8.2 Simulation of Ballistic Resolutioning of Helium from Bubbles in Iron by Molecular Dynamics — R. E. Stoller (Oak Ridge National Laboratory)

OBJECTIVE

The objective of this research is to develop an understanding of the mechanisms and processes that control the evolution of helium-stabilized cavities in fusion structural materials.

SUMMARY

Helium generation and accumulation is important under DT fusion irradiation conditions. Ballistic resolutioning of He from bubbles could limit bubble growth by ejecting gas atoms back into the metal matrix. Molecular dynamics simulation has been used to study this process in iron as a surrogate for structural materials. A newly developed Fe-He interatomic potential was employed. The primary variables examined were: irradiation temperature (100 and 600K), iron knock-on atom energy (5 and 20 keV), bubble radius (~0.5 and 1.0 nm), and He-to-vacancy ratio in the bubble (0.25, 0.5 and 1.0). Helium ejection by high-energy iron recoils was clearly observed on a time scale consistent with a ballistic mechanism. The results are summarized.

PROGRESS AND STATUS

Introduction

The evolution of gas-stabilized bubbles in irradiated materials is inherently a dynamic process, involving a balance of growth and shrinkage mechanisms. Simplistically, the bubble volume will grow in units of atomic volume by absorbing vacancies and shrink by either emitting vacancies or absorbing interstitials. Absorption or emission of gas atoms will also change the bubble volume, although the incremental change is generally less than an atomic volume. The absolution volume change is dependent on the ratio of gas atoms to vacancies (i.e. pressure) in the bubble. In addition to the thermal and kinetic processes such as diffusion that lead to He absorption and emission from bubbles, the potential for high-energy recoils to remove gas atoms from bubbles has also been discussed and, to a limited extent, investigated [1-3]. This ballistic resolutioning mechanism is illustrated in Fig. 1. The conditions investigated in the present study are summarized in Table 1, and extend range of results of obtained previously and in Ref. 2. A more complete report on the results is being prepared for publication in the Journal of Nuclear Materials based on a presentation at the 15th International Conference on Fusion Reactor Materials.

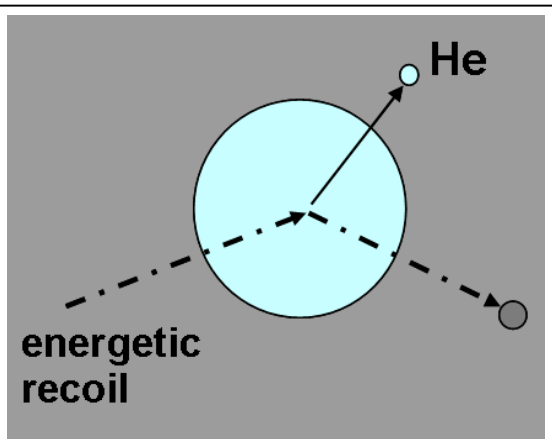

Fig. 1. Illustration of ballistic gas resolutioning from a bubble by an energetic recoil.

Table 1. Simulation conditions investigated				
Temperature (K)	Cascade energy (keV)	Bubble size		He to vacancy ratio
		Number of vacancies	Radius (nm)	
100	5	40	0.48	0.25, 1
	5	339	1.0	0.25, 0.5, 1
	20	40	0.48	0.25, 1
	20	339	1.0	0.25, 0.5, 1
600	5	40	0.48	0.25, 1
	5	339	1.0	0.25, 0.5, 1
	20	40	0.48	0.25, 1
	20	339	1.0	0.25, 0.5, 1

Approach

The basic computational approach employed in this investigation follows that published previously [2]. A newly developed Fe-He interatomic potential has been employed [4-6], with the iron matrix described by the potential of Ackland and co-workers from 1997 [7]. Constant pressure, periodic boundary conditions were employed in a cubic simulation cell of 70 or 80 lattice parameters, corresponding to 686k or 1024k atoms. Before initiating a ballistic event, a bubble of the desired size was created by removing the necessary number of iron atoms in an approximately spherical volume, and the number of helium atoms required to obtain the desired He-to-vacancy ratio shown in Table 1 were placed within the volume. Then, the atom block was thermally equilibrated at the specified temperature for approximately 25 ps. Consistent with the strong He-He and He-vacancy binding observed in previous work with these potentials, no thermal resolutioning was observed. The equilibrated atom configuration was saved and used as the starting point for the subsequent simulations. The ballistic cascade simulations were initiated by giving one of the Fe atoms located near the bubble a defined amount of kinetic energy and an initial direction oriented toward the bubble. Based on previous experience with the statistical nature of cascade simulations, between ten and twenty simulations were carried out for each of the conditions listed in Table 1, with variability ensured by the different PKA locations and in some cases by further equilibration of the starting configuration.

Each MD cascade simulation was continued until variables such as the number of defects, and the average kinetic and potential energy had stabilized for a few ps. The time required to reach this new pseudo-equilibrium depended on the PKA energy and irradiation temperature, varying between about 15 to 25 ps. The final atom configuration was then characterized by locating the He atoms and measuring the distance between any ejected He atoms and the

initial bubble surface, and by counting the number and distribution of the point defects (vacancies and interstitials) created by the cascade.

Results

The results are summarized in Figures 2 and 3. The red, blue, and green curves in Fig. 2 show the total number of He atoms displaced from the bubble surface by at least 1 lattice parameter, more than 10 lattice parameters, and between 5 and 10 lattice parameters, respectively. The rapid evolution of helium resolutioning is quite clear with the maximum number of He atoms ejected being reached by <40 fs. This time is quite short on the time scale of displacement cascade evolution in which the peak number of displaced atoms is not reached until >0.5 ps. This is shown by the black curve in Fig. 2, which plots the number of Frenkel defects created. This number is still increasing rapidly well after the number of He ejected has saturated. This is in contrast to the results observed by Parfitt and Grimes [3] for He bubbles in UO_2, where a delayed emission process was observed that arose from thermal mixing near the bubble surface.

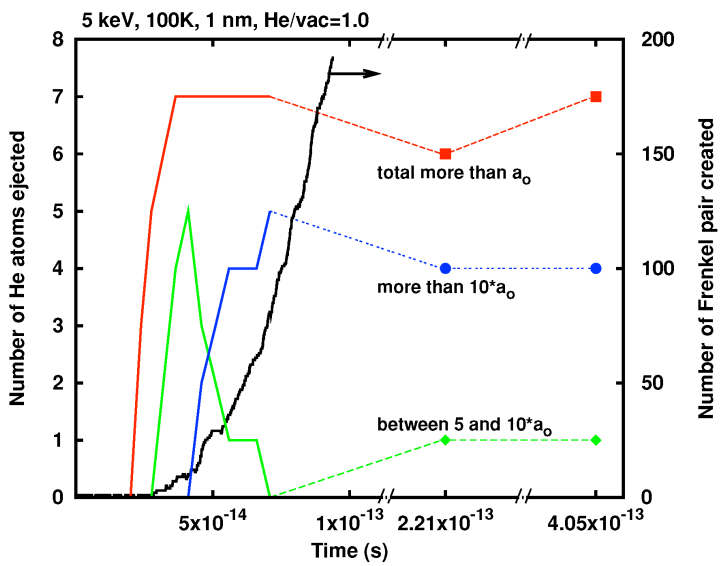

Fig. 2. Time dependence of He ejection from a 1 nm bubble and point defect formation in a 5 keV cascade at 100K. He/vacancy ratio is 1.0.

The dependence of He resolutioning on the irradiation conditions are shown in Fig.3 for a 1 nm bubble size (339 vacancies). The data points indicate the mean value and the error bars are the standard error of the mean. The trends are quite clear. At both 100 and 600K there is less resolutioning from 20 keV cascades than from 5 keV cascades. This seems somewhat counter-intuitive, but us a result of the reduced elastic scattering cross section as the particle energy increases. At either cascade energy, resolutioning is reduced at the higher temperature. This is consistent with the greater thermal motion of the He atoms making it more difficult for collisions which transfer large amounts of energy in elastic collisions. Lastly, it is clear that bubble pressure, represented by the He/vacancy ratio, has a strong influence of the number of He atoms ejected.

FURTHER WORK

Ongoing analysis of these results will provide guidance for developing ballistic resolutioning parameters that can be employed in reaction rate theory models of He-vacancy cluster dynamics. The use of atomistic-based resolutioning parameters will improve the fidelity of the higher length and time scale models used to predict microstructural evolution and the swelling and hardening produced by cavities in irradiated materials.

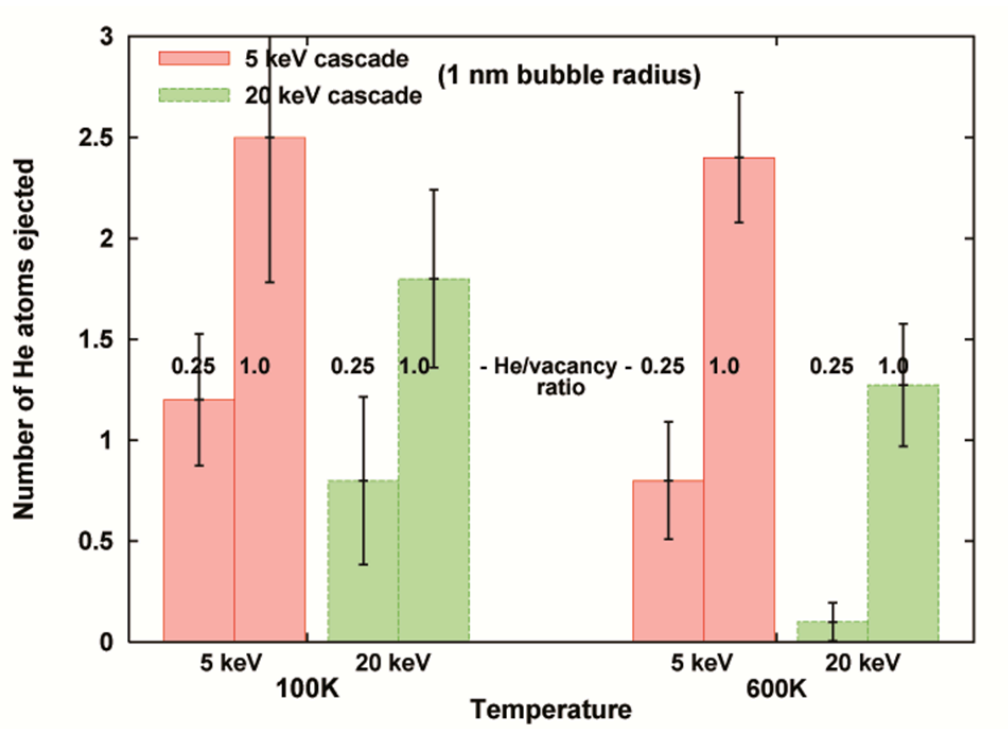

Fig. 3. Summary of ballistic He resolutioning from 1 nm He bubbles in iron as a function of temperature, cascade energy, and He/vacancy ratio.

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