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.

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.

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1. Introduction

Tungsten (W) has the highest melting point (3410 °C) and the lowest vapor pressure ($1.3 \times 10^{-7}$ 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...
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, δ=(ρ_2−ρ_1)/ρ_1×100%). 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 number of point defects. 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.

![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.](image-url)
number of atoms (Tables 1 and 2). $E_{\text{PKA}}$ is determined by the elastic collision formula

$$E_{\text{PKA}} = \frac{4m_1m_2E_0}{(m_1 + m_2)^2}$$

where $E_0$ represents the kinetic energy of the neutron, $m_1$ and $m_2$ represent the mass of the neutron and the PKA, respectively. Substituting values for $E_0$, $m_1$ and $m_2$, equation (1) becomes $E_0 = 46.05\ E_{\text{PKA}},$ so $E_{\text{PKA}}$ of $3$ and $5$ keV used in this work corresponds to a neutron energy of $138.45$ and $230.25$ keV, respectively.

MD simulation was divided into four stages, namely, the simulation system construction, the relaxation, the radiation damage and the defect analysis. In the simulation system construction stage, different sizes of simulation boxes were established according to the simulation conditions such as $E_{\text{PKA}}$ (Tables 1 and 2). In the relaxation stage, the simulation system was relaxed for about 10 ps under the canonical (NVT) ensemble. In the defect analysis stage, the lattice matching analysis method (LMA) [25] was used to determine the number and distribution of radiation-induced point defects. It should be noted that the GB region was not included in the calculation of the number of interstitials or vacancies, due to its irregular arrangement of atoms.

**3. Results and discussion**

### 3.1. Effect of GB on the number of irradiation-induced vacancies and interstitials

Fig. 2 shows the variation of the number of surviving vacancies and interstitials formed in the GI at different $d$ with $E_{\text{PKA}}$ of $3$ or $5$ keV. For single crystal W, the average number of interstitials or vacancies (equal in number) is $7.28$ and $10.04$ when $E_{\text{PKA}}$ is $3$ and $5$ keV, respectively.

Table 3 shows the difference in the volume of the simulation box ($V$), the total number of atoms ($N$), the energy of PKA ($E_{\text{PKA}}$), the atomic density of the GB region before ($\rho_1$) and after ($\rho_2$) irradiation and the increased percentage of the atomic density after irradiation ($\delta$) of GB-W systems.

<table>
<thead>
<tr>
<th>GB system</th>
<th>N</th>
<th>$E_{\text{PKA}}$ (keV)</th>
<th>$\rho_1$ (atoms/nm$^3$)</th>
<th>$\rho_2$ (atoms/nm$^3$)</th>
<th>$\delta$ (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Sigma$ [001] [120]</td>
<td>94400</td>
<td>5</td>
<td>59.73</td>
<td>59.81</td>
<td>0.14</td>
</tr>
<tr>
<td>$\Sigma$ [001] [130]</td>
<td>212400</td>
<td>5</td>
<td>59.20</td>
<td>59.26</td>
<td>0.10</td>
</tr>
<tr>
<td>$\Sigma$ [011] [150]</td>
<td>78720</td>
<td>5</td>
<td>61.69</td>
<td>61.74</td>
<td>0.08</td>
</tr>
<tr>
<td>$\Sigma$ [011] [230]</td>
<td>70800</td>
<td>3</td>
<td>61.18</td>
<td>61.24</td>
<td>0.10</td>
</tr>
<tr>
<td>$\Sigma$ [011] [140]</td>
<td>78800</td>
<td>3</td>
<td>60.68</td>
<td>60.77</td>
<td>0.15</td>
</tr>
<tr>
<td>$\Sigma$ [011] [150]</td>
<td>209400</td>
<td>5</td>
<td>60.73</td>
<td>60.80</td>
<td>0.12</td>
</tr>
</tbody>
</table>

There are two main mechanisms at work from Fig. 3 (b) to 3 (c): (1) the interstitials and vacancies recombine, (2) the interstitials and vacancies diffuse towards GB. The first mechanism makes the number of defects significantly reduced. The second mechanism results in...
enrichment of vacancies within the GI, due to reduced vacancy-interstitial recombination. Understanding the second mechanism is as follows. The diffusion energy barrier of interstitial (0.002 eV) is much lower than that of vacancy (1.8 eV) in W\(^{[27]}\). The interstitials can also migrate at a very low temperature (1.5 K)\(^{[26]}\). However, it is reasonable to regard vacancies as immobile in the time scale of ps at the temperature of 300 K, which can be verified in the early work that our group has done on single W\(^{[28]}\). Therefore, interstitials can migrate a long distance towards GB and are absorbed by GB due to low diffusion energy barrier, which is a main reason why the GB has a bias-absorption effect on interstitials compared with vacancies.

The diffusion capacity of interstitials is further enhanced due to the presence of the GB. The research results of Li et al.\(^{[29]}\) show that the diffusion capacity of interstitials is enhanced at a certain distance from the GB, and interstitials are directly absorbed by the GB at several atomic layers of distance from the GB. Visual observation in Fig. 3 (c) shows that there are some vacancies and interstitials in the region next to the GB, which we define as local extension of GB.

Now we analyze two exception data with arrow marks in Fig. 2 (d). When we account the numbers of point defects in GI, the assumption that the GB width does not change is taken. It is the GB local extension, as shown in Fig. 3 (c), that leads to the two exception data in Fig. 2 (d), as well as the data of number of vacancy outside the blue trend line in Fig. 2 (a) and (c). From more visualization of our most simulation cases and the analysis of data in Fig. 2, this GB local extension accounts for a small proportion.

### 3.3. The interaction between the GB and the PDZ

The peak defect zone (PDZ), formed during collision cascades with the highest number of point defects, has a strong effect on the number and spatial distribution of the final point defects in the process of collision cascade, which had also been seen in single crystal W\(^{[28]}\). In polycrystalline, it is significant to clearly understand the interaction between the GB and the PDZ. Taking $\Sigma 5$ [001] [120] GB system as an example, the calculational tests of different $d$ values ($d$ is 0.5, 1.0, 1.3, 1.6, 2.0, 2.3, 2.6, 3.0, 4.0 and 5.0 nm) are designed to observe the evolution of point defects at different cases, PDZ passes through GB, PDZ overlaps with GB, and PDZ is not in contact with GB when $E_{PKA}$ is 3 keV, see some cases in Fig. 4.

<table>
<thead>
<tr>
<th>$d$ (nm)</th>
<th>1.0</th>
<th>1.3</th>
<th>1.6</th>
<th>2.0</th>
<th>2.3</th>
<th>2.6</th>
<th>3.0</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta N_v$</td>
<td>4.28</td>
<td>1.02</td>
<td>6.31</td>
<td>3.30</td>
<td>3.82</td>
<td>5.99</td>
<td>5.06</td>
</tr>
<tr>
<td>$\Delta N_i$</td>
<td>2.29</td>
<td>0.22</td>
<td>5.01</td>
<td>2.50</td>
<td>0.86</td>
<td>1.76</td>
<td>1.19</td>
</tr>
</tbody>
</table>

Table 4: The difference of the number of average surviving vacancies $\Delta N_v$ and the difference of the average surviving number of interstitials $\Delta N_i$ in GI for symmetric tilt GB-W systems when $E_{PKA}$ changes from 5 to 3 keV.

Fig. 2. The variation of the number of surviving defects formed in GI of GB-W at different $d$ with $E_{PKA}$ of 3 or 5 keV. (a) Vacancies, $E_{PKA} = 3$ keV; (b) Interstitials, $E_{PKA} = 3$ keV; (c) Vacancies, $E_{PKA} = 5$ keV; (d) Interstitials, $E_{PKA} = 5$ keV. The corresponding horizontal red solid lines are the average number of interstitials or vacancies (their numbers are equal) in the single crystal with horizontal red dash lines presenting its error bars. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)
Fig. 4 shows the visualization of distribution of point defects in the PDZ and at the stable stage in $\Sigma 5[001](120)$ GB-W system. Table 5 lists the number of surviving vacancies and interstitials, $N_V$ and $N_I$, at different $d$ values in $\Sigma 5[001](120)$ GB-W system with $E_{\text{PKA}}$ of 3 keV.

When the PDZ is not in contact with the GB, for example, $d$ is 5.0 nm (Fig. 4 (g) and (h)), it looks there is no interaction between the GB and the PDZ, and the existence of GB seems not change the number of formed point defects. Thus, the GB-W system should be equivalent to the single crystal W system in this case. However when we check from Table 5 at $d = 5.0$ nm, $N_V$ is almost equal to that in single crystal W ($7.28 \pm 0.17$), but $N_I$ is less than that in the single crystal W ($7.28 \pm 0.17$). These imply that interstitials which are not nearby the GB are still able to diffuse towards GB and are absorbed by GB, while vacancies not.

When the PDZ comes into contact with the GB, for example, $d$ is 1.6 and 3.0 nm (Fig. 4 (c), (d), (e) and (f)), there is interaction between the GB and the PDZ with different overlapping. From Table 5 at the range 1.6–2.0 nm of $d$, the number of defects especially $N_V$ is
relatively low, corresponding to the overlapping area between the GB and the PDZ is larger as shown in Fig. 4 (c) and (d). Similar results were observed in Cu [20] and TiO2 [30], when the PDZ overlaps with the GB region maximally, the number of point defects formed in the GI is least. Let d goes small further for example, d is 0.5 nm (Fig. 4 (a) and (b)), the PDZ passes through the GB, both NV and NI increase again. Thus we can draw the conclusion that the ratio of GB region overlaps with PDZ is larger, the number of surviving point defects in the GI is statistically relative smaller.

3.4. The variation of the number of surviving point defects with distance from GB

As mentioned above, the existing studies [19–21] only gave the total number of surviving vacancies and interstitials for different GB systems at different d values. However, it is an interesting issue to detect the effect of GB on the variation of defect number with distance from GB. In this paper, the calculational test scheme is designed and the main ideas are: Counting the number of surviving vacancies and interstitials at different distance from the GB, analyzing their variation, and considering the effect of E_{PKA}.

The schematic diagram of calculational test scheme is shown in Fig. 1 (c). The widths of the GBs are about 0.9 nm. The fixed d value is 3.0 nm, and E_{PKA} is 3 or 5 keV. The distance of 3.0 nm to the edge of GB was divided into six equal bins, and the numbers of vacancies and interstitials in the bin 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 were counted.

Fig. 5 shows that the variation of the number of surviving vacancies and interstitials formed in GI with distance from the GB of W at different E_{PKA}. It should be noted that if there is no vacancy or interstitial in some bin, the height of the histogram is zero. In the following analysis we first neglect the special data points marked by circles in Fig. 5, which will be analyzed later. It can be seen from Fig. 5 (a) and (b) that the number of vacancies varies with the distance from the GB whenever E_{PKA} is 3 or 5 keV, but there is a common distribution trend: vacancy-intensive region exists. When E_{PKA} is 3 keV (Fig. 5 (a)), the number of vacancies which distribute in the bin of 1.0–2.0 nm is more than other bins; when E_{PKA} is 5 keV (Fig. 5 (b)), the similar bin is 0.5–1.5 nm. In other words, the distribution of vacancies is affected by E_{PKA}, and the vacancy-intensive region tends to move forward (towards GB) with the increase of E_{PKA}.

On the whole, the vacancy-intensive area is formed nearby the GB. We understand this from the diffusion energy barrier of the vacancy. The diffusion energy barrier of the vacancy is 1.8 eV in the single tungsten [27], but its value starts to decrease, from 1.8 eV to 1.2 eV, 0.7 eV, 0.5 eV or even smaller in several layers near the GB [2]. Therefore, the vacancies near the GB may become mobile, and may diffuse towards the GB or even are absorbed by the GB due to the decrease of the diffusion energy barrier. Finally, the number of surviving vacancies in the thickness of several atomic layers (within 0.5 nm) from the GB is relatively smaller than those in the vacancy-intensive region. In Fig. 5, the PKA is set at d = 3.0 nm, and the PDZ is located at between GB and PKA as shown in Fig. 3 (b), very near GB region, leading to few vacancies in the vicinity of d of 3.0 nm, as shown in Fig. 3 (c).

It can be seen from Fig. 5 (c) and (d) that either E_{PKA} is 3 or 5 keV, no matter the number or the variation of interstitials is relatively less in the range of 0–3.0 nm from the GB compared with that of vacancies, and is affected by the E_{PKA} far less than the situation of vacancy. This is quantitatively evidence that the interstitials are easier to diffuse and are absorbed by GB than vacancies, mainly attributing to the big difference of the diffusion energy barrier of interstitial and vacancy in W (0.002 eV vs 1.8 eV).

There are six special points in Fig. 5 which are marked by green or red circles. Five of them are marked by green circles, one in Fig. 5 (a), (b) and (c) respectively, and two in Fig. 5 (d). By visualizing them one by one, the GB local extension is observed in these five cases and ignored these data in analysis. The case marked by red circle in Fig. 5 (d) is also visualized. In incidence more number of interstitials (2.5) locally sites in the bin of 1.5–2.0 nm.

Fig. 5. The variation of the number of surviving vacancies and interstitials formed in GI with distance from the GB of W, d = 3.0 nm, the distance of PKA from the center of GB. (a) Vacancies, E_{PKA} = 3 keV; (b) Vacancies, E_{PKA} = 5 keV; (c) Interstitials, E_{PKA} = 3 keV; (d) Interstitials, E_{PKA} = 5 keV.
with less number in its adjacent two bins. In this study, we found the GB local extension in Z5 [001] [120], $\Sigma 17$ [001] [350] and $\Sigma 13$ [001] [230] GB systems. We calculate the atomic density of the GB region before ($p_1$) and after ($p_2$) irradiation for the symmetric tilt GBs, which is shown in Tables 1 and 2. It reads that $p_1$ is related to the GB type, and less than the atomic density of the single crystal. No matter which grain boundary system is, $p_2$ is always greater than $p_1$ and the increased percentage of the atomic density after irradiation, $\delta$, is 0.08–0.15%. This result indicates that a portion of the interstitials is absorbed by GB after irradiation, which may be the reason for the GB local extension. Li et al. [2] studied the role of the GB in W in heating radiation damage, the $E_{PKA}$ is 6 keV and the simulated temperature is 600 K. They found that the semi-influence range of the GB extends to about 10 Å locally from 5 Å of the pristine GB in the Z5 [001] [130] GB system. Zhang et al. [31] studied the GB sink strength under prolonged electron irradiation. They constructed two sets of twist GBs of high energy and large angle, $E_{PKA}$ was 40 eV and the simulated temperature was 2000 K. They found that high-energy GBs which were served as “sinks” for the irradiation-induced point defects did not saturate in BCC Mo, at least for nanograins. Moreover, the analysis of GB structure showed that the atomic density and width of the GBs remain unchanged after the absorption of point defects. Therefore, more calculation data will be needed to understand of the extent of the GB absorption point defects and the change of the GB structure after GB interacting with the radiation-induced defects.

4. Conclusion

In this paper, the atomic evolution view of interaction between GB and irradiation-induced point defects is given by using molecular dynamics method with taking six symmetric tilt GB structures of tungsten. It is found that the GB has a bias-creation effect on interstitials compared with vacancies by studying the effect of GB on the number of irradiation-induced vacancies and interstitials. The number of surviving vacancies is statistically increasing with the increase of the distance between the PKA and the center of the GB, but the number of interstitials changes little and is less than that of the single crystal. The number of surviving vacancies in the GI is more than that of interstitials. The visualization and quantitative analysis of the data of surviving vacancies and interstitials show that during the whole collision cascade process two main mechanisms played synergistic role in the reduction of the number of point defects in the recombination stage, which were the recombination of vacancies and interstitials and the diffusion of interstitials towards the GB. By analyzing the various extent of interaction between the GB and the PDZ, it is found that the ratio of the GB region overlaps with PDA is larger, and the number of surviving point defects in the grain interior is statistically relative smaller. When the GB region almost does not overlap with PDZ, the vacancies-intensive area is formed near the GB, and tends to move forward (towards the GB) with the increase of $E_{PKA}$. But the distribution of interstitials is relatively uniform, which is affected by the $E_{PKA}$ far less than the situation of vacancy. This gives quantitative evidence that the irradiation-induced interstitials are easier to diffuse longer distance and be absorbed by GB than vacancies, resulting in that the GB has a bias-creation effect on interstitials. The GB local extension after irradiation is observed for which the interstitials absorbed by the GB may be responsible. The evolutionary details of the interaction between the symmetric tilt GB and irradiation-induced point defects provide more insight into its physical picture. The designed scheme of calculation test is completely applicable to studies of the effect of other types of GBs on irradiation-induced point defects.

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