8.3 OBJECT KINETIC MONTE CARLO SIMULATIONS OF RADIATION DAMAGE IN BULK TUNGSTEN

— G. Nandipati, W. Setyawan, H. L. Heinisch, K. J. Roche, R. J. Kurtz (Pacific Northwest National Laboratory) and B. D. Wirth (University of Tennessee)

OBJECTIVE

The objective of this work is to study the damage accumulation in pure crystalline bulk tungsten (W) during irradiation using the object kinetic Monte Carlo (OKMC) method.

SUMMARY

We used our recently developed lattice based OKMC code; *KSOME* [1] to carry out simulations of radiation damage in bulk W. We study the effect of dimensionality of self-interstitial atom (SIA) diffusion, i.e. 1D versus 3D, on the defect accumulation during irradiation with a primary knock-on atom (PKA) energy of 100 keV at 300 K for dose rates of 10^{-5} and 10^{-6} dpa/s. As expected 3D SIA diffusion significantly reduces damage accumulation due to increased probability of recombination events. In addition, dose rate, over the limited range examined here, appears to have no effect in both cases of SIA diffusion.

PROGRESS AND STATUS

Results

Simulation conditions used in the present simulations are exactly the same as reported in Ref. [2]. Figure 1 shows the total number of vacancies and vacancy clusters and average vacancy clusters for 1D and 3D SIA cluster diffusion as a function of the dose at 300 K in W irradiated with 100 keV cascades at the dose rates of 10^{-5} dpa/s and 10^{-6} dpa/s. In both cases of SIA cluster diffusion, there is no effect of dose rate on the densities of vacancies and vacancy clusters, or on the average vacancy cluster size (see Figure 1(a-c)) This behavior is not surprising because of the fact that SIA clusters diffuse very fast and are quickly absorbed at grain boundaries and vacancies are immobile at 300 K, and all this occurs in a very short time interval. This time-interval is very small when compared to the time-interval between two cascade insertions for the dose rates studied in this report. To see any effect of dose rate, the cascade insertion rate has to be faster than the damage evolution. In addition, the average vacancy cluster size does not appear to change with dose for both cases of SIA cluster diffusion (see Figure 1(c)). As expected, due to the higher probability for recombination events, the number density of vacancies for 3D SIA diffusion is lower by an order of magnitude when compared to 1D SIA diffusion. Surprisingly, the average vacancy cluster size of the 3D SIA diffusion case is slightly larger than for 1D SIA diffusion. From Figure 1(a), the number density of vacancies appears to grow linearly for 3D SIA diffusion with a growth rate (slope) of 13,660 vacancies/dpa, while for 1D SIA diffusion it appears to grow as $DPA^{0.21}$, a power law growth rate.

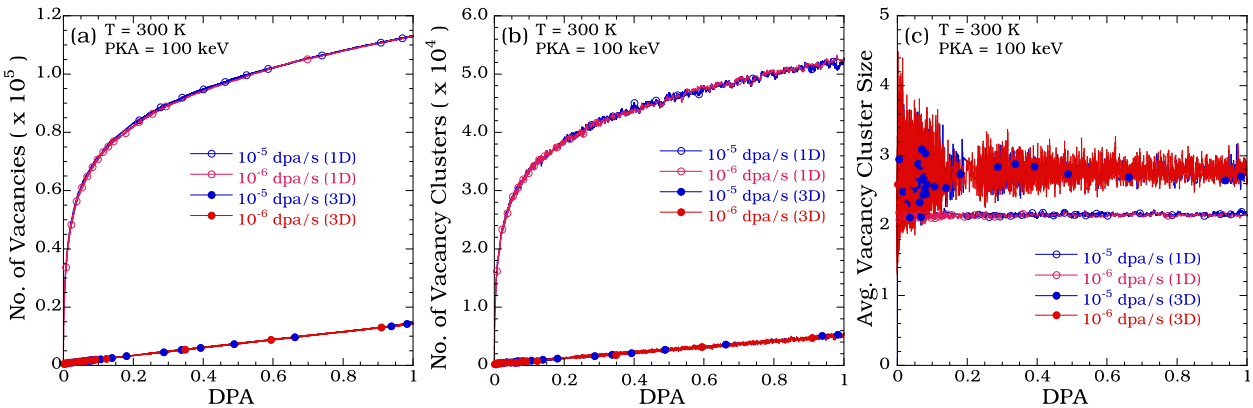

Figure 1. Comparison of damage accumulation at 300 K when SIA clusters diffuse in 1D and 3D at dose rate of 10^{-5} and 10^{-6} dpa/s using 100 keV cascades. (a) number density of vacancies (b) number density of vacancy clusters (c) average vacancy cluster size.

Figure 2 shows snap shots of the vacancy cluster distributions at 1 dpa. The radius of each sphere in a snap shot is scaled by the vacancy cluster size as $(\text{cluster size})^{1/3}$. To aid the visualization the radius of each sphere is increased by 5 times. The coloring scheme for each sphere is based on the increased radius. It can be seen from Figure 2 that the scale runs from 5 to 26.39, which corresponds to vacancy cluster sizes from ranging from 1 to 147 vacancies. Both for 1D and 3D SIA diffusion, most of the vacancies exist as mono-vacancies. As expected, Figs 1 and 2 show that 3D SIA diffusion significantly inhibits damage accumulation.

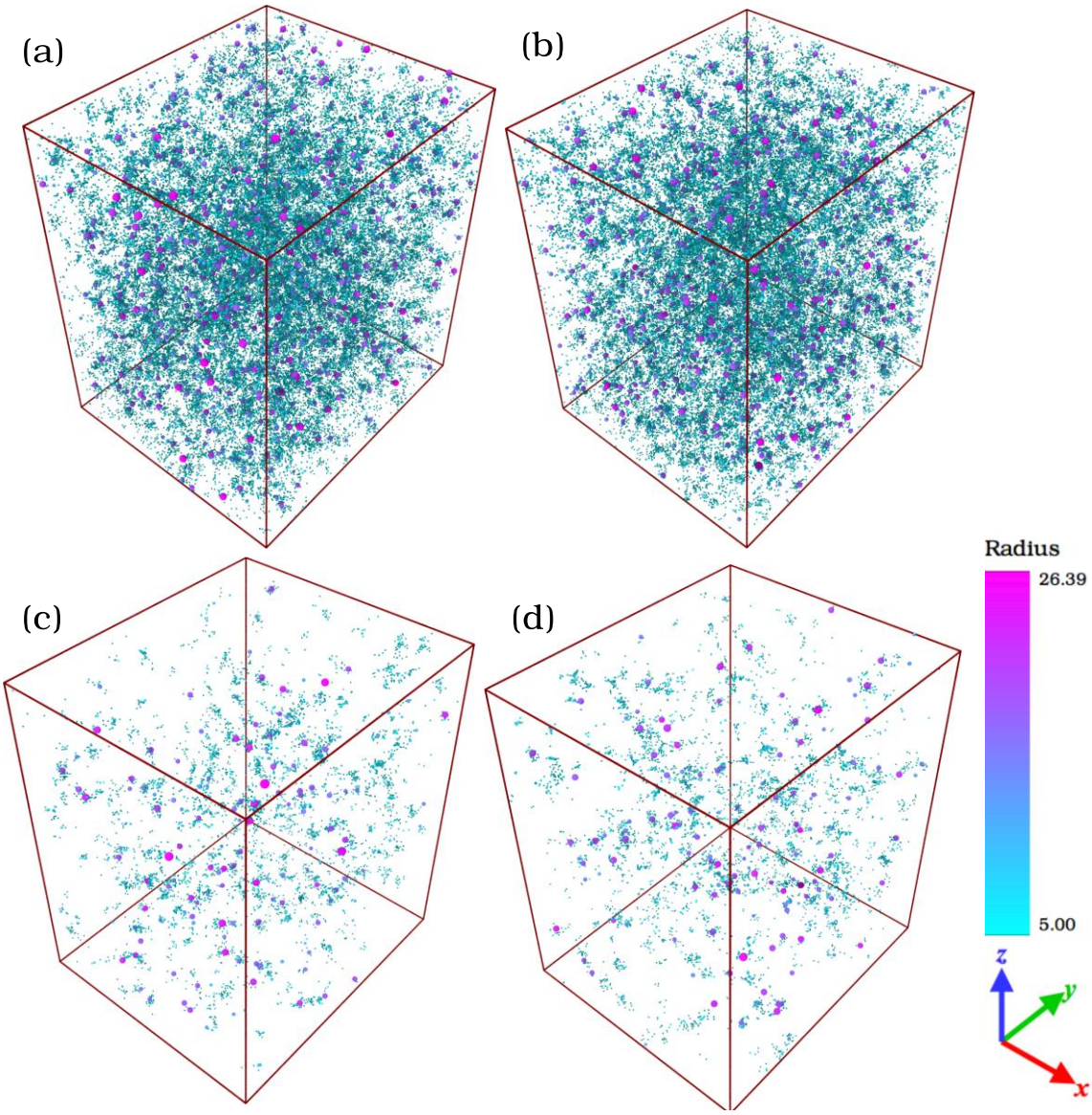

Figure 2. Snap shots of vacancy cluster microstructure at a dose of 1dpa at 300 K. (a) 10^{-5} dpa/s, SIAs diffuse 1D (b) 10^{-6} dpa/s, SIAs diffuse 1D (c) 10^{-5} dpa/s, SIAs diffuse 3D (d) 10^{-6} dpa/s, SIAs diffuse 3D (Radius = 5 x (vacancy cluster size)$^{1/3}$)

Future Work

We are carrying out further simulations to understand defect accumulation at various dose rates, PKA energies, temperatures, simulation cell and grain size, and also at different PKA spectrums. In addition we also intend to carry out sensitivity studies to understand the effect of kinetic parameters and, SIA and vacancy clustering.

Acknowledgement

All computations were performed either on HOPPER or CARVER at National Energy Research Scientific Computing Center (NERSC) and Argonne National Lab, MCS Workstations.

References

[1] G. Nandipati *et al* Semiannual Progress Report DOE/ER-0313/54, Jun (2013), 179-183
[2] G. Nandipati *et al* Semiannual Progress Report DOE/ER-0313/57, Dec (2014), 160-165