Scripta Materialia 112 (2016) 50–53

Contents lists available at ScienceDirect

Scripta Materialia

journal homepage: www.elsevier.com/locate/scriptamat

Grain size effects on dislocation and twinning mediated plasticity in magnesium

Haidong Fan [a,b,*], Sylvie Aubry [c], Athanasios Arsenlis [c], Jaafar A. El-Awady [a]

[a] Department of Mechanical Engineering, Johns Hopkins University, Baltimore, MD 21218, USA
[b] Department of Mechanics, Sichuan University, Chengdu, Sichuan 610065, China
[c] Materials Science Division, Lawrence Livermore National Laboratory, Livermore, CA 94551-0808, USA

ARTICLE INFO

Article history:
Received 1 May 2015
Received in revised form 1 August 2015
Accepted 7 September 2015
Available online 20 September 2015

Keywords:
Discrete dislocation dynamics
Size effects
Dislocation–twin boundary interactions
Magnesium
Twinning plasticity

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

* Corresponding author at: Department of Mechanical Engineering, Johns Hopkins University, Baltimore, MD 21218, USA.
E-mail addresses: haidongfan8@foxmail.com (H. Fan), jelawady@jhu.edu (J.A. El-Awady).

http://dx.doi.org/10.1016/j.scriptamat.2015.09.008
1359-6462/

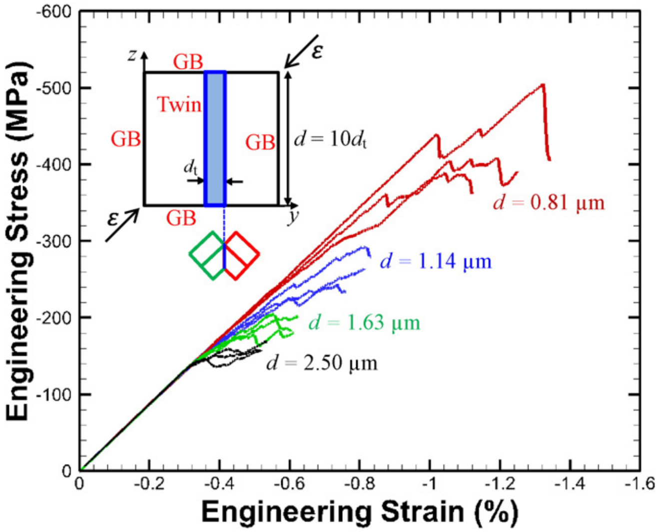

Fig. 1. Stress–strain responses of twinned polycrystals having different grain sizes. The inset shows a cross-section on the *yz* plane of the simulation cell having edge length *d*. A twin lamella having thickness $d_t = 0.1d$ is introduced at the center of the grain. Periodic boundary conditions are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

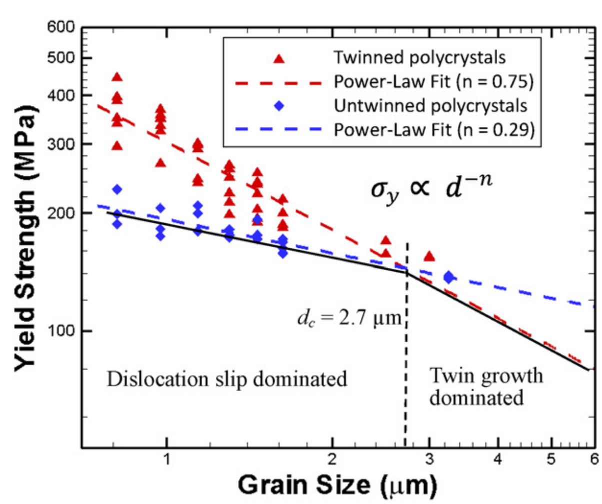

Fig. 2. Yield strength as a function of grain size from simulations of twinned and untwinned polycrystals.

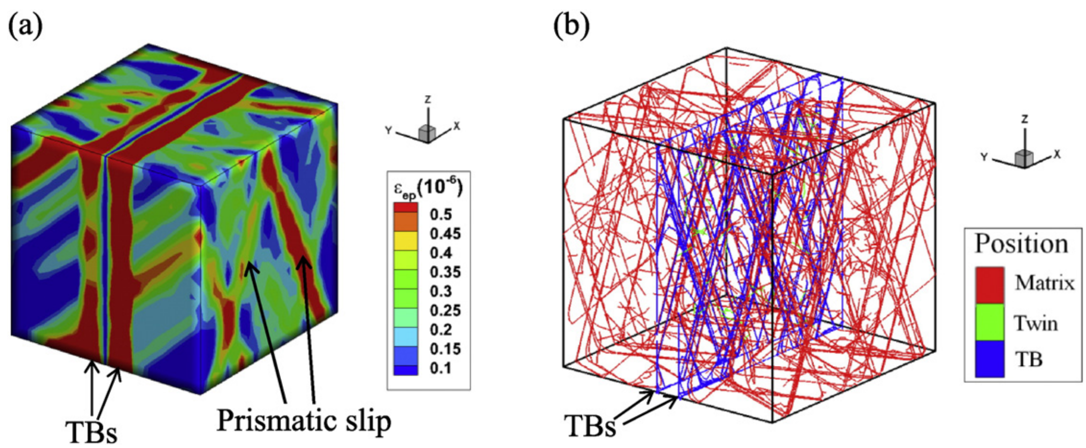

Fig. 3. (a) Contours of the effective plastic strain and (b) dislocation configuration in a $d = 3.0$ μm twinned grain at −0.2% plastic strain.

is in good agreement with the critical grain size of 2.7 μm reported experimentally for pure Mg [7].

To reveal the deformation mechanism in the twinned polycrystals, the contours of the effective plastic strain, as well as the dislocation configuration for grain size $d = 3.0$ μm are shown in Fig. 3. The evolutions of the effective plastic strain and dislocation microstructure are also shown online in Supplementary Movie I. As observed in Fig. 3(a), the plastic strain in the matrix is mediated by <a> dislocation slip on prismatic planes. In addition, considerable plastic deformation is also observed along the twin boundaries, while few dislocation activities are observed in the twin due to the small twin volume fraction as shown in Fig. 3(b).

According to the dislocation–TB interaction model [18], the following dislocation decomposition takes place for the activated prismatic <a> dislocations when they intersect the twin boundary:

$$\langle a \rangle \rightarrow \boldsymbol{b}_r + \boldsymbol{b}_t. \tag{1}$$

This decomposition is also similar to that reported experimentally [31,32], and from MD simulations [33–35]. Note this process could occur spontaneously because this decomposition is energetically favorable. In Eq. (1), the dislocation $\boldsymbol{b}_r = 0.5 < c + a >$ is a residual dislocation on the TB, which is sessile because of its special core structure, while the twinning dislocation, $\boldsymbol{b}_t$, can glide freely on the TB. Due to the high mobility of twinning dislocations [28,29] and the high Schmid factor of ~0.5 on the TB, twinning dislocations are highly glissile, as observed in the online Supplementary Movie I. This leads to considerable plastic strain on the TB, as shown in Fig. 3(a). On the other hand, the sessile residual dislocation induces a repulsive back stress on the subsequent incident dislocations, which contributes to the dislocation pileups near the TB. This is one possible reason for the strong barrier effect of the TBs.

In a previous DDD study of the effects of orientation and grain size on dislocation mediated plasticity in Mg, the grain size effects were reported to be largely controlled by the Peierls stress of the active dislocations [8]. A strong grain size effect with an exponent of 1.16 was reported for basal slip with suppressed twinning [8], which applies as well to the current twinning dislocations since they have the same low Peierls stress. Furthermore, the prismatic slip of polycrystals with suppressed twinning exhibits a weak grain size effect with an exponent of 0.29. On the other hand, for twinned polycrystals an intermediate grain size effect with an exponent of 0.75 is observed. This intermediate exponent can be rationalized based on the two types of active dislocations in these twinned polycrystals, namely, prismatic dislocations and twinning dislocations.

While the glide of the twinning dislocations on the TB leads to TB migration [33–35], in literature atomic shuffling was also proposed as a necessary assisting mechanism during the TB migration process [29]. However, atomic shuffling is accompanied by negligible macroscopic deformation [29,36]. Thus it can be expected that its effect would be minimal on the current predictions. To further understand the effect of grain size on twinning mediated plasticity, Fig. 4 shows the plastic strain induced by twinning dislocations (or TB migration/twin growth) versus the total plastic strain and grain size. The initially flat TB and the predicted TB at the end of the simulations for a grain size of $d = 3.0$ μm are also shown in the inset and online Movie I. It is observed that plastic strain mediated by TB migration in larger grains is significantly larger, i.e. up to 50% at yielding for $d = 2.50$ μm, indicating that twinning deformation is favorable in such larger grains. On the other hand, plastic strain mediated by TB migration in smaller grains is significantly smaller.

Finally, the critical grain size, below which a transition from twinning deformation to dislocation slip occurs, can be explained as the following. The presence of a twin can be argued to have two main roles. On the one hand, TB leads to strengthening through residual dislocations, which block subsequently incident dislocations, as shown in Fig. 3(b). On the other hand, twinning dislocations lead to weakening through considerable twin growth, as shown in Fig. 3(a). In Mg polycrystals with grain sizes <2.7 μm, TB migration is difficult due to the

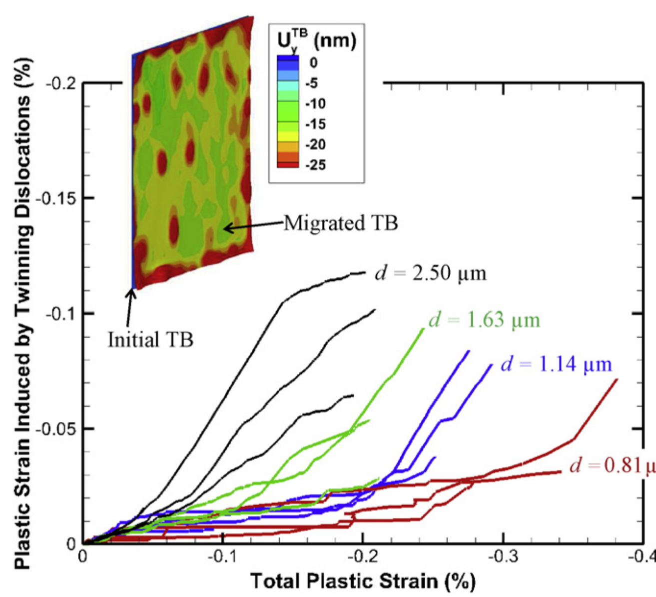

Fig. 4. Plastic strain induced by twinning dislocations versus the total plastic strain. The insert shows the initial and migrated TB from a $d = 3.0$ μm simulation. The displacement contours, U_y^{TB}, are overlaid on the migrated TB.

strong suppression of twinning dislocation activity by the grain size, as shown in Fig. 4. As a result, it would be expected that plasticity would be dominated by dislocation slip in untwinned grains, as shown in Fig. 2. Furthermore, for polycrystals with grain sizes >2.7 μm, plasticity would be dominated by twin growth. Therefore, the critical grain size is a result of the competition between the TB induced strengthening and twin growth induced weakening, which agrees well with previous predictions [18]. Although the critical grain size in the current simulations agrees well with the experimental observations, other factors, such as GB misorientation, twin position, number of twins per grain, as well as the loading direction, could all possibly change the critical grain size slightly from the currently predicted value. In addition, here, twin growth was only mediated by twinning dislocations as a result of dislocation–TB interactions. It is worth noting that nucleation of twinning dislocations from TBs (not modeled here) could also be possible [37].

In summary, the grain size effects on both the dislocation slip and twinning deformation are studied by the discrete dislocation dynamics simulations. Our simulation results show that the twinning deformation displays a stronger grain size effect than dislocation slip. In addition, a critical grain size of 2.7 μm exists, below which a transition from twinning deformation to dislocation slip occurs. Our analysis indicates these phenomena are a result of the competition between the TB induced strengthening and twin growth induced weakening.

This research was sponsored by the Army Research Laboratory (#W911NF-12-2-0022). The views and conclusions contained in this document are those of the authors and should not be interpreted as representing the official policies, either expressed or implied, of ARL or U.S. Government. The U.S. Government is authorized to reproduce and distribute reprints for Government purposes notwithstanding any copyright notation herein. This work was performed in part under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344. HF also acknowledges the financial support of the National Natural Science Foundation of China (11302140), Program for Innovative Research Team (IRT14R37) and Fundamental Research Funds for the Central Universities.

Supplementary data to this article can be found online at http://dx.doi.org/10.1016/j.scriptamat.2015.09.008.

References

[1] J.A. Sharon, Y. Zhang, F. Mompiou, M. Legros, K.J. Hemker, Scr. Mater. 75 (2014) 10–13.
[2] D.V. Wilson, J.A. Chapman, Philos. Mag. 8 (1963) 1543–1551.
[3] G.S. Rao, Y.V.R.K. Prasad, Metall. Mater. Trans. A 13 (1982) 2219–2226.
[4] N. Ono, R. Nowak, S. Miura, Mater. Lett. 58 (2004) 39–43.
[5] H.J. Choi, Y. Kim, J.H. Shin, D.H. Bae, Mater. Sci. Eng. A 527 (2010) 1565–1570.
[6] Z. Trojanová, Z. Száraz, A. Mielczarek, P. Lukáč, W. Riehemann, Mater. Sci. Eng. A 483–484 (2008) 477–480.
[7] J. Li, W. Xu, X. Wu, H. Ding, K. Xia, Mater. Sci. Eng. A 528 (2011) 5993–5998.
[8] H. Fan, S. Aubry, A. Arsenlis, J.A. El-Awady, Scr. Mater. 97 (2015) 25–28.
[9] M.R. Barnett, Z. Keshavarz, A.G. Beer, D. Atwell, Acta Mater. 52 (2004) 5093–5103.
[10] R. Lapovok, P.F. Thomson, R. Cottam, Y. Estrin, J. Mater. Sci. 40 (2005) 1699–1708.
[11] M.R. Barnett, Scr. Mater. 59 (2008) 696–698.
[12] M.A. Meyers, O. Vöhringer, V.A. Lubarda, Acta Mater. 49 (2001) 4025–4039.
[13] A. Arsenlis, W. Cai, M. Tang, M. Rhee, T. Oppelstrup, G. Hommes, T.G. Pierce, V.V. Bulatov, Model. Simul. Mater. Sci. Eng. 15 (2007) 553–595.
[14] C.C. Wu, P.W. Chung, S. Aubry, L.B. Munday, A. Arsenlis, Acta Mater. 61 (2013) 3422–3431.
[15] H. Fan, Z. Li, M. Huang, Scr. Mater. 66 (2012) 813–816.
[16] Z. Li, C. Hou, M. Huang, C. Ouyang, Comput. Mater. Sci. 46 (2009) 1124–1134.
[17] H. Fan, Z. Li, M. Huang, X. Zhang, Int. J. Solids Struct. 48 (2011) 1754–1766.
[18] H. Fan, S. Aubry, A. Arsenlis, J.A. El-Awady, Acta Mater. 92 (2015) 126–139.
[19] Y. Tang, J.A. El-Awady, Acta Mater. 71 (2014) 319–332.
[20] S.R. Agnew, Ö. Duygulu, Int. J. Plast. 21 (2005) 1161–1193.
[21] H. Fan, J.A. El-Awady, J. Appl. Mech. 82 (2015) 101006-101006.
[22] S. Groh, E.B. Marin, M.F. Horstemeyer, D.J. Bammann, Model. Simul. Mater. Sci. Eng. 17 (2009) 075009.
[23] H. Fan, J.A. El-Awady, Mater. Sci. Eng. A 644 (2015) 318–324.
[24] H. Conrad, W.D. Robertson, Trans. Metell. Soc. AIME 209 (1957) 503.
[25] R.E. Reed-Hill, W.D. Robertson, Acta Metall. 5 (1957) 717–727.
[26] A. Staroselsky, L. Anand, Int. J. Plast. 19 (2003) 1843–1864.
[27] Y. Tang, J.A. El-Awady, Mater. Sci. Eng. A 618 (2014) 424–432.
[28] A. Serra, R.C. Pond, D.J. Bacon, Acta Metall. 39 (1991) 1469–1480.
[29] H. Khater, A. Serra, R. Pond, Philos. Mag. 93 (2013) 1279–1298.
[30] I.J. Beyerlein, L. Capolungo, P.E. Marshall, R.J. McCabe, C.N. Tomé, Philos. Mag. 90 (2010) 2161–2190.
[31] M. Hyong Yoo, C.-T. Wei, Philos. Mag. 14 (1966) 573–587.
[32] D.I. Tomsett, M. Bevis, Philos. Mag. 19 (1969) 129–140.
[33] J. Wang, I.J. Beyerlein, C.N. Tomé, Int. J. Plast. 56 (2014) 156–172.
[34] A. Serra, D.J. Bacon, Philos. Mag. A 73 (1996) 333–343.
[35] H. El Kadiri, C.D. Barrett, J. Wang, C.N. Tomé, Acta Mater. 85 (2015) 354–361.
[36] A. Ostapovets, P. Molnár, Scr. Mater. 69 (2013) 287–290.
[37] L. Leclercq, L. Capolungo, D. Rodney, Mater. Res. Lett. 2 (2014) 152–159.