Atomistic Modeling of Grain Boundaries and Dislocation Processes in Metallic Polycrystalline Materials

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The objective of this review article is to provide a concise discussion of atomistic modeling efforts aimed at understanding the nanoscale behavior and the role of grain boundaries in plasticity of metallic polycrystalline materials. Atomistic simulations of grain boundary behavior during plastic deformation have focused mainly on three distinct configurations: (i) bicrystal models, (ii) columnar nanocrystalline models, and (iii) 3D nanocrystalline models. Bicrystal models facilitate the isolation of specific mechanisms that occur at the grain boundary during plastic deformation, whereas columnar and 3D nanocrystalline models allow for an evaluation of triple junctions and complex stress states characteristic of polycrystalline microstructures. Ultimately, both sets of calculations have merits and are necessary to determine the role of grain boundary structure on material properties. Future directions in grain boundary modeling are discussed, including studies focused on the role of grain boundary impurities and issues related to linking grain boundary mechanisms observed via atomistic simulation with continuum models of grain boundary plasticity. [DOI: 10.1115/1.3183776]

Keywords: grain boundaries, atomistic simulation, dislocations, plasticity

1 Introduction

Experiments on polycrystalline metallic samples have indicated that grain boundary structure can affect many material properties related to fracture and plasticity, such as grain boundary energy, grain boundary mobility, crack nucleation, and ductility [1,2]. Although several authors have proposed correlations between material properties and grain boundary misorientation [2–5] (quantified via the Σ value of a boundary in the coincident site lattice (CSL) notation [6]), agreement between published experimental results in the literature does not yet point to a universal relationship. Instead, based on experimental evidence, grain boundaries are typically classified as having either "desirable" or "undesirable" performance or properties with respect to each behavior of interest.

This qualitative approach has been used in conjunction with the concept of grain boundary (GB) engineering [7], the goal of which is to increase the percentage of desirable grain boundaries or interfaces within the GB character distribution and to reduce the number and connectivity of undesirable boundaries through material processing techniques. Reducing the connectivity of undesirable boundaries is particularly important, as polycrystalline samples with a properly oriented continuous path of undesirable boundaries would be susceptible to failure in terms of desired GB network properties regardless of the percentage of desirable interfaces [8]. For example, several authors have shown that the fraction of low-order CSL boundaries can be increased through sequential straining and annealing cycles [2]. As a result, enhancements in corrosion resistance [4], creep resistance [9], and crack nucleation and growth resistance under various loading conditions [10] have been observed experimentally. Of particular effectiveness is the introduction of $\Sigma 3$ (111) annealing twins [11]. These twins are reckoned to lead directly to an increase in the fraction of desirable boundaries and to a reduction in the connectivity of the undesirable boundaries within the network. In addition, crack growth may be arrested at triple junctions that contain at least two $\Sigma 3$ boundaries.

Although experiments are of critical importance, quantitative information aimed at identifying the nanoscale mechanisms that promote grain boundary influences on dislocation slip transfer is currently inaccessible to experiments, aside from very limited in situ high-resolution transmission electron microscopy (TEM) studies [12,13]. Inherently, grain boundaries are interfaces with nanoscale thickness comprised of ordered defect structures and some degree of disordered atomic arrangement, depending on the extent of prior nonequilibrium processing and/or deformation. Their influence on material properties extends across multiple higher length scales. Atomistic simulations have provided an avenue to study the underlying mechanisms associated with plasticity, such as dislocation nucleation, dislocation migration, dislocation slip transfer, grain boundary migration and sliding, grain rotation, and atom shuffling.

The objective of this article is to provide a concise review of atomistic modeling efforts aimed at understanding the nanoscale behavior and the role of grain boundaries in plasticity of metallic polycrystalline materials. The common goal of the atomistic modeling efforts discussed in this article is to enhance predictive models for failure in metallic materials, such as those presented by Ashmawi and Zikry [14,15], Bieler and co-workers [16–18], and Yamakov and co-workers [19,20]. For example, Bieler et al. [18] proposed a fracture initiation parameter in limited ductility metallic materials. This parameter is constructed as a criterion for damage nucleation, accounting for slip interaction and incompatibilities at a grain boundary. The accuracy of such a model could be enhanced significantly with additional knowledge of grain boundary structure and its potential influence on dislocation mechanisms in the local neighborhood of the grain boundary.

Contributed by the Materials Division of ASME for publication in the JOURNAL OF ENGINEERING MATERIALS AND TECHNOLOGY. Manuscript received February 2, 2009; final manuscript received April 3, 2009; published online August 27, 2009. Assoc. Editor: Hanchen Huang.

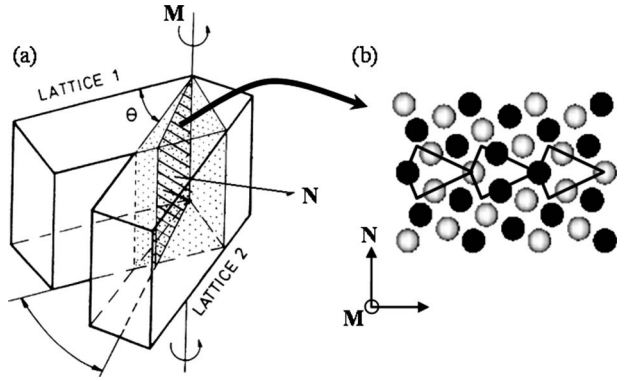

Fig. 1 (*a*) **Schematic diagram of the five macroscopic degrees of freedom associated with a grain boundary (adapted from Ref. [1]). (*b*) Atomic structure of a symmetric tilt Σ5 (210) ×⟨001⟩ interface. Translations parallel and perpendicular to the interface plane result in a periodic repeating structure at the interface.**

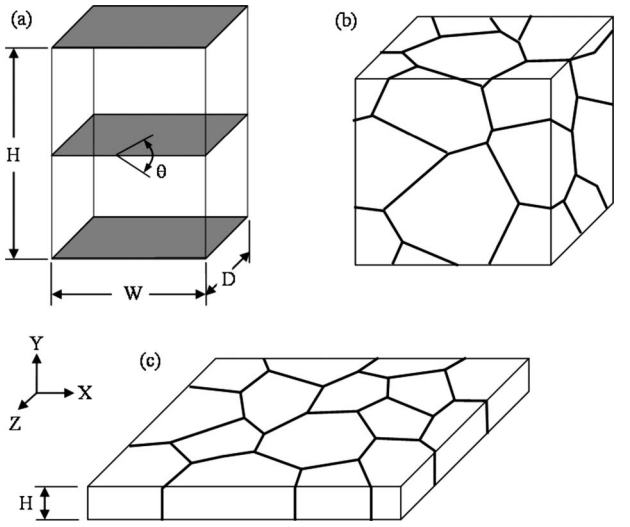

Fig. 2 Schematic illustration of (*a*) a bicrystal grain boundary model, (*b*) a 3D periodic nanocrystalline model, and (*c*) a columnar nanocrystalline model. Periodic boundary conditions are typically applied in all directions for each model to avoid the influence of free surfaces on the mechanisms associated with dislocation activity. For the bicrystal model, this results in a repeating planar defect in the *Y*-direction.

2 Grain Boundaries in Metallic Materials

Grain boundaries are planar defects with nanoscale thickness, which accommodate misorientation of adjoining regions of uniform (or nearly uniform) crystallographic orientation. In ductile coarse-grain metals, the migration of dislocations (which are nucleated at Frank–Read sources within the grain interiors) is arrested by grain boundaries due to slip incompatibility between neighboring grains. Both Hall [21] and Petch [22] envisioned dislocation "pile-up" at the grain boundaries based on experimental evidence and proposed that yield occurred in ductile polycrystalline materials once the stress exerted on the neighboring grain by the dislocation pile-up reaches a critical value, resulting in the Hall–Petch equation [23]. In metallic materials with poor ductility, grain boundaries may serve as nucleation sites for microvoids and the path for crack propagation during fracture. For example, Watanabe [7] envisioned a connected network of undesirable grain boundaries within a brittle material as the path of least resistance for crack propagation. In most work on GB engineering, as discussed previously, undesirable boundaries are viewed as weaker than others using arguments based on geometry (neighboring grain orientations and CSL designation) or composition (presence of impurities).

From a geometric perspective, interfaces between crystal lattices have five "macroscopic" and three "microscopic" degrees of freedom [1,6,24,25]. Four macroscopic degrees of freedom are accounted for by two orientation vectors, while the fifth is defined by an interface angle. For example, one method to characterize the macroscopic geometry of a grain boundary is via a misorientation angle, a misorientation axis vector, and the normal vector to the interface plane, as shown in Fig. 1(*a*). Boundaries for which the normal to the interface plane is perpendicular to the misorientation axis are defined as "tilt" interfaces, whereas boundaries for which the normal to the interface plane is parallel to the misorientation axis are defined as "twist" interfaces. In general, grain boundaries in actual polycrystals have both tilt and twist components. Interfaces between crystal lattices also have three microscopic degrees of freedom associated with the mutual translation of the opposing lattice regions parallel and perpendicular to the interface plane. These translations lead to a description of the atomic level geometry of a GB associated with unrelaxed atomic arrangements [25]. Finally, nanoscale movements of individual atoms at the GB occur to minimize the interface energy for a given GB geometry leading to structure at the interface, as shown in Fig. 1(*b*).

Specific grain boundary angle/axis combinations result in an array of coincident lattice points between the two crystalline regions [1,6,24]. This array of lattice points is known as the CSL, while the inverse density of coincident lattice points is defined as Σ. The CSL notation is considered as a tool to characterize grain boundary geometry because the pattern of coincident atomic sites leads directly to a definable periodic geometry at the interface. Atomistic simulations by Sutton and co-workers [26–29] showed that the structure of symmetric tilt interfaces in face-centered cubic (FCC) metals may be viewed as a linear combination of "structural units." With this tool, several authors attempted to correlate character and/or distribution of the interface structural units to material properties or specific dislocation mechanisms. Unfortunately, several limitations of the structural unit model (SUM) limit the success of such correlations. First, it is difficult to identify structural units with three-dimensional character, as is commonly the case with twist boundaries. Second, the SUM has limited applicability for interfaces with mixed tilt and twist characteristics or if high index misorientation axes are examined [30]. Third, it is difficult to quantify the degree of elastic distortion of the structural units necessary for geometric compatibility in polycrystals, and it is unclear what role elastic distortion plays in plastic deformation [25]. Finally, the SUM fails to describe interfaces with delocalized structural units, as is prevalent in materials with low to moderate intrinsic stacking fault energies. Rittner and co-workers [31–33] showed that for materials with low stacking fault energies, grain boundary dislocations tend to dissociate, leading to short intrinsic stacking fault facets that extend from the interface plane. Rittner and Seidman [32] also showed that if the delocalization of the interface is severe, the structural units may not change continuously between two favored boundaries. For these reasons, the SUM has not been extended to characterize polycrystalline microstructures, even though structural features similar to those proposed in Refs. [26–29] are often observed during atomistic simulation of nanocrystalline geometries (Secs. 3.2 and 3.3).

3 Atomistic Modeling of Dislocation Nucleation

Atomistic simulation of dislocation activity and grain boundary behavior during plasticity has focused on three distinct configurations: (i) bicrystal models, (ii) columnar nanocrystalline models, and (iii) 3D nanocrystalline models. A schematic drawing of each simulation geometry is shown in Fig. 2. The purpose of this section is to discuss advantages and disadvantages of each simulation

configuration and to identify common grain boundary mechanisms that occur during plastic deformation. This section will focus on results of molecular dynamics (MD) simulations presented in the literature; for a review of MD theory and interatomic potentials, the reader is directed toward texts by Allen and Tildesley [34] and Haile [35].

3.1 Bicrystal Models. Bicrystal models have been used in the literature to study intergranular fracture [36,37], grain boundary sliding and shear-driven grain boundary migration [38–49], and dislocation nucleation [19,50–56]. The advantage of bicrystal models is that the grain boundary geometry and structure can be precisely specified, promoting correlations between grain boundary structure and material properties. For example, Sansoz and Molinari [43,44] were able to directly correlate individual failure mechanisms to the presence of certain structural units along the interface plane using the quasicontinuum method. In tension, failure of the grain boundary occurred via partial dislocation nucleation and grain boundary cleavage. In shear, Sansoz and Molinari reported three different failure modes, depending on the interface structure: grain boundary sliding by atomic shuffling, nucleation of partial dislocations from the bicrystal interface, and grain boundary migration. Atomic shuffling occurred during shear deformation only for interfaces that contained the E structural unit, which is associated with the symmetric tilt $\Sigma 9\ (221)\langle 110\rangle$ interface [32]. Sansoz and Molinari proposed that the free volume inherent to this structural feature was responsible for triggering the atomic shuffling event during shear. Mishin and co-workers [46–49] showed analogous results using MD simulation, providing correlations between the shear stresses applied to a grain boundary, the structure of the grain boundary (in terms of structural units), and normal motion of the grain boundary.

Spearot et al. [50–53] and Tschopp et al. [54–56] used MD simulations to examine the role of interface structure on the nucleation of dislocations from copper and aluminum bicrystal boundaries subjected to tension and compression normal to the interface. These simulations focused on the evolution of the grain boundary structure during partial dislocation nucleation and the resulting structure of the grain boundary after full dislocation emission. Motivated by these simulation results, Spearot et al. [52] developed a model to correlate interface geometry and structure with the tensile stress required for dislocation nucleation. The proposed model utilized a description of slip system orientation in the adjoining lattice regions to account for GB geometry and a characterization of the average porosity at the interface to correlate interface structure and dislocation nucleation during a uniaxial tensile deformation. This model was successful in capturing the influence of the grain boundary structure on dislocation nucleation for many $\langle 100\rangle$ and $\langle 110\rangle$ symmetric tilt grain boundaries (e.g., Figure 7 in Ref. [52]); however, the proposed model was unable to capture the severe reduction in tensile strength for boundaries, which contained the E structural unit, which has a substantial free volume per unit boundary surface area.

Spearot et al. [52] originally proposed that the interface strength model may be extended to symmetric tilt grain boundaries with the E structural unit by including (i) a more advanced description of the interface porosity, including the role of gradients or connectivity of free volume within the interface region, and (ii) a crystallographic characterization, which accounts for the alignment of the E structural unit with respect to the primary slip systems for dislocation nucleation. Tschopp et al. [57] examined the distribution of free volume within the grain boundary region for a range of $\langle 110\rangle$ symmetric tilt grain boundaries between 109.5 deg and 180 deg (all of which contain the E structural unit); they computed two-point correlation and lineal path statistics, providing a more complete understanding of the porosity distribution within the interface region. Their analysis provides a means to correlate the interface structure and the tensile stress required for dislocation nucleation within the misorientation range considered.

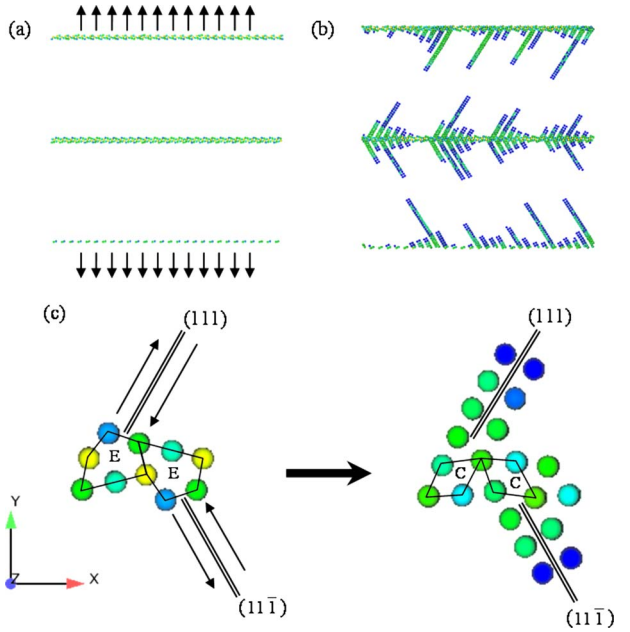

Fig. 3 (*a*) Bicrystal interface model for a $\Sigma 9\ (221)\langle 110\rangle$ symmetric tilt grain boundary after thermodynamic equilibration at 10 K. (*b*) Partial dislocations emitted from the grain boundary during a uniaxial tensile deformation. (*c*) Mechanism by which the E structural unit collapses during the partial dislocation nucleation event. Atoms are colored by the centrosymmetry parameter; atoms in a perfect FCC arrangement are removed. Reproduced with permission from Ref. [53].

However, a characterization of the connectivity of interface porosity by itself does not appear sufficient to explain the severe drop in tensile strength for boundaries which contain the E structural unit.

Porosity configuration with respect to crystallographic orientation of the primary slip systems is also of first order importance as shown by Spearot [53]. Using uniaxial and constrained tension boundary conditions, Spearot showed that the natural conformation of the interface porosity with respect to the primary dislocation slip systems is responsible for the ease of emission of Shockley partial dislocations during uniaxial tension from boundaries, which contain the E structural unit. Specifically, the emission of Shockley partial dislocations was facilitated by the collapse of the free volume at the interface, which is positioned at the termination of the primary slip planes. The mechanisms associated with the emission of partial dislocations from a $\Sigma 9\ (221)\langle 110\rangle$ bicrystal interface are shown in Fig. 3. These mechanisms are consistent for all $\langle 110\rangle$ symmetric tilt grain boundaries within misorientations between 109.5 deg and 180 deg. Spearot [53] also reported that tensile stresses parallel to the interface plane (multiaxial state of stress) can diminish the severity of the E structural unit on the dislocation nucleation process by postponing the collapse of the free volume within the E structural unit. Although delayed, the mechanisms by which the E structural unit collapsed during deformation and the mechanisms associated with partial dislocation nucleation were consistent with uniaxial tension simulations. Accordingly, one can comprehend the process of emission of partial dislocations in terms of stress-state dependent stability criteria of structural units of the boundary.

The disadvantages of the kinds of bicrystal models that have been pursued in previous efforts are (i) that configuration and boundary conditions can isolate individual mechanisms associated with plastic deformation (this is an advantage if fundamental studies of plasticity are desired but is considered a disadvantage here with respect to understanding the deformation of polycrystalline materials); (ii) that important aspects of the microstructure, such as triple junctions, are not considered; (iii) that they are energy

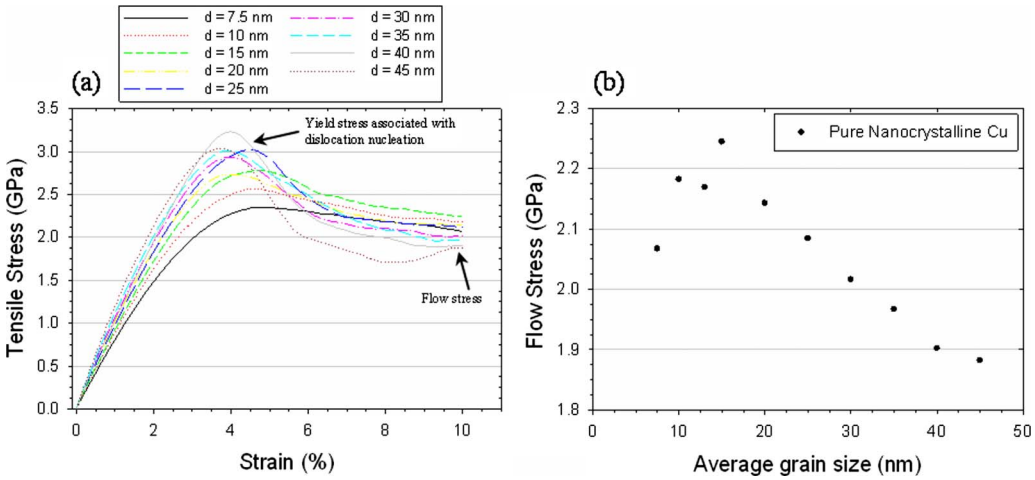

Fig. 4 (*a*) Stress-strain diagrams generated during uniaxial tensile deformation of a pure Cu nanocrystalline sample. Simulations contain approximately 20×10^6 atoms and are performed at 300 K. (*b*) Flow stress versus grain diameter for pure nanocrystalline Cu showing a maximum strength around 15 nm.

minimized and therefore representative of near equilibrium structures, excluding potential effects of prior deformation and absorption of dislocations; and (iv) that they do not typically involve multiple dislocation reactions or slip transfer events, focusing on individual processes of absorption or desorption of dislocations. Item (iii) and to some extent (iv) are also limitations of 2D and 3D models of nanocrystalline structures with MD. It is often observed in MD simulations of 3D nanocrystalline models that multiple atomic scale mechanisms are coupled during plastic deformation, such as atomic shuffling in the presence of triple junctions and partial dislocation nucleation (Sec. 3.3). However, it is possible to isolate each of these individual mechanisms by using bicrystal models with specific boundary conditions, as observed in Sansoz and Molinari [43,44]. Thus, while atomistic simulation of plasticity and fracture using bicrystal models provides significant insight into the role of individual features of the GB on deformation, the interrelationships between mechanisms associated with plasticity are critical in actual polycrystalline microstructures. To date, such interrelationships have not been fully elucidated using MD and bicrystal geometries.

3.2 Columnar Nanocrystalline Models. Columnar nanocrystalline models have been used to study grain boundary diffusional creep [58], dislocation activity [59,60], and deformation twinning [61,62]. The advantages of columnar models are (i) that triple junctions and geometric compatibility characteristics of polycrystalline samples are naturally included and (ii) that larger grain sizes than those used typically in fully 3D nanocrystalline models (Sec. 3.3) can be studied via the use of a small periodic dimension in the columnar direction. With regard to the last point, it can be envisioned that large enough grains can be explored to move well into the microcrystalline region of substantial practical importance, say above 50–100 nm mean grain size. Certainly, this is an important consideration in quantifying GB engineering concepts. For example, Yamakov et al. [59–62] studied several aspects associated with plastic deformation of a columnar nanocrystalline Al sample. Aluminum was chosen for their simulations with the hypothesis that the higher intrinsic stacking fault energy (as compared with copper and nickel), which leads to a shorter stacking fault width, would facilitate the emission of trailing partial dislocations, which were not observed in earlier simulations in 3D nanocrystalline models (Sec. 3.3). Yamakov et al. used a columnar microstructure with a thickness of only 10 $(1\bar{1}0)$ atomic planes in order to simulate larger nanoscale grain sizes. They identified the stacking fault width as a critical length scale parameter necessary to describe the crossover between extended partial dislocation and full dislocation emission from grain boundaries in nanocrystalline metals.

The primary disadvantage of columnar nanocrystalline models is that the imposed periodic boundary in the columnar direction may impart image forces on dislocations as an artifact as they are nucleated during deformation. For thin columnar samples, on the order of that used by Yamakov et al. [59], dislocations are restricted to form only on certain slip systems, with dislocation cores parallel to the columnar axis. This may result in (i) an overabundance of one particular type of dislocation (such as the infinitely straight edge dislocations observed by Yamakov et al.) and (ii) dislocation nucleation on secondary slip systems, depending on grain orientation. Relaxing these restrictions may result in different structures or kinetics for the observed dislocation, twinning, or creep mechanisms. For example, Van Swygenhoven and coworkers [63,64] argued that it is insufficient to interpret the crossover between regimes involving only the emission of the leading partial dislocation and both leading and trailing partial dislocations in terms of the intrinsic stacking fault energy. Such an approach implicitly assumes (i) the existence of pre-existing partial dislocations and (ii) that partial dislocation cores are infinitely long and straight [63]. Neither assumption is true in 3D nanocrystalline geometries (Sec. 3.3). Van Swygenhoven et al. argued that the entire generalized stacking fault energy curve must be taken into consideration and proposed that the ratio of the unstable and intrinsic stacking fault energies is more appropriate to describe the observed dislocation activity in 3D nanocrystalline models. If this ratio is close to unity, emission of the trailing partial dislocations are anticipated during the deformation process; conversely, if this ratio is high, extended leading partial dislocations are expected within the nanocrystalline grains.

3.3 3D Nanocrystalline Models. Three-dimensional nanocrystalline models have been used to study intergranular fracture [65,66], dislocation emission from grain boundaries [63,67–80], the role of twin boundaries on plasticity [81–83], temperature and stress-assisted grain boundary migration [84,85], and the inverse Hall–Petch effect [86–89]. Simulations by Schiotz et al. [87] showed that molecular dynamics is capable of capturing the softening behavior of materials below a critical grain diameter if certain definitions are made regarding the plastic deformation of the material. Specifically, two critical stresses are defined from the stress-strain diagrams generated via molecular dynamics, as illustrated in Fig. 4 [90]: (i) a "yield stress" associated with the emis-

sion of partial dislocations in an originally dislocation starved system, which corresponds to the maximum in the stress-strain diagram; and (ii) a "flow stress," which is assumed to capture the role of grain size on dislocation migration and which corresponds to the plateau region in the stress-strain diagram. The flow stress is then used to examine the inverse Hall–Petch behavior. In pure nanocrystalline Cu, a maximum in the flow stress occurs for a mean grain size around 15 nm, as shown in Fig. 4(*b*). This diameter is generally considered as the critical length scale in which grain boundary mediated processes become dominant, although dislocation activity can still be active in grains with sizes below this critical grain diameter (e.g., Fig. 1 in Ref. [86] or Fig. 9 in Ref. [78]).

Van Swygenhoven and co-workers [63,67–78,81–83] focused predominantly on the mechanisms associated with dislocation nucleation from grain boundaries in nanocrystalline metals. They reported that dislocation activity is "partial mediated," in that Shockley partial dislocations are nucleated one at a time from the grain boundaries [78]. Ledges or other grain boundary irregularities served as heterogeneous sites for partial dislocation nucleation [83], analogous to bicrystal simulations presented by Capolungo et al. [91]. Through detailed analysis of the grain boundary structure [70,74,76], nucleation of the first partial dislocation in nanocrystalline metals was shown to be assisted by atomic shuffling in the local neighborhood of triple junctions (regions of excess free volume). In addition, grain boundary sliding was always present for boundaries, which are subjected to a shear stress acting on the grain boundary plane. In Cu and Ni, the trailing (second) partial dislocation was often not emitted from the grain boundary; as a result, an extended intrinsic stacking fault (which was typically longer than the equilibrium spacing between partial dislocations due to the high excess energy of the nanocrystalline system) remained within the grain. In Al on the other hand, the trailing partial dislocation was usually observed soon after the initial dislocation nucleation event.

The disadvantages of 3D nanocrystalline models are (i) that due to the necessary computing power, smaller grain sizes are considered as compared with columnar nanocrystalline models, and (ii) that construction of "realistic" grain boundary networks can be challenging owing to the substantial constraints placed on finding minimum energy configurations by virtue of the 3D network of boundaries. It is observed that ledges or other regions of misfit act as heterogeneous sources for partial dislocation nucleation; accordingly, decisions that influence grain size distribution and the construction of the grain boundary network in 3D nanocrystalline samples have a first order effect on the observation of dislocation activity during deformation. Naturally, if a large number of grains are considered (which requires millions of atoms for polycrystalline models with grain diameters above 10 nm), then the grain size distribution created during Voronoi construction will be log-normal. Gross and Li [92] argued that this is not sufficient in some cases and developed a sequential method to skew the grain size distribution toward a desired "input" function, which could be either hypothetical or experimentally motivated. Furthermore, during construction of a nanocrystalline model, a decision must be made regarding the initial "spacing" between atoms at the grain boundaries. This decision can dramatically influence the structure of the boundary. The current authors believe that this is an open area for future research, which is necessary to advance correlations between porosity-driven atomic shuffling, partial dislocation nucleation, and nanocrystalline plasticity.

4 Atomistic Modeling of Dislocation Slip Transfer Reactions

By comparison, fewer atomistic studies have focused on dislocation slip transfer reactions within or across grain boundaries [93–97]. This reference list does not include many studies in the literature that focus on the transmission of lattice dislocations through bi-material interfaces, such as those in Cu–Ni by Hoagland and co-workers [98–100] for use in understanding the mechanisms associated with plastic deformation in nanolaminate structures. Boundary conditions for dislocation slip transfer calculations can be challenging, as dislocations with defined type and structure must first be introduced into the model and then propagated toward the grain boundary via an applied deformation. Thus, many studies focus on simplified bicrystal geometries. Slip transmission criteria that have been proposed in the past have been based on limited high-resolution transmission electron microscopy (HRTEM) observations and concepts based on slip of full dislocations. Details of grain boundary partial dislocations and excess free volume migration have not yet been fully considered. The slip transmission criteria of Lee et al. [13], Robertson and Birnbaum [101] and Clark et al. [102] have highlighted the role of relative orientation of slip planes across the interface, as well as orientation of the primary slip plane and the residual Burgers vector in the boundary following transmission. Such qualitative criteria require updating as more quantitative information becomes available from atomistic studies involving multiple mediation events.

In seminal MD work, de Koning et al. [94] examined the interaction between dislocation loops nucleated from a crack tip and six low-order symmetric tilt CSL boundaries. Depending on the boundary geometry, dislocations could either pass easily through the boundary ($\Sigma 13$) or be completely obstructed by the interface ($\Sigma 29$). Ultimately, de Koning et al. concluded that resistance to slip transmission could be posed as a function of three variables: (i) the ratio of resolved stress on the primary slip systems on either side of the boundary, (ii) the magnitude of residual Burgers vector content in the grain boundary, and (iii) the orientation of the primary slip planes relative to the grain boundary. Jin et al. [95] examined the interaction of screw dislocations with a coherent (111) twin boundary in Al, Cu, and Ni. They reported two dislocation/grain boundary interaction mechanisms: (i) the screw dislocation could propagate into the opposing grain by cutting through the coherent twin boundary and (ii) the dislocation could be absorbed into the grain boundary, dissociating into partials along the grain boundary plane. The activation of each mechanism was dependent on the applied shear strain used to drive the dislocation toward the boundary and on the energetic barrier associated with the formation of Shockley partial dislocations.

Employing a 3D nanocrystalline model, Hasnaoui et al. [97] used molecular dynamics to study the interaction between dislocations nucleated during nanoindentation and grain boundaries beneath the surface of the nanocrystalline sample. Grain boundaries served as both sinks for the homogenously nucleated dislocations beneath the indenter and as sources for new dislocations, which migrate back into the plastic zone beneath the nanoindenter. The behavior of each individual grain boundary beneath the indenter appeared to depend on local grain boundary structure and stress state. Hasnaoui et al. [97] did not observe direct transmission of dislocations through any of the grain boundaries in their nanocrystalline model. A quantitative understanding of connections between transmission, absorption, and desorption mechanisms is, to date, unknown and thus a rich area for future research.

MD simulations are limited in terms of the combined length and time scales in addressing the processes involved in absorption and desorption of multiple dislocations contributed from a pile-up into a grain boundary. Some understanding has been gained in conjunction with high-resolution TEM imaging of dislocations [12,13]. To characterize dislocation slip transfer reactions with grain boundaries associated with dislocation pile-ups in FCC crystals, the coupled atomistics and dislocation dynamics (CADD) framework of Shilkrot et al. [103,104] is promising and has been employed recently by Dewald and Curtin [105] to study dislocation-grain boundary reactions of edge dislocations impinging on a $\Sigma 11$ (113) tilt boundary in Al, including pile-ups. In the CADD framework, dislocations are passed from a continuum domain to the fully atomistic domain to resolve the interface reac-

tions. A useful multiscale modeling approach invoking domain decomposition, CADD is presently limited to straight dislocation lines due to the complexity of criteria and means of passing mixed dislocations through the continuum-atomistic interface. Such approaches have the potential to improve understanding of the evolution of grain boundaries as multiple dislocations are absorbed and desorbed, including cases in which they may move within the boundary, increase the energy, and release it upon desorption, perhaps at sites other than those of absorption. Such studies will indeed be crucial to support continuum models for slip transfer at grain boundaries. Indeed Dewald and Curtin [105] further modified slip transmission criteria based on their simulations, which uncovered certain complexities in the process.

Processes of dislocation nucleation at bicrystal boundaries are surprisingly complex, often involving a sequence of grain boundary structure rearrangement steps prior to nucleation of dislocations into the lattice. The notion that grain boundary structure evolves during successive slip transfer events motivates development of constitutive models for behavior of grain boundaries as distinct evolving entities. Energetic pathways for structure rearrangement during processes of nucleation, absorption, and desorption form the basis of a natural link between atomistic and continuum modeling concepts. Ma and co-workers [106,107] suggested an energetic approach to modeling grain boundary penetration of dislocations, specifically based on the elastic energy of formation of misfit dislocations that remain as debris following slip penetration. However, no mechanism is proposed to account for change in GB structure after penetration. Such an activation energy barrier concept has been pursued in a recent multiscale continuum model for nanocrystalline metals by Capolungo et al. [91]. Warner et al. [108] similarly introduced a model for nanocrystalline metals that considers nucleation and absorption of dislocations, with the grain boundary dependent source strength characterized by a critical resolved shear stress on the primary system of nucleated dislocations. Suffice it to say that development of multiscale modeling approaches for coupling long range fields for arrays of curved dislocations interacting with grain boundaries is a matter of high importance to clarifying these issues for polycrystals above the scales of grain size characterizing most nanocrystalline simulations to date.

5 Modeling Effects of Impurities and Nonequilibrium Grain Boundaries

Over the last decade, most of the work on grain boundary modeling via MD simulation has focused on pure systems, largely due to the lack of accurate interatomic potentials for use in a wide range of alloys. Representing a step forward, Jang et al. [109,110], Elsener et al. [111], and Rajgarhia et al. [90] recently presented MD simulations aimed at understanding the role of dopants or impurities at grain boundaries in nanocrystalline Al and Cu. Molecular dynamics simulations by Rajgarhia et al. [90] are motivated by theoretical predictions that dopants at the grain boundaries in nanocrystalline materials can retard grain growth at elevated temperatures [112,113]. Recent results by Rajgarhia et al. [90] for a nanocrystalline Cu–Sb solid-solution alloy with 12 nm average grain diameter are presented in Fig. 5. As a first approximation, Sb is assumed to be positioned only at the grain boundaries and no attempt is made to tailor the Sb concentration at specific interfaces. Figure 5 shows two snapshots of dislocation activity during uniaxial tensile deformation at 300 K. MD simulations on Cu indicated that Shockley partial dislocations are nucleated from the grain boundaries and propagate across the grain interiors (leaving a trailing stacking fault in their wake), in agreement with previous MD simulations by Van Swygenhoven et al. (Sec. 3.3). Interestingly, grain boundary sources for partial dislocation nucleation appear to correlate qualitatively with regions of Sb at the grain boundaries; a precise quantification of the role of Sb dopant atoms is currently in progress [114].

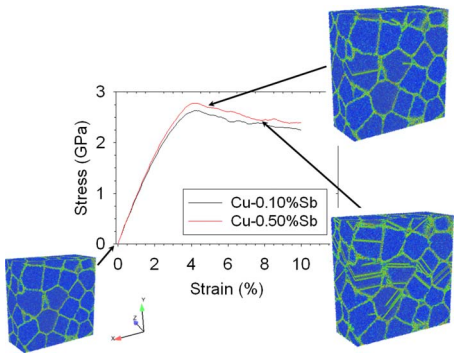

Fig. 5 Stress-strain response of nanocrystalline Cu–Sb solid-solution alloys with 0.1 at. % and 0.5 at. % Sb at the grain boundaries. Nanocrystalline samples are deformed in uniaxial tension at 300 K. Partial dislocation sources at the grain boundaries correlate qualitatively with regions of Sb concentration.

Most MD calculations to date for grain boundaries (bicrystals or polycrystals) have neglected the role of excess defects (dislocations and free volume) at grain boundaries induced by prior cold work. Ungar and co-workers [115–118] showed increasing dislocation density levels and vacancy concentrations with plastic deformation, with deformation-induced vacancy production in polycrystalline Cu greater than that in single crystal Cu. Atomistic calculations to support understanding of these measurements have been lacking, partly due to the length and time scales involved, and also to the challenges in computing heavily deformed nonequilibrium grain boundary structures using atomistic simulations, since the time scales involved in establishing these structures by reactions with lattice dislocations greatly exceed MD capabilities. Hence, some sort of biased Monte Carlo scheme is likely necessary to build the grain boundary structure and must be validated against experimentally characterized boundaries.

6 Concluding Remarks

As evident from the above discussion, atomistic simulation has provided significant insight into the role of grain boundaries in plasticity, particularly in the case of homogeneous nanocrystalline metals. Quantitative understanding related to dislocation nucleation and slip transfer reactions at grain boundaries is extremely difficult to access experimentally, representing an ideal opportunity for molecular dynamics simulation or other atomistic-level calculations. Yet, significant progress still needs to be made, primarily in the areas of extending the number of slip transfer events to realistically large numbers, modeling nonequilibrium grain boundaries (which are potentially more characteristic of GBs in heavily deformed metallic polycrystalline samples), and understanding dislocation activity in polycrystalline metals with heterogeneous compositions (e.g., impurities at grain boundaries or metallic alloys with heterophase interfaces). Progress on this front has been slowed by limitations inherent to atomistic simulation methods, such as the development of accurate, computationally-efficient interatomic potentials for alloy systems, limited length scales, and the short time scales associated with finite temperature molecular dynamics simulations. The latter limitation has motivated accelerated MD methods, as recently discussed by Derlet et al. [119], although their application to date has focused primarily on dislocation nucleation in nanoscale single crystals (nanowires) rather than metallic polycrystals.

Acknowledgment

DES is supported, in part, by the Ralph E. Powe Junior Faculty Enhancement Award from Oak Ridge Associated Universities. DLM is grateful for the support of the Carter N. Paden, Jr. Distinguished Chair in Metals Processing and the NSF under Grant No. CMMI-0758265.

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