

Article

Evolution of Irradiation Defects in W and W-Re Systems: A Density Functional Theory and Rate Theory Study

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Abstract: In a fusion environment, tungsten, a plasma-facing material in a reactor, is subject to the irradiation of high-energy neutrons, generating a large amount of displacement damage and transmutation products (such as rhenium, Re). We studied the evolution of defects under irradiation in W and W-Re systems using the density functional theory (DFT) and rate theory (RT) method. The results indicate that the evolution of irradiation defects is mainly affected by the irradiation dose, dose rate, and temperature. During irradiation, loops form first in W, followed by the generation of voids, which are due to the different migration energies of point defects. Higher dose rates result in a higher density and larger size of defects in tungsten. Higher temperatures cause a decrease in void density and an increase in size. The results obtained at 600 °C were in good agreement with the reported TEM data. In W-Re alloys, it is indicated that the formation of loops is delayed because Re suppresses the nucleation of loops. The dynamic introduction of Re in W stabilizes the growth of defects compared to W-Re alloys, suggesting that transmuting elements have less detrimental effects on irradiation than alloying. As defect densities and sizes were quantified under different irradiation conditions, the results provide data for the multi-scale simulation of the radiation damage and thermal/mechanical properties in plasma-facing materials under fusion conditions.



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Keywords: tungsten; irradiation defects; rate theory; transmutation

1. Introduction

Magnetic confinement fusion is a promising method for achieving controllable thermonuclear fusion. However, the choice of material for plasma-facing components remains a key challenge [1]. Tungsten (W) is a promising candidate due to its high melting temperature (3380 °C) and low neutron-capture cross section [2]. It will be possible to use it as a plasma-facing material (PFM) in most Tokamak devices in the future [3]. Currently, the major obstacle is the irradiation swelling and embrittlement due to the generation of defects in W under high-energy neutron exposure [4], which might shorten the service life of reactor components. Meanwhile, nuclear transmutation reactions, e.g., (n, 2n) and (n, γ) [5,6], occur in pure tungsten irradiated by 14 MeV fusion neutrons, resulting in the accumulation of transmutation elements, such as rhenium (Re) and osmium (Os) [7]. According to research, it is estimated that the concentration of Re in the wall materials of ITER and DEMO reactors can reach 6% under high-dose neutron irradiation (>30 dpa) [8]. After 50 dpa irradiation, calculations predicted that pure W would change into a W-18Re-3Os alloy at the first wall [9]. Therefore, it is necessary to consider the effect of Re in W.

Since the 1970s, several studies have been conducted on the evolution of irradiation defects in W and W-Re systems [10–16]. It was found that a large number of micro-voids and dislocation loops could appear in pure W irradiated by neutrons around 0.1 dpa, while the presence of Re could reduce the formation of micro-voids and produce certain

precipitates. It was found that these precipitates included a χ phase (W-Re₃) and a σ phase (W-Re), which consisted of a core rich in Re and was surrounded by a less dense Re-rich cloud [17]. To investigate their micro-mechanism, researchers carried out simulations to explore the interaction between defects. Suzudo et al. [18] calculated the binding energies of Re atoms with vacancies and self-interstitials (SIAs) in W using DFT and proved the strong attraction between point defects and Re atoms. Gharaee [19] further evaluated the interaction between W interstitial atoms and solute Re and confirmed the view of Suzudo that the role of W-Re mixed interstitial atoms in solute transport should not be neglected. It is the mixed interstitial atoms that promote the accumulation of Re, which leads to the formation of irradiation-induced precipitates.

To make comparisons with the experimental data, researchers began to simulate the reaction between irradiation defects and transmutation atoms on a larger scale. Huang [20] constructed two models using the Monte Carlo (MC) method to study the thermodynamics of W-Re alloys. The formation mechanism of Re clusters was elaborated, and the important role of substituted Re in solute transport was confirmed. Moreover, a KMC model was established to simulate the formation of irradiation defects and precipitates under different conditions [21]. Li et al. [22] found a formation mechanism of void lattices in tungsten under neutron irradiation using the MD + OKMC method, and the simulation results matched the experimental observations. Recently, Hu [23] reviewed the microstructural evolution of W under neutron irradiation comprehensively and noted that whether the performance of W in a real fusion neutron irradiation environment can be predicted is still an open question.

Indeed, predicting irradiation defects quantitatively in W and W-Re systems is still very difficult. Even the difference between the results of the input parameters, such as SIA migration energy, was found to be more than one magnitude [24–27]. In addition, the most stable structures and the optimal migration paths of SIAs and W-Re mixed interstitial atoms are still controversial. Therefore, our study aims to investigate the diffusion mechanism of interstitial atoms in W and W-Re systems in DFT; establish the rate theory model; simulate the evolution of irradiation defects under different radiation doses, dose rates, and temperatures; and try to draw comparisons with experimental observation data on defects that have been reported.

2. Computational Methodology

The material is damaged by neutron irradiation quickly after irradiation at a microsecond or even nanosecond time scale, while the subsequent evolution of defects will occur over a longer time scale, such as several days. The size of defects spans a wide scale, from the atomic level to the mesoscopic level. Therefore, we hope to use a multi-scale simulation method combining the atomic scale and the mesoscale to study the nucleation and growth process of irradiation-induced defects [28].

In our work, we first used the first-principles method to calculate the energy parameters, then established the evolution model of irradiated defects in tungsten based on the rate theory method, and finally brought the energy parameters into the rate theory model to carry out the numerical solution calculations to obtain the evolution data on irradiated defect sizes and number densities in different irradiation conditions.

2.1. Calculation of Energy Parameters

The first-principles method is based on density functional theory (DFT), and the Vienna Ab initio Simulation Package (VASP) was used [29]. The projector-augmented wave (PAW) potential was used to describe the interaction between the electron and the nucleus, and the Perdew–Burke–Ernzerhof (PBE) functional was used to describe the interaction between the electrons. We used the $4 \times 4 \times 4$ supercell containing 128 lattice points for SIAs and the $3 \times 3 \times 3$ supercell containing 54 lattice points for W-Re mixed interstitial atoms. After the convergence tests, we used a cut-off energy of 350 eV for the plane-wave basis, and the lattice constant of W was set to be 3.176 Å. The Monkhorst–Pack k-point grid

density was sampled as $3 \times 3 \times 3$. The electron self-consistent iteration converged to an accuracy of 1×10^{-5} eV, and each nucleus was relaxed until the force on it was less than -0.01 eV/Å. During the optimization process, all the atoms were completely relaxed until the convergence precision was reached, and the shape and volume of the supercell were also relaxed.

The formation energies of SIAs were calculated via

$$E_{\text{SIAs}}^f = E_{(N+1)W} - \frac{N+1}{N} E_{\text{NW}} \quad (1)$$

where $E_{(N+1)W}$ and E_{NW} were the total energy of the system with and without SIAs, respectively.

The formation energies of W-Re mixed interstitial atoms were calculated via

$$E_{X-W}^f = E_{\text{NW}+X} - E_{\text{NW}} - E_X \quad (2)$$

where $E_{\text{NW}+X}$ was the total energy of the system with W-Re mixed interstitial atoms, E_{NW} was the total energy of the system without the Re atom, and E_X was the energy of a single Re atom in the supercell.

The migration energies were obtained using the nudged elastic band (NEB) method [30] and defined as the difference between the highest energy point and the lowest energy point on the curve.

2.2. Rate Theory Model

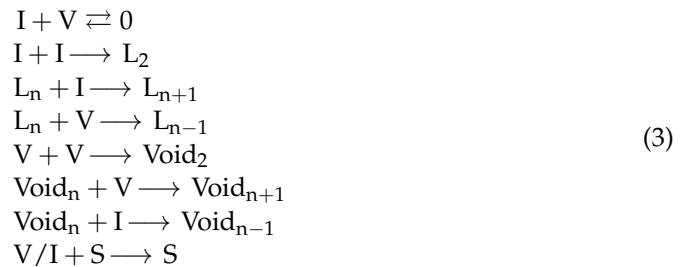
In this work, a numerical simulation method based on rate theory is used to simulate radiation damage in tungsten. The original point defects considered in the models include self-interstitial atoms (I), vacancies (V), and Re atoms. Re atoms are assumed to be either in the lattice position as the substituent atom (ReV) or in interstitial sites as Re interstitials (Re_i). The symbols and meanings of irradiation defects are listed in Table 1.

Table 1. Symbols and meanings of irradiation defects.

Symbol	Definition
I	Self-interstitial atoms
L ₂	Interstitial clusters
L _n	Interstitial loops
V	Vacancies
Void ₂	Vacancy clusters
Void _n	Micro-voids
S	Sinks
ReV	Re substitutes
Re _i	Re interstitials
Re ₂	Re clusters
Re _{i(n)}	Precipitates

Model I in this study only focuses on the evolution of vacancies, self-interstitials, and their clusters in pure tungsten [31,32]. In the beginning, neutron irradiation induces a large number of vacancies and self-interstitial atoms. Movable point defects will diffuse and form clusters, and clusters will grow into more complex defects, such as voids and loops, through a series of interactions. The detailed reaction types in defect evolution are displayed in Formula (3): the production and recombination of point defects, the generation of interstitial clusters (L₂) and interstitial loops (L_n), the reaction of interstitial loops and vacancies, the generation of vacancy clusters (Void₂) and micro-voids (Void_n), the reaction

of micro-voids and self-interstitial atoms, and the reaction of point defects and sinks (grain boundaries, dislocations, etc.) [33,34].



The variation in the concentration of interstitials C_i is expressed using the following equation [35,36]:

$$\frac{dC_i}{dt} = P - (D_i^m + D_v^m)C_iC_v - 2D_i^mC_i^2 - D_i^m\sqrt{C_{Li}C_L}C_i - 2D_i^mC_i\sqrt[3]{C_{void}^2C_{voidV}} - D_i^mC_iC_s \tag{4}$$

P is the production rate of Frenkel pairs, D_i^m and D_v^m are the mobility of single interstitials and single vacancies. Their value is characterized by migration energy $D_{i,v}^m = \nu \exp(-E_{i,v}^m/kT)$, where ν is the atomic vibration frequency, $E_{i,v}^m$ means the migration energy of interstitial atoms and vacancies, k is the Boltzmann constant, and T is the temperature. C_v means the concentration of vacancy. C_L is the concentration of interstitial-type dislocation loops, and C_{Li} is the concentration of interstitials already absorbed on the loops with a concentration of C_L . C_{void} is the concentration of voids, and C_{voidV} is the concentration of vacancies already absorbed on the voids having a concentration of C_{void} . C_s is the concentration of permanent sinks, such as dislocations and grain boundaries.

The concentration of interstitials C_v is expressed using the following equation:

$$\frac{dC_v}{dt} = P - (D_i^m + D_v^m)C_vC_i - 3D_v^mC_v^3 - D_v^m\sqrt{C_{Li}C_L}C_v - 2D_v^mC_v\sqrt[3]{C_{void}^2C_{voidV}} - D_v^mC_vC_s + EMIT\nu C_{void} \tag{5}$$

Ab initio calculations show that the vacancy cluster is unstable. The binding energy of a vacancy to a vacancy cluster becomes positive only when the final cluster size is larger than 3. Therefore, the nucleation of vacancy clusters is optimized compared with that of interstitial clusters. In addition, in order to consider the high-temperature behavior, the evaporation of vacancies from a void should be considered, which is expressed via $EMIT\nu C_{void}$. Its value is characterized via binding energy $EMIT\nu = \nu \exp(-E_v^b/kT)$. E_v^b is the binding energy between a void₂ vacancy cluster and a vacancy.

The concentration of interstitial loops C_L and interstitials aggregated in the loops C_{Li} could be expressed as:

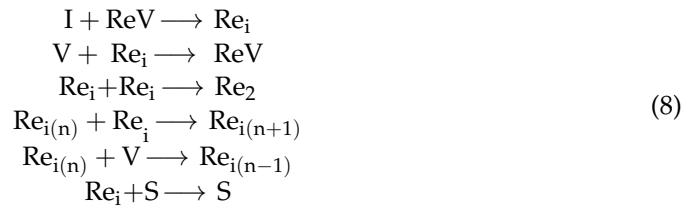
$$\frac{dC_L}{dt} = D_i^mC_i^2 + 0.000001P\frac{dC_{Li}}{dt} = D_i^m(C_{Li}C_L)^{1/2}C_i - D_v^m(C_{Li}C_L)^{1/2}C_v \tag{6}$$

The concentration of voids C_{void} and vacancies aggregated in the voids C_{voidV} could be expressed as:

$$\begin{aligned}
 \frac{dC_{void}}{dt} &= D_v^mC_v^2 + 0.000001P \\
 \frac{dC_{voidV}}{dt} &= D_v^m(C_{voidV}C_{void}^2)^{1/3}C_v - D_i^m(C_{voidV}C_{void}^2)^{1/3}C_i
 \end{aligned} \tag{7}$$

In Model II, transmutation products (Re) are considered. Initially, they occupy the lattice position, which is regarded as substitutes (ReV). In irradiation conditions, ReV will trap interstitial atoms to form Re_i and form a symmetrical dumbbell configuration (Re-W dumbbell) together with the W atom [15]. It has been demonstrated that the migration barrier of Re-interstitial complexes is much lower than that of Re-vacancies, so the interstitial

diffusion mechanism is dominant [26]. The added reaction types in defect evolution are displayed in Formula (8): the reaction of interstitials and Re-substitutes (ReV), the reaction of vacancies and Re interstitials (Re_i), the generation of Re clusters (Re₂) and precipitates (Re_{i(n)}), the reaction of micro-voids and self-interstitial atoms, and Re interstitials absorbed by sinks.



C_i in this model is expressed as:

$$\frac{dC_i}{dt} = P - (D_i^m + D_v^m)C_iC_v - 2D_i^mC_i^2 - D_i^m\sqrt{C_{Li}C_L}C_i - D_i^mC_iC_s - 2D_i^mC_i\sqrt[3]{C_{void}^2C_{voidV}} - D_i^mC_iC_{ReV} \tag{9}$$

where C_{ReV} is the concentration of Re substitutes.

C_v in this model is expressed as:

$$\begin{aligned}
 \frac{dC_v}{dt} = P - (D_i^m + D_v^m)C_vC_i - 3D_v^mC_v^3 - D_v^m\sqrt{C_{Li}C_L}C_v - 2D_v^mC_v\sqrt[3]{C_{void}^2C_{voidV}} \\
 - D_v^mC_vC_s + EMITvC_{void} - (D_v^m + D_{Rei}^m)C_vC_{Rei} - D_v^mC_v\sqrt[3]{C_P^2C_{Px}}
 \end{aligned} \tag{10}$$

In the equation, C_{Rei} is the concentration of Re interstitials. C_P is the concentration of Re precipitates, and C_{Px} is the concentration of Re atoms already absorbed on the Re precipitates with a concentration of C_P .

C_{Rei} in this model is expressed as:

$$\frac{dC_{Rei}}{dt} = D_i^mC_iC_{ReV} - (D_v^m + D_{Rei}^m)C_vC_{Rei} - 2D_{Rei}^mC_{Rei}C_{Rei} - D_v^mC_v\sqrt[3]{C_P^2C_{Px}} - D_{Rei}^mC_{Rei}C_s \tag{11}$$

In the equation, Re_i is produced via the recombination of interstitials and Re substitutes and it will be absorbed by vacancies, Re interstitials, Re clusters, and sinks.

In order to obtain more information on the evolution of defects, the size needs to be obtained along with the calculation of the concentration. Here, we obtain the average radius of the loops and voids using

$$R_L = 0.2\sqrt{3/4\pi a^2 C_{Li}/C_L}, R_V = 0.2 \times \sqrt[3]{9\sqrt{3}/32\pi a^3 C_{VoidV}/C_{Void}} \tag{12}$$

In the equation, Re_i is produced through the recombination of interstitials and Re substitutes and it will be absorbed by vacancies, Re interstitials, Re clusters, and sinks.

3. Results and Discussion

There is a consensus that the key energy parameters in the rate theory model above include the vacancy mobility energy, the SIA mobility energy, etc. The value of the vacancy mobility energy is about 1.66 eV [24], which has not attracted much controversy. In the following part, the mobility energy of the self-interstitial atoms (SIAs) in tungsten was obtained using DFT calculations.

3.1. Energy Parameter Calculation in W

In the body-centered cubic (bcc) structure of W, the possible structures of SIAs are mainly divided into two categories. One is the dumbbell structure formed by the SIAs and the normal atom originally at the lattice point, including <111> dumbbell, <110> dumbbell, <100> dumbbell, and <11h> dumbbell (h~0.5), as shown in Figure 1. The other is the interstitial structure where an SIA comes into the interstitial site of the lattice, such as the tetrahedral interstitial and octahedral interstitial, as shown in Figure 2. In addition, it may

also occur that an SIA shares the same lattice point with the normal atom originally at the lattice point, forming $\langle 111 \rangle$ crowdion, as shown in Figure 3.

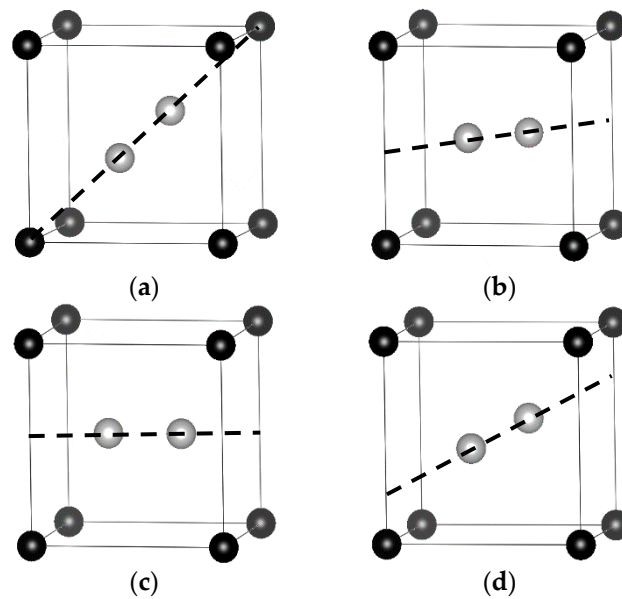


Figure 1. The dumbbell structure of SIAs: (a) $\langle 111 \rangle$ dumbbell, (b) $\langle 110 \rangle$ dumbbell, (c) $\langle 100 \rangle$ dumbbell, and (d) $\langle 11h \rangle$ dumbbell ($h \sim 0.5$).

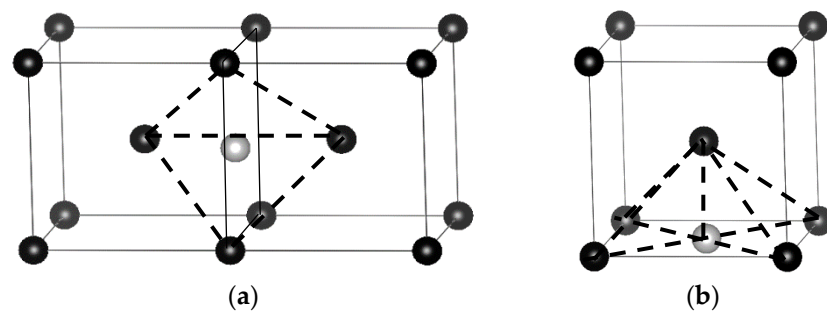


Figure 2. The interstitial structure of SIAs: (a) tetrahedral interstitial, and (b) octahedral interstitial.

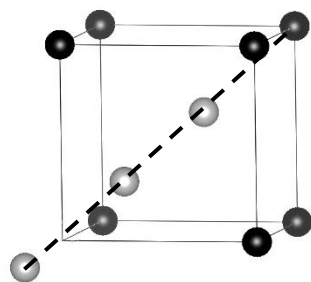


Figure 3. The $\langle 111 \rangle$ crowdion structure of SIAs.

Figure 4 shows the formation energies of different SIA structures. The most stable structures are $\langle 111 \rangle$ crowdion and $\langle 11h \rangle$ dumbbell ($h \sim 0.5$), with formation energies of 9.87 eV and 9.88 eV, respectively. The formation energy of $\langle 111 \rangle$ dumbbell is 9.92 eV, which is the metastable structure. The formation energies of $\langle 110 \rangle$ dumbbell, tetrahedral interstitial, $\langle 100 \rangle$ dumbbell, and octahedral interstitial are 10.26 eV, 11.52 eV, 12.00 eV, and 12.12 eV, which are significantly higher than that of $\langle 111 \rangle$ dumbbell, so they are less likely to exist.

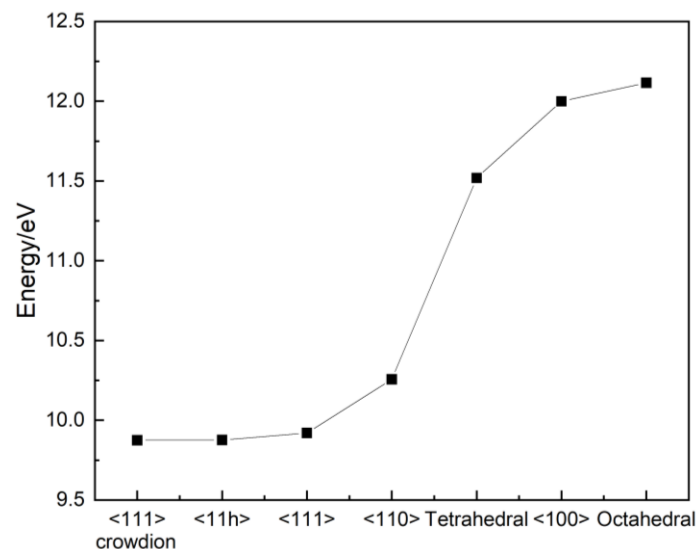


Figure 4. The formation energies of different SIA structures.

The metastable structure of SIAs is $\langle 111 \rangle$ dumbbell, whose formation energy is only 0.04~0.05 eV higher than that of $\langle 111 \rangle$ crowdion and $\langle 11h \rangle$ dumbbell ($h \sim 0.5$). In the high-temperature environment of the practical application of W materials, such a small energy difference is almost meaningless, so we choose $\langle 111 \rangle$ dumbbell to calculate the migration and rotation energy of SIAs.

The one-dimensional translation along the $\langle 111 \rangle$ direction of the $\langle 111 \rangle$ crowdion structure of SIAs is shown in Figure 5, and its NEB curve is shown in Figure 6. It shows that the one-dimensional migration energy of the $\langle 111 \rangle$ crowdion structure of SIAs is 0.11 eV.

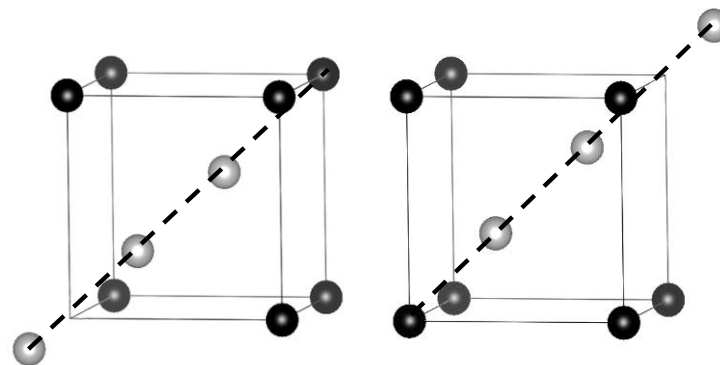


Figure 5. The one-dimensional translation along the $\langle 111 \rangle$ direction of the $\langle 111 \rangle$ crowdion SIA structure.

The rotation path $\langle 111 \rangle \rightarrow \langle 110 \rangle \rightarrow \langle 11\bar{1} \rangle$ of the $\langle 111 \rangle$ dumbbell structure of SIAs is shown in Figure 7, and its NEB curve is shown in Figure 8. The $\langle 11h \rangle$ dumbbell structure ($h \sim 0.5$) with lower energy and more stability will be formed during the rotation process of the $\langle 111 \rangle \rightarrow \langle 110 \rangle \rightarrow \langle 11\bar{1} \rangle$ path because $\langle 111 \rangle$ dumbbell is not the most stable structure. Therefore, neither the starting point nor the ending point in Figure 8 is the lowest point, which forms two “valleys” on the curve. By calculating the difference between the highest point and the lowest point on the curve, we find that the rotation energy of the $\langle 111 \rangle$ dumbbell structure of SIAs in the $\langle 111 \rangle \rightarrow \langle 110 \rangle \rightarrow \langle 11\bar{1} \rangle$ path is 0.38 eV, which is approximately equal to the difference between the formation energy of $\langle 111 \rangle$ dumbbell and $\langle 110 \rangle$ dumbbell.

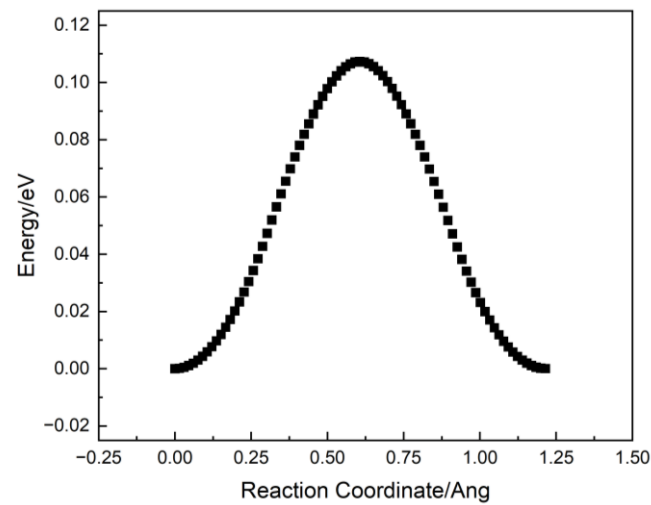


Figure 6. The NEB curve of the translation of SIAs.

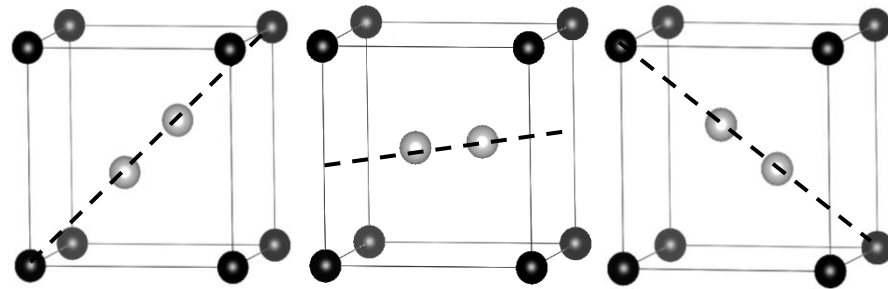


Figure 7. The rotation path $\langle 111 \rangle \rightarrow \langle 110 \rangle \rightarrow \langle 11\bar{1} \rangle$ of the $\langle 111 \rangle$ dumbbell structure of SIAs.

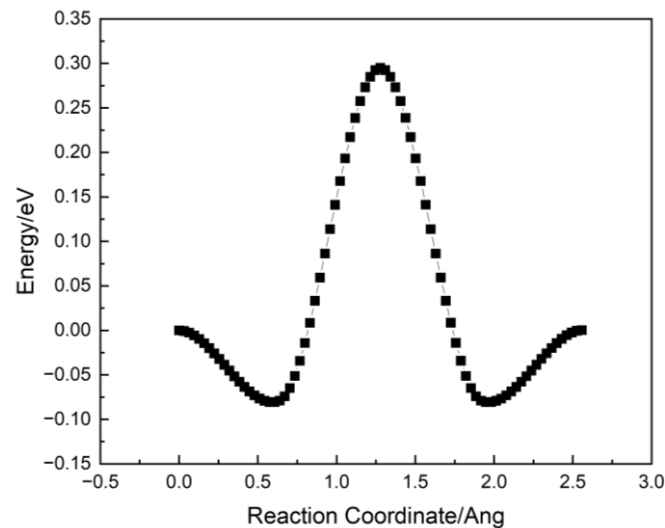


Figure 8. The NEB curve of the rotation of SIAs.

Since the rotation energy is much larger than the migration energy, SIAs in W mainly go through one-dimensional translation in the $\langle 111 \rangle$ direction. It is worth noting that the difference between the formation energy of $\langle 111 \rangle$ dumbbell and $\langle 11h \rangle$ dumbbell ($h \sim 0.5$) is extremely small, so SIAs may also rotate in the $\langle 111 \rangle \rightarrow \langle 11h \rangle$ ($h \sim 0.5$) path, which impedes one-dimensional translation along the $\langle 111 \rangle$ direction.

3.2. Energy Parameter Calculation in W-Re

In the body-centered cubic (bcc) structure of W, the possible structures of W-Re mixed interstitial atoms are mainly divided into two categories. One is the dumbbell structure formed by the interstitial atom Re and the normal atom originally at the lattice point, including $\langle 111 \rangle$ dumbbell, $\langle 110 \rangle$ dumbbell, $\langle 100 \rangle$ dumbbell, and $\langle 11h \rangle$ dumbbell ($h \sim 0.45$), as shown in Figure 9. The other is the interstitial structure, where the interstitial atom Re comes into the interstitial site of the lattice, such as the tetrahedral interstitial and octahedral interstitial, as shown in Figure 10.

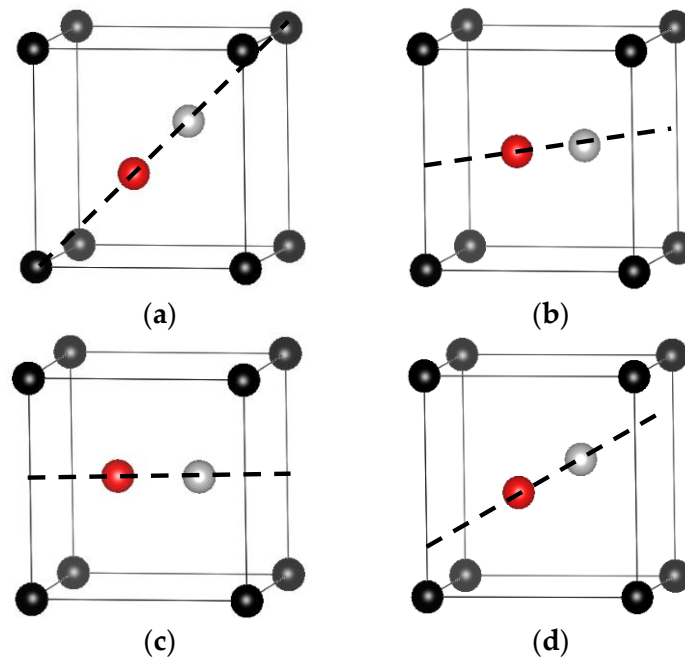


Figure 9. The dumbbell structure of W-Re mixed interstitial atoms: (a) $\langle 111 \rangle$ dumbbell, (b) $\langle 110 \rangle$ dumbbell, (c) $\langle 100 \rangle$ dumbbell, and (d) $\langle 11h \rangle$ dumbbell ($h \sim 0.45$).

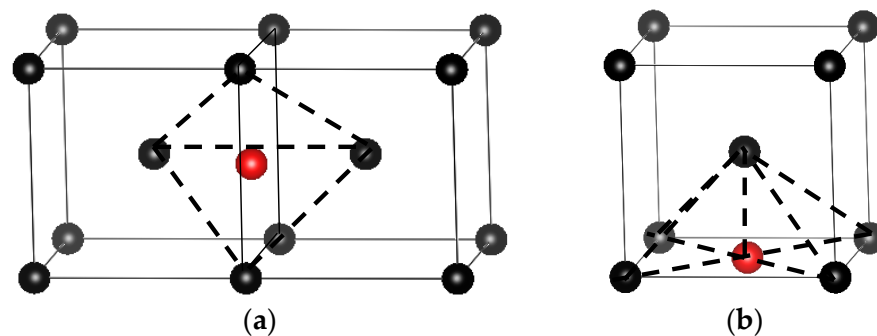


Figure 10. The interstitial structure of W-Re mixed interstitial atoms: (a) tetrahedral interstitial, (b) octahedral interstitial.

Figure 11 shows the formation energies of different structures of W-Re mixed interstitial atoms. The most stable structures are $\langle 111 \rangle$ dumbbell and $\langle 11h \rangle$ dumbbell ($h \sim 0.45$) with the formation energies of 8.65 eV. The formation energies of $\langle 110 \rangle$ dumbbell, tetrahedral interstitial, $\langle 100 \rangle$ dumbbell, and octahedral interstitial are 8.70 eV, 9.98 eV, 10.63 eV, and 10.80 eV, which are significantly higher than that of $\langle 111 \rangle$ dumbbell and $\langle 11h \rangle$ dumbbell ($h \sim 0.45$), so they are less likely to exist.

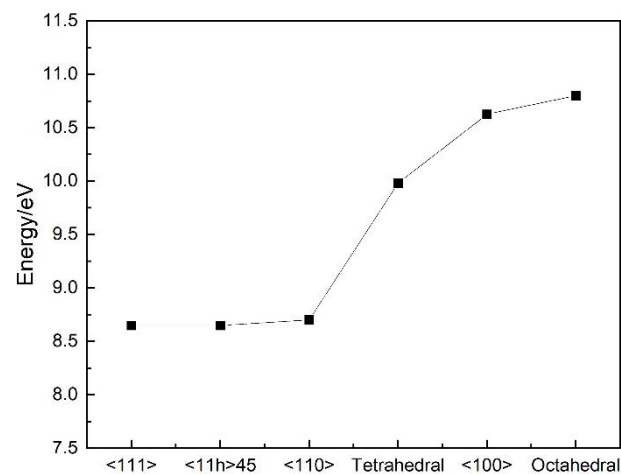


Figure 11. The formation energies of different structures of W-Re mixed interstitial atoms.

The $\langle 111 \rangle$ dumbbell and $\langle 11h \rangle$ dumbbell ($h \sim 0.45$) structures are the most stable structures of W-Re mixed interstitial atoms. Since $\langle 11h \rangle$ dumbbell ($h \sim 0.45$) is a relatively asymmetric structure, and $\langle 111 \rangle$ dumbbell is a symmetric structure, we choose $\langle 111 \rangle$ dumbbell to calculate the migration and rotation energy of W-Re mixed interstitial atoms.

The one-dimensional translation along the $\langle 111 \rangle$ direction of the $\langle 111 \rangle$ dumbbell structure of W-Re mixed interstitial atoms is shown in Figure 12, and its NEB curve is shown in Figure 13.

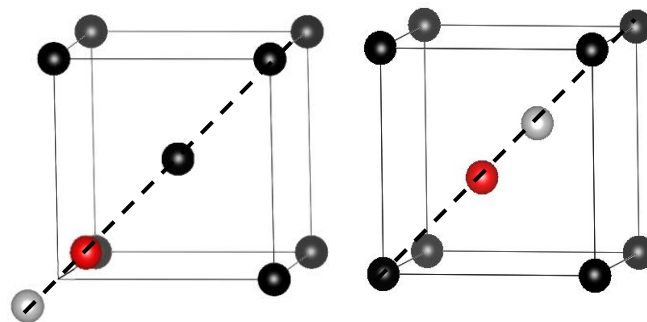


Figure 12. The one-dimensional translation along the $\langle 111 \rangle$ direction of the $\langle 111 \rangle$ dumbbell structure of W-Re mixed interstitial atoms.

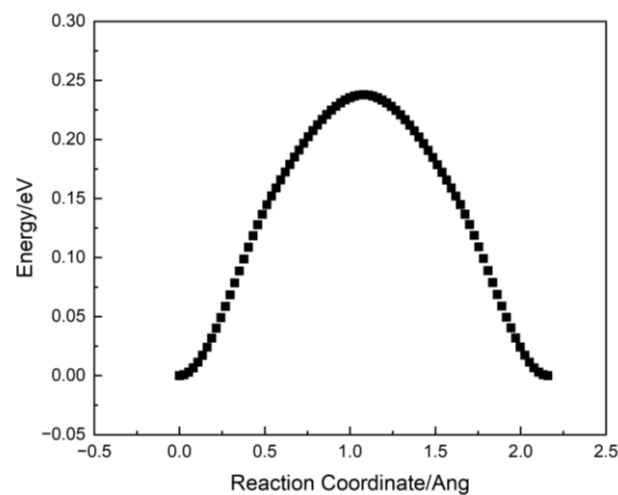


Figure 13. The NEB curve of the translation of W-Re mixed interstitial atoms.

Figure 13 shows that the one-dimensional translation energy of the $\langle 111 \rangle$ dumbbell structure of W-Re mixed interstitial atoms in the $\langle 111 \rangle$ direction is 0.24 eV.

The rotation path $\langle 111 \rangle \rightarrow \langle 110 \rangle \rightarrow \langle 11\bar{1} \rangle$ of the $\langle 111 \rangle$ dumbbell structure of W-Re mixed interstitial atoms is shown in Figure 14, and its NEB curve is shown in Figure 15.

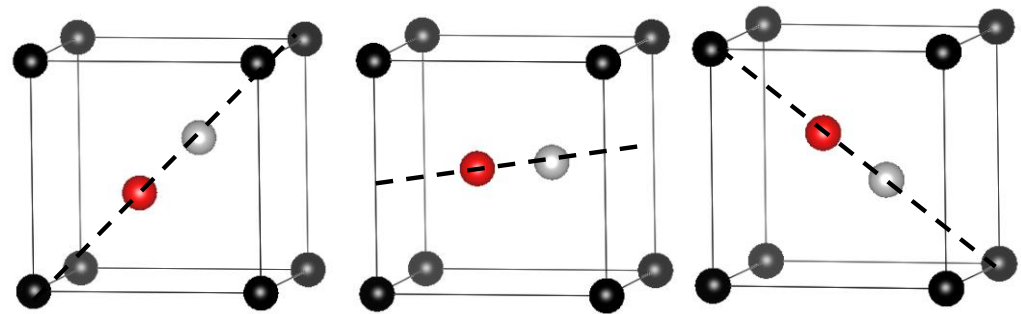


Figure 14. The rotation path $\langle 111 \rangle \rightarrow \langle 110 \rangle \rightarrow \langle 11\bar{1} \rangle$ of the $\langle 111 \rangle$ dumbbell structure of W-Re mixed interstitial atoms.

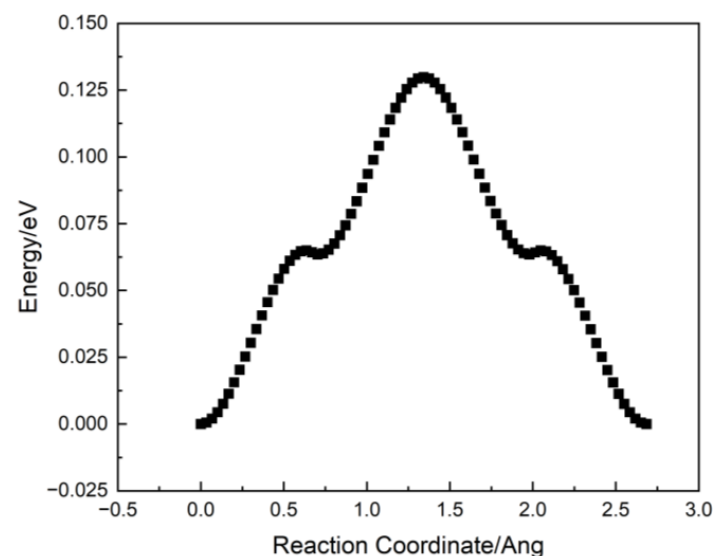


Figure 15. The NEB curve of the rotation of W-Re mixed interstitial atoms.

Except for $\langle 111 \rangle$ dumbbell, $\langle 11h \rangle$ dumbbell ($h \sim 0.45$) is the most stable structure, and will be formed during the rotation process of the $\langle 111 \rangle \rightarrow \langle 110 \rangle \rightarrow \langle 11\bar{1} \rangle$ path. Therefore, the curve is not a perfect peak, and there are two small peaks in addition to the main peak. By calculating the difference between the highest point and the lowest point on the curve, we find that the rotation energy of the $\langle 111 \rangle$ dumbbell structure of W-Re mixed interstitial atoms in the $\langle 111 \rangle \rightarrow \langle 110 \rangle \rightarrow \langle 11\bar{1} \rangle$ path is 0.13 eV.

The motions of W-Re mixed interstitial atoms are not the same as that of SIAs. If W-Re mixed interstitial atoms only go through the one-dimensional translation in the $\langle 111 \rangle$ direction, then the Re atom will be trapped between two W atoms until W-Re mixed interstitial atoms dissociate, which is a rare event. There is little difference between the translation energy and the rotation energy, and even the rotation energy is less than the migration energy. Therefore, W-Re mixed interstitial atoms will change their direction frequently via rotation, so that the Re atom is no longer trapped between two W atoms. In a word, W-Re mixed interstitial atoms mainly move in a coordinated way through one-dimensional translation in the $\langle 111 \rangle$ direction and rotation in the $\langle 111 \rangle \rightarrow \langle 110 \rangle \rightarrow \langle 11\bar{1} \rangle$ path, forming a three-dimensional free diffusion.

3.3. Rate Theory Calculation for W

The parameters used in rate theory calculations are listed in Table 2. Displacement defects, primarily vacancies, and interstitials result largely from high-energy neutron irradiation. Their production rate is estimable using SPECTRA [37,38].

Table 2. Parameters involved in the models.

Parameters	Symbol	Value
Temperature	T	600–1200 °C
Dose rate	P	10^{-8} – 10^{-6} dpa/s
SIA migration energy	E_i^m	0.11 eV [this work]
SIA rotation energy	E_i^r	0.38 eV [this work]
Vacancy migration energy	E_v^m	1.66 eV [24]
Alloy content in W-Re systems	x	1~10 at. %
W-Re mixed interstitial atomsmigration energy	E_{Re}^m	0.24 eV [this work]
W-Re mixed interstitial atomsmrotation energy	E_{Re}^r	0.13 eV [this work]
Density of sinks	C_s	10^{-10} [36]
Atomic vibration frequency	ν	10^{13} [39]
Lattice constant	a	3.176×10^{-10} m

Through employing the rate theory model, equations were solved using the Gear method. This approach enabled the simulation of the evolution of microscopic defects in materials due to neutron irradiation, thereby determining the concentration and size of point defects, loops, and voids [40]. Given the known lattice constant of tungsten, these concentrations would be converted into number densities.

The results, including reported data [23,41,42], are depicted in Figure 16. Section 3.1 of our study yielded a migration energy of 0.11 eV. However, incorporating this value into the model did not align with the experimental data. Consequently, the sum of migration and rotation energies (0.49 eV) was proposed as a revised migration energy. Figure 16a illustrates that the density of interstitial loops increases with a prolonged irradiation time, and at a higher dose rate, the density escalates under both migration energies. At lower SIA migration energies, the loop density is significantly reduced compared to at higher SIA migration energies. This highlights the influence of SIA migration energy on loop density. Figure 16c shows a wave-like progression in loop size over time. Fluctuations in mean loop size are more pronounced at lower SIA migration energies, attributed to greater mobility causing faster movement of interstitial atoms. The irradiation dose rate marginally affects the size but slows the evolution rate of these fluctuations. Comparatively, the solid line in Figure 16a,c aligns more closely with TEM data. This suggests that the actual migration energy of SIA in the experimental material tungsten might exceed the DFT-calculated value for pure tungsten. Figure 16b,d reveal that voids emerge later during irradiation, with their density rising with increased irradiation dose and rate. Notably, void density remains relatively unchanged across different SIA migration energies, indicating a minor correlation with interstitial atomic migration energy. When compared to TEM data, the simulation results show good congruence with experimental findings, particularly at higher irradiation dose rates.

Figure 17 depicts the number density of loops and voids at varying irradiation temperatures, juxtaposed with the corresponding TEM data under similar conditions. In Figure 17a, the impact of temperature on loop density appears negligible. The solid-line data ($E_m = 0.49$ eV) at 600 °C and the dotted line ($E_m = 0.11$ eV) at 800 °C align with experimental findings. However, at 1200 °C, the simulated results for both migration energies diverge significantly from the TEM data, with the simulation values being several orders of magnitude higher. This discrepancy suggests that at high temperatures, the actual number of loop nucleation events is substantially lower than simulated. The probable causes of this discrepancy include the omission of interstitial loop embryo dissociation at elevated temperatures and the potential underestimation of SIA mobility in the model. The model

assumes constant migration energy for interstitial atoms at high temperatures, whereas the actual mobility energy at 1200 °C could be lower than 0.11 eV.

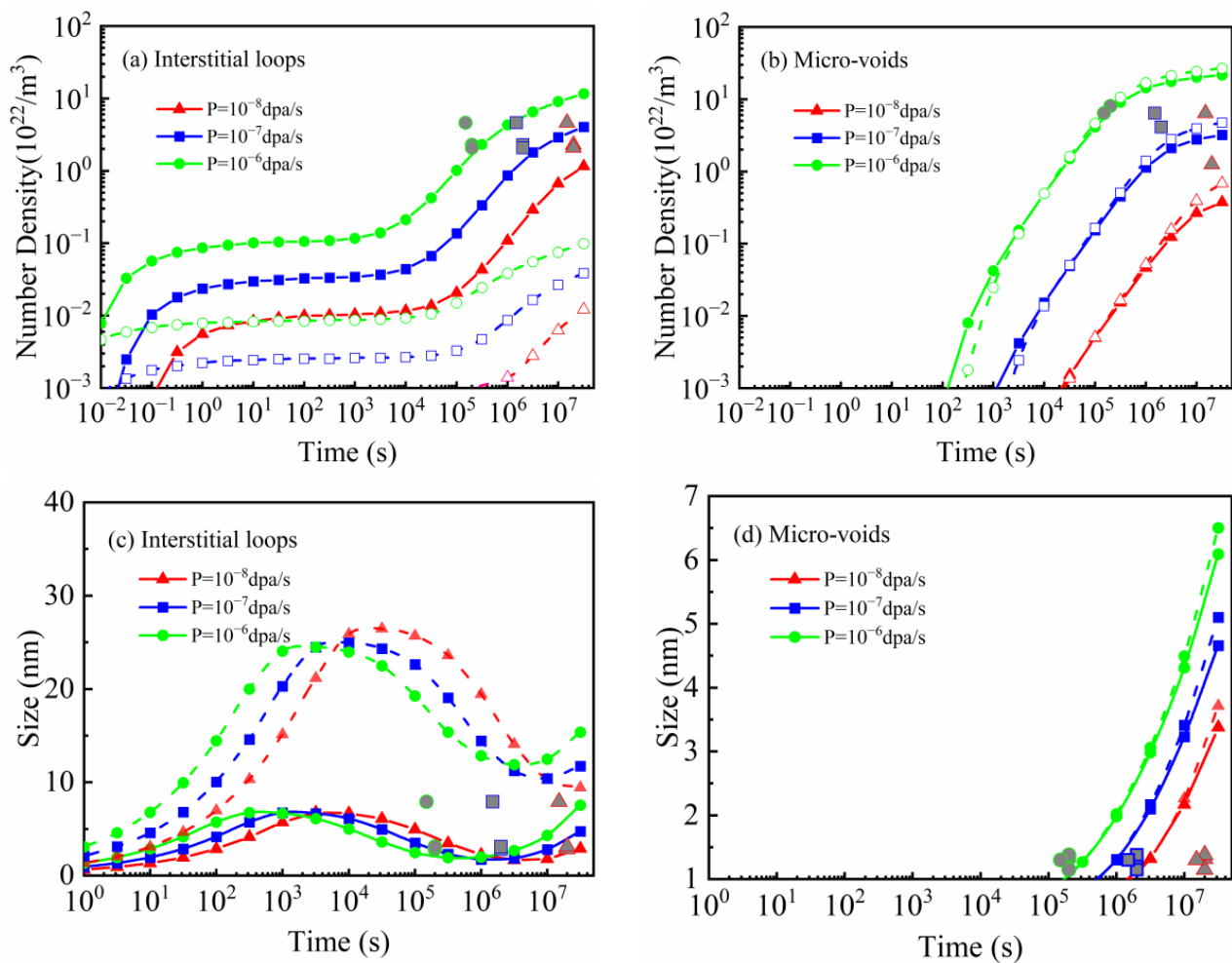


Figure 16. Number density and size of loops and voids caused by high (10^{-6} dpa/s), medium (10^{-7} dpa/s), and low (10^{-8} dpa/s) dose rate of neutron irradiations of W at 600 °C, when the migration energy value is 0.11 eV (dashed line) and 0.49 eV (solid line), respectively. Gray symbols mean reported densities and sizes of TEM-observed defects in references (data from Refs. [23,41,42]).

Figure 17b illustrates a decrease in void density with rising temperatures. The model's predictions align well with TEM data at 600 °C, but not at 800 °C or 1200 °C. Experimental evidence [41] suggests that temperature has a minimal effect on void nucleation density, hinting at potential shortcomings in the model's void density evolution equation at extremely high irradiation temperatures. This discrepancy could be attributed to the model's inclusion of void nuclei dissociation at high temperatures.

Figure 17c indicates that temperature exerts a minimal influence on loop size. Consistency with experimental data [42] is observed for the solid line data ($E_m = 0.49$ eV) at 600 °C and the dotted line ($E_m = 0.11$ eV) at 800/1200 °C. In contrast, Figure 17d reveals an increase in void size with temperature, which aligns well with TEM experimental findings.

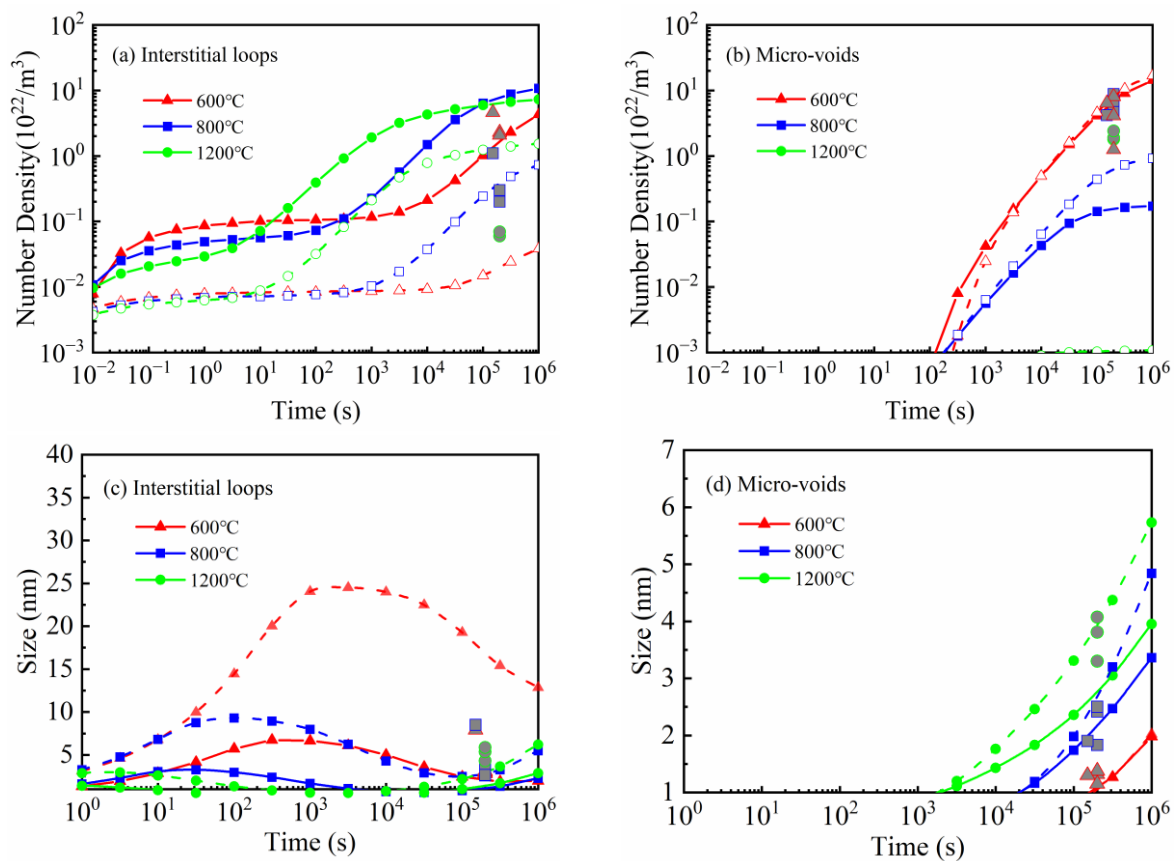


Figure 17. Number density and size of loops and voids at different temperatures (600–1200 °C), where the neutron irradiation dose rate (P) is 10^{-6} dpa/s. The migration energy value is 0.11 eV (dashed line) and 0.49 eV (solid line), respectively. Gray symbols mean reported densities and sizes of TEM-observed defects in references (data from Refs. [23,41,42]).

3.4. Rate Theory Calculation for W-Re

By solving the rate equation of Model II, we determined the number density and size of loops, voids, and Re precipitates.

Figure 18a reveals that in W-Re alloys, the loop number density is significantly lower than in pure tungsten. Despite some accumulation following irradiation, the size of these loops does not increase. This phenomenon might be a result of the added rhenium atoms, which could potentially elevate the recombination likelihood of interstitial atoms. Moreover, similar to pure tungsten, the loop density in W-Re increases with the irradiation dose rate. Figure 18b,e indicate that adding rhenium slightly reduces the density of voids but significantly increases their size. Notably, the lower the irradiation dose rate, the larger the void size. This observation suggests that rhenium introduction inhibits void nucleation while promoting its growth in size. This outcome contrasts with experimental observations in pure tungsten, where the presence of rhenium is known to reduce micro-void formation [43]. We hypothesize that this discrepancy could be attributed to rhenium attaching to the void surfaces, forming complexes that lead to the observed reduction in void number density in experiments [44]. Figure 18c,f show an increase in Re precipitates over time, with their size also enlarging as the irradiation dose increases. Like voids, the size of these precipitates increases as the irradiation dose rate decreases. We infer that this pattern might be due to a higher probability of point defect nucleation at increased dose rates, resulting in smaller voids and secondary phase sizes.

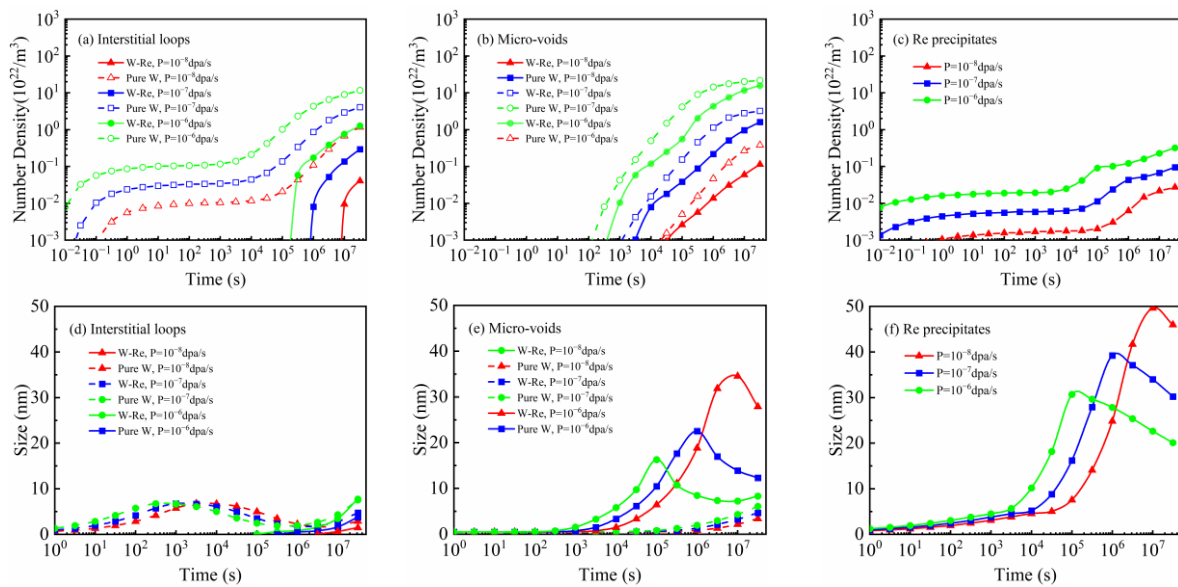


Figure 18. Number density and size of loops, voids, and precipitates caused by a high (10^{-6} dpa/s), medium (10^{-7} dpa/s), and low (10^{-8} dpa/s) dose rate of neutron irradiations in W-1%Re alloy.

Figure 19 demonstrates that both loop density and size at 800 °C exceed those at 600 °C and are nearly negligible at 1200 °C. Consistent with the behavior observed in pure tungsten, the void density diminishes as the irradiation temperature increases. Conversely, the density of Re precipitates rises while their size diminishes with elevated temperatures.

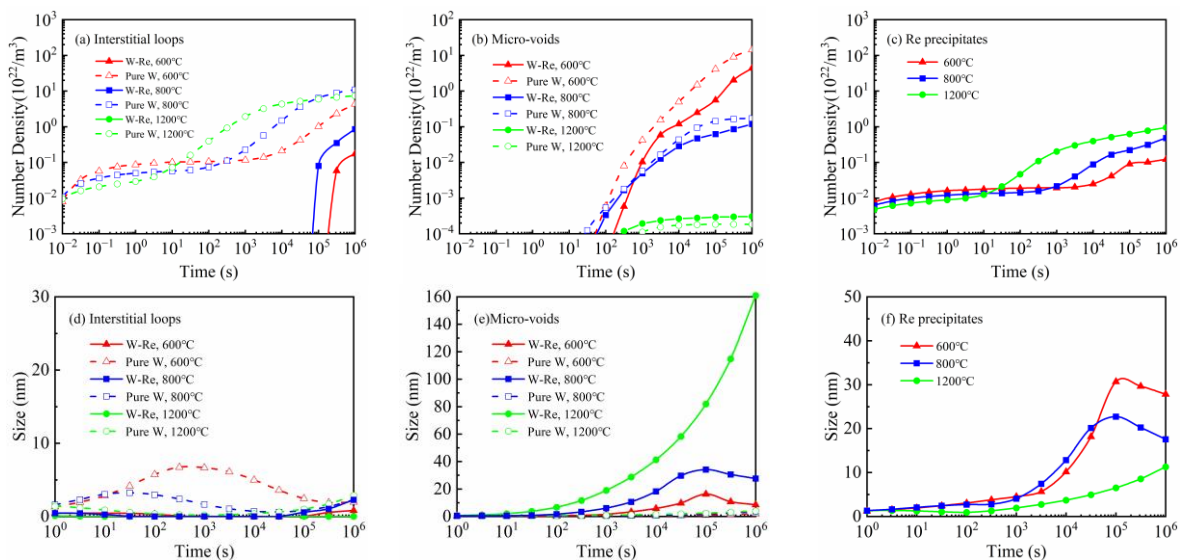


Figure 19. Number density and size of loops, voids, and precipitates in W-1%Re alloy at different temperatures (600–1200 °C), where the neutron irradiation dose rate (P) is 10^{-6} dpa/s.

Figure 20 highlights that in various W-Re alloys, the loop density is markedly lower compared to pure tungsten, with a corresponding reduction in loop size. Both the void size and Re precipitate dimensions increase with rising Re content. While the Re content does not influence the nucleation of irradiation defects, it does impact their growth. This effect can be attributed to the increase in ReV, leading to the $\text{ReV} + \text{I} = \text{Re} + \text{V}$ reaction. As vacancies and Re atoms accumulate, growth in the size of voids and Re precipitates is observed, but the nucleation of these defects diminishes as the self-interstitial atoms are depleted.

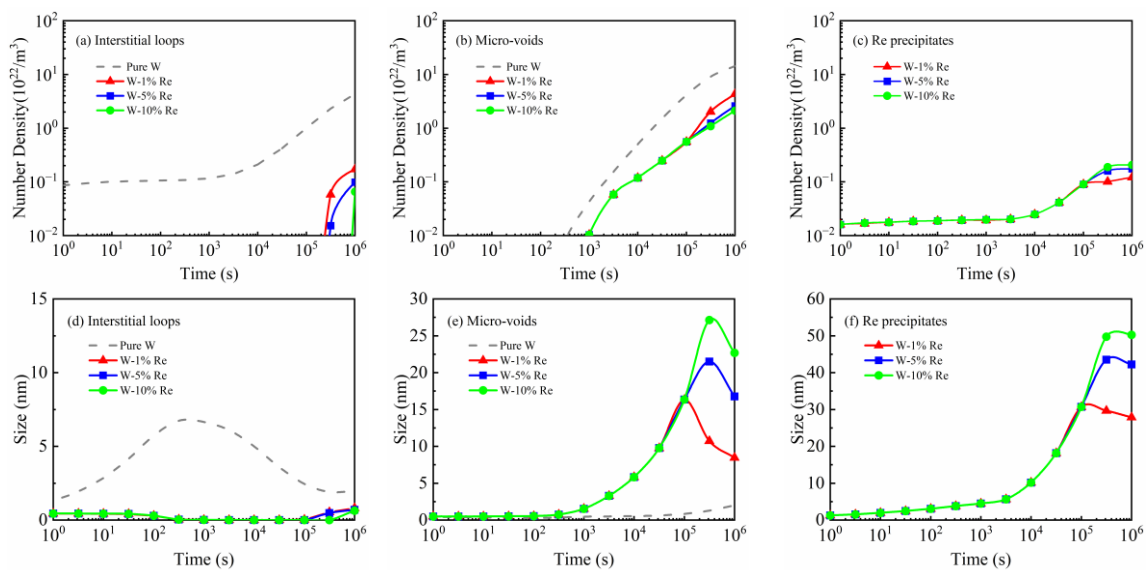


Figure 20. Number density and size of loops, voids, and precipitates in Pure W, W-1%Re, W-5%Re and W-10%Re at 600 °C, where the neutron irradiation dose rate (P) is 10^{-6} dpa/s.

In fusion reactor operational conditions, rhenium does not exist in tungsten initially prior to irradiation but accumulates with an increased irradiation dose. The yield of Re can be calculated using the linear chain method [45,46]. It is estimated that the transmutation yields in plasma-facing materials for the fusion demonstration reactor (DEMO) and high-flux isotope reactor (HFIR) are approximately 500 and 30,000 appm/dpa [47], respectively. Consequently, the Re yield parameters in Models II and III are set to be 10^{-4} appm/s and 10^{-2} appm/s. To enhance model accuracy, we discard the assumption of the pre-irradiation W-Re alloy and incorporate the transmutation yield to simulate the dynamic transmutation process.

Figure 21 illustrates the evolution of various irradiation defects at different transmutation yields ($P_{\text{Re}} = 0, 10^{-4}$ appm/s, 10^{-2} appm/s). The W-1% Re alloy serves as the control group, as the final accumulated Re content reaches 1% when $P_{\text{Re}} = 10^{-2}$ appm/s. The gray symbol represents experimental data [23,48] under HFIR conditions (700 °C, 0.44 dpa). As depicted in Figure 21a, the loop density in dynamic transmutation scenarios decreases compared to non-transmutation cases, but this reduction is delayed. This effect can be attributed to the minimal accumulation of Re elements in the early stages of irradiation, which does not significantly consume interstitial atoms. Observation of the gray symbol positions indicates that the dynamic transmutation model aligns more closely with experimental data. In Figure 21b, a transmutation rate of 10^{-4} appm/s has a negligible effect on void density. However, both $P_{\text{Re}} = 10^{-2}$ appm/s and the direct addition of 1% Re elements reduce the density. When compared to experimental data, the alloy model more accurately reflects in-reactor conditions. Figure 21c shows that dynamic transmutation leads to the earlier formation of Re precipitates. We hypothesize that this is due to dynamic transmutation producing Re elements at a slower rate, thereby hindering cluster nucleation. Moreover, the density of Re precipitates differs considerably from experimental data, possibly because the model only considers the interstitial-mediated migration of Re. An interesting observation is made in Figure 21d: the dynamic addition of Re elements causes loop growth to extend midway through irradiation but diminish toward the end. This is likely because the presence of dynamic Re elements temporarily influences loop nucleation, resulting in a temporary increase in average size. Analysis of TEM data in Ref. [23] shows that introducing Re slightly reduces the loop size, aligning with our calculations. Figure 21e demonstrates that dynamically introducing Re atoms impacts void growth. A gradual addition slows void growth compared to adding all the Re elements in one stream. The presence of Re precipitates leads to a slight increase in void size, explained via our model

at the mechanistic level: Re atoms deplete self-interstitial atoms (SIAs), reducing their recombination with voids. Lastly, dynamic transmutation fosters uniform growth in Re clusters, influencing the size of Re precipitates. The positioning of the experimental data suggests that precipitate size under low-dose dynamic transmutation may more accurately reflect real-world engineering scenarios.

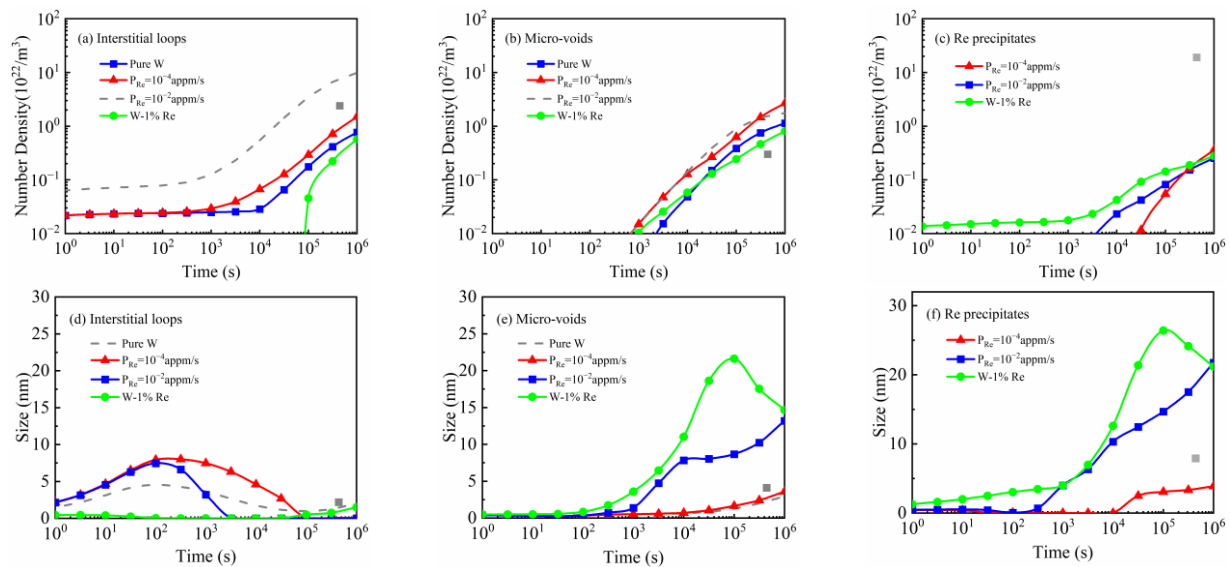


Figure 21. Number density and size of loops, voids, and precipitates at different transmutation yields ($P_{\text{Re}} = 0, 10^{-4} \text{ appm/s}, 10^{-2} \text{ appm/s}$), where the neutron irradiation dose rate (P) is 10^{-6} dpa/s and the temperature is 700°C . Gray symbols mean reported densities and sizes of TEM-observed defects in references (data from Refs. [23,48]).

4. Conclusions

A computational model, integrating density functional theory (DFT) calculations and rate theory (RT), was developed in this study to analyze the evolution of defects in tungsten (W) and tungsten-rhenium (W-Re) systems under neutron irradiation. We examined the effect of varying neutron irradiation doses, dose rates, temperatures, and alloy compositions on the formation of loops, voids, and precipitates, comparing our findings with experimental results from transmission electron microscopy (TEM) studies.

In pure tungsten systems, higher irradiation dose rates lead to increased defect formation. When the mobility of interstitial atoms is set to 0.49 eV, our simulation results align closely with those reported in the references. The effect of the irradiation temperature on loops is not obvious, but the effect on voids is as follows: the higher the irradiation temperature, the lower the number density, and the larger the size. In the W-Re alloy, the introduction of Re inhibits the nucleation of loops and voids, and we speculate that this is due to the fact that Re promotes the combination of point defects. While the irradiation temperature has a negligible effect on loop formation, its impact on voids is significant: higher temperatures result in fewer but larger voids. In W-Re alloys, the addition of rhenium inhibits the nucleation of loops and voids. We hypothesize that this inhibition is due to rhenium's facilitation of point defect recombination. The dynamic addition of the Re element to W seems to stabilize the growth of loops, voids, and precipitates more effectively than in W-Re alloys, indicating that transmutation elements may have a lesser detrimental impact on irradiation than alloying elements. Our model is proficient in calculating defect evolution under high-dose irradiation over extended periods, aiding the computation of mechanical properties such as irradiation hardening [49–51] and key parameters like thermal conductivity [52], and providing essential data for developing new nuclear fuels and materials. This model shows promising applicability in reactor engineering.

Future work should focus on optimizing and improving the model by analyzing more irradiation data, so as to provide guidance for the design of radiation-resistant materials.

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