided by the system volume (see Fig. 3).

In summary, developing a simple efficient scheme, we have studied dislocation dynamics in binary alloys under simple shear deformations. Their gliding motion along the Burgers vector is preferentially into the softer regions. Therefore, the composition dependence of the elastic moduli in Eq. (6) (elastic inhomogeneity) is essential in our theory. Note that our simulation times are much shorter than the time scale of the composition evolution. As has been confirmed in our previous two-dimensional simulation, there should eventually appear a compositional Cottrell atmosphere around each dislocation core also in three dimensions, which can affect dislocation dynamics and phase separation on long time scales. We will examine in future how dislocations influence various phase transitions in solids. In addition, in one phase states, dislocations tend to be formed close to preexisting dislocations and shear bands, where strains are localized, thicken with decreasing the shear rate in the plastic flow. Simulation of dislocation formation under uniaxial deformations is also under way.

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17. A \( \pi/2 \) rotation around the \( y \) axis gives \( e'_1 = e_1/2 + \sqrt{3} e_3/2 \), \( e'_2 = \sqrt{3} e_2/2 - e_3/2 \), \( e'_3 = -e_3 \), \( e'_4 = e_4 \), and \( e'_5 = -e_5 \). The rotation around the \( z \) axis reduces to that in 2D and is rather trivial (Ref. 13).
18. In terms of the usual elastic moduli \( C_{11}, C_{12} \) and \( C_{44} \) we have \( \mu_2 = (C_{11} - C_{12})/2 \) and \( \mu_3 = C_{44} \).
19. More generally, we need to use the convective time derivative \( \partial \bar{\sigma} / \partial t + \mathbf{v} \cdot \nabla \) in Eqs. (7) and (8) for large strains.
20. For \( \gamma = 10^{-3} \) the separation of the slip planes has become 1.5 longer than for \( \gamma = 10^{-4} \) in Fig. 2.
21. Around dislocations produced by shear strain, \( \Phi \) is typically 10% of \( \Psi \).
23. The elastic energy of edge dislocations per unit length is \( \alpha^2 \mu_2 \ln(\ell/a)/(4\pi(1-\nu)) \) in isotropic elasticity, where \( \ell \) is the distance among the dislocations and \( \nu \) is the Poisson ratio. Then we obtain a rough estimation of the dislocation line density \( \sim \ell \) in the text.
24. Shear bands have been observed from nanometer scales to macroscopic scales particularly in metallic glasses. The dynamics of their growth is still not well understood.