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The evolution of interaction between grain boundary and irradiation-induced point defects: Symmetric tilt GB in tungsten

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HIGHLIGHTS

- The phenomenon of local extension of GB was observed.
- The influence of GB on distribution of surviving defects was discussed.
- The designed scheme of calculational tests is versatile.

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ABSTRACT

Molecular dynamics method is used and scheme of calculational tests is designed. The atomic evolution view of the interaction between grain boundary (GB) and irradiation-induced point defects is given in six symmetric tilt GB structures of bcc tungsten with the energy of the primary knock-on atom (PKA) E_{PKA} of 3 and 5 keV and the simulated temperature of 300 K. During the collision cascade with GB structure there are synergistic mechanisms to reduce the number of point defects: one is vacancies recombine with interstitials, and another is interstitials diffuse towards the GB with vacancies almost not move. The larger the ratio of the peak defect zone of the cascades overlaps with the GB region, the statistically relative smaller the number of surviving point defects in the grain interior (GI); and when the two almost do not overlap, vacancy-intensive area generally exists nearby GBs, and has a tendency to move toward GB with the increase of E_{PKA}. In contrast, the distribution of interstitials is relatively uniform nearby GBs and is affected by the E_{PKA} far less than the vacancy. The GB has a bias-absorption effect on the interstitials compared with vacancies. It shows that the number of surviving vacancies statistically has increasing trend with the increase of the distance between PKA and GB. While the number of surviving interstitials does not change much, and is less than the number of interstitials in the single crystal at the same conditions. The number of surviving vacancies in the GI is always larger than that of interstitials. The GB local extension after irradiation is observed for which the interstitials absorbed by the GB may be responsible. The designed scheme of calculational tests in the paper is completely applicable to the investigation of the interaction between other types of GBs and irradiation-induced point defects.

1. Introduction

Tungsten (W) has the highest melting point (3410 °C) and the lowest vapor pressure (1.3×10^{-7} Pa) in all metals as well as the advantages of good thermal conductivity and not formation of hydride [1]. Thus, W is considered to be the most promising candidate materials for plasma-facing materials (PFMs) [2–6] and divertor materials [7–11] in future nuclear fusion reactors. As a plasma-facing material, W will be exposed directly to the high-energy neutron particle flow and heat flow from the plasma [12]. Many physical properties of W are changed significantly under such a severe irradiation environment. When neutrons

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passing through the material, they will collide with the lattice atoms [13]. A lot of point defects form during the collision cascades, and they will further develop into extended defects, such as dislocations loops, stacking fault tetrahedrons and vacancy voids [2]. Furthermore, the interaction between certainly existed GB and radiation-deduced point defects has a significant effect on the performance of polycrystalline W.

Currently experimental observation of the formation of point defects in collision cascades is almost impossible due to its very short time and very small space scale (ps and nm), as well as the GB effect. Molecular dynamics (MD) method is an effective way to study the collision cascades [7,8,14,15]. Many of the research work done by MD on single crystal W [16–18] are very helpful in understanding the evolution process of collision cascades during which a lot of point defects, i.e. vacancies and interstitials form and recombine, leaving some defects survived. It is generally believed that GBs can be served as "sinks" for point defects and there have been researches to support this conclusion. Some studies such as bi-crystal W structure [19], copper [20] and nickel [21] have found that in the GB structures, the number of surviving interstitials in the GI is less than that in the single crystal and is related to the distance between the GB and the PKA. However, there also have been divergent results. For example, the study of radiation damage in nano-crystalline W [22] by MD reported that in the stable stage, the number of interstitials in nano-crystalline W is twice as large as that in single crystal W, which contradicts the above prevailing view. The contradictory results reflect the lack of awareness of interaction between GBs and radiation-induced defects. Therefore, clearly understanding the interaction mechanism between GBs and irradiation-induced defects is still much needed, which will be helpful for the deeper insight of effect of GBs and guidance in regulating size and orientation of grain to improve the resistance property and performance of materials on radiation damage.

In general, in order to know the effects of GBs, the total number of vacancies and interstitials are calculated with PKA at different d (the distance between the PKA and the center of the GB) in different GB systems [19–21]. It has been well known that in single crystal W the progress of collision cascades is divided into three stages: the ballistic stage, the recombination stage and the stable stage, and the mechanisms of each stage have been explored [16]. For the W system with GB structure, the existence of GB has an effect on the formation and evolution of the three stages, which directly affects the number and distribution of surviving point defects. However, the more detailed observations remain unclear, for instance, how different extent of effects of GB on vacancies and interstitials respectively? Whether or not the GB regions change after the interaction? It has been known that there is influence of GBs on the number of surviving point defects, whereas is there influence on distribution of surviving defects? And how the effects are?

To explore the above issues, in this paper, MD method is used and scheme of calculational tests is designed. Taking the six groups of symmetric tilt GB structures of body-centered cubic W as objects, the atomic evolution view of the interaction between GB and irradiation-induced point defects is given by visualization and quantitative calculation of the number of the point defects distribution. This paper focuses on the following parts: exploring the more detailed effect of GB on the number of irradiation induced vacancies and interstitials; visualizing the process of collision cascades; studying the interaction between the GB and the peak defect zone (PDZ); quantitatively analyzing the distribution of the number of point defects nearby GB.

2. Methodology

2.1. Theoretical model

In this study, we established two single crystal structures with different volumes and six common symmetric tilt GB structures in W. The six symmetric tilt GBs are Σ5 [001](120), Σ5 [001](130), Σ13 [001](150), Σ13 [001](230), Σ17 [001](140) and Σ17 [001](350) GB, where Σ represents the coincident site lattice parameter, [uvw] represents the rotation axis, and (hkl) represents the symmetry plane. In order to eliminate the instability of the GB structure, one of the two atoms in the GB with a distance of less than 0.8a (a is the lattice constant of W, and a is 0.316 nm) was removed.

Fig. 1 (a) is the stable structure of Σ5 [001](120) GB-W, which is selected as the representative symmetric tilt GB in this work. For a single crystal system, periodic boundary conditions were applied in all three directions. While for the GB systems, only two directions parallel to the GB interface imposed periodic boundary conditions. The energy of atoms in the GB is quite different from that in the GI. Therefore, the GB width of these six GB systems could be obtained by atomic energy distribution at different distances from the center of the GB. And then the GB energy was obtained by calculation. Table 1 and Table 2 list the basic information of structures for two single crystals and six GBs, including the volume of simulation region (V), the total number of atoms (N), the energy of PKA (E_{PKA}), the atomic density of the single crystal (ρ), the atomic density of the GB region before (ρ_1) and after (ρ_2) irradiation, and the increased percentage of atomic density after irradiation (δ, $\delta=(\rho_2-\rho_1)/\rho_1 \times 100\%$). Table 3 shows the information related to the six GB systems, including the symmetry plane (n), the angle of rotation (Φ), the coincident site lattice parameter (Σ), the GB width (H) and the GB energy (E).

2.2. The details of MD simulation

MD method was used in this work to study the interaction between symmetric tilt GBs and irradiation-induced point defects in W. The potential used in the MD simulations was the 2NN MEAM potential [23] coupled with the ZBL potential [24]. All simulations were carried out at 300 K. E_{PKA} is 3 and 5 keV, and the bigger the E_{PKA}, the larger the volume of the system and the greater the total

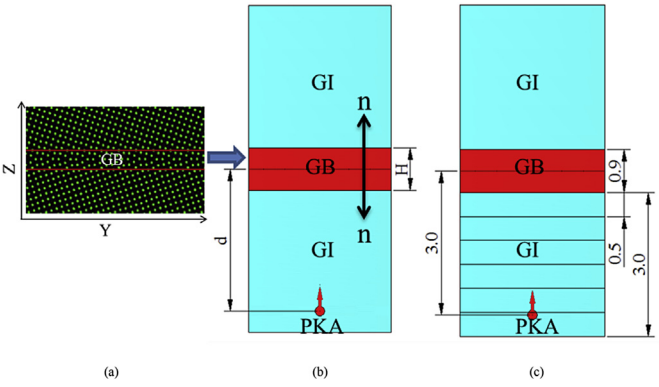

Fig. 1. Schematic diagrams of GBs. (a) The stable structure of the Σ5 [001](120) GB in bcc W. (b) Simulation setup. n represents the symmetry planes of the GBs. The PKA atom is launched towards the center of GB from a distance d with energy E_{PKA} is 3 and 5 keV, the width of the GB is H. (c) The scheme of calculational test, and the unit is nm. The widths of the GBs are about 0.9 nm, the distance of PKA from the center of GB is 3.0 nm. Counting the numbers of vacancies and interstitials in the range of 0–0.5, 0.5–1.0, 1.0–1.5, 1.5–2.0, 2.0–2.5 and 2.5–3.0 nm from the GB.