ATOMIC STRUCTURE OF GRAIN BOUNDARIES IN NANOSTRUCTURED TUNGSTEN

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Grain boundaries (GBs) have significant effects on the mechanical properties of a wide range of polycrystalline nanostructural materials. The role of GBs in these materials is enhanced due to the extremely increased fraction of atoms near GBs. The study of atomic-level structure of GBs has usually been confined to coherent coincidence site lattice (CSL) boundaries. In a field ion microscope (FIM), inherent possibility of atom-by-atom dissection of the specimen by field evaporation ensures three-dimensional reconstruction of the positions of the atoms. It was shown that the misorientation distribution of GBs in heavily drawn tungsten demonstrates a tendency for high-angle GBs to have significant populations at certain misorientation angles around the [110] axis [1].

A crystallographic consideration shows that these misorientations are related to a special type of GBs terminated by a low index plane and the medium index complements to this surface. When one grain is terminated by a close-packed plane, the complementary grain can be terminated by a low- or medium-index plane at the condition that misorientation angle is equal to a half of the CSL misorientation angle. A mathematical modeling showed that the calculated cleavage energy is a function of the misorientation angle for these GBs: incommensurate GB's with a special misorientation angles have comparatively high cohesive energies.

We have demonstrated that random GBs are well structured at the atomic scale, i.e., the lattices retain their identity right up to the GB plane. FIM images have also shown that there are a few GB atoms which showed considerable relaxation in the direction perpendicular to the (110) plane. The role of large individual atomic relaxation displacements corresponding to formation of the self-interstitial atoms may be regarded as an optimization of local atomic settings.

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2. I.M. Mikhailovskij, E.V. Sadanov, T.I. Mazilova, O.V. Dudka, V.A. Ksenofontov, O.I. Lugovska Atomic structure of random grain boundaries in tungsten // Materials Letters, 2012, v. 70, p. **60–62**.