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Stacking fault emission from grain boundaries: Material dependencies and grain size effects

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ABSTRACT

When load is applied to fcc nanograins, leading partial dislocations nucleate at grain boundary steps and propagate into the grain, leaving stacking faults behind. The extent to which these faults expand before a trailing partial is emitted generally does not equal the equilibrium separation distance of the corresponding full dislocation. Here we use a density functional theory – phase field dislocation dynamics model to study the effect of applied stress, 3D grain size, material stacking fault energies, and grain boundary ledge size on the stress-driven emission of leading and trailing partial dislocations from a grain boundary. The calculation accounts for the nucleation and glide of leading and trailing partial dislocations by incorporating the entire material γ-surface into the formulation. We show that the nucleation stress for a Shockley partial from a grain boundary is controlled by the size of the grain boundary ledge, scales with the unstable stacking fault energy γ_U, and is insensitive to grain size. We also reveal a gigantic γ-surface effect where small changes in $\gamma_I/\mu b$ can lead to large changes in the extent of the stacking fault region. Last, we find that the stacking fault region increases with grain size and eventually saturates at larger grain sizes, which our analyses suggest can be attributed to local grain boundary stresses. These findings can provide insight into transitions in the mechanical behavior of nanostructured metals.

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1. Introduction

Due to increasing applications for nano-scale devices, the growing need to ensure reliability and predictive modeling capabilities has motivated extensive research and discussion on the mechanical behavior and deformation mechanisms in nano-crystalline materials. Experimental studies and atomistic simulations have shown that unlike at the coarse-grained scale, grain boundary driven mechanisms, such as grain boundary accommodation, dislocation emission and absorption at grain boundaries, grain boundary sliding, and deformation twinning [1–11], become dominant at the nanoscale. They also find that as grain size reduces to nanoscale dimensions, partial-mediated slip, and concomitantly stacking faults, become more prevalent. This grain-size induced transition to partial-mediated slip from conventional slip in turn alters many elementary dislocation processes, such as cross-slip, nucleation, lock formation, and grain boundary mobility [12–16]. For instance, deformation twinning in nanocrystals can be attributed to the higher propensity for the formation and glide of partial dislocations [17,10,18,5,19]. Because of the growing importance of fcc nano-materials in many technological uses, understanding the intrinsic and extrinsic conditions under which partial-mediated slip arises are of great importance.

Molecular dynamics (MD) simulations have shown that when nano-grains are deformed, the grain boundaries emit and absorb partial dislocations [1,8,20,6]. Both the leading and trailing partial dislocations can be produced, with the former partial forming the stacking fault. The instant the trailing partial is emitted and glides, the stacking fault produced by the leading partial is removed. Thus the extent to which the leading partial can glide into the grain before the trailing partial is emitted is the maximum width of the stacking fault, denoted here as w_{max}. In certain cases, the leading partial is able to propagate to the opposing grain boundary without the trailing partial being emitted. Then the stacking fault spans the entire grain cross-section [1], and w_{max} equals the grain diameter D. The size of w_{max} relative to D can be related to the transition from full- to partial-dislocation mediated plasticity observed in fcc crystals [21,14].

To date, the conditions that determine the size of w_{max} originating at grain boundaries are not well understood. It has been reported or proposed that small grain sizes, certain values of stacking fault energies intrinsic stacking fault energy, SFE, unstable SFE, and/or large applied stresses favor partial emission and production of wide w_{max} [21,14,6,22–24,1]. Furthermore, in most experimental and

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numerical systems studied, many of these factors are coupled. For instance, higher applied stresses are associated with smaller grain sizes or with higher unstable stacking fault energies. Such interdependencies have made gaining insight into the conditions that control the extent of w_{max} a challenge both experimentally and numerically.

A number of modeling and simulation techniques have been used to study the width and the expansion of stacking faults in fcc metals. MD and density functional theory (DFT), for instance, have been employed as mentioned; however, the range of grain sizes and strain rates that can be used to study this phenomena are limited. As an alternative means, much effort has been invested in developing analytical models where the dependencies on some of these factors are given explicitly. Perhaps the most well known models of this class are those based on dislocation theory, which include the widening or narrowing of the stacking fault width due to applied stress [25] and relativistic effects [26–28]. While these models account for several forces on the partial dislocations (drag, repulsive elastic forces, attractive stacking fault force) they do not include the effect of grain size or the presence of grain boundaries. Continuum scale models for polycrystalline materials have also been developed for both extended dislocations and grain size effects [31,30,32–34]. All the above-mentioned analytical models thus far only include the intrinsic stacking fault energy (SFE) in their calculations. Yet, it has been emphasized by a number of all-atom numerical and experimental studies that it is important to also account for other SFEs, such as the unstable SFE [22,23,35,32].

A relatively new technique for predicting stacking fault behavior in fcc metals is phase field dislocation dynamics (PFDD). Traditionally phase field methodologies have been used to study phase transformations in materials. More recently, this energy-based formulation has been developed to model dislocation glide and the interactions between dislocations into what is now called PFDD [36,37]. Over the past decade, PFDD has proven to be capable of modeling a number of elementary dislocation processes, such as dislocation nucleation, annihilation, dislocation–dislocation interactions, and dislocation–obstacle interactions [37–40]. In these formulations, the dislocations modeled were full, not partial, dislocations. To overcome this limitation, PFDD has been advanced to model the development of extended dislocations by direct incorporation of the material γ-surface for defect energy into the governing free-energy functional [41,36]. In these prior works, the γ-surfaces were derived from either DFT or MD [41–43]. With an atomistically informed PFDD, partial dislocation loops, stacking fault regions, and the dynamic behavior of one or many interacting dislocations are all natural outcomes. As a testament to its capability, it has been shown that the DFT-PFDD model can predict equilibrium stacking fault widths w_0 for a wide range of fcc metals in agreement with available results from DFT or MD alone [44,41,42]. With an MD-PFDD version, Shockley partial emission from grain boundaries was studied in nano-sized Ni fcc grains [45]. It was found that the maximum extent w_{max} was much greater than w_0 and it increased with grain size. This result further emphasizes the importance of grain size effects on stacking fault behavior.

In this work, we employ the DFT-PFDD model to understand the key variables controlling w_{max}. The variables we choose to explore here are grain size, grain boundary step sizes, and stacking fault energies. We show that the threshold stress for partial emission σ_{th} increases with unstable SFE. We also reveal a gigantic γ-surface effect in which small changes in intrinsic stacking fault energy $\gamma_I/\mu b$ can lead to large changes in stacking fault expansion. For a broad range of fcc metals, we show that w_{max} increases with grain size to a point of saturation. We present analyses that suggest that this positive grain size effect may arise from differences in the internal stress state between smaller and bigger grains. Specifically we show that the grain boundaries generate a heterogeneous stress state in their vicinity that contains additional stress components not present within the grain interior. Thus, in smaller grains, more of the grain volume is significantly affected by the stress fields from neighboring grain boundaries.

2. 3D density functional theory-phase field dislocation dynamics model formulation

In this section we describe the DFT-PFDD model formulation. First, we present a description of the different energetic contributions accounted for within the phase field portion (PFDD) of the model. For further details on the PFDD formulation, we refer the reader to [37,36,41,38–40]. In the second part of this section, we discuss integration of PFDD with DFT, which permits modeling of partial dislocations and extended core regions of full dislocations.

2.1. PFDD formulation

In the crystalline systems of interest here, plastic deformation is carried out by the motion and interaction of partial and full dislocations. The PFDD model is formulated to account for these processes by introducing a scalar phase field variable $\zeta_n^\alpha(x,t)$ for each slip system (α, n), where α refers to the slip plane and n the Burgers vector direction. This phase field variable tracks the sign and the number of dislocations that cross an active slip plane at position x and time t [37].

In the case of most fcc metals, slip planes and slip directions belong to the family of $\{111\}\langle 110\rangle$ slip systems. There are 12 independently oriented slip systems and hence the model has 12 phase field variables. Partial dislocations correspond to the $\{111\}\langle 112\rangle$ family of slip systems. A partial dislocation on a given slip plane can be represented by a linear combination of the phase field variables on that same plane.

In PFDD, the evolution of dislocation dynamics in the system is governed by the minimization of the total system energy, E, according to Ginzburg–Landau [37,38,36]:

$$\frac{\partial \zeta_n^\alpha(x,t)}{\partial t} = -L\frac{\delta E}{\delta \zeta_n^\alpha(x,t)}. \tag{1}$$

The total energy E is the sum of two energy components: the elastic energy, E^{elas}, and the generalized stacking fault energy, E^{gsfe}. E^{elas} accounts for both short- and long-range interactions between dislocations in addition to dislocation interactions with any externally applied stress. The E^{gsfe} is similar to the Peierls energy in the sense that it describes the energy needed to move a dislocation core through the crystal lattice [41,46–48]. Both of these energy terms can be expressed as functions of the phase field variables ζ [37,39,41].

The elastic strain energy is related to the difference between the total strain energy and the plastic strain energy. The phase field variables ζ_n^α can be directly related to the plastic distortion by summing over all active slip systems [36,49]:

$$\beta_{ij}^p(x,t) = \sum_{n=1}^{3}\sum_{\alpha=1}^{4} b^\alpha \zeta_n^\alpha(x,t)\delta_n s_i^\alpha m_j^n, \tag{2}$$

where the Burgers vector of each system is defined as b^α, and s_i^α and m_j^n are the slip direction and slip plane normal, respectively. Finally, δ_{n_α} is a Dirac distribution supported on the slip plane α that describes the density of the active slip systems [50].

Using Eq. (2), a Fourier transform and other simplifications, the elastic energy E^{elas} can be expressed in terms of the phase field