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Orientation influence on grain size-effects in ultrafine-grained magnesium

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Abstract: The mechanical behavior of ultrafine-grained magnesium was studied by discrete dislocation dynamics (DDD) simulations. Our results show basal slip yields a strong size effect, while prismatic and pyramidal slips produce a weak one. We developed a new size-strength model that considers dislocation transmission across grain boundaries. Good agreement between this model, current DDD simulations and previous experiments is observed. These results reveal that the grain size effect depends on 3 factors: Peierls stress, dislocation source strength and grain boundary strength.

***Keywords**:* Discrete dislocation dynamics; Size-effect; Ultrafine-grained magnesium

As the lightest structural metal, magnesium (Mg) and its alloys are utilized in many applications in automotive, aerospace and other industries. Due to the low symmetry of hexagonal closed packed (HCP) crystals, Mg and its alloys display a strong anisotropic behavior [1], which was also observed in Mg polycrystals having strong texture. Size-affected strengthening in polycrystalline Mg can be characterized into three groups according to the texture [2]: (1) weak grain size-effects for basal textured polycrystals tested in tension with the *c*-axis under contraction, resulting in deformation by compression twining, pyramidal and prismatic slips [2, 3]; (2) intermediate size-effects during the deformation of weak/randomly textured polycrystals, deforming through basal slip and tension twining in a fraction of the grains [3-5]; and (3) strong size-effects in basal texture tested in compression with the *c*-axis under tension, which leads to predominate tension twining deformation [6-8]. The intensities of the orientation dependent size-effects are similar to FCC (strong effect) and BCC (weak effect) materials [9], and were attributed to the variations in

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the Peierls stress [10]. However, this conflicts with the Hall-Petch relationship, which assumes a constant power law exponent of –0.5 that is independent of the Peierls stress. That is to say, the Hall-Petch relationship does not address the effect of orientation or texture directly.

Here we conduct a parametric study on the influence of orientation on the grain size-effects of ultrafine-grained Mg using three-dimensional discrete dislocation dynamics (3D-DDD) simulations. In particular, all simulations were performed using the ParaDiS code [11, 12]. Fig. 1(a) shows the representative cubical simulation cell, having edge length *d*, with periodic boundary conditions (PBCs) along the three directions. All six surfaces of the simulation cell are considered as representative grain boundaries (GBs). The cell size is varied such that, 800 nm $\leqslant d \leqslant$ 1.5 μm. The basic Mg properties chosen for the simulations are: shear modulus, G = 17 GPa; Poission ratio, ν = 0.29; magnitude of the <*a*> dislocation Burgers vector, b = 0.325 *nm*; axial ratio, *c/a* = 1.6236; and mass density, ρ = 1738 kg/m^3.

In polycrystalline Mg, twinning was shown to be strongly dependent on grain size. In AZ31, Barnett et al. [13] showed that the percentage of twinned grains decreases with decreasing grain size. The stress-strain response was also shown to change from a concave shape to a convex one when the grain size is ~4 μm. This is a direct indication of the absence of twinning deformation for such small grain sizes. Lapovok et al. [14] also pointed out that the transition grain size below which twinning is absent is 3~4 μm for ZK60. More recently, in pure magnesium polycrystals, Li et al. [8] revealed that the transition grain size is about 2.7 μm, below which dislocation-slip dominates. A rational for this transition from twinning to dislocation-slip was discussed in [15]. Many studies show that twinning exhibits a stronger grain size-effect than dislocation-slip in FCC, BCC and HCP materials [16]. That's to say, the critical stress to activate twinning increases faster with decreasing grain size. As a result, there exists a transition grain size, below which dislocation-slip dominates. This transition grain size is ~3 μm, which is consistent with the range of grain sizes studied here. Subsequently, the current DDD simulations not accounting for twinning should adequately capture the main deformation mechanism in the

considered grain size regime.

The grain orientation was chosen such that the *c*-axis makes a 46.85° angle with respect to the *z*-axis of the simulation cell (see Fig. 1(a)). Using this representative grain model, the orientation of each grain in the bulk materials is identical, which corresponds to a strong basal texture in polycrystalline Mg samples. However, the misorientation between the *a*-axes in neighboring grains is not accounted for here. Nevertheless, in the current simulations, the GB is introduced as an artificial interface/barrier to dislocation motion. Dislocations trapped at the GB can be transmitted into neighboring grains if the shear stress on the dislocation exceeds the GB strength. This approximation was successfully adopted by DDD simulations of polycrystalline FCC materials [17]. The GB transmission strength is largely governed by the misorientation angle [18-20], θ_{mis}, which can be approximated as $\tau_{GB} = 2Gsin^2(0.5\theta_{mis})$. Experimental characteristics of as-received pure Mg shows that the majority of GBs are low angle GB, while for ECAP Mg samples the fraction of high angle GBs exceeds that of low angle GB after the 8th pass [21]. Thus, in the current simulations, we choose an intermediate case with a nominal misorientation angle, $\theta_{mis} = 15°$, and nominal GB transmission strength, $\tau_{GB} = 580$ MPa.

Initially, Frank-Read (FR) dislocation sources of length $l_{\mathrm{src}} = 800b$ were randomly distributed within the simulation cell, with an initial dislocation density of $\rho_{\mathrm{src}} = 5\times10^{12}$ m^{-2}. The slip system of each FR source was chosen randomly to have either <*a*> Burgers vector on the basal, prismatic or pyramidal I planes or ⟨*c*+*a*⟩ Burgers vector on pyramidal II planes. These slip systems typically produce most of the dislocation-mediated plasticity in deformed Mg crystals [22, 23], and have been commonly chosen in previous crystal plasticity and DDD simulations [12, 24]. To account for the possible statistics of dislocation distributions, each grain size was simulated using at least three different initial dislocation distributions. The experimentally measured Peierls stresses for dislocations on the basal (0.52 MPa) prismatic (39.2 MPa) and pyramidal (105 MPa) planes were prescribed in the simulations [25]. Finally, since the *c*-axis resides in the *yz* plane, deformation under four representative loading orientations was investigated: 1) along (010) direction, or

y loading; 2) along (001), or z loading; 3) along (011), or yz loading; 4) along $(01\bar{1})$, or $y\bar{z}$ loading. Thus, deformation is expected to be dominated by basal slip during y and z loading, prismatic slip during yz loading, and pyramidal slip during $y\bar{z}$ loading. The strain rate imposed in all simulations was $\dot{\varepsilon}$ = –5000/s.

The compressive engineering stress-strain responses of d = 1.3 μm grains loaded in the four orientations are shown in Fig. 1(b). The responses of single crystal simulations are also shown for comparison. In Figs. 1(c)-(f), the effective plastic strain contours showing the active slip traces from bulk single crystal simulations are shown. It should be noted that while twinning was reported in bulk single crystal experiments [26, 27], it is not accounted for in current DDD simulations due to difficulties in incorporating twinning plasticity within DDD. Nevertheless, the single crystalline simulations are beneficial to revealing the dislocation mechanisms under different loading directions. Besides, comparing these simulations with the polycrystalline simulations qualitatively addresses the effect of GBs on dislocation mediated plasticity in ultrafine-grained Mg.

The single crystal stress-strain responses under y or z uniaxial loadings are effectively similar since these directions make 46.85° and 43.15° angles with respect to the basal plane. Thus, plasticity is mostly facilitated by basal slip, as evidenced by the effective plastic strain counter in Figs. 1(e) and 1(f). Furthermore, the stress-strain responses of these two orientations are distinct with multiple stress drops followed by linear elastic loading intervals. These drops could be linked to source-nucleation [18], since basal dislocations have a low Peierls stress and high mobility. Another possible reason is PBCs, which might lead to spurious dislocation annihilation. However, the spurious annihilation is suppressed in polycrystal simulations due to the presence of GBs. On the other hand, under yz and $y\bar{z}$ loadings, the Mg single crystal exhibits higher yield stresses. In the yz case, the loading axis is nearly perpendicular to the c-axis, and plasticity is predominately accommodated by prismatic slip, as shown in Fig. 1(d). In the $y\bar{z}$ case, the loading axis nearly coincides with the c-axis and plasticity is predominantly accommodated by pyramidal II slip. Recent HCP 2D-DDD simulations are qualitatively consistent with the current single crystal simulations [28].

In addition, for polycrystals, similar increases in the strength as a function of loading orientation are observed. Finally, while all the single crystal simulations show no hardening, a strong hardening is observed from all the polycrystal simulations. This is a direct consequence of GB strengthening.

Fig. 2 shows the yield stress as computed from current DDD simulations versus grain size for the different loading orientations. In order to investigate the orientation-dependence of the size-effect intensity a power law $\sigma_y \propto d^{-n}$ is used to fit the results. The prismatic and pyramidal slip dominated orientations exhibit a weak grain size-effect with an exponent n = 0.2, which agrees well with experimental results [2]. On the other hand, the basal slip orientation demonstrates a much stronger size-effect with an exponent n = 1.16, which is higher than the 0.5 exponent reported experimentally [3]. This might indicate that the current initial dislocation density (5×10^{12} m^{-2}) is much lower than that in experiments [29], which would lead to a stronger size-effect.

Experimental studies have suggested that the orientation influence is mainly driven by the anisotropy in the Peierls stresses [2]. To investigate this, the Peierls stress ($\sigma_0 = \tau_0/P$, where τ_0 is the Peierls stress, and P is the Schmid factor) was subtracted from the yield stress to formulate a "Hall-Petch" power law relationship in the form $(\sigma - \sigma_0) \propto d^{-n}$, as shown in Fig. 2(b). It is clear that the exponent for pyramidal slip changes from 0.2 to 0.52, and for prismatic slip from 0.22 to 0.42. These exponents are still considerably lower than that for basal slip, conveying that anisotropy in the Peierls stress cannot alone explain the orientation dependence, and other factors influencing grain size-effects must be accounted for.

Many GB modeling studies showed that dislocation transmission across GBs plays an important role in the overall mechanical behavior [18-20, 30], which is also often experimentally observed [31, 32]. Therefore, the polycrystal yielding can be characterized by two conditions: (a) the activation of pre-existing dislocation sources (grain yielding); and (b) dislocation transmission across GB into neighboring grains due to dislocation pileups (GB yielding). The latter can be expressed mathematically as:

$$k\tau_y = \tau_{GB} \tag{1}$$

where τ_y is yield shear stress or critical resolved shear stress (CRSS), and k is the number of dislocations in the pileup. Furthermore, a dislocation source at the grain center will experience a back stress τ_b from dislocation pileups at the GB. Thus, the shear stress required to activate a source can be expressed as

$$\tau_{src} = \tau_y - \tau_b \tag{2}$$

where τ_{src} is the dislocation source activation strength. In the following, we assume that the length of the dislocation pileups is considerably smaller than the grain size, so that the distance between dislocation source and any pileup dislocation is approximately $d/2$. Thus, the back stress from the pileups is

$$\tau_b = 4kD/d \tag{3}$$

where $D = Gb/2\pi(1-\nu)$. Solving equations (1-3), the yield strength can be expressed as:

$$\tau_y = \frac{1}{2}\left(\tau_{src} + \sqrt{\tau_{src}^2 + 16D\tau_{GB}/d}\right). \tag{4}$$

Equation (4) is a dislocation pileup and transmission model that accounts for the strength of pre-existing sources as well as the GB strength. When τ_{src} is small (i.e. large grains) or τ_{GB} is high (high angle GB),

$$\tau_y \approx \tau_{src} + 2\sqrt{D\tau_{GB}}d^{-0.5}, \tag{5}$$

which is equivalent to the traditional Hall-Petch relationship. On the other hand, if $\tau_{GB} = 0$, then the yield strength is governed only by the strength of pre-existing dislocation sources, $\tau_y = \tau_{src}$, which is the case of single crystals. In general, both τ_{src} and τ_{GB} should be accounted for adequately. The dislocation source strength can be expressed by [33, 34]

$$\tau_{src} = \tau_0 + \beta Gb\sqrt{\rho_{dis}} + \alpha Gb/\bar{\lambda}_{max} \tag{6}$$

where $\bar{\lambda}_{max}$ is the statistically maximum dislocation source length, which is also a function of grain size [17]. Thus, the grain size-effect depends on three factors: Peierls stress, dislocation source activation stress, and GB strength. $\bar{\lambda}_{max}$ and its standard deviation for polycrystalline materials were given by [17]

$$\bar{\lambda}_{max} = \int_0^{\frac{d}{2}} P(\lambda_{max})\, \lambda_{max}\ d\lambda_{max} \tag{7}$$

$$\sigma_{\lambda_{max}} = (\int_0^{\frac{d}{2}} P(\lambda_{max}) \lambda_{max}^2\, d\lambda_{max} - \bar{\lambda}_{max}^2)^{1/2}. \tag{8}$$

Here, $P(\lambda_{max}) = n\frac{4(d-2\lambda_{max})}{d^2}(1-\frac{(d-2\lambda_{max})^2}{d^2})^{n-1}$, the number of dislocation pining points n = 2 Integer[$r_{mob}\rho_{src}V/l_{\mathrm{src}}$], and r_{mob} is the percentage of mobile dislocations. A similar model was also used for single crystalline magnesium [35].

The proposed model in equations (4), (6), (7) and (8) is plotted in Fig. 3 versus the current DDD simulations and some published experimental results. In the model, the following parameters were used [36]: $\beta = 0.35$; $\alpha = 0.6$; and r_{mob} = 1/12, 1/6, and 1/4 for basal, prismatic and pyramidal slips, respectively. It is clear from Fig. 3(a) that the proposed dislocation pileup and transmission model agrees well with the current DDD simulations. Both DDD and the model show a stronger size-effect for basal slip. In Fig. 3(a), the single-arm source model for polycrystalline materials (i.e. only equations (6)-(8) without consideration of dislocation transmission across GBs) [17], is also shown. It is clear that this model on its own fails to capture the grain size-effects, indicating that dislocation transmission across GBs plays an important role in the response of ultrafine-grained Mg and cannot be ignored. Fig. 3(b) shows that the current model and DDD simulations agree well with experimental predictions, with the exception of a single experimental data point for grain size below 200 nm. This could be due to the deformation mechanisms other than dislocation pileup and transmission in such size regime, like GB gliding [6] and stress-driven grain growth [37].

In summary, discrete dislocation dynamics simulations were employed to investigate the orientation and grain size-effects in ultrafine grained Mg crystals. The grain size-effects were shown to be strongly orientation dependent. Strong size-effects were observed for basal slip, while weak ones for prismatic and pyramidal slips. A new dislocation pileup and transmission model was also developed. This model shows that the grain size-effect is a function of three factors: Peierls stress, dislocation source strength, and grain boundary strength. Finally, good agreement among this model, current DDD simulations and published experimental results was observed.

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