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An atomistic study of resistance offered by twist grain boundaries to incoming edge dislocation in FCC metals

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ABSTRACT

We explored 45 twist grain boundaries (GBs), spanning a broad range of misorientation angles ($0° < \theta < 180°$), to quantify the resistance offered to incoming lattice edge dislocation in different FCC metals (Al, Cu and Ni). The results provide corroborative evidence of the fact that GBs with higher energy offer strong resistance to incoming edge dislocation. Consequently, it has been found that: (1) the dislocation absorption resistance (stress at which dislocation is absorbed in the GB) follows a power-law relationship with the grain boundary energy, (2) grain boundary absorption resistance in FCC materials follow a simple statistical distribution, (3) the absorption resistance for the particular material is governed by the non-dimensional parameter $\gamma_s/\mu b_p$, where γ_s is the stacking fault energy, μ is the shear modulus and b_p is the Burgers vector of partial dislocations. It is envisioned that crystal plasticity based models could use this information to choose and define more realistic constitutive equations for grain boundaries.

1. Introduction

Grain boundaries (GBs) are important microstructural features of polycrystalline materials that impact their bulk properties [1]. This fact has motivated everlasting efforts to understand the behavior of GBs to predict deformation and failure of engineering materials. An important task in this quest is to quantify the GB resistance to lattice dislocations, and establish, if possible, some trends between GB properties and material's crystallography. This would help in improved predictions of material behavior using microstructure-based models that take into account the GB effects on plasticity [2,3]. In view of this, numerous studies have been taken up at the atomistic level to link the GB properties and simple descriptors of boundary like GB angle, energy etc. and study the interaction of GBs with dislocations for various tilt [4,5] and twist [6,7] boundaries. While these studies have revealed some trends between GB descriptors and properties, the trends remain, till date, inclusive [8].

Recently, there has been a resurgence of interest in studying and quantifying the resistance offered by various GBs to incoming lattice dislocations in crystalline materials [9,10]. Such studies are motivated from the previous attempts to include dislocation-GB formalism in the continuum framework [11,12]. In these formulations, the stress at which dislocation enters the GB is an input to the simulation. This information can only be gleaned from atomistic simulations, which provide a detailed real-time monitoring of the events occurring at the nanoscale. In a companion paper, we also had quantified the absorption resistance (AR) offered by 6 different twist GBs to an incoming edge dislocation in Al [7] . Here, we performed a broad study on 45 twist GBs to report general trends in dislocation-GB interactions prevailing in different FCC materials (Al, Cu and Ni). This makes this study, to the authors' knowledge, the most extensive of its kind and its findings are expected to inform microstructure based models to include grain boundary strength given crystallographic data, which can, nowadays, be measured using electron backscatter diffraction techniques [13].

2. Computational methodology

The bi-crystal structures in this study were simulated using LAMMPS code [14] employing the embedded-atom method potentials for FCC Al [15], Cu [16] and Ni [15]. The left grain of the simulation cell (Fig. 1) had its x-, y- and z-axis oriented along $[1\bar{1}0]$, $[\bar{1}\bar{1}1]$ and $[\bar{1}\bar{1}\bar{2}]$ crystal directions, respectively. To create various twist GBs, the right grain was rotated along x-axis ($[1\bar{1}0]$) to various misorientation angles ($0° < \theta < 180°$) to form different twist

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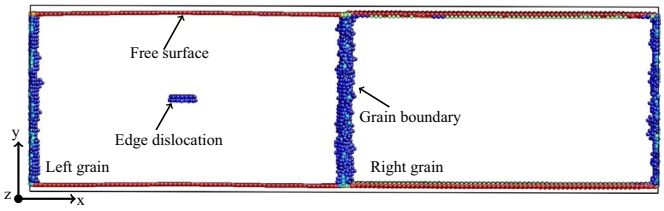

Fig. 1. MD simulation cell showing the edge dislocation-twist GB configuration. Only atoms in non-centrosymmetric environment are shown.

Table 1.
GB energies (mJ/m^2) and orientations of right grain of simulation cell for various GBs investigated in this study.

Sr. No.	Angle (deg.)	y-	z-	Al energy	Cu energy	Ni energy
1	8.05	[3̄ 3̄ 4]	[4̄ 4̄ 6̄]	403.76	531.02	674.05
2	11.42	[2̄ 2̄ 3]	[3̄ 3̄ 4̄]	521.78	631.78	756.65
3	19.47	[1̄ 1̄ 2]	[2̄ 2̄ 2̄]	586.13	721.63	849.11
4	25.24	[4̄ 4̄ 1]	[1̄ 1̄ 8̄]	582.54	712.75	853.10
5	29.49	[1̄ 1̄ 3]	[3̄ 3̄ 2̄]	565.20	692.93	835.96
6	35.26	[1̄ 1̄ 0]	[0 0 2̄]	621.99	763.15	906.08
7	45.29	[4̄ 4̄ 1̄]	[1 1 8̄]	607.64	755.38	900.91
8	54.73	[0 0 1]	[1̄ 1̄ 0]	543.08	728.67	887.17
9	60.51	[3̄ 3̄ 2̄]	[2 2 6̄]	558.82	766.72	909.71
10	62.79	[1 1 10]	[1̄0̄ 1̄0̄ 2]	576.76	800.06	942.16
11	66.16	[1 1 7]	[7̄ 7̄ 2]	569.38	773.71	906.30
12	69.15	[2 2 11]	[1̄1̄ 1̄1 4]	600.07	799.19	943.19
13	74.21	[1 1 4]	[4̄ 4̄ 2]	570.78	761.58	899.32
14	76.74	[2 2 7]	[7̄ 7̄ 4]	594.36	810.44	953.44
15	79.97	[1 1 3]	[3̄ 3̄ 2]	616.91	824.11	967.10
16	81.95	[2̄ 2̄ 3̄]	[3 3 4̄]	638.32	855.53	998.52
17	84.23	[2 2 5]	[5̄ 5̄ 4]	582.75	781.06	924.06
18	87.47	[5 5 11]	[1̄1 1̄1 10]	595.73	795.82	941.48
19	90.00	[1 1 2]	[1̄ 1̄ 1]	614.08	810.37	963.68
20	93.68	[4 4 7]	[7̄ 7̄ 8]	651.88	832.09	1013.92
21	96.21	[5 5 8]	[8̄ 8̄ 10]	670.21	857.40	1023.80
22	98.04	[2 2 3]	[3̄ 3̄ 4]	684.76	865.77	1039.86
23	100.03	[5 5 7]	[7̄ 7̄ 10]	697.91	879.11	1066.16
24	103.26	[4 4 5]	[5̄ 5̄ 8]	645.10	856.79	1036.10
25	105.79	[1̄ 1̄ 4̄]	[4 4 2̄]	673.41	873.94	1058.30
26	109.47	[1 1 1]	[1̄ 1̄ 2]	688.34	881.11	1050.10
27	112.98	[8 8 7]	[7 7 16]	638.33	856.42	1001.95
28	115.24	[1̄ 1̄ 8̄]	[8 8 2̄]	658.87	885.48	1038.73
29	119.49	[3 3 2]	[2̄ 2̄ 6]	672.81	893.26	1077.77
30	125.26	[0 0 3̄]	[3 3 0]	649.88	877.13	1009.81
31	131.47	[3 3 1]	[1̄ 1̄ 6]	660.25	894.06	1050.10
32	133.32	[7 7 2]	[2̄ 2̄ 14]	612.43	907.10	1055.23
33	135.29	[1 1 8̄]	[4 4 1]	502.23	867.17	1020.67
34	141.06	[1 1 5̄]	[5 5 2]	525.35	817.75	971.05
35	144.74	[1 1 0]	[0 0 1]	552.28	844.84	1019.56
36	147.27	[3̄ 3̄ 4]	[4̄ 4̄ 6]	610.42	867.96	1047.17
37	150.50	[7 7 1̄]	[1 1 14]	631.94	930.92	1092.05
38	152.47	[4 4 1̄1]	[11 11 8]	600.51	908.08	1056.14
39	154.76	[4 4 1̄]	[1 1 8]	614.86	947.46	1095.59
40	157.99	[3 3 1̄]	[1 1 6]	578.60	904.22	1062.71
41	160.53	[1 1 2̄]	[2 2 2]	606.32	939.68	1087.82
42	164.21	[2 2 1̄]	[1 1 4]	577.63	893.26	1059.52
43	166.74	[7 7 4̄]	[4 4 14]	610.77	925.35	1068.29
44	169.97	[3 3 2̄]	[2 2 6]	553.37	853.83	996.82
45	173.79	[14 14 1̄1]	[11 11 28]	522.98	823.42	966.59

GBs. The corresponding y- and z-axis of right grain, and GB energy for Al, Cu and Ni are displayed in Table 1. The lengths of simulation cell were approximately 11 nm in y- and 9 nm in z-directions, with x-direction length varying as 40 nm for Al, 110 nm for Cu and 85 nm for Ni. These dimensions ensured no attraction or repulsion of the dislocation from GB during static relaxation. The corresponding no. of atoms in the system were approximately 3×10^6, 7×10^6 and 6×10^6 for Al, Cu and Ni, respectively. The validity of the GB structures was confirmed by comparing the GB energies with literature, wherever possible (for ex., Cu energies were found to be similar to the energies computed by Wolf [17] using an EAM potential), and also by confirming a linear relation between boundary energy and free volume, an observation consistent with previous atomistic studies [8].

An edge dislocation was introduced (using the procedure described by Osetsky and Bacon [18]) at the center of left grain, and the system was relaxed using conjugate-gradient algorithm using a timestep of 1 fs. The bi-crystal was periodic along x- and z-directions, and free surfaces (two to three layers of atoms) were created along y-direction to facilitate the application of shear stress. The temperature of the system was kept at 10 K under the micro-canonical (NVE) ensemble. Initial relaxation was carried out for 25 ps, following which the shear stress was applied by adding external force on top layer of atoms along x-direction (Burgers vector), keeping the lower layer of atoms fixed. The applied stress was increased gradually in different MD runs until the dislocation was absorbed in the GB. For more details on the simulation conditions and twist GB structure, the reader is referred to Ref. [7].

3. Results and discussion

The general interaction observations between edge dislocation and all twist boundaries were same as detailed in Ref. [7] (movement of edge dislocation towards the GB under shear stress, increase in stacking fault width upon reaching the boundary, absorption in the boundary and consequent formation of a GB step). Upon plotting the AR offered by the boundary to incoming edge dislocation against boundary energy, a power law relationship of the form $y = ax^b$ was observed for all the considered FCC materials. The negative value of exponent b in the scaling relation (Fig. 2) implies that the resistance offered by the twist GB decreases with GB energy, a finding that is consistent with the current thoughts on dislocation-GB interactions [7,9,10]. We also unsuccessfully tried to fit our data to other grain boundary descriptors like GB angle, and also with other anisotropic elasticity material properties.

The AR values for the studied FCC materials were found to be in the range of 40–240 MPa for Al, 120–360 MPa for Cu and 250–450 MPa for Ni for all the GBs. In order to smear out this effect, we chose to plot the normalized AR (AR of a boundary divided by the average AR of all boundaries for a particular material) as a stochastic variable. A histogram of the normalized AR was plotted (shown in Fig. 3), which depicts the total number of GBs that have their normalized AR within a given range. Apparent from Fig. 3 is the fact that twist GB AR in FCC materials follows a simple normal distribution (solid lines in Fig. 3, which represent a normal fit to the histogram data). This finding holds weather one considers the frequency of normalized AR (as defined above), or the frequency of absorption resistance normalized with respect to minimum/maximum resistance value for the particular material. Having said that, it can be observed that there is quite a large variation in the GB AR values for the cases examined here.

The results presented in the previous paragraph suggest that it should be possible to use the same distribution function (normal distribution), albeit with different mean and standard deviation parameters, for GB AR in materials with FCC crystal structure. This information can be used in polycrystal microstructural models of crystal plasticity (CP) to prescribe GB resistance, which can vastly improve the predictions on interpretation of GBs on the impedance of deformation, thereby offering a strong contribution to