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The role of partial mediated slip during quasi-static deformation of 3D nanocrystalline metals

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ABSTRACT

We present dislocation simulations involving the collective behavior of partials and extended full dislocations in nanocrystalline materials. While atomistic simulations have shown the importance of including partial dislocations in high strain rate simulations, the behavior of partial dislocations in complex geometries with lower strain rates has not been explored. To account for the dissociation of dislocations into partials we include the full representation of the gamma surface for two materials: Ni and Al. During loading, dislocation loops are emitted from grain boundaries and expand into the grain interiors to carry the strain. In agreement with high strain rate simulations we find that Al has a higher density of extended full dislocations with smaller stacking fault widths than Ni. We also observe that configurations with smaller average grain size have a higher density of partial dislocations, but contrary to simplified analytical models we do not find a critical grain size below which there is only partial dislocation-mediated deformation. Our results show that the density of partial dislocations is stable in agreement with in situ X-ray experiments that show no increase of the stacking fault density in deformed nanocrystalline Ni (Budrovic et al., 2004). Furthermore, the ratio between partial and extended full dislocation contribution to strain varies with the amount of deformation. The contribution of extended full dislocations to strain grows beyond the contribution of partial dislocations as the deformation proceeds, suggesting that there is no well-defined transition from full dislocation- to partial dislocation-mediated plasticity based uniquely on the grain size.

1. Introduction

Nanocrystalline (nc) materials and metallic nanolayers have received extensive research attention over the last few decades due to their superior mechanical properties (Kumar et al., 2003; Wolf et al., 2005; Meyers et al., 2006; Wang and Misra, 2011). There is general consensus that grain boundaries (GBs) and interfaces play a prominent role in deformation behavior, including strength, hardening and failure. These interfaces act as sources, sinks and barriers for dislocations leading to the Hall–Petch relationship (Hall, 1951; Petch, 1953), which states that the yield strength is inversely proportional to the square root of the grain size. When the average grain size is in the 10–40 nm range there is a transition to an inverse

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Hall–Petch effect in which the yield stress decreases with grain refinement. This transition is also attributed to GB-mediated deformation mechanisms. Initially, this transition was linked only to the average grain size, while now simulations have shown that the GB energetics also plays a fundamental role. High-energy GBs are able to accommodate deformation by GB sliding and grain agglomeration (Shan et al., 2004), while in materials with lower energy GBs, dislocation mechanisms are relatively more important (Koslowski et al., 2011; Vo et al., 2008; Lebensohn et al., 2007).

Currently, there is no such consensus on the nucleation and propagation of partial dislocations from GBs and their impact on deformation twinning and hardening. While strain-hardening arises from a loss of dislocation mobility due to the interaction with the forest dislocations in coarse-grained polycrystals and single crystals, hardening in nc metals has been linked to the intrinsic stacking fault energy, γ_{sf}. Yamakov et al. (2004) observed in atomistic simulations that in materials with high γ_{sf}, such as Al, a trailing partial is emitted after the leading partial, forming an extended full dislocation. Conversely, in materials with low γ_{sf}, like Au and Ag, the trailing partial does not nucleate and the stacking fault left behind by the leading partial extends over the entire grain. The increase in hardening is attributed to the lack of emission of trailing partials in the latter case.

Transmission electron microscopy (TEM) experiments by Chen et al. (2003) confirmed the presence of deformation twinning created by the nucleation of leading partial dislocations from GBs in nc Al. In their work (Chen et al., 2003) stacking faults are explained using a line tension approximation by comparing the critical shear stress needed to nucleate a dislocation and the corresponding critical length with the average grain size. Yamakov et al. (2004) also suggest that the critical size criterion is related to the stacking fault width relative to the grain size. Chen et al. and Yamakov et al. reported that the transition from full dislocation dominated- to partial dislocation dominated deformation occurs at a critical grain size that is inversely proportional to the γ_{sf}. Recent experiments in nc Pd (Ivanisenko et al., 2009) observed extensive full dislocation activity at large applied strain. In addition, recent molecular dynamics (MD) and dislocation dynamics simulations suggest that assuming a dependency on γ_{sf} may not be enough (Frøseth et al., 2004; Hunter et al., 2011, 2013). The ability to nucleate the trailing dislocation to form an extended partial depends on the unstable stacking fault energy (γ_{usf}), the applied strain, and the strain rate.

In this paper we perform quasi-static simulations of the evolution of dislocations using a phase field dislocation dynamics (PFDD) approach (Koslowski et al., 2002). We focus on the nucleation and evolution of partial dislocations in grain structures with grain sizes in the range of 10–50 nm. To this end, we incorporate the material gamma surface (Vitek, 1968) calculated with atomistic simulations (Lee et al., 2011) into the PFDD model to account for dislocations dissociating into partials in Al and Ni. GB mediated deformation mechanisms, such as grain boundary sliding (Koslowski et al., 2011), that become of importance in nc structures with grain sizes below 10 nm or at high temperatures are not included in the present work. The comparison of Al with Ni shows that the gamma surface has a large impact on dislocation behavior. The high $\gamma_{sf}/\mu b$ in Al enforces the stacking fault ribbon between the leading and trailing partials to be narrower than in Ni. The grain size influences the relative density of partial and extended full dislocations with initially more extended full dislocations in grain structures with larger grain size. Our simulations show that the contribution to strain of extended full dislocations grows beyond the contribution of partial dislocations at higher applied strain. This tendency was observed in atomistic simulations that show that the density of partial dislocations reaches a plateau (Vo et al., 2008) or decreases (Tucker et al., 2012) while the density of extended full dislocations increases monotonically.

This paper is organized into the following sections. Section 2 describes the formulation of the PFDD model including the implementation of the gamma surface, the strain-controlled loading condition and the GB structure. In Section 3, we apply our method to investigate effects of the gamma surface, grain size and strain rate on dislocation behavior. In Section 4, we present a summary and concluding remarks.

2. Numerical method

In the PFDD approach, dislocations are represented by a set of phase field variables $\xi^{\alpha}(\boldsymbol{r})$. Each phase field is assigned to one of the 12 slip systems, α, in face-centered cubic (fcc) metals. An integer jump on the value of $\xi^{\alpha}(\boldsymbol{r})$ in the slip plane indicates the location of a dislocation. The plastic strain $\epsilon^{p}_{ij}(\boldsymbol{r})$ is related to the phase fields through (Koslowski et al., 2002)

$$\epsilon^{p}_{ij}(\boldsymbol{r}) = \sum_{\alpha}^{12} \frac{1}{2}\xi^{\alpha}(\boldsymbol{r})(b^{\alpha}_{i}m^{\alpha}_{j} + b^{\alpha}_{j}m^{\alpha}_{i})\delta_{\alpha}, \tag{1}$$

where $\boldsymbol{m}^{\alpha}$ is the slip plane normal, $\boldsymbol{b}^{\alpha}$ is the Burgers vector and δ_{α} is a Dirac delta function confining the slip on the slip plane. The phase fields can be related to local and average quantities such as strain, stress and dislocation density. The local strain can be calculated using the isotropic elastic Green's function, $G(\boldsymbol{r})$, (Koslowski et al., 2002; Mura, 1987) as

$$\epsilon_{ij}(\boldsymbol{r}) = \bar{\epsilon}_{ij} - C_{klmn}\epsilon^{p}_{mn,\,l}(\boldsymbol{r}) * \frac{1}{2}(G_{ik,j}(\boldsymbol{r}) + G_{jk,i}(\boldsymbol{r})), \tag{2}$$

where $\bar{\epsilon}$ is the homogeneous part of the strain, C_{klmn} are the components of the stiffness tensor and $*$ represents the convolution operator. In strain-controlled deformation, $\bar{\epsilon}$ equals the applied strain $\epsilon^{\mathrm{applied}}$, while in stress-controlled deformation $\bar{\epsilon}$ follows (Lei and Koslowski, 2011)