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Relationship between monolayer stacking faults and twins in nanocrystals

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Abstract—A density functional theory–phase field dislocation dynamics model is used to study stress-induced emission of defects from grain boundaries in nanoscale face-centered cubic (fcc) crystals under ambient conditions. The propensity for stable stacking fault formation and the maximum grain size D_{SF} below which a stacking fault is stable are found to scale inversely with the normalized intrinsic stacking fault energy, $\gamma_I/\mu b$, where μ is the shear modulus and b is the value of the Burgers vector. More significantly, we reveal that a grain size smaller than D_{SF} is a necessary but not sufficient condition for twinning. Rather, it is shown that deformation twinning additionally scales with $\Delta_{SFE} = (\gamma_U - \gamma_I)/\mu b$, where γ_U is the unstable stacking fault energy. The combined effects of the material γ-surface and nanograin size for several pure fcc metals are presented in the form of a twinnability map. The findings may provide useful information in controlling nanostructures for improved mechanical performance.
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1. Introduction

Deformation twinning has a marked effect on the structural properties of nanocrystalline face-centered cubic (fcc) metals [1]. In such fine, nanometer-sized grains, twins, as well as stacking faults and perfect dislocations, are emitted from the grain boundaries [2]. For fcc crystals, perfect dislocations, stacking faults and twins have a number of features in common. They are constrained to {1 1 1} planes, are stable in the fcc crystal and can accommodate mechanical strain [3–6]. However, these defects are structurally very different. Perfect dislocations are linear defects that do not change the lattice orientation as they glide. Shockley partial dislocations create stacking faults as they glide, and these stacking faults are planar defects in which the fcc stacking sequence has been altered. Twins are also planar defects but are comprised of at least two adjacent stacking faults [7]. They reorient the lattice and introduce a twin boundary [1,5]. Consequently, for the same strain, these three defects do not lead to the same texture, slip activity and deformation response.

Over the years, extensive experimental, theoretical and numerical studies have been dedicated to understanding which intrinsic properties, such as the stacking and twin fault energies, and extrinsic properties, such as grain size and grain boundary properties, control which defect is emitted, whether it be perfect dislocations, stacking faults or twins. Analytical models based on dislocation theory have attempted to dissect the development of stacking faults or twins from grain boundaries step by step. Most of them assume that partials are emitted from the same boundary via sequential glide of the same Shockley partial on adjacent planes (referred to as monotonic activation of partials, MAP [8,9]). When a single leading partial is emitted and propagates across the grain to the opposing grain boundaries without subsequent nucleation of the trailing partial, then a monolayer stacking fault has formed. On the other hand, when the trailing partial nucleates from the same source, it corrects the stacking fault and recovers the original stacking. The net displacement corresponds to the glide of a perfect dislocation. However, if, instead of the trailing partial, a second leading partial is emitted on the adjacent plane, then a nascent two-layer twin forms.

Validating these defect kinetics has mainly been performed indirectly via post-mortem characterization of deformed nanocrystalline materials and static and dynamic atomic-scale simulations of defect structure or emission. Taken together, observations and atomic-scale simulations clearly indicate that crystal orientation, nanocrystalline grain size, fault energies or the entire γ-surface can influence which of these defects is emitted from grain boundaries [2,10–17]. In general, when the intrinsic stacking fault energy, γ_I, is low enough, or the nanocrystal small enough, and/or the crystal orientation is situated to promote nucleation of the second leading partial nucleation over nucleation of the trailing partial, then twinning becomes likely.

Despite the progress made, many basic questions on twinning in nanocrystals still remain. First, which defect prevails from grain boundaries has yet to be clarified. Further, while it has been shown that both the material γ-surface and grain size play a role in this selection, their

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relationship remains elusive [18]. In addition, the relative importance of various fault energies, such as the unstable stacking fault energy or twin fault energy, is still not well understood. Last, to date, questions regarding the kinetic pathways taken by defects after they have been emitted from grain boundaries cannot be answered easily via in situ observation. For this information, modeling and simulation have been employed.

Molecular dynamics (MD) simulations and density functional theory (DFT) have been the most common numerical tools used for relating the γ-surface to stacking fault formation and twinning. However, both are well known to be limited by very small length and short time scales. In MD, for instance, usually very fine grain sizes ($<$100 nm) and high rates (10^8 s^{-1}) are simulated. Therefore, while MD simulations have been insightful, it is still desirable to explore stacking fault and twin formation at larger length scales and longer time scales consistent with experiments, where different principles or kinetic pathways can operate. Some mesoscopic simulation tools, such as discrete dislocation dynamics, can attain greater length and time scales than MD; however, they tend to make use of rules to model partial dislocations [19,20].

Here we employ a novel mesoscale model, called density functional theory–phase field dislocation dynamics (DFT-PFDD), to explore the collaborative role that the material γ-surface and grain size play in stress-induced grain boundary emission of stacking faults and twins into nanocrystals. In the DFT-PFDD calculations, the nucleation and motion of discrete dislocations on crystallographic slip planes are predicted as driven by the minimization of the system energy. No rules are imposed that could bias which pathways should be followed. To describe the core energy of the defects emitted, this model incorporates the full 3-D γ-surface from DFT into the free energy functional on which the phase field formulation is based. The result is that the most energetically favorable defect and its motion are predicted for a given material and grain size. Whether a leading partial is nucleated and how far it extends are determined by the energetics formulated into the simulation, which involves the strain energy, dislocation core energy and external work. Likewise, whether a twin forms is governed by the same governing energetic function. An important benefit of DFT-PFDD is that dislocation motions within large 3-D nanocrystals ($\sim$100 nm side length) over long periods of time ($\sim$1 to several 1000 s) can be simulated.

1.1. The alternate emission (AE) mechanism for twinning

In prior work, we used the DFT-PFDD technique [21–23] to study dislocation emission from grain boundaries ledges in 3-D crystals. From these calculations emerged an energetically favorable grain-boundary-driven twinning pathway in a 3-D grain. We revealed an alternative mechanism for stacking fault and twin formation where a two-layer twin forms via partial emissions from opposing grain boundaries. This twinning mechanism accommodates strain yet eliminates backstress. In these respects, this alternate emission (AE) pathway for grain-boundary-driven deformation twinning is distinct from other twinning mechanisms, such as the MAP or random activation of partials (RAP) mechanisms. In MAP, a twin is constructed from sequential glide of identical twinning dislocations emitted onto adjacent planes. MAP can leave ever increasing steps in the grain boundary, and consequently backstresses develop as the twin expands. RAP, the zero-strain twinning mechanism [24], addresses this problem. In RAP, the twinning dislocations emitted from the same boundary have different Burgers vectors that sum to zero. Although no grain boundary backstresses or steps would develop, the RAP mechanism also does not accommodate strain, unlike MAP. The AE mechanism has the potential to be more favorable than MAP or RAP since it both accommodates strain and has an inherent mechanism for removing backstresses.

In this article, we explore the dependencies of the AE twinning mechanism on grain size and intrinsic material properties (γ-surface). We show that their effects are in agreement with experiments, yet different from those of other grain-boundary-driven mechanisms. In particular, we show that combinations of grain sizes and γ_I that lead to stable stacking fault formation do not necessarily lead to two-layer twinning. For twinning, the $\Delta_{SFE} = (\gamma_U - \gamma_I)/\mu b$ also needs to be sufficiently high.

2. Model formulation

We begin by briefly reviewing some essential elements of the DFT-PFDD model as it applies to fcc metals. Details on the general formulation and derivation of the energy terms can be found in Refs. [25–28,23].

A DFT-PFDD calculation is based on energy minimization. It predicts, not prescribes, the energetically favorable response that gliding dislocations within a crystal will choose to accommodate the mechanical driving force. Such responses include dislocation nucleation, expansion and interactions [23,29–32].

To model fcc dislocations as partial and full dislocations, the full 3-D γ-surface for a given fcc metal is incorporated into the formulation. In this work, the γ-surfaces for the materials in this study are calculated from DFT using the same Perdew–Burke–Ernzerhof (PBE) [33] exchange correlation functional and the projector-augmented wave (PAW) potential for the electron–ion interactions [34,35]. A Monkhorst–Pack scheme [36] was used to construct the Brillouin zone, and the Methfessel–Paxton smearing method (0.2 eV smearing width) was employed for the integration over the zone [37]. The simulation cells were built using 16$\{1\,1\,1\}$ layers, in which the upper eight layers were rigidly shifted in the $\langle 1\,1\,2\rangle$ and $\langle 1\,1\,0\rangle$ directions. Following each shift, the system was relaxed along the $\langle 1\,1\,1\rangle$ direction by minimizing the Hellman–Feynman forces on each atom. For all the metals modeled, the energies for each point converged to 10^{-6} eV atom^{-1}, and a cut-off energy of 600 eV was adopted. These calculations used a sufficient thickness of vacuum surrounding the shifted slabs, with relaxation in the normal direction of the atomic positions. For more details see Ref. [38]. Together, the DFT-PFDD technique permits the study of a wide range of dislocation core properties of fcc metals based on DFT calculations [21,22], but at length and time scales much greater than those of DFT or MD alone.

2.1. Phase field dislocation dynamics

In general, phase field models track the evolution of one or more scalar order parameters. Specifically in