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Grain boundary energies in body-centered cubic metals

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Abstract—Atomistic simulations using the embedded atom method were employed to compute the energies of 408 distinct grain boundaries in bcc Fe and Mo. This set includes grain boundaries that have tilt, twist, and mixed character and coincidence site lattices ranging from Σ3 to Σ323. The results show that grain boundary energies in Fe and Mo are influenced more by the grain boundary plane orientation than by the lattice misorientation or lattice coincidence. Furthermore, grain boundaries with (1 1 0) planes on both sides of the boundary have low energies, regardless of the misorientation angle or geometric character. Grain boundaries of the same type in Fe and Mo have strongly correlated energies that scale with the ratio of the cohesive energies of the two metals.

Keywords: Grain boundaries; Grain boundary energy; bcc metals; Atomistic calculations

1. Introduction

Because grain boundaries have a significant influence on the physical properties of polycrystalline solids [1–4], their properties, including energy, have been the subjects of extensive experimental and computational study. In annealed polycrystals, the grain boundary energy distribution (GBED) is known to be inversely correlated to the grain boundary character distribution (GBCD), defined as the relative areas of grain boundaries distinguished by lattice misorientation and grain boundary plane orientation [5,6]. Morawiec [7] developed a technique to determine the GBED from three-dimensional electron backscatter diffraction (3D-EBSD) data, and this has been applied to measure grain boundary energies in a number of ceramics and metals including MgO [8,9], Y_2O_3 [10], Ni [11], a Ni-based alloy [12], a ferritic steel [13], and an austenitic steel [14]. This method requires large amounts of data because there are no assumptions about the functional form of the GBED, and the number of unknown energies scales with the discretization of the system. Furthermore, the results are relative, rather than absolute, values of the grain boundary energies. Nevertheless, to the extent that comparisons of the measured and calculated energies have been possible, there has been satisfactory agreement between experiment and simulation, especially for the most frequently observed grain boundaries in the materials examined (Σ3 and Σ9 boundaries) [15,16].

The agreement between grain boundary energies derived from experiment and simulation suggests that both methods are reliable when properly applied [16]. Therefore, computer simulations by the embedded atom method (EAM) can be utilized to survey and compare a large number of grain boundary energies [17,18]. For example, Holm et al. [17] recently showed that the grain boundary energies in Al, Au, Cu, and Ni, which share the face-centered cubic (fcc) crystal structure, are correlated and scale with the shear modulus. One purpose of the present study is to determine whether or not body-centered cubic (bcc) metals exhibit the same phenomenon; we therefore employ similar methods.

There have been a number of atomistic simulations of grain boundary energies in bcc metals [19–25]. Wolf [22–24] showed that the energy anisotropies of Fe and Mo were similar for symmetrical tilt boundaries, twist boundaries on (1 0 0) and (1 1 0) planes, and certain general grain boundaries. Morita and Nakashima [20] investigated the boundary energy of <0 0 1> symmetric tilt boundaries in Mo, producing results consistent with the boundary energies calculated by Wolf [22–24] and with experimental boundary energies measured by the thermal grooving

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method [18]. Tschopp et al. [21] examined a large data set of grain boundary energies in Fe using molecular statics. Kim et al. [19] used molecular statics calculations to populate a grain boundary energy database that uniformly samples the five parameter grain boundary space for bcc Fe. While these simulations uniformly covered misorientation space in 10° increments, the discretization of the grain boundary plane space was coarser.

Recently, Yesilleten and Arias [25] showed that the boundary energies of <1 1 0> symmetric tilt boundaries in Mo were influenced by the incorporation of vacancies. Specifically, the coherent twin boundary energy increased from 0.61 J/m^2 to 2.13 J/m^2 when half of the atoms in the plane adjacent to the grain boundary were removed. This result illustrates the significant influence that the atomic structure of the interface can have on the computed energy. In general, if only one starting configuration is considered, there is no guarantee that the minimized energy of that boundary corresponds to the global minimum boundary energy. In their study of grain boundaries in fcc metals, Olmsted et al. [18] addressed this difficulty by minimizing the energies of hundreds or more of crystallographically identical boundaries that had different microscopic starting configurations. This exploration of microscopic configurations provides a greater likelihood that an energy near the minimum is reached. In general, one would expect that the naturally occurring boundaries have sufficient time and ample supply of point defects to reach a minimum of their free energies in the grand canonical ensemble.

The database created by Kim et al. [19] contains far more grain boundary energies for a bcc material than any of the other calculations. However, they considered only one initial configuration for each grain boundary type, so it is not obvious that these energies represent the minimum energy states. The purpose of this paper is to report the results of the calculation of 408 grain boundary energies in Fe and Mo. For this survey, between 100 and 10,000 different initial microscopic states were considered for each type of boundary and we report the minimum energy. We chose Fe and Mo because these materials are widely used in the polycrystalline form and there are previous reports to which we can compare subsets of the results. We also examine the correlation between the grain boundary energies in Fe and Mo and consider the extent to which isomorphic materials have correlated grain boundary energies.

2. Methods

This work considers the grain boundaries in all bicrystals that can be constructed in a periodic cell with dimensions less than or equal to $20a_0/2$, measured parallel to the grain boundary, where a_0 is the lattice spacing. The 408 boundaries that fit within this cell have 80 different misorientations and a range of characters; 176 are twist boundaries, 381 are tilt boundaries, and 20 are neither pure tilt nor pure twist boundaries. Note that 169 of the boundaries are both twist and tilt, depending on the choice of axis [26–28]. The 408 boundaries are not evenly distributed throughout the space of possible grain boundaries and do not provide complete coverage. For example, there are 40 Σ3, 27 Σ5, 21 Σ7, and 29 Σ9 grain boundaries, meaning that 29% of the 408 grain boundaries are concentrated at four misorientations. Because these grain boundaries were selected based only on a maximum periodicity condition, they are of relatively high symmetry and are not expected to mimic the actual distribution of grain boundary types in real polycrystals.

Grain boundary energies were computed by minimizing system energy using the conjugate-gradient method in the LAMMPS code [29] at $T = 0$ K with embedded-atom method (EAM) interatomic potentials. The computational cell has periodic boundary conditions in the y and z directions with a minimum length of $17a_0/2$. The minimum length in the x direction, which is normal to the plane of grain boundary, was $20a_0/2$. The computational scheme is similar to prior studies of the grain boundary energy for fcc metals, which has been described in detail elsewhere [17,18]. The Mendelev potential 2 was used for Fe [30] and the Finnis–Sinclair potential was used for Mo [31]. These potentials were selected because they reproduced the lattice constants and the elastic constants of Fe and Mo (see Table 1), and have also been used to simulate grain boundary energies [21–24] For each macroscopic grain boundary structure, the energies of 100–10,000 initial configurations were minimized. These initial configurations were generated using a method similar to that described by Olmsted et al. [18] with a modification to the step where atoms are removed if they were too close together. Before removing atoms, each atom in the grain boundary region was perturbed by a very small distance in a random direction. This displacement should have little or no effect in the

Table 1. Selected materials properties for Fe and Mo.

Materials properties	Mendelev Fe EAM2[a]	Experimental values of Fe[b]	Finnis–Sinclair Mo EAM[c]	Experimental values of Mo[b]
Lattice constant a_0 (Å)	2.8553	2.8664	3.1472	3.1470
Melting point T_m (K)	1773	1811	3062.6 ± 7.6	2896
Cohesive energy E_{coh} (eV)	4.122	4.28	6.82	6.82
Coherent twin energy (mJ/m^2)	26.2	–	38.9	–
Bulk modulus B (GPa)	177.8	168.7	262.6	259.8
Voigt average shear modulus μ_{voigt} (GPa)	89.28	86.8	125.98	126.7
C' (GPa)	49.2	43	151.6	153.0
C_{11} (GPa)	243.4	226	464.7	463.7
C_{12} (GPa)	145.0	140	161.5	157.8
C_{44} (GPa)	116.0	116	108.9	109.2

[a] Simulated materials properties of Fe are from Refs. [30,37,39].
[b] Experimental materials properties of Fe and Mo are from Ref. [40] except for E_{coh} from Ref. [41].
[c] Simulated materials properties of Mo are from Ref. [31] except for T_m from Ref. [42].