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Binding energy of self-interstitial atoms to grain boundaries: An experimental approach

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ABSTRACT

The energies of formation and binding of self-interstitial atoms at grain boundaries in tungsten have been found out using the field evaporation phenomenon. The binding-energy distribution for interstitials at the high-angle GB of general type is characterized by a broad characteristic energy spectrum energy spectrum with a full width at half maximum of 1.98 eV. Our experimental results are compared with published theoretical data on the interaction of interstitials with grain boundaries and found to be qualitatively reliable.

1. Introduction

Grain boundaries (GBs) are important structural elements of polycrystal materials for a variety of technological applications. One of the long-standing issues for materials science and engineering is the nature of interaction between point defects and grain boundaries in polycrystals [1,2]. For current development of materials for advanced applications, it is crucial to know the magnitude of the formation and binding energies of point defects at the GBs [3]. Nonetheless, in spite of this large body of theoretical research, there are hitherto no experimental data available for the GB energetics of point defects to probe and validate the numerical simulation results.

In this decade, the experimental approach to the determination of the formation energy of self-interstitial atoms (SIAs) was opened using the phenomenon of low-temperature field evaporation [4]. The advanced technique for direct *in situ* energetic characterization was applied to tungsten monocrystals saturated with the interstitial atoms produced during the bombarded with accelerated helium atoms in the chamber of a field ion microscope (FIM). The objective of the present work is to experimentally investigate the formation and binding energies of SIAs interacting with high-angle GBs in tungsten using field ion microscopy.

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2. Experimental

The experimental determination of the formation and binding energies of SIAs interacting with high-angle GBs in tungsten was carried out using a two-chamber helium field ion microscope with samples cooled to (25±2) K at the residual gas pressure of about 10^{-7} Pa [4]. The specimens were prepared from 0.15 mm tungsten wires of 99.98 at% with a fiber structure. After placement in the FIM, the studied region of the specimen was cleaned and polished in the electric field [5] of 57–58 V/nm until an atomically smooth surface was formed.

The experiments have been performed in the FIM supplied with a source of neutral helium atoms with energy of 5 keV [4]. The neutral helium atoms produced by charge exchange do not deflect by a high FIM operating voltage, so the direct atomic-scale observation of elementary radiation events was allowed in our experiments. The irradiation was carried out in the direction perpendicular to the specimen axis which in most cases coincided with the $<110>$ crystallographic direction.

3. Results and discussion

We investigate the energetics of SIAs interacting with high-angle GBs in tungsten created by irradiation with 5 keV He atoms at fluences of 10^{16}–10^{17} atoms/m^2. Fig. 1 shows the FIM patterns of the tungsten nanobicrystal with the radius of curvature of 36 nm obtained at the operating voltage of 5.84 kV corresponding to the

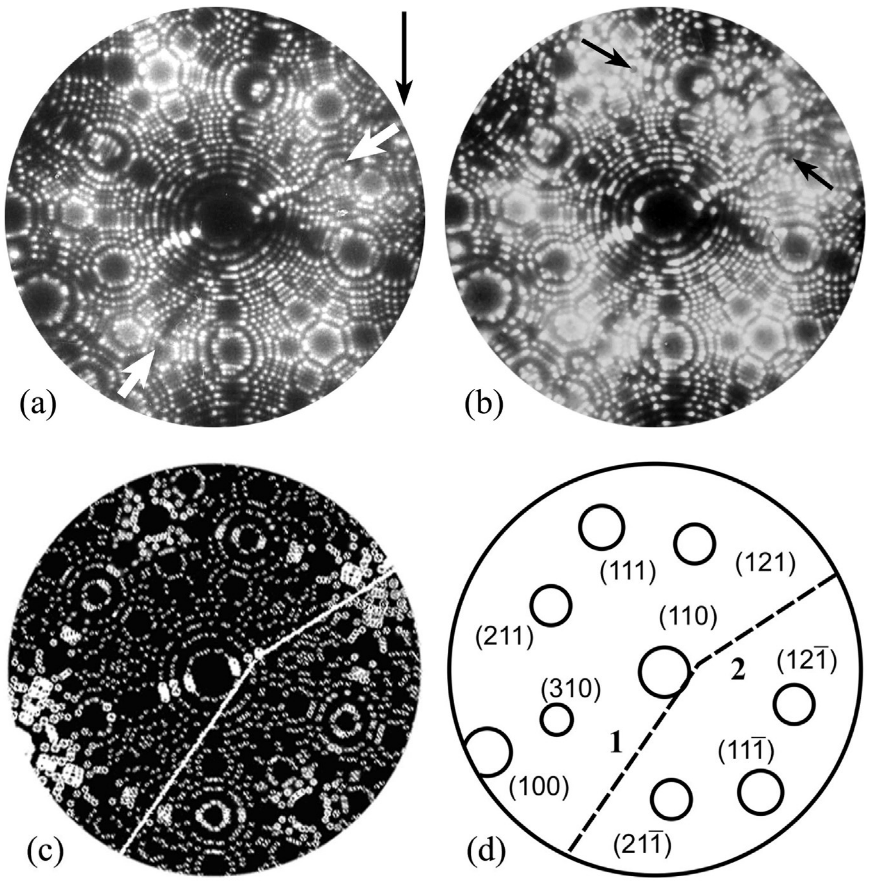

Fig. 1. FIM images of the tungsten bicrystal (a) before and (b) after the irradiation by helium atoms with an energy of 5 keV to a fluence of 3.0×10^{16} atoms/m^2, and (c) simulation pattern with (d) corresponding stereographic projection. White arrows show the GB track; black arrows indicate (a) the irradiation direction and (b) surface vacancies.

best image condition at field strength of 44.0 V/nm [5] (a) before and (b) after irradiation with fluence of 3.0×10^{16} atoms/m^2 at elevated field strength of 52.38 V/nm; simulation image (c), and corresponding stereographic projection (d). The crystallographic analysis shows that the bicrystal contains a tilt GB a general type [1] with the misorientation matrix

$$\hat{R} = \begin{pmatrix} 0.981 & 0.019 & 0.192 \\ 0.019 & 0.981 & 0.192 \\ -0.192 & 0.192 & 0.962 \end{pmatrix},$$

which generates the misorientation axis $<110>$ with the angle of $15.80°$. The interface planes are $(3\bar{3}7)/(1\bar{1}5)$ for the microfacet (1) and $(1\bar{1}5)/(001)$ for the microfacet (2) shown in Fig. 1(d).

Fig. 2 shows the field ion images of the same specimen as in Fig. 1 acquired after field polishing by field evaporation (a) and further bombardment at 6.00 kV corresponding to the field strength of 46.22 V/nm. The arrow in Fig. 2(a) points the irradiation direction. The comparison of FIM images in Figs. 1 and 2 obtained at different field strengths exhibits in both cases formation of surface vacancies. One of the numerous surface vacancies is shown in Fig. 2(b) by the black arrow. In contrast to the radiation experiments at higher field strengths illustrated by Fig. 1, there is

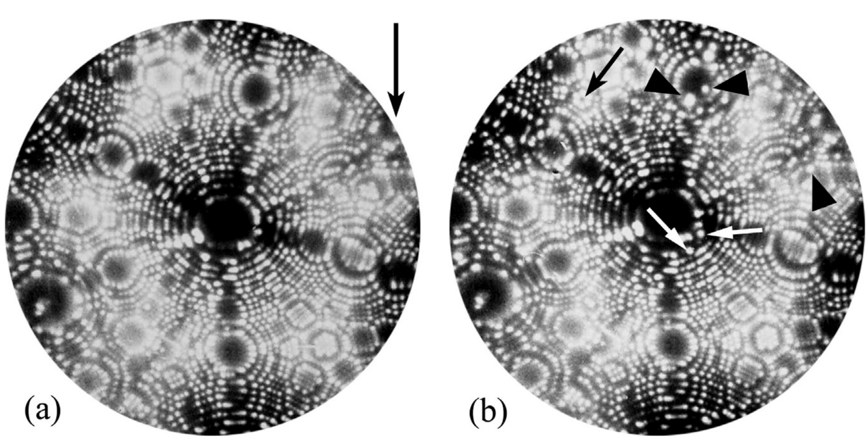

Fig. 2. FIM images of the same bicrystal as in Fig. 1(a) before and (b) after the bombardment by helium atoms at a fluence of 3.0×10^{16} atoms/m^2. The arrow (a) shows the beam direction, the white arrows point the adatoms at the GB and the black arrow indicates the surface vacancy.

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