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The influence of dislocation climb on the mechanical behavior of polycrystals and grain size effect at elevated temperature

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ABSTRACT

The mechanical behavior of a polycrystalline aluminum in tension was modeled using a climb-assisted discrete dislocation dynamics (DDD) technique. Special focus was on how dislocation climb influences the flow stress of the polycrystalline aluminum with regard to selected grain sizes at elevated temperature. A periodical representative cell (PRC) consisting of given number of grains was used in the simulations. Results showed that, at the high temperature considered, dislocation climb plays an important role in defining the mechanical behavior of the polycrystalline crystal. Specifically, dislocation climb decreases significantly the flow stress and hardening rate while increases the dislocation density by relieving the dislocation pile-ups against the grain boundaries (GBs). In addition, the grain size effect on the yield stress of polycrystalline aluminum is significantly weakened by dislocation climb, especially when the grain size falls in the range of submicron. Another interesting result is that, at high temperature, when both dislocation climb and glide are considered, the grain size effect seems to be insignificant with regard to the applied strain rate, although the strength of material increases with enhanced loading rate.

1. Introduction

With rapid development of micron/nanometer technology, small sized specimens or structures are extensively used in various NEMSs/MEMSs. The size effect introduced by decreasing specimen size has become a hot topic in both academia and industry. Unlike plastic deformation behavior of macro-sized specimens, the plastic deformation of micron/submicron-sized specimens is usually size-dependent, i.e. the smaller is the stronger. This size effect has been captured by several typical micromechanical tests, such as thin wire torsion (Fleck et al., 1994; Dunstan et al., 2009; Liu et al., 2013), thin film tension (Espinosa et al., 2004), and micro/nano pillars compression or tension (Uchic et al., 2004; Greer et al., 2005; Kim et al., 2012), where the strength of micro-sized specimens follows a power-law relation $\sigma \propto D^{-n}$, with D being the exterior characterize size (Dunstan and Bushby, 2014). In addition to the specimen size, various interior microstructural sizes, such as grain size of polycrystals (Hall, 1951; Petch, 1953), layer thickness of multilayer (Misra et al., 2005), twin thickness of nano-twinned metals (Lu et al., 2009), are also shown to strongly influence the strength of materials and follow a similar power-law relation $\sigma \propto d^{-n}$, with d being the interior characterize size. Therefore, a power scale law $\sigma \propto l^{-n}$ seems to be able

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to describe both specimen size effect and microstructural size effect (Greer and DeHosson, 2011). However, there may be significant differences in the underlying mechanisms in these size effects, which require further investigation.

Physically, size effect on the mechanical behavior of materials stems from exterior and interior constraints (Arzt, 1998; Greer and DeHosson, 2011; Fan et al., 2011, 2012; Zhu et al., 2013). Hall (1951) and Petch (1953) first studied the influence of interior GB constraint on the strength of polycrystals, and used a power law $\sigma = \sigma_0 + kd^{-n}$ (usually called as H–P relation) to relate the strength σ of polycrystalline metals to the grain size d, with σ_0 being the friction stress for mobile dislocations or yield stress for materials with sufficiently large grain sizes, n the scaling exponent and k the H–P slope. In this well-known relation, both n and k characterize the intensity of grain size effect, which are closely related to the grain boundary (GB) constraint effect on dislocation motion (Li et al., 2009). By assuming that GB is rigid wall for gliding dislocations and only one single-ended/double-ended pile-up exists in an isolated grain, it can be deduced that the power exponent n equals to 0.5 (Hall, 1951; Petch, 1953; Hirth, 1972). However, a series of experiments and simulations indicated that there are some uncertainties in the Hall–Petch exponent n, i.e. within possible ranges between 0 and 1 (Dunstan and Bushby, 2013), 1/3 and 1 (Baldwin, 1958; Kocks, 1970; Flinn et al., 2001), 0.5 and 1 (Hirth, 1972; Biner and Morris, 2002; Ohno and Okumura, 2007; Li et al., 2009), 0.82 and 1.25 (Evers et al., 2004), 1.19 and 1.50 (Borg, 2007), or 0.5 and 1.5 (Balint et al., 2008). These deviations from the classical Hall–Petch relation with $n = 0.5$ perhaps originate from a number of differences including initial dislocation density (Balint et al., 2008), grain boundary constraint (Li et al., 2009) and high-order stress/slip gradient near GBs (Ohno and Okumura, 2007). For different GB structures, dislocation pile-up interacts with GBs by different manners, including dislocation pinning, reflection, absorption, emission and transmission (Shen et al., 1986, 1988). Evidently, the "rigid-GB" assumption made by many researchers may over-estimate the constraint effect of GB on dislocation motion (Li et al., 2009), which may lead to both over-estimated grain size effect and strain hardening rate of polycrystals. Recent experimental and computational observations showed that the build-up of long dislocation pile-ups near the compliant GBs is effectively prevented due to absorption or transmission of dislocations at GBs (Li et al., 2009; Danas et al., 2010; Fan et al., 2011, 2012; Abuzaid et al., 2012). As a result, strong back-stress on the dislocation sources and follow-up dislocations induced by dislocation pile-ups is relieved, rendering the scaling exponent n to deviate from 0.5. Besides dislocation absorption and transmission at the compliant GBs, several other dislocation relaxation mechanisms, including dislocation cross-slip (Brown, 1997; de Sansal et al., 2009) and dislocation climb (Ayas et al., 2014; Danas and Deshpande, 2013), can also effectively prevent the build-up of long dislocation pile-ups against GBs (Ayas et al., 2012) and significantly change the extent of the size effect. Unlike dislocation glide and cross-slip, climb of edge dislocations requires vacancy diffusion, thus significant dislocation climb can only be readily observed at temperatures above $0.3T_m$, where T_m is the melting temperature of materials (Ayas et al., 2014). Recent uniaxial compression of Indium micro-pillars at room temperature by Lee et al. (2011) exhibited much weaker size effect than that of Au (Greer et al., 2005), Ni and Ni_3Al (Uchic et al., 2004). A possible explanation is that the occurrence of dislocation climb weakens the size effect as room temperature is above $0.3T_m$ for lower melting-point Indium. In addition, there is also some circumstantial evidence that elevated temperature can weaken the dependence of flow stress on grain size for several polycrystalline metals (Singh, 2004; Ono et al., 2003; Atwell et al., 2012; Hagihara et al., 2013). Although these experiments showed directly or indirectly that elevated temperature can influence the size effect, there seem few studies on how dislocation climb at high temperature influences the grain size effect (i.e. H–P relation).

In addition to experiments, DDD simulation, which treats plastic deformation as the evolution of a large number of dislocations, has been used in capturing size effect and its underlying mechanisms at micron/submicron scale. To study the H–P effect of polycrystals and its underlying mechanisms, a series of DDD simulations have been performed, including 2D-DDD (Biner and Morris, 2002, 2003; Balint et al., 2005, 2006a, 2008; Li et al., 2009; Fan et al., 2011; Ahmed and Hartmaier, 2010), 2.5D-DDD (Lefebvre et al., 2005, 2007) and 3D-DDD (Espinosa et al., 2006; Ohashi et al., 2007; de Sansal et al., 2009; Fan et al., 2012). Several factors influencing the mechanical behavior of polycrystals and its grain size effect (H–P relation) have been carefully investigated, including the number of slip systems, the grain arrangement, the dislocation source density and the range of grain sizes (Balint et al., 2005, 2006a, 2008; Biner and Morris, 2002, 2003), the density of grain boundaries (Kumar et al., 2009), dynamic recovery at GBs and GB diffusion (Ahmed and Hartmaier, 2011), dislocation penetrating GB (Li et al., 2009; Kumar et al., 2010; Fan et al., 2011, 2012), dislocation curvature (Ohashi et al., 2007) and cross-slip (de Sansal et al., 2009). However, most of these simulations limit the dislocation motion on their fixed slip planes, except the modeling of GB-dislocation climb by Ahmed and Hartmaier (2011). More recently, several schemes have been developed to incorporate dislocation climb into the 2D-DDD and 3D-DDD simulations (Keralavarma et al., 2012; Davoudi et al., 2012; Danas and Deshpande, 2013; Ayas et al., 2012, 2014; Ahmed and Hartmaier, 2011; Haghighat et al., 2013; Gao et al., 2011, 2013). By a climb-enabled DDD method, Davoudi et al. (2012) studied the response of an aluminum thin film under uniaxial tension, showing that fewer pile-ups form against the passivation layer and the number of dislocations in formed pile-up also decreases due to dislocation climb. Climb-assisted DDD simulation on smooth and passivated single crystal films by Ayas et al. (2012, 2014) shows that dislocation climb significantly changes the size effect and Bauschinger effect of thin film, since climb breaks up the dislocation pile-ups against passivated surfaces. From these simulations it seems that dislocation climb could break up the formation of long dislocation pile-ups against GBs, thus significantly influencing the grain size effect on the strength of polycrystalline materials in a high temperature environment. To our best knowledge, studies of the influence of dislocation climb on grain size effect or Hall–Petch relation are lacking in published literature.

The objective of this work is to perform a climb-enabled 2D-DDD simulation on the tensile response of a polycrystalline aluminum. The emphasis is on the influence of dislocation climb on the grain size dependent responses and its underlying mechanisms. This paper is organized as follows: Section 2 gives a brief introduction to the climb-enabled 2D-DDD method