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Simulations of stress-induced twinning and de-twinning: A phase field model

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Abstract

Twinning in certain metals or under certain conditions is a major plastic deformation mode. Here we present a phase field model to describe twin formation and evolution in a polycrystalline fcc metal under loading and unloading. The model assumes that twin nucleation, growth and de-twinning is a process of partial dislocation nucleation and slip on successive habit planes. Stacking fault energies, energy pathways (γ surfaces), critical shear stresses for the formation of stacking faults and dislocation core energies are used to construct the thermodynamic model. The simulation results demonstrate that the model is able to predict the nucleation of twins and partial dislocations, as well as the morphology of the twin nuclei, and to reasonably describe twin growth and interaction. The twin microstructures at grain boundaries are in agreement with experimental observation. It was found that de-twinning occurs during unloading in the simulations, however, a strong dependence of twin structure evolution on loading history was observed.

Keywords: Phase field method; Partial dislocation; Deformation twin; Polycrystal deformation

1. Introduction

Deformation twinning is a major plastic deformation mode in some cubic and in most non-cubic materials [1–4]. For example, in hcp crystals, where deformation by slip along some directions either is not possible or requires very high stresses, twinning is a dominant deformation mechanism. Although plastic deformation predominantly occurs via dislocation nucleation and slip in coarse grained fcc metals and alloys with medium to high stacking fault energies, deformation twinning becomes important in nanocrystalline materials as grain sizes decreases [5–9]. Twin formation during crystal growth from the melt due to crucible contact stresses or growth stresses can be problematic in the processing of single crystals, such as CdTeZn growth via the vertical gradient freeze method [10,11]. A fundamental understanding of the effect of microstructure, defects and external stresses on twin nucleation and growth is helpful in designing advanced or improving existing materials and materials processing methods.

Experiments and atomistic simulations show that deformation twinning in nanocrystalline fcc metals forms and evolves via partials dislocations emitted from grain boundaries [5–9]. The stacking fault energy and energy pathways are predicted using first principle calculations [12–14]. Molecular dynamics (MD) simulations have been successfully used to investigate how grain boundary structure influences dislocation nucleation and in examining the twinning mechanisms [9,15,16]. Stacking fault core fields in fcc metals have been analyzed by MD simulations and continuous models [17]. The critical twinning stress was estimated using a continuous mechanical model [3,12], which suggests that the shear stress on the habit plane and slip direction of the twin controls twin nucleation. In addition, one of the commonly accepted mechanisms in both coarse grained and nanocrystalline fcc metals is that a twin nucleates and evolves via the nucleation and slip

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of partial dislocations with the same Burgers vectors. In the present work we assume that twin nucleation, growth and de-twinning is a process of partial dislocation nucleation and slip on successive habit planes under internal and external stresses. A phase field model is proposed to describe the dynamics of partial dislocations and to study both stress-induced partial dislocation nucleation and twin structure evolution. Compared with atomistic simulation methods, the main advantage of the mesoscale phase field method is that it permits simulations at relatively large length and long time scales. Furthermore, it is possible to incorporate the effect of long-range elastic interactions on deformation twin evolution due to second phases, such as inclusions/precipitates, once the elastic constants and lattice mismatches are known. The capability of our model is demonstrated by modeling twin microstructure evolution in a polycrystalline fcc solid.

2. Phase field model

Fig. 1 illustrates the formation of the thinnest possible twin in the matrix formed by the nucleation and passage of three partial dislocation loops on successive planes. Since the partial dislocation is the smallest unit cell in the twin structure, we study twin evolution using partial dislocation dynamics similar to the phase field model of dislocation dynamics [18–20]. In this work an arbitrary fcc crystal is used as an example. With the assumption that a twin consists of partial dislocations with the same Burgers vectors there are 12 twin variants in a single fcc crystal related to 12 distinct partial dislocations with slip planes $\{1\,1\,1\}$ and dislocation Burgers vectors $\langle 1\,1\,\bar{2}\rangle$, respectively. Twelve order parameters $\eta_{\alpha\beta}(r, t)$ ($\alpha = 1,2,3,4$; $\beta = 1,2,3$) are used to describe the partial dislocations and their time evolution, where α denotes the four $\{1\,1\,1\}$ slip planes and β denotes the three Burgers vectors on each of the slip planes. Considering a partial dislocation loop, the discontinuous displacement across the slip plane is described as $\mathbf{u} = \eta_{\alpha\beta}(r, t)\mathbf{b}_{\alpha\beta}$, where $\mathbf{b}_{\alpha\beta}$ is the partial dislocation Burgers vector. The order parameter $\eta_{\alpha\beta}(r, t)$ is equal to 1 inside the partial dislocation loop (or in the stacking fault) and $\eta_{\alpha\beta} = 0$ outside the partial dislocation loop (outside of the stacking fault). The order parameter $\eta_{\alpha\beta}$ changes smoothly from 0 to 1 across the dislocation core. Since dislocation density is proportional to the gradient of the discontinuous displacement, the partial dislocation in the phase field model is described by distributed small dislocations, as in the Peierls–Nabarro model [21]. Such a description correctly gives the dislocation stress field far from the dislocation core and removes the non-physical singular stress in the theoretical solution. Next we discuss the energy change of the system during partial dislocation formation, glide and twin growth. The energy change includes crystalline energy, interfacial energy and elastic energy.

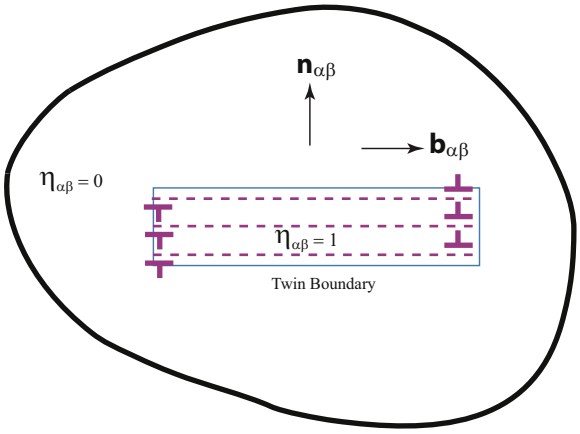

Fig. 1. A schematic view of a twin nucleus.

2.1. Crystalline energy

The twin formation in Fig. 1 involves the generation and slip of three partial dislocation loops on successive planes. The nucleation and slip of a partial dislocation loop accompanies energy changes, including crystalline energy, stacking fault energy, elastic energy, and the core energy of two partial dislocations. The crystalline energy is the energy barrier which a partial dislocation must overcome during slip. Fig. 2a, which is reproduced from the first principles calculation for Al [12], shows the energy pathway during the formation of an infinite stacking fault or a partial dislocation loop in which the two partial dislocations are separated by an infinite distance. The energy pathway does not include the elastic and core energies of two partial dislocations. The horizontal axis of the figure is exactly the same as the order parameter $\eta_{\alpha\beta}$ in our phase field model. It can be seen that the energy pathway has two local minima at the perfect crystal $\eta_{\alpha\beta} = 0$ and the crystal with infinite stacking fault $\eta_{\alpha\beta} = 1$ (or an infinite partial dislocation loop). The energy of the perfect crystal at $\eta_{\alpha\beta} = 0$ is 0 and is taken as the reference state. The energy at $\eta_{\alpha\beta} = 1$ is equal to the stacking fault energy. Fig. 2b shows the energy pathway during the formation and growth of an infinite twin [12]. When $\eta_{\alpha\beta} \leqslant 1$ the energy pathway is the same as that shown in Fig. 2a. However, when $\eta_{\alpha\beta} > 1$ the energy pathway plots the energy change during the passage of partial dislocations on successive planes. Comparing the energy changes of one stacking fault, two stacking faults and a twin structure shown in Fig. 2a and b, it was found that the stacking fault energy is very close to the energy of two twin boundaries. If we view the stacking fault energy as the interfacial energy of the partial dislocation or twin boundaries, the crystalline energy of a partial dislocation can be obtained by subtracting the stacking fault energy from the energy pathway as shown in Fig. 3. Fig. 3b plots the crystalline energy $f(\eta_{\alpha\beta})$ of the partial dislocation by subtracting $\gamma_{st}\eta_{\alpha\beta}$ from Fig. 3a, which is for a stacking fault. Such a double well potential can also be obtained by subtracting $2\gamma_{\text{twin}}$ from the energy change ($i < \eta_{\alpha\beta} < i + 1$, $i \geqslant 1$) shown in Fig. 2b.