8.8 HELIUM EFFECTS ON DISPLACEMENT CASCADES IN TUNGSTEN — W. Setyawan, G. Nandipati, K. Roche, H. Heinisch, R. J. Kurtz, (Pacific Northwest National Laboratory); and B. D. Wirth (University of Tennessee)

OBJECTIVE

The objective of this research is to support the prediction of helium effects on irradiation damage properties of tungsten-based materials using computational methods.

SUMMARY

Molecular dynamics (MD) simulations were performed to investigate He effects on displacement cascades in W. Helium content, proportion of interstitial and substitutional He and temperature were varied to reveal the various effects. The effect of interstitial He on the number of self-interstitial atoms (SIAs) produced during cascade damage appears to be insignificant. However, interstitial He tends to fill a vacancy (V). Nevertheless, this process is less favorable than SIA-V recombination particularly when excess SIAs are present before a cascade. The efficiency of He filling and SIA-V recombination increases as temperature increases due to increased point defect mobility. Likewise, substitutional He is more susceptible to displacement during a collision cascade than W. This susceptibility increases towards higher temperatures. Consequently, the number of surviving V is governed by the interplay between displaced substitutional He and SIA-V recombination. The temperature dependence of these processes results in a minimum number of V reached at an intermediate temperature.

PROGRESS AND STATUS

Introduction

Tungsten is a primary material choice for divertor components in future fusion reactors due to its low sputtering coefficient, excellent thermal conductivity, relatively low neutron activation and good mechanical strength. Tungsten will be exposed to a flux of He escaping the plasma as well as He produced from transmutation. The presence of He degrades the intended materials properties. Some studies have been done on He diffusion and retention [1-3], bubble formation [4, 5], He-related nano voids formation [6, 7] etc. However, the effects on primary displacement cascade damage have not been explored in detail. An earlier work was done to study the effects on cascade damage at 300 K with relatively low primary-knock-on atom (PKA) energy up to 20 keV [8]. The current work is intended to investigate He effects on cascade damage at higher PKA energies. Different He concentrations and initial proportion of substitutional versus interstitial He, and temperatures up to 2050 K are included.

Formalism

Molecular dynamics (MD) simulations were performed to investigate He effects on displacement cascade evolution in W. A combination of empirical potentials was employed. For the W-W interaction, the Finnis-Sinclair type of potential developed by Ackland and Thetford [9] was taken, in which the short-range part was then modified to harden the repulsion at small interatomic distances [10]. Modification was also done at distances relevant to self-interstitial configurations to improve defect formation energies. A new W-He pair potential from Ref. [10] was used. The potential reproduces simple He defect energetics and structures in excellent agreement with ab initio results. The calculated interstitial He atom migration energy with the

new W-He potential is 0.2 eV. For He-He interaction, the Beck potential [11] with short-range modification by Morishita [12] was used.

The simulations were performed using LAMMPS software [13]. Before He atoms were added, the pure tungsten system was thermalized in the *NPT* ensemble for 30 ps. Then He atoms were placed at random interstitial positions at least 1.6 Å from W or any previously placed He. This is the starting configuration to generate three He compositions, namely 100% interstitial (100I), 50% substitutional (50I50S) and 100% substitutional (100S). To create substitutional He, random interstitial He were swapped with random W. All compositions were further thermalized in *NPT* for 5 ps before displacement cascade was initiated. The short thermalization time was intended to randomize the velocity of He atoms without allowing clustering to occur.

A displacement cascade was simulated using a 75-keV tungsten primary-knock-on atom (PKA) randomly chosen from the central region of the simulation cell. The PKA was given a random initial direction. At the beginning, the cascade was performed in *NVE* using an adaptive time step with maximum displacement of 0.005 Å per step. The cascade events and cooling were followed for ~10 ps, afterwards the system was thermalized to a target temperature in *NVT* and defect migration was followed for a total simulation time of 55 to 60 ps. Periodic boundary conditions were applied to a cubic cell of size $100a \times 100a \times 100a$ containing 2M W atoms in a bcc lattice.

Results

In the absence of a displacement cascade, clustering of He atoms was first investigated. The 100I composition with He content of 134, 460, 2300 and 4600 appm was thermalized at 300, 1025 and 2050 K. Note that 1025 and 2050 K represent 0.25 and 0.5 of tungsten's melting temperature respectively. The clustering was followed for 200 ps. The number of self-interstitial atoms (SIAs) at 50, 100, 150 and 200 ps is summarized in Table 1. Note that the number of SIAs in Table 1 is given in appm for easy comparison with the He content. At room temperature, He clustering of size up to five occurred. However, no SIAs were observed for all concentrations presumably due to limited mobility of the clusters to form large enough clusters to displace W from the lattice sites (kick-out mechanism). At 1025 and 2050 K, large enough clusters formed and produced SIAs. The minimum He cluster size to start a kick-out mechanism is 7 atoms at 1025 K. The minimum size decreases to 5 atoms at 2050 K. Therefore, at lower temperatures, not only that the cluster mobility is more limited, the W atoms themselves are more stable at the lattice sites compared to at elevated temperatures.

Table 1. Number of SIAs in appm due to He clusters (initially interstitial) displacing W from the lattice sites. Each set of four values corresponds to the number of SIAs at 50, 100, 150 and 200 ps simulation time.

	134 appm	460 appm	2300 appm	4600 appm
300 K	0,0,0,0	0,0,0,0	0,0,0,0	0,0,0,0
1025 K	0,0,0,0	0,0,0,0	0,2,8,15	6,36,96,153
2050 K	0,0,0,0	0,0,2,2	21,76,137,181	151,360,507,605

The clustering study is also useful in estimating the number of SIAs produced by kick-out mechanism in addition to those produced during the displacement cascade. In all cases of cascade simulations reported here, there are no kick-out SIAs within the simulation time of ~60 ps. The number of surviving V in pure tungsten was calculated to be 80.9 at 1025 K (Table 2). This number slightly increases at lower temperatures and vice versa. Note that results from all displacement cascades are averaged from 15 simulations. Helium effects on the cascade damage are first studied at 1025 K as a function of He level and composition. The results are summarized in Table 3. Three legends are used to label vacancies for discussion purposes. V_W denotes tungsten-vacant sites that may or may not be occupied by He. Sites that are occupied by neither W nor He are simply denoted as V. Helium-filled vacancies are denoted as V^{He}. Note that there can be more than one He occupying a V^{He}. Therefore, to discuss the He effects on the vacancy and SIA production, V^{He} is used instead of the number of substitutional He.

The effects of interstitial He are the following (see the top portion of Table 3). At 134 appm, the number of SIAs is only +2 compared to pure W. This value increases to 87.7 (+7 from pure case) with 460 appm. However, at 2300 appm, the number decreases to 81.7, which is only +1 from pure case. Therefore, it appears that the small variation in the number of SIAs is a statistical effect and that interstitial He has insignificant effect on SIA production. On the other hand, the effect on the number of vacancies is significant. Up to 460 appm, the number of V is 81.3 (approximately the same as in pure case) with 134 appm and 80.1 (-1 from pure case) with 460 appm, and decreases to 47.1 (-34 from pure case) with 2300 appm. Clearly, interstitial He atoms start to fill some of the vacancies produced during the cascade. The corresponding V^{He} are 1.7, 7.6 and 34.6 with 134, 460 and 2300 appm.

The effects of substitutional He can be seen from the 460 appm data in Table 3. The number of new V^{He} (additional number relative to the initial number before cascade) decreases from 7.6 to -44.5 (with 50I50S) and to -157.3 (with 100S). This indicates that some of the initial V^{He} are now occupied by initial SIAs. However, it is unclear to what proportion that this process occurs during the cascade compared to during the SIA migration after the cooling stage. Further analysis is needed. On the other hand, the number new SIAs are 87.7, 20.1 and -91.1 with 100I, 50I50S and 100S respectively. This indicates that there is a critical composition where the number of new SIAs would be zero, i.e., the number of SIAs produced by cascade is balanced by the number of initial SIAs filling the vacancies created by the cascade. Note that at the critical composition, the number of vacancies is not necessarily zero even though there are no new SIAs created. The number of V is 80.1, 64.7 and 66.3 with 100I, 50I50S and 100S respectively. These surviving vacancies may come from the initial V^{He} where the He atoms get displaced during the collision cascade. It is also interesting to note that the number of surviving V saturates at ~65 as the proportion of substitutional He is increased. The critical composition and the minimum number of surviving vacancies are expected to depend on factors such as PKA energy (damage volume), He content and temperature.

Table 2. Number of surviving vacancies (V) in pure tungsten after damage from 75-keV PKA as a function of temperature.

	300 K	1025 K	2050 K
V	81.5	80.9	77.1

Table 3. Number of point defects after damage from 75-keV PKA at 1025 K as a function of He content and initial He composition, i.e., substitutional (S) and interstitial (I). V_W denotes the number of sites that are not occupied by W. V^{He} denotes the number of vacancies (V) occupied by He.

appm	$He(S)_{init}$	$He(I)_{init}$	SIA_{init}	V	V_W	SIA_{new}	V^{He}_{new}
134	0	268	0	81.3	82.9	82.9	1.7
460	0	918	0	80.1	87.7	87.7	7.6
2300	0	4590	0	47.1	81.7	81.7	34.6
134	134	134	134	74.6	203.0	69.0	-5.6
460	459	459	459	64.7	479.1	20.1	-44.5
2300	2295	2295	2295	65.1	1784.0	-511.0	-576.1
460	918	0	918	66.3	826.9	-91.1	-157.3

The effects of temperature are studied using 460 appm He. The results for different He compositions are presented in Table 4. First, the number of new V^{He} with 100I increases with temperature due to increased He mobility. The increase is from 6.8 at 300 K to 7.6 at 1025 K and to 15.3 at 2050 K. However, when initial SIAs are present, the number of new V^{He} decreases with temperature. This decrease is more significant compared to the increase in the 100I case indicating the more dominant process of SIA filling vacancies than He filling vacancies. The SIA-V recombination is enhanced towards higher temperature. The consequence on the critical composition in which no new SIAs created is that as the temperature increases, it requires a smaller proportion of interstitial He in the initial composition to balance the damage-produced SIAs.

Next is temperature effect on the minimum number of vacancies. At 300 K, increasing the proportion of substitutional He does not change the number of surviving V which is ~86. At 1025 K, the number of surviving V decreases from ~80 at 100I composition to (and saturates at) ~65 towards 100S as previously discussed. At 2050 K, a reverse trend occurs, i.e., the number of V increases: 67, 73 and 79 for 100I, 50I50S and 100S respectively. The results show that the number of surviving vacancies in the presence of substitutional He reaches a minimum at an intermediate temperature (in this study is 1025 K). This can be understood from the following. When initial V^{He} are present, the substitutional He atoms are more susceptible to displacement during collision cascade than W. Some of the initial V^{He} are then filled by initial SIAs. Hence the number of surviving V is determined by the interplay between the increased number of damage-created vacancies from V^{He} and the increased SIA-V recombination. At low temperatures, SIA-V recombination is not as effective, while at high temperatures the instability of initial substitutional He is more than the increased SIA-V recombination, resulting in a minimum number of V at an intermediate temperature.

Table 4. Number of point defects after damage from 75-keV PKA with 460 appm He as a function of temperature (T) and initial He composition, i.e., substitutional (S) and interstitial (I). V_W denotes the number of sites that are not occupied by W. V^{He} denotes the number of vacancies (V) occupied by He.

T (K)	$He(S)_{init}$	$He(I)_{init}$	SIA_{init}	V	V_W	SIA_{new}	V^{He}_{new}
300	0	918	0	86.3	93.1	93.1	6.8
1025	0	918	0	80.1	87.7	87.7	7.6
2050	0	918	0	65.9	81.2	81.2	15.3
300	459	459	459	87.4	516.5	57.5	-29.9
1025	459	459	459	64.7	479.1	20.1	-44.5
2050	459	459	459	73.0	458.5	-0.5	-73.5
300	918	0	918	85.9	895.1	-22.9	-108.8
1025	918	0	918	66.3	826.9	-91.1	-157.3
2050	918	0	918	79.3	758.0	-160.0	-239.3

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