Postprint: Molecular Dynamics Study of Early-Stage W Irradiation Damage

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Abstract

Molecular dynamics simulations were employed to investigate the atomic mechanisms of irradiation-induced defect formation and evolution in bcc-W during the early stages of neutron irradiation. Primary knock-on atom (PKA) energies of 1.0–25.0 keV were selected, with simulation temperatures ranging from 100 to 900 K, to study the number and distribution of defects produced by displacement cascades in W, the influence of PKA direction and temperature on the number of stable Frenkel pairs, defect clusters, and the displacement threshold energy of W. The results show that if cascade-induced defects exhibit a nearly spherical dense distribution at the peak stage, the number of Frenkel pairs in the stable stage is relatively small; conversely, if defects exhibit a non-spherical, relatively dispersed distribution, the number of Frenkel pairs in the stable stage is relatively large. The number of stable Frenkel pairs is not significantly affected by PKA direction and shows a decreasing trend with increasing temperature. In comparison, the fraction of interstitial atom clusters is higher than that of vacancy clusters, while vacancy clusters tend to form larger clusters. The average displacement threshold energy of W is less affected by temperature and exhibits certain anisotropy.

Full Text

Molecular Dynamics Study of Initial Radiation Damage in Tungsten

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Abstract

Tungsten is a candidate material for the first wall and divertor in a tokamak fusion reactor, where it must withstand high neutron irradiation. The defects created in displacement cascades form the primary state of damage, and their subsequent evolution leads to important changes in microstructure and engineering properties. However, the evolution and aggregation of radiation-induced defects at the atomic level cannot be observed experimentally to date. In this work, the molecular dynamics (MD) method was used to explore the microstructural processes and atomic mechanisms of defect formation and evolution in bcc-W during the initial stage of radiation. The primary knock-on atom (PKA) energy range was 1.0–25.0 keV, and the simulation temperature range was 100–900 K. We investigated the number and distribution of defects produced by displacement cascades, the influence of PKA direction and temperature on the number of stable Frenkel pairs, defect clusters, and the displacement threshold energy of W. The results showed that if the cascade-induced defects exhibit a nearly spherical and dense distribution at the peak stage, the number of stable Frenkel pairs is relatively small; conversely, if the defects show a non-spherical and relatively dispersed distribution, the number of stable Frenkel pairs is relatively large. The number of stable Frenkel pairs is insensitive to PKA direction and tends to decrease with increasing temperature. Comparatively, the fraction of interstitial clusters is higher than that of vacancy clusters, while vacancies tend to form larger clusters. The average displacement threshold energy of W is less affected by temperature and exhibits certain anisotropy. The results of this work can provide data for analyzing the behavior of W materials under nuclear environments.

KEYWORDS W, molecular dynamics (MD), displacement cascade, steady Frenkel pairs number, displacement threshold energy

Introduction

In both the International Thermonuclear Experimental Reactor (ITER) Tokamak and future Demonstration Fusion Reactor (DEMO), the first wall must withstand high neutron fluxes (2.5×10^{22} n/cm^2) and severe thermal fluxes (10

MW/m^2 in ITER)[?]. Therefore, the protective layer material for the first wall, the so-called plasma-facing material, must be selected based on its performance under harsh radiation conditions. Tungsten has become a leading candidate for plasma-facing materials in future fusion reactors due to its high thermal conductivity, low sputtering yield, high melting temperature[?], and low hydrogen retention[?]. The divertor, which can remove H isotopes, He, and impurities from the plasma, also tends to be made of W or tungsten alloys, and all-W divertors already exist. In He-cooled divertor designs, W is also considered as a structural material[?]. Therefore, understanding the performance of W under irradiation conditions is a critical issue for nuclear energy development. However, the formation and aggregation of irradiation-induced point defects occur at spatiotemporal scales of picoseconds (ps) and nanometers (nm), which cannot be measured by current experimental techniques. Consequently, computer simulation plays a key role in studying irradiation effects[?]. Among these methods, molecular dynamics (MD) is widely used because it provides details of atomic dynamic processes, tracks structural evolution as a function of time, and describes spatial and temporal scales consistent with those of irradiation-induced displacement cascades.

When irradiation neutrons enter the material lattice, they transfer part of their energy to W atoms. This W atom becomes the primary knock-on atom (PKA), which triggers a series of collisions in W called a collision cascade, resulting in irradiation displacement damage and the formation of interstitials and vacancy defect pairs (Frenkel pairs), vacancy clusters, interstitial clusters, dislocation loops, vacancy tetrahedra, and other irradiation defects. In the initial stage of irradiation damage, displacement cascades first produce a large number of Frenkel pairs, which reach a peak in a short time and then gradually decrease and stabilize under the thermal spike effect[?]. In recent years, W has received increasing attention due to its potential excellent properties. Xu et al.[?] used MD to study vacancy diffusion behavior in irradiated W and found that vacancy migration threshold energy and W atom recoil energy depend on PKA direction, and that recoil atoms interact not only with nearest-neighbor vacancies but also with second-nearest-neighbor vacancies. Li et al.[?] used MD to study irradiation damage from low-energy (20.0–200.0 eV) He atoms bombarding W surfaces at different temperatures, finding that surface damage can occur below the commonly assumed threshold energy, and that increasing substrate temperature increases the likelihood of W atoms stacking on the surface, with the most probable energy range for this surface damage being 50.0–80.0 eV. Caturla et al.[?] studied cascade efficiency and defect distribution in W under 1.9 GeV proton irradiation, showing that vacancies in W are isolated and no vacancy clusters form under 30.0 keV PKA. Troev et al.[?] studied defect properties in W containing H and He through quantum mechanical calculations of positron lifetime, finding that H and He atoms are absorbed in vacancies and nanovoids in W, and their presence in larger nanovoids significantly reduces positron lifetime. Park et al.[?] studied the distribution direction of dumbbell interstitials, concluding that stable dumbbell interstitials all align along the

[111] direction, and that during irradiation damage, [111]-oriented dumbbell interstitials recombine with vacancies faster than those in other directions. As interest in W materials continues to grow, a deeper understanding of defect formation mechanisms and various properties of W under irradiation conditions is of great significance for nuclear energy development.

This work uses the molecular dynamics method to systematically understand the formation mechanisms of vacancies, interstitials, and their clusters induced by neutron irradiation in W at the microscopic atomic scale, calculating defect numbers and distributions, and analyzing the influence of temperature, irradiation energy, PKA incident direction, and other factors. Additionally, this work calculates the displacement threshold energy E_d of W.

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1 Computational Methods and Conditions

Tungsten has two allotropes, α and β. At standard temperature (0 °C, 273.15 K) and normal pressure (1.01×10^5 Pa), α-W is stable with a bcc structure. β-W only appears in the presence of oxygen, is stable below 630 °C, and transforms back to α-W above 630 °C in an irreversible process. The research object of this work is α-W, i.e., bcc-W.

This work employs the molecular dynamics method to study defect formation and evolution in bcc-W during the initial stage of irradiation damage. The PKA energy E_{PKA} is obtained from the elastic collision formula between a W atom (mass m_2) and a neutron (energy E_{01}, mass m_1): $E_{\mathrm{PKA}} = \frac{4m_1m_2E_{01}}{(m_1+m_2)^2}$. The approximate relationship is $E_{01} = 46.05E_{\mathrm{PKA}}$. Therefore, the maximum PKA energy studied in this work is 25.0 keV, corresponding to approximately 1151.25 keV neutron energy. The 14.0 MeV neutron energy in a fusion reactor corresponds to approximately 306.0 keV PKA energy[**?**]. Fast neutrons transfer energy to PKA atoms in W in the range of 1.0 to 100.0–200.0 keV, and most defects in fusion materials are produced by PKA energies less than 100.0 keV[**?**]. Based on available computational resources, the PKA energy in this work was set to 1.0–25.0 keV, and the simulation system size ranged from approximately 20,000 to 130,000 atoms depending on the PKA energy. The PKA incident directions were mainly [100] and [135]; simulation temperatures were 100, 500, and 900 K. The potential function was constructed by coupling the Ziegler–Biersack–Littmark (ZBL) potential[**?**] with the 2NN MEAM potential proposed by Lee et al.[**?**], which better reproduces high-energy particle collisions. This type of potential function was also used in reference[**?**].

First, the model was relaxed for about 10 ps in the isothermal–isobaric (NPT) ensemble at the target temperature to bring the system energy to its lowest state under the set conditions, obtaining a stable structure (Structure 1), which served as the reference structure for defect analysis. Then, a specific atom in Structure 1 was selected as the PKA and assigned a new initial velocity according to the set simulation energy and direction, while the velocities and directions

of other atoms remained unchanged. This structure (Structure 2) served as the initial structure for irradiation damage simulation, and cascade collision simulations were performed in the canonical (NVT) ensemble for a certain period. The simulation time for a single cascade depends on the system size, PKA energy, and potential function; this work simulated atomic motion behavior occurring within 10–30 ps. A Berendsen thermostat was applied outside the system to maintain the simulation temperature at the set value, and periodic boundary conditions were applied throughout the simulation system. After irradiation, statistical analysis was performed on the results, primarily using the lattice matching analysis (LMA) method[**?**] to determine the number and distribution of point defects induced by cascade collisions. At least 6 simulations with different PKAs were performed under each specific energy and temperature condition, and the results were statistically averaged.

The displacement threshold energy E_d is defined as the minimum energy transferred to a lattice atom to cause displacement and produce permanent defects. For E_d calculations, the model contained 4032 atoms, and E_d was calculated for 3 temperatures (100, 500, and 900 K) and 3 directions ([100], [110], and [111]). Under a given temperature and direction, the selected PKA atom was given energy in a range of 15 eV, increasing in 1 eV increments. Within this energy range, the minimum PKA energy that produced a stable Frenkel pair was defined as E_d for that atom in the selected direction. This simulation was performed 75 times, each time selecting a different PKA, and the average of the 75 calculations was taken as the E_d of W at that temperature and direction. The same procedure was followed for other temperatures and directions, with a total of 675 calculations for E_d.

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2 Results and Discussion

2.1 Temporal Evolution and Morphology of Frenkel Pairs During W Irradiation

[Figure 1: see original paper] shows the evolution curves of the number of Frenkel pairs in W over time under different PKA energies (5.0, 15.0, and 25.0 keV) at 100 K. The curve characteristics are consistent with previous research results[**?**, **?**, **?**]. At the initial moment, Frenkel pairs increase rapidly to a peak (the ballistic phase), then decrease quickly (the recovery phase), and finally reach a stable stage (10–30 ps). It can be seen that both the time to reach the peak and the time to reach a stable state increase with PKA energy (1.0–25.0 keV). [Figure 2: see original paper] shows the distribution of point defects at the peak moment and stable stage when the PKA energy is 10.0 keV. Black atoms represent vacancies, mainly distributed at the cascade center; white atoms represent interstitials, mostly distributed at the edges of the cascade center. It can be observed that after the cascade passes the peak stage, a large number of interstitials recombine with vacancies under the thermal spike effect, causing

the number of Frenkel pairs to drop rapidly, leaving fewer Frenkel pairs at the stable stage.

Simulation results show that when the energy exceeds 10.0 keV, the variation in cascade distribution morphology during the defect peak stage caused by different PKAs becomes significant, which affects the final number and distribution of Frenkel pairs, as shown in [Figure 3: see original paper]. Generally, the peak defect morphology can be divided into two types: nearly spherical dense type and non-spherical relatively dispersed type. If the defects at the peak moment show an approximately spherical dense distribution, the peak defect number is usually large. Because the separation distance between vacancies and interstitials is relatively small and the thermal spike effect lasts longer, defect recombination is relatively easy, leading to a high probability of fewer Frenkel pairs at the stable stage, as shown in [Figure 3a: see original paper]. If the defects at the peak moment show a non-spherical relatively dispersed distribution, the peak defect number is relatively small, the thermal spike stage is relatively short, and the separation distance between interstitials and vacancies is larger, which is not conducive to defect recombination, resulting in more residual Frenkel pairs, as shown in [Figure 3b: see original paper]. This trend is not significantly affected by PKA direction.

When the defects at the peak moment are of the non-spherical relatively dispersed type, an alternating sequence of vacancies and interstitials along the close-packed [111] direction can sometimes be observed, as shown in the circled part of [Figure 3b: see original paper]. Interstitials migrate to positions far from the cascade center through this form, making them less likely to recombine and also leading to more Frenkel pairs.

2.2 Number of Frenkel Pairs at Stable Stage

The relationship between the number of stable Frenkel pairs N_{FS} calculated in this work and PKA energy is shown in [Figure 4: see original paper], which follows the empirical formula recommended by Bacon et al.[**?**]:

$$N_{\mathrm{FS}} = aE_{\mathrm{PKA}}^{b}$$

where a and b are constants less affected by irradiated material type and temperature. Fitting the MD data yields $a = 3.433$ and $b = 0.697$, similar to results from references[**?**] ($a = 3.706, b = 0.590$) and[**?**] ($a = 3.335, b = 0.602$). [Figure 4: see original paper] also shows the estimation of Frenkel pair numbers $N_{\mathrm{FS(NRT)}}$ using the Norgett–Robinson–Torrens (NRT) formula[**?**]:

$$N_{\mathrm{FS(NRT)}} = 0.8\frac{E_{\mathrm{dam}}}{2E_d}$$

where E_{dam} refers to damage energy rather than PKA energy. However, since MD simulations do not consider ionization energy loss, using E_{PKA} to approx-

imate E_{dam} for comparison with MD-simulated N_{FS} predictions is appropriate[**?**, **?**]. E_d was selected as 85 eV[**?**, **?**].

As shown in [Figure 4: see original paper], the N_{FS} produced by MD-simulated cascades is significantly lower than the NRT predicted values. This is because only a small fraction of interstitials produced in cascades migrate to distant locations through focused collision chains, while most interstitials are generated at the edges of the irregular cascade region. These interstitials are very close to vacancies at the defect center, and the cascade defect center has high kinetic energy during the thermal spike stage, which facilitates interstitial–vacancy recombination, resulting in a significant reduction in Frenkel pairs. Similar results were obtained for W in reference[**?**] and for various metals including Fe, Cu, and Zr in reference[**?**]. These two methods for estimating irradiation damage defects lead to the concept of cascade efficiency.

Cascade efficiency is defined as $\eta = N_{\mathrm{FS}}/N_{\mathrm{FS(NRT)}}$[**?**, **?**]. As PKA energy increases, cascade efficiency shows a decreasing trend, eventually stabilizing at approximately 0.3 ([Figure 5: see original paper]), consistent with the value obtained in reference[**?**]. Bacon et al.[**?**] also showed that cascade efficiencies for different metals typically stabilize between 0.2 and 0.4.

2.3 Relationship Between N_{FS} and PKA Incident Direction

The arrangement period and density of atoms differ along different crystal directions in a crystal, leading to anisotropic properties. Therefore, bcc-W will also exhibit anisotropic irradiation performance in cascade collisions. shows the number of Frenkel pairs in the stable stage and the variation of Frenkel pair numbers with direction under different PKA directions in W.

The variation in Frenkel pair numbers is calculated using the following formula:

$$F = 100\% \times \frac{(N_i - N_{\mathrm{ave}})}{N_{\mathrm{ave}}}$$

where F represents the variation of Frenkel pair numbers with different PKA directions, N_i represents the stable Frenkel pair number for each direction, and N_{ave} represents the average of Frenkel pair numbers for 5 directions. The results show that the data fluctuation is only about 10% at most, as shown in . It can be seen that the stable Frenkel pair numbers for the 5 directions studied in this work differ very little at 3.0 keV energy.

Therefore, at low energies, PKA direction has no obvious effect on the number of stable Frenkel pairs in bcc-W cascade collisions. Similar results were obtained in reference[**?**] for hcp-Ti with PKA energies of 0.3–5.0 keV and in reference[**?**]. It should be noted that to enhance the accuracy of simulation results, at least 3 simulations with different PKAs were performed for each direction in this work, and the simulation results were statistically averaged.

2.4 Relationship Between N_{FS} and Temperature

To study the effect of temperature on irradiation defect generation, simulations were performed at PKA energy of 3.0 keV and temperatures of 100, 500, and 900 K, with 9 calculations performed at each temperature. The results are shown in [Figure 6a: see original paper]. It can be seen that N_{FS} decreases slightly with increasing temperature. To verify this at different energies, cases at 5.0, 10.0, and 15.0 keV were also calculated, as shown in [Figure 6b: see original paper]. Overall, N_{FS} shows a slight decreasing trend with increasing temperature, similar to results in references[**?**, **?**, **?**], with a decrease amplitude between 7% and 40%. This may be because increasing temperature enhances W atomic mobility and thermal spike duration, both of which promote interstitial–vacancy recombination to some extent, leading to more defect annihilation and thus reducing the number of Frenkel pairs remaining at the stable stage. Another possible reason is that increased temperature shortens the replacement collision sequence (RCS) length in cascades, causing cascades to exist in a more compact form, resulting in smaller separation distances between vacancies and interstitials, which facilitates recombination.

2.5 Defect Clusters

Defect clusters affect the migration direction and ease of point defects and may also influence the recovery and annihilation of point defects in cascades and the evolution of material properties after irradiation, so their role cannot be underestimated. Cluster fraction f_{cl} is defined as the ratio of the number of defects forming clusters N_{cl} to the total number of defects of that type N_{tot}:

$$f_{cl} = \frac{N_{cl}}{N_{tot}}$$

For example, the interstitial cluster fraction f_{cli} is the ratio of the number of interstitials forming interstitial clusters N_{cli} to the total number of interstitials N_{toti}. [Figure 7: see original paper] shows the variation of interstitial cluster fraction f_{cli} and vacancy cluster fraction f_{clv} with PKA energy at 100 K at the stable stage.

As shown in [Figure 7: see original paper], defect cluster fractions are roughly between 0.15 and 0.40, similar to references[**?**, **?**, **?**], indicating that cluster fractions are not high. Thus, most defects in W still exist as single defects, but in most cases f_{cli} is higher than f_{clv}, consistent with results in references[**?**, **?**, **?**]. These studies show that most single interstitials or interstitials in clusters have high mobility within the MD simulation time scale. According to literature reports, the migration activation energy of W atoms in the [111] direction is (0.03 ± 0.002) eV[**?**], (0.047 ± 0.01) eV[**?**], 0.03 eV[**?**], and 0.061 eV[**?**], while the vacancy migration energy of W is 1.44 eV[**?**], 1.78 eV[**?**], and 2.054 eV[**?**], with an average vacancy migration energy of (3.1 ± 0.05) eV[**?**]. It can be seen that interstitial migration energy is much smaller than vacancy migration energy,

and smaller migration energy makes migration easier, thus facilitating cluster formation. Moreover, studies have shown that once formed, vacancies are not easily mobile. For example, Fikar et al.[**?**] introduced one Frenkel pair in a large system at 1000 K, and MD simulation for 50 ps showed that interstitials migrated 15 lattice distances along the [111] direction while the vacancy did not move. Bai et al.[**?**] also concluded that vacancies are not easily mobile in their study of Cu. This work also visualized the stable stage of the cascade process and found that W vacancies basically do not move after formation ([Figure 8: see original paper]).

Therefore, interstitials may more easily form clusters due to their higher mobility. The calculation results of this work also show that under low-energy PKA (less than 5.0 keV), it is difficult for either interstitials or vacancies to form clusters. When PKA energy increases, single defects still account for a large proportion of total defects. However, as shown in [Figure 9: see original paper], compared with interstitial clusters, although vacancy clusters with size (i.e., number of vacancies in a cluster) of 4 or less are relatively fewer, vacancies are more prone to form large clusters, forming vacancy clusters with more than 5 vacancies, even creating a large cluster containing 12 vacancies. Interestingly, research results on W vacancy clusters are highly controversial. Reference[**?**] observed vacancy clusters at 5 ps in cascades with 20.0 keV PKA energy, but the clusters disappeared at 30 ps. Proton irradiation studies of W[**?**] showed that W vacancies are isolated, and no vacancy clusters formed even at 30.0 keV PKA energy. However, reference[**?**] concluded that large vacancy clusters can be generated at 10.0 keV PKA energy. Therefore, the issue of vacancy clusters in W under irradiation requires further in-depth study.

2.6 Displacement Threshold Energy

Both experiments and simulations have studied the E_d of W, but the results vary greatly. Moreover, experiments can only measure secondary effects of defect formation (resistivity or dislocation loops), making the true E_d difficult to measure experimentally. Molecular dynamics simulation is an ideal method for calculating E_d because it can directly "control" individual displacement events of specific atoms in specific directions of the lattice without interference from other events. [Figure 10: see original paper] shows the calculated E_d of W in the [100], [110], and [111] directions at temperatures of 100, 500, and 900 K, with results from other researchers[**?**, **?**, **?**, **?**, **?**] included for comparison. It can be seen that the simulation results of this work are basically within the range of previous studies. The average E_d values (averaged over 3 directions) at 100, 500, and 900 K are 62.17, 62.77, and 59.47 eV, respectively. It is evident that E_d is not significantly affected by temperature, showing a slight decrease at 900 K. However, from the perspective of individual directions, E_d in the close-packed [111] direction increases slightly with temperature, while E_d in the [100] and [110] directions decreases slightly.

The increase in E_d with temperature may be due to the following reasons: Defect

generation in the system is mainly caused by collision chains and RCS that easily form along close-packed directions after collisions. High temperature intensifies atomic thermal vibrations, shortening RCS length and reducing the average separation distance between vacancies and interstitials, making recombination more likely. At the same time, recovery of interstitials and vacancies other than RCS is also promoted, requiring more energy to produce stable Frenkel pairs, thus increasing E_d. The decrease in E_d with temperature may be because high temperature not only promotes recovery but also provides opportunities for some interstitials to thermally activate and migrate to positions far from the cascade center, leading to a decrease in E_d.

Based on the above analysis, the effect of temperature on E_d is the result of two competing mechanisms with opposite effects. Whichever mechanism dominates will determine the corresponding temperature effect on E_d.

[Figure 11: see original paper] is a box plot of the relationship between E_d and PKA incident direction. It can be seen that PKA incident direction has a significant effect on E_d, consistent with many previous studies. The average E_d shows a maximum value in the [110] direction (80.0 eV) and a minimum value in the close-packed [111] direction (40.0 eV). The relatively small E_d in the close-packed direction may be because RCS along this direction makes it easier for interstitials to migrate far from vacancies, producing more Frenkel pairs. Calculation results for Cu in reference[**?**] and for V in reference[**?**] also showed that E_d in close-packed directions is relatively small compared to other directions. The [100], [110], and [111] directions calculated in this work are all low-index directions, with maximum E_d of about 90.0 eV. Reference[**?**] calculated E_d for Cu and found that low-index directions had lower E_d (only about 25.0 eV in [100] and [110] directions), while high-index directions had relatively high E_d (up to 180.0 eV). It can be seen that E_d exhibits certain anisotropy.

It is evident that temperature (100–900 K) has little effect on the average E_d, which decreases slightly by about 3.0 eV at 900 K. The decrease in E_d indicates that less energy is required to produce stable defects, meaning that more defects will be generated in the system under the same irradiation energy (several keV). This seems to contradict the earlier statement that the number of stable Frenkel pairs shows a decreasing trend with increasing temperature. Moreover, E_d is affected by direction, which seems to contradict the earlier statement that the number of stable Frenkel pairs is insensitive to PKA direction at 3.0 keV. This is because, in addition to atomic collision displacement, the accompanying thermal spike effect cannot be ignored in cascade collision processes. The thermal spike has a significant impact on point defect recovery, thereby affecting irradiation-induced stable Frenkel pairs. The fact that the number of Frenkel pairs produced by MD-simulated cascades is much smaller than the NRT predicted value is a typical manifestation of the thermal spike effect. In displacement threshold energy calculations, because the applied PKA energy is very small (tens of eV), the thermal spike effect is minimal, so the comprehensive effect of temperature on E_d is mainly reflected in defect pair separation, leading to a slight decrease

in E_d with increasing temperature. The effect of direction on E_d shows certain anisotropy due to different lattice arrangement periods and densities. Therefore, although E_d is an important parameter affecting interstitial and vacancy defect formation, the final number of stable Frenkel pairs cannot be simply judged by E_d alone.

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3 Conclusions

1. For the simulated PKA energy range (1.0–25.0 keV) and temperature range (100–900 K) in bcc-W, cascade defect distributions at the peak stage generally exhibit two morphologies: nearly spherical dense type and non-spherical relatively dispersed type. In most cases, when peak defects show a nearly spherical dense distribution, the number of stable Frenkel pairs is relatively small; conversely, when they show a non-spherical relatively dispersed distribution, the number of Frenkel pairs is relatively large.
2. At PKA energy of 3.0 keV and temperature of 100 K, the number of stable Frenkel pairs is not significantly affected by PKA incident direction (this work calculated [100], [110], [111], [112], and [135]), with maximum variation of about 10% among directions. At PKA energies of 3.0–15.0 keV, the number of stable Frenkel pairs decreases slightly with increasing temperature (100–900 K).
3. Under PKA (1.0–25.0 keV), most defects in W exist as single defects, making it difficult to form defect clusters, with cluster fractions mostly between 0.15 and 0.40. Comparatively, the interstitial cluster fraction is higher than the vacancy cluster fraction. At 25.0 keV PKA, interstitial clusters with 4 or fewer defects per cluster are more numerous than vacancy clusters, while clusters with more than 5 defects per cluster are only vacancy clusters, indicating that vacancies tend to form larger clusters.
4. The displacement threshold energy is less affected by temperature, with the threshold energy in three directions [100], [110], and [111] being around 60.0 eV at 100, 500, and 900 K. The displacement threshold energy shows certain anisotropy: at 100 K, the minimum E_d occurs in the close-packed [111] direction with an average value of 40.0 eV, while the maximum E_d occurs in the [110] direction with an average value of 80.0 eV.

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