



Radiation damage production in massive cascades initiated by fusion neutrons in tungsten



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ABSTRACT

Neutrons in fusion reactors produce primary radiation damage from displacement cascades in tungsten (W) at an average PKA energy of 150 keV. We find, using molecular dynamics simulations, that cascades at this energy do not break up into subcascades. The massive amount of energy concentrated in the liquid-like heat spike facilitates a fairly high rate of formation of large dislocation loops and other defect structures, of sizes readily visible in today's electron microscopes. We investigate the structures and distribution of the cascade debris in W predicted by different interatomic potentials. In particular, our simulations show the formation of (100)-type dislocation loops, in agreement with recent experiments and in contradiction to the earlier held view that only 1/2(111)-type loops occur in W.

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1. Introduction

Tungsten (W), with its unique combination of properties including good thermal conductivity and high melting point, combined with resistance to erosion and low neutron activation, is a candidate material for both structural and plasma-facing components in current and future fusion reactors. However, the brittleness of tungsten poses a problem, and in addition little is currently known on the radiation embrittlement from the long-term effects of high neutron doses. The precise nature of defect structures formed in cascades constitutes a key factor determining microstructural evolution of the material, and is crucial for predicting the performance of components during the lifetime of the reactor.

The high-energy neutrons produced by the D–T fusion plasma [1] give rise to primary recoils in tungsten with average energies of around 150 keV. Recent *in situ* TEM observations [2] of 150 keV self-ion irradiated W have shown the occurrence of novel cascade damage from single ion impacts. These experiments offer a unique opportunity for direct comparison of cascade simulations to experiment. For this purpose we have performed molecular dynamics (MD) simulations of 150 keV collision cascades in W, comparing the predictions of different interatomic potentials.

Cascade damage has been extensively studied by MD methods, and in particular, it has been shown that damage production becomes a linear function of recoil energy after the onset of subcascade break-up [3]. However, cascade damage in W has

previously been studied by MD methods for energies only up to 100 keV [4]. The simulations described in this work show that even at 150 keV, break-up is not complete. The high energy density in the compact cascades gives rise to collective effects which have a significant effect on damage production. The precise nature of defect structures provides input for models aimed towards predicting defect evolution in tungsten.

There are still large uncertainties considering the numbers of defects produced in W. The SRIM recommended value for the threshold displacement energy (TDE) used in the NRT model is $E_d = 90$ eV, whereas experiment [5] gives a lower TDE, suggesting that the rate of defect production should be higher than what the SRIM/NRT model predicts. This is unusual, for example cascade simulations in iron predict defect numbers significantly lower than the NRT model. The full MD simulations of cascades in W performed in this work cast light on this issue.

2. Methods and analysis

MD simulations of collision cascades from 150 keV recoils have been performed using the PARCAS code [6]. Simulations were performed at 0 K to include only athermal processes in defect creation. Cubic simulation cells with periodic boundaries, of 48 nm to a side and containing over 6 million atoms, were used for each cascade. A Berendsen thermostat [7] was applied to cell borders, and each cascade was simulated for 40 ps, at which point the cell had cooled to an average temperature of only a few K.

Three different potentials were compared. Most simulations were done using the modified EAM potential by Derlet et al. [8]

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(hereafter denoted by D–D), with the repulsive part given by the universal Ziegler–Biersack–Littmark potential [9], fitted by Björkas et al. [10]. These were compared to simulations using Ackland–Thetford EAM potential (A–T) [11], and a more recent Tersoff-type potential by Ahlgren et al. (A–H) [12]. The predicted TDE for the latter two potentials was determined by the method described in Ref. [13]. Simulation cells with 38,400 atoms, initially with half liquid and half crystal structure, were used to find the melting points for the D–D and A–T potentials.

The simulations incorporate electronic energy losses in the form of electronic stopping (ES) given by SRIM [14]. This is implemented as a friction term, and requires the use of a lower energy threshold T_c , below which the friction term is not applied, else all thermal modes are quickly quenched. To check the effect of this, the value of T_c was varied from 1 eV to 100 eV in simulations using the D–D potential.

Defects were detected with two methods which were then compared to each other and found to agree completely. On the one hand atoms were filtered according to potential energy, and those with 0.2 eV higher than the potential's predicted cohesive energy were singled out. This was compared to defects identified using an automated Wigner–Seitz cell method [15].

Large irregular defect structures were relaxed separately at 600 K for 100 ps.

The size and shape of a cascade was determined by analysing the liquid atoms at the time the liquid-like area was largest, approximately after the first 300 fs. An atom was determined to be liquid when the average energy of the atom and its neighbors exceeded the energy corresponding to the melting temperature.

3. Results and discussion

3.1. Defect numbers

Collective effects occurring in the cascade heat spike, such as recombination, play an important role in defect production. Although thermally activated recombination is not included in these simulations, nevertheless the number N_{FP} of surviving Frenkel pairs (FP) is far less than the number N_{NRT} predicted by the NRT model [16].

N_{NRT} is a function of damage energy T_d , i.e. the amount of energy which has gone to the ionic system. In these simulations, T_d is given by the initial PKA energy minus the energy which is removed from the system as a result of electronic stopping. In cascades simulated with the D–D potential and $T_c = 10$ eV, $T_d \approx 110$ keV (see Table 1), and the efficiency, calculated as N_{FP}/N_{NRT} , is 0.4. Here we use the NRT recommended value $E_d = 90$ eV to determine N_{NRT} . The same efficiency is predicted when $T_c = 1$ eV, with lower defect numbers balancing the lower T_d , while $T_c = 100$ eV gives an efficiency of 0.5. The direction-specific TDEs predicted by the D–D potential agree well with the experimental values, while the average over all directions is very close to the higher NRT value [10], since E_d is higher in higher index directions. These simulations are thus consistent with both the experimental TDE and the NRT recommended value.

The TDE predicted by the A–H potential is also in reasonable agreement with experiment, with $E_d = 39 \pm 1$, 69 ± 1 and 59 ± 1 in the $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ directions, respectively. However, the efficiency predicted by cascade simulations is only 0.2. With the A–T potential the efficiency is 0.3, although the predicted TDE is higher ($E_d = 57 \pm 1$, 103 ± 1 and 89 ± 1 in the $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$ directions, respectively). The efficiency is thus sensitive to the potential for other reasons than the predicted TDE.

Rather, N_{FP} is affected by the difference in cluster sizes appearing in the cascade debris. Simulations with the D–D potential give the largest SIA clusters, and correspondingly the highest average number of defects. This is due to the fact that large SIA clusters involve large defect numbers, while cascades with only small clusters also have fewer defects in total. Although the Tersoff-type A–H potential tested in this work has lower TDEs than the other two potentials, it produces no large clusters, and has an average of only 90 Frenkel pairs per cascade. The A–T potential predicts roughly 30% fewer Frenkel pairs than the D–D potential, and accordingly the SIA clusters are slightly smaller.

3.2. Effects of the electronic stopping threshold

The time plot in Fig. 1 of the cumulative ES energy losses shows no difference during the first 250 fs for different T_c . This is the ballistic phase of the cascade, when recoils are very energetic, and the number of atoms with kinetic energy less than 100 eV is negligible. Thus the energy lost to ES is derived almost exclusively from atoms with energies above 100 eV. As a result, the use of a low-energy cut-off, and the choice of its value, does not affect the development of the cascade until the very end of the ballistic phase, when lower energy atoms begin to appear.

After the ballistic phase is over, during the thermal phase, the subsequent electronic energy losses for different T_c values above 5 eV are minimal, since most atoms at this point have energies below 5 eV. However, with $T_c = 1$ eV, a large amount of energy is still lost to the electronic system during the thermal phase, due to the large number of atoms in this phase that have energies just above 1 eV. The energy losses affect the formation of defect clusters, with only small clusters forming when $T_c = 1$ eV, and large clusters appearing when $T_c \geq 5$ eV (see Fig. 2).

3.3. Cascade morphology

The relatively short distance of propagation of even the highest-energy recoils in W, combined with the lower energy disturbance caused by their passage, results in a continuous liquid area which occasionally gives rise to large interstitial clusters. These are found around the perimeter of the liquid area, suggesting that they have formed by the liquid isolation mechanism [15]. The occurrence of very large SIA clusters is accompanied by a vacancy-rich core, often containing a large vacancy cluster, and in general the larger the SIA cluster is, the closer it lies to the accompanying vacancy cluster. Large clusters appear in areas of cascades that are compact and almost spherical. These also take the longest to recrystallize as the surface-to-volume ratio is the smallest.

Table 1
Defect numbers N_{FP} , the size of the largest vacancy (CI_{max}^{vac}) and SIA cluster (CI_{max}^{SIA}), and the fraction of vacancies (F_{vac}) and SIAs (F_{SIA}) in clusters larger the 4, for different ES cut-off energy T_c and using the D–D potential. The total energy E_{ES} lost to electronic stopping during the simulation is given in the last column.

T_c (eV)	N_{FP}	CI_{max}^{vac}	CI_{max}^{SIA}	F_{vac}	F_{SIA}	E_{ES} (keV)
1	122.2 ± 2.9	5	54	0.00	0.47 ± 0.03	82.5 ± 1.2
5	182.8 ± 27.9	118	164	0.21 ± 0.07	0.71 ± 0.07	47.6 ± 0.65
10	179 ± 21.0	96	175	0.19 ± 0.06	0.72 ± 0.06	42.9 ± 0.6
20	183 ± 18.1	72	94	0.16 ± 0.06	0.81 ± 0.01	39.1 ± 0.227
100	257 ± 49.7	177	224	0.28 ± 0.10	0.81 ± 0.05	34.6 ± 1.55

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