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Grain size effects on dislocation and twinning mediated plasticity in magnesium

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ABSTRACT

Grain size effects on the competition between dislocation slip and $\{10\bar{1}2\}$-twinning in magnesium are investigated using discrete dislocation dynamics simulations. These simulations account for dislocation–twin boundary interactions and twin boundary migration through the glide of twinning dislocations. It is shown that twinning deformation exhibits a strong grain size effect; while dislocation mediated slip in untwinned polycrystals displays a weak one. This leads to a critical grain size at 2.7 μm, above which twinning dominates, and below which dislocation slip dominates.

Due to the low symmetry of hexagonal closed packed (HCP) crystals, both dislocation mediated slip and twinning are important deformation modes. It has been reported from textured polycrystalline magnesium (Mg) experiments that both twinning and dislocation plasticity are grain size dependent. The extent of the grain size effect is strongly influenced by the texture orientation. This dependence can be characterized into three groups [1]: (1) weak grain size effects for deformation by compression twinning, pyramidal and prismatic slips [1,2]; (2) intermediate size effects for basal slip and tension twinning [2–4]; and (3) strong size effects for predominant tension twinning deformation [5–7]. For dislocation slip, recent discrete dislocation dynamics (DDD) simulations showed that grain size effects are governed by three factors [8]: dislocation Peierls stress, dislocation source strength, and grain boundary strength. However, to date, the effects of grain size on twinning deformation are still not well understood.

The grain size also influences the expected predominant deformation mode. In AZ31, Barnett et al. [9] showed that the stress–strain response changes from a concave shape into a convex shape when the grain size is on the order of 3 to 4 μm. This is a result of the absence of twinning deformation in the polycrystals with smaller grain sizes. Furthermore, Lapovok et al. [10] suggested that there exists a critical grain size below which twinning is suppressed, and this critical grain size is 3–4 μm for ZK60. More recently, in pure Mg polycrystals, Li et al. [7] showed that this critical grain size is about 2.7 μm, and for smaller grains dislocation mediated plasticity dominates. Barnett [11] rationalized the existence of such a critical grain size below which twinning deformation is suppressed by suggesting that the sensitivity of twinning to grain size is greater than that for dislocation mediated plasticity. This is also in agreement with the experimental observations in FCC, BCC and HCP materials [12].

In the current work, to quantify the grain size effects on twinning deformation in Mg, the mechanical behavior of twinned polycrystals is modeled using three-dimensional discrete dislocation dynamics simulations. All simulations are performed using the DDD code ParaDiS [13,14]. The inset in Fig. 1 shows the cross-section of the 3D cubical simulation cell with an edge length *d*. Periodic boundary conditions (PBCs) are employed along all three directions. The six surfaces of the simulation cell are considered to be grain boundaries (GBs). This simulation cell is a representative grain in a bulk polycrystal with identical orientation in each grain, which resembles the strong texture in Mg and its alloys [9]. A $\{10\bar{1}2\}$ tension twin lamella of thickness d_t is introduced at the center of the grain, and the grain size is varied between $d = 0.81$ and 3.25 μm, with $d_t = d / 10$ in all simulations.

The GB is treated as an interface barrier to dislocation motion [15–17]. As dislocations are gliding towards the GB, they will be trapped. As a result, subsequent dislocations pile up at the GB, leading to an increased shear stress on the leading dislocation. Once this shear stress exceeds the GB barrier strength, the leading dislocation can be transmitted across the GB. Due to the PBCs, this dislocation would be transmitted back into the simulated grain in a periodic manner. Note the image force associated with GBs is not considered, since no

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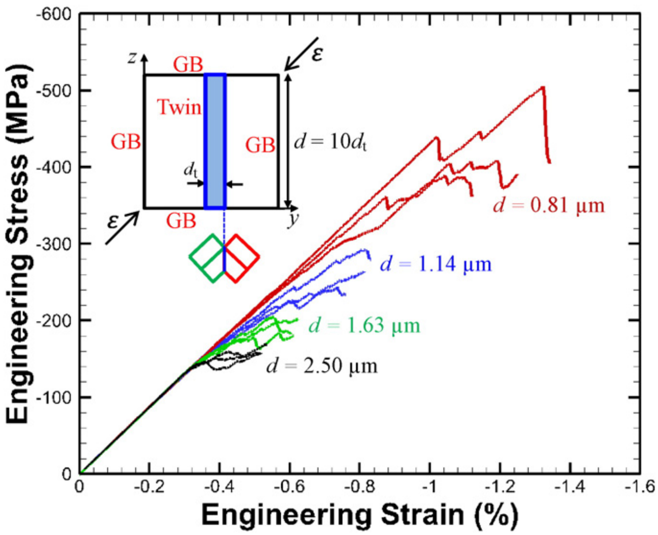

Fig. 1. Stress–strain responses of twinned polycrystals having different grain sizes. The inset shows a cross-section on the *yz* plane of the simulation cell having edge length *d*. A twin lamella having thickness $d_t = 0.1d$ is introduced at the center of the grain. Periodic boundary conditions are applied along all three directions.

misorientation is introduced. Further details regarding the dislocation–GB interactions were discussed elsewhere [8,18]. In the current simulations, the GB barrier strength is $\tau_{GB} = 580$ MPa, which was shown to agree well with experimental results of textured polycrystalline ZK60 [18].

For dislocation interactions with $\{10\bar{1}2\}$ tension TBs, we utilized the interaction model we recently proposed in Ref. [18]. In this model, geometric and power dissipation rules were specified to identify the dislocation interaction outcomes (i.e. twinning, residual, and transmitted dislocations). All the possible incident dislocations ($\langle a \rangle$, $\langle c \rangle$ and $\langle c + a \rangle$) on any slip plane (basal, prismatic, pyramidal I and pyramidal II planes) were considered. In addition, the TB migration induced by gliding twinning dislocations is also accounted for here.

Initially, Frank–Read (FR) dislocation sources of length $l_{src} = 800b$ were randomly distributed within the simulation cell, in both the grain and twin, with a total initial density of $\rho_{src} = 5 \times 10^{12}$ m^{-2}. Note the FR source length is usually chosen according to the mean free slip path of dislocation sources controlled by the dislocation source density [15]. The slip system of each FR source was chosen randomly to be either an $\langle a \rangle$ Burgers vector on the basal, prismatic or pyramidal I planes; or $\langle c + a \rangle$ Burgers vector on pyramidal II planes. These slip systems have been reported to typically produce most of the dislocation-mediated plasticity in Mg [19–21]. The dislocation mobility for each dislocation type is a bi-linear function of stress, which was fitted to molecular dynamics (MD) results of Mg [18,22,23]. The experimentally measured Peierls stresses for dislocations on the basal (0.52 MPa [24]), prismatic (39.2 MPa [25]), and pyramidal (105 MPa [26]) planes were used, which are also in good agreement with MD estimates [22,23,27]. Recent MD simulations have also shown that twinning dislocations (dislocations gliding on the twin boundary) are highly glissile [28,29], but the exact mobility law has not been reported yet. In the current simulations, the mobility and Peierls stress for twinning dislocations were set to equal those for basal dislocations, as a first approximation. The basic Mg parameters used in the current simulations include: shear modulus, $G = 17$ GPa; Poisson ratio, $\nu = 0.29$; magnitude of $\langle a \rangle$ dislocation Burgers vector, $b = 0.325$ nm; axial ratio, c/a = 1.6236; and mass density, $\rho = 1738$ kg/m^3.

Tension twins occur under two typical strain paths, namely, contraction perpendicular to the *c*-axis and extension parallel to the *c*-axis. To mimic this, thus, a uniaxial compressive load with a constant strain rate of $\bar{\varepsilon} = -5000$ s^{-1} was imposed at a 45° angle counterclockwise from the positive *y*-axis (i.e. contraction perpendicular to the *c*-axis of the grain (matrix)), as observed in the inset in Fig. 1. Since the computational burden of DDD simulations is very heavy, especially for the large samples, the relatively high strain rate could accelerate our simulations.

The engineering stress–strain responses for a subset of the simulated twinned polycrystals having different grain sizes, are shown in Fig. 1. Due to the heavy computation burden, each simulation was performed up to a plastic strain of −0.2%. It is observed that the yield strength increases significantly with decreasing grain size. In addition, a significant amount of scatter is seen on the curves for a given grain size, as a result of the random assignments of the dislocation source positions, slip planes and Burgers vectors.

The yield strengths from all the current DDD simulations for the twinned Mg polycrystals are shown in Fig. 2 as a function of grain size. To further characterize the grain size effects on twinning, the yield strengths as predicted from simulations of Mg polycrystals with no twin lamella (mimicking a suppressed twinning case) are also shown. It is observed that the strengths from the simulations with twinning or with suppressed twinning both separately display a power law relationship with grain size ($\sigma_y \propto d^{-n}$). The best fitting exponent from the suppressed twinning simulations is 0.29, while that for the twinning simulations is 0.75. This indicates that when twinning is suppressed, the grain size effect for dislocation slip only is significantly weaker than that when both dislocations and twinning are active. We can see the twinning deformation exhibits a stronger grain size effect than dislocation slip, which agrees well with the experimental observations [9, 12]. Note that twinning plasticity is assisted by TB migration (or twin growth), which is accommodated in the current simulations by the glide of twinning dislocations on the twin boundary. These twinning dislocations are produced from matrix dislocation interactions with the twin boundary. In addition, it should be noted that although twin nucleation from GBs has not been accounted for here, it is grain size independent as indicated by EBSD observations showing that the twin thickness and fraction of twinned grains are weakly controlled by the grain size [30].

It is also interesting to observe from Fig. 2 that the power laws fitted from the simulations with twins or suppressed twins intersect at a critical grain size 2.7 μm. Below this critical grain size, dislocation slip would be expected to be favorable, since it commences at a low applied stress. On the other hand, twinning mediated plasticity is expected to dominate above this critical grain size. This predicted critical grain size

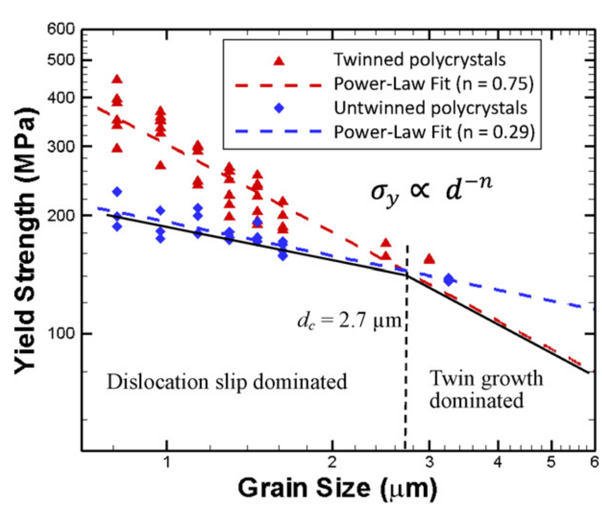

Fig. 2. Yield strength as a function of grain size from simulations of twinned and untwinned polycrystals.