Scripta Materialia 116 (2016) 108–111

Contents lists available at ScienceDirect

Scripta Materialia

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

Symmetric tilt boundaries in body-centered cubic tantalum

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ARTICLE INFO

Article history:
Received 8 September 2015
Received in revised form 22 January 2016
Accepted 25 January 2016
Available online xxxx

Keywords:
Coincidence lattice
Grain boundary structure
Grain boundary energy
Molecular dynamics (MD)
Transition metals

ABSTRACT

Grain boundaries can play a significant role in the mechanical response of materials. Atomistic simulations are used to investigate 79 coincidence site lattice grain boundary structures and energies in tantalum, a model body-centered cubic transition metal. Quasi-symmetric Σ3, Σ5, Σ7, Σ13, and Σ27 boundaries are observed, of which Σ3 and Σ7 also exist as traditional mirror-symmetry conserving boundary structures. These results are supported by previous observations of similar phenomena in other bcc transition metal Σ5 boundaries. Metastable low energy Σ3 boundary structures in tantalum could influence the formation and stability of deformation twins and abnormal growth grain favoring Σ3 boundaries.

Grain boundaries play a critical role in the determination of mechanical, chemical, and thermal properties of polycrystalline materials. Specifically, the internal structure and energy can strongly determine grain boundary (GB) stability and influence the deformation response by affecting dislocation nucleation, dislocation motion, grain boundary sliding, diffusion, and radiation damage processes [1–7]. The distribution and character of grain boundaries are critical in controlling the strength of metals [8], especially tantalum [9–11]. The nature of grain boundaries is inherently complex because their energy is dependent on their character, which depends on five degrees of freedom. To these, one could add translation, which also changes the nature of the boundaries and has been shown to be particularly important for bcc metals [12]. A number of analytical approaches have been developed to treat GB structures: coincidence site lattice (CSL), displacement shift complete, and other topological treatments e.g., [13]. To investigate the dependence of deformation mechanisms on GB structural details, we first must understand the structural and energetic landscape of GBs as in recent surveys of face-centered cubic (fcc) [14] and some body-centered cubic (bcc) [15] materials.

Supporting these surveys, there have been numerous reports using both simulations and experiments to understand the GB structure and energies of fcc materials [14,16,17]. These studies have included both symmetric and asymmetric tilt boundaries on (111), (100), (110) and (113) planes [14,18]. In contrast, only a handful of studies exist on bcc transition metals including the work of Wolf on Fe/Mo [12,19], Yeşilleten and Arias on Mo [20], Ratanaphan et al. on Fe/Mo [15], and Shibuta et al. on Fe [21]. There are few experimental and/or simulation reference points for atomistic GB structures in tantalum; the principal reference is the structure of the Σ5 (310)/[001] CSL tilt boundary investigated both experimentally and theoretically by Campbell et al. [22,23]. Hence, there is clearly a deficiency in available data for GBs in Ta within the current literature.

In the present work, we investigate GB structures in bcc tantalum and their associated energies using molecular dynamics (MD). Seventy-nine grain boundaries of varying tilt axis and misorientation (as described by the CSL model) are evaluated. The accompanying 'Data in Brief' details complete tilt axis ⟨*abc*⟩, grain boundary normal (*hkl*), CSL Σ index, misorientation, and conversion of these values into appropriate simulation basis for four tilt axes: ⟨001⟩, ⟨011⟩, ⟨111⟩, and ⟨112⟩. We use the MD code LAMMPS [24] to generate and relax bicrystal structures based on the scheme of Tschopp et al. [18,25,26]. Briefly, within a fully periodic system, one crystal is sequentially shifted with respect to another along its γ-surface; atoms that exceed overlap criteria are selectively removed; and the boundary is relaxed in the GB normal direction. The grain boundary energy (GBE) is calculated by evaluating the excess energy of the system per grain boundary area, taking into account that each simulation contains two parallel grain boundaries. The embedded atom model (EAM) potential developed by Ravelo et al. [27] is principally employed, but the importance of the Σ3 coherent twin boundary to deformation behavior warranted a "quantum accurate" investigation using a spectral neighbor analysis potential (SNAP) developed by Thompson et al. [28]. Depending on the boundary orientations, between hundreds and thousands of possible atomic arrangements containing up to fifty thousand atoms were sampled to produce each minimum energy configuration, thus neither density functional theory (DFT) nor extended use of SNAP is practical for the present study.

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http://dx.doi.org/10.1016/j.scriptamat.2016.01.038
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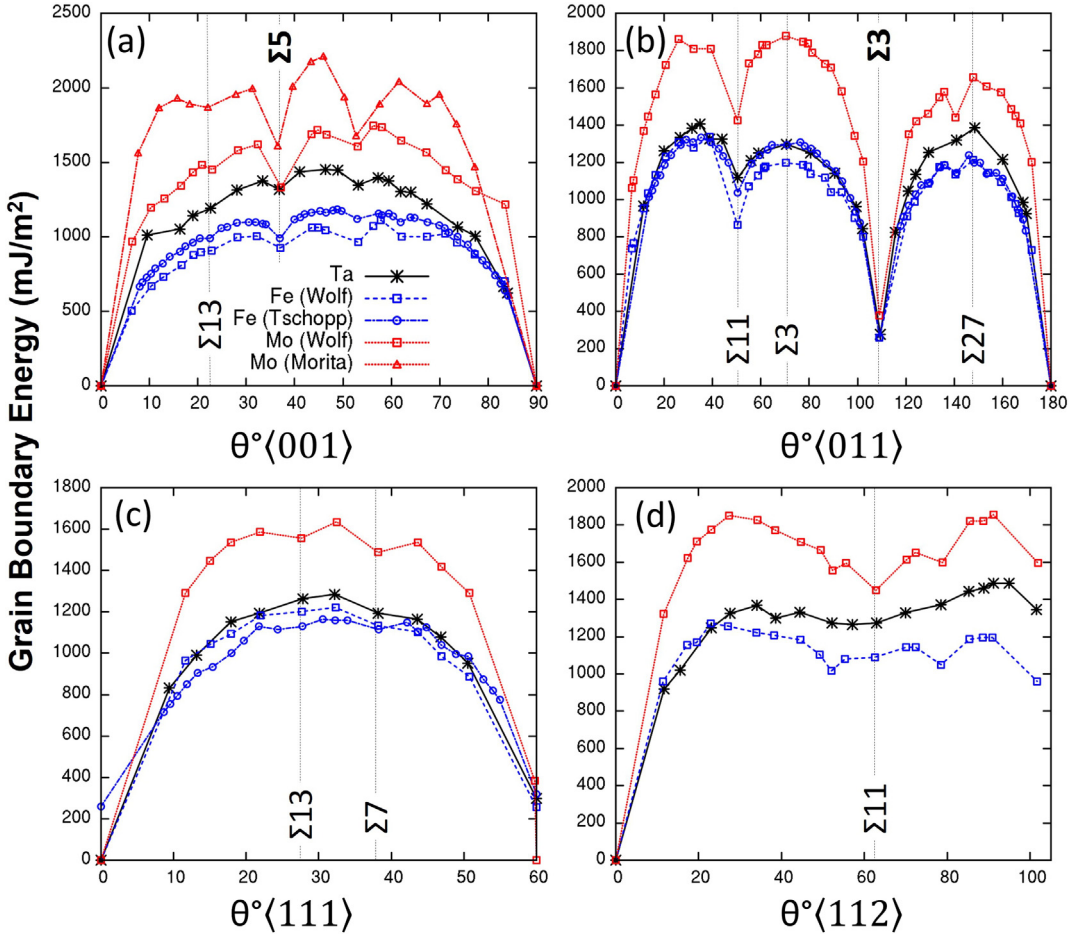

Fig. 1. Grain boundary energy as a function of misorientation for four tilt axis. GBEs for Ta are shown as black asterisks (GBE values can be found in the supplemental material). Also provided is relevant data for bcc Fe (blue) and bcc Mo (red) from empirical potentials (Wolf [12,19], Morita and Nakashima [31], and Tschopp et al. [6]) illustrating similar trends. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Fig. 1 shows the calculated GBEs as a function of misorientation angle alongside previous results for other bcc elements. GB structures presented in subsequent figures are indicated by vertical dashed lines. Based on calculations of surface energies for bcc transition metals, the energy of tantalum interfaces are bracketed between iron and molybdenum [29]. We note that it is to be expected that GBEs calculated in this work will be slightly lower than those calculated by tight binding or ab-initio methods [17,30].

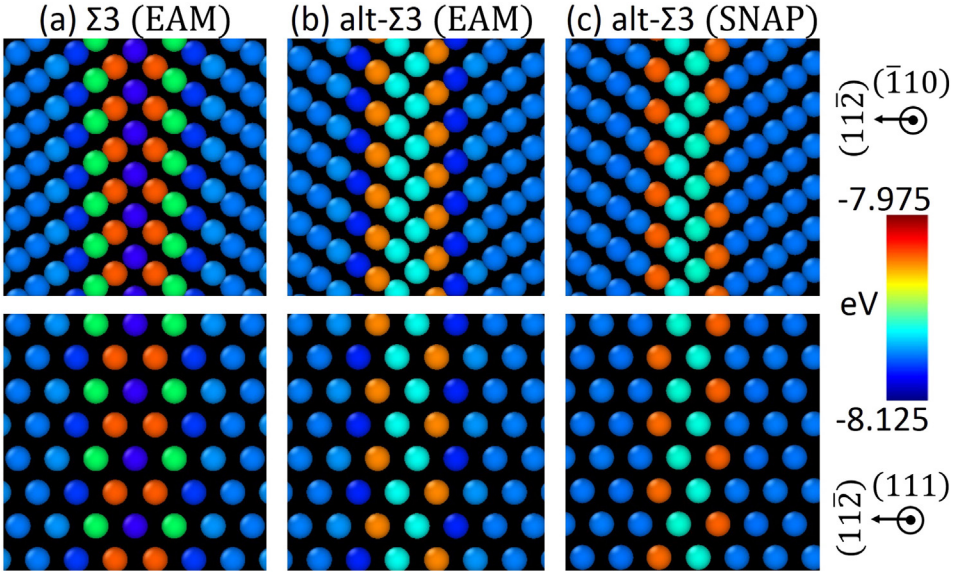

Fig. 2. Configurations of Σ3⟨011⟩ boundaries colored by eV/atom shown for two projections. In each projection the GB normal is horizontal. (Left) EAM symmetric twin boundary. (Middle) EAM quasi-symmetric boundary with broken mirror symmetry in both (110) and (111) projections. (Right) SNAP quasi-symmetric boundary.