Dislocation formation in alloys

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Dislocation formation under applied strain and phase transition is studied by a phase field model. The main difficulty of constructing a field theory for plastic deformation is arising from nonlinear properties of crystals, for example the periodicity and the crystal symmetry. In our theory, the nonlinear elastic energy is a periodic function of local strains, which is reflecting the periodicity of crystals as follows.

$$f_{\rm el} = \frac{1}{2}Ke_1^2 + \Phi(e_2, e_3) + \Psi(e_4, e_5, e_6), \quad (1)$$

$$\Phi = \frac{\mu_2}{4\pi^2}\left[3 - \cos 2\pi\left(\frac{e_2}{\sqrt{2}} - \frac{e_3}{\sqrt{6}}\right) - \cos 2\pi\left(\frac{e_2}{\sqrt{2}} + \frac{e_3}{\sqrt{6}}\right) - \cos\left(\frac{4\pi e_3}{\sqrt{6}}\right)\right], \quad (2)$$

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

where $\Phi(e_2, e_3)$ is a uniaxial elastic energy and $\Psi(e_4, e_5, e_6)$ is a shear elastic energy. Strain components are defined as $e_1 = \nabla\cdot\mathbf{u}$, $e_2 = \nabla_x u_x - \nabla_y u_y$, $e_3 = (2\nabla_z u_z - \nabla_x u_x - \nabla_y u_y)/\sqrt{3}$, $e_4 = \nabla_x u_y + \nabla_y u_x$, $e_5 = \nabla_y u_z + \nabla_z u_y$, and $e_6 = \nabla_z u_x + \nabla_x u_z$. e_1 is local dilation strain, e_2 and e_3 are local uniaxial strains, and e_4, e_5 and e_6 are local shear strains. In two phase alloys, free energy density is written as

$$f(\psi, \mathbf{u}) = f_{\rm BW}(\psi) + \alpha e_1\psi + f_{\rm el}, \quad (4)$$

where ψ is a composition of two alloys. We numerically solved Cahn-Hilliard equations using above free energy functional.

Snapshots in Fig.1 are dislocation formation of two phase alloys under the stretching. Initially, we put a spherical hard metal on the center of the system. The elastic field is spontaneously deformed at the interface region, and network dislocations are preferentially gliding into the soft region. Due to the symmetry of the deformation along the [0 0 1] direction, slips along (0 1 1) and (1 0 1) planes, which are sort of symmetry breaking, are observed.

Snapshots in Fig.2 are dislocation formation around a preexisting circular slip toward the [0 1 0] direction. Because this slip plane initially breaks the symmetry with respect to the xy plane, proliferation of dislocation is observed only along (0 1 1) plane.

In this presentation, we also show the spontaneous dislocation by phase separation of two phase alloys and mechanical response of the applied strain in preexisting elastic inhomogeneity of two phase alloys.

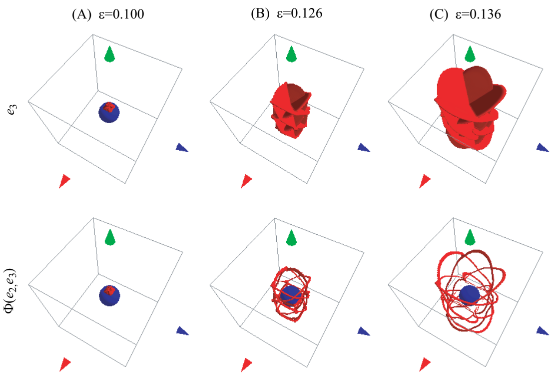

Figure 1: Dislocation formation of two phase alloys under the extension along the z axis (green arrow). A blue surface is an interface between two metals.

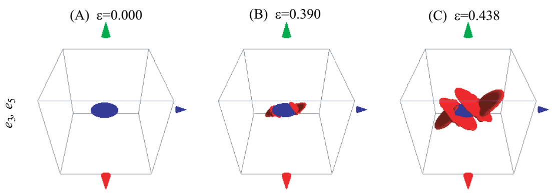

Figure 2: Dislocation formation around a preexisting circular dislocation loop (Blue plane) slipping toward the [0 1 0] axis (Blue arrow).

References

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