8.1 Molecular Dynamics Modeling of Atomic Displacement Cascades in 3C-SiC —

G. D. Samolyuk, Y. N. Osetskiy, and R. E. Stoller (Oak Ridge National Laboratory)

OBJECTIVE

The objective of this research is to investigate the damage in 3C-SiC induced at fusion irradiation condition and describes microscopic origin of these experimentally observed phenomena.

SUMMARY

A set of atomic displacement cascades was simulated using popular SiC Tersoff interatomic potentials. The types of created defects and their dynamics were analyzed. The validity of existing interatomic potentials was investigated by comparison of typical point defect diffusion barriers obtained using these potentials with first principles results.

PROGRESS

The purpose of this work is to develop a basic understanding of defect formation and evolution SiC. Initial 10 keV cascade simulations were carried out at a range of temperatures and indicated that in-cascade recombination seemed to be much lower than in metals. Simulations at 50 keV have shown the same behavior as indicated in Fig. 1. Fig. 1a shows the time dependence of defects obtained in a 50 keV SiC cascade at 600, and Fig. 1b shows typical results for similar simulations in iron. Note that the ratio of the peak defect count to the stable defect count at t>10 ps is less than a factor of two in SiC and almost two orders of magnitude in iron.

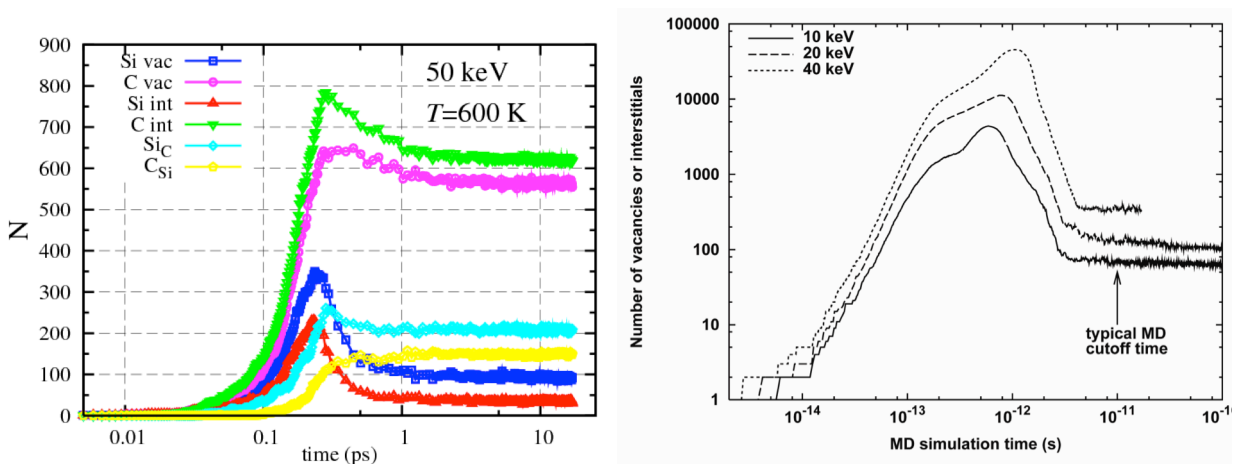

Fig. 1. Time dependence of the number of point defects observed in MD displacement cascade simulations: (a) 50 keV SiC cascade at 600 K and (b) 10, 20, and 40 keV cascades in iron.

Point defects in SiC consist of interstitials (I) and vacancies (V) of both carbon and silicon, as well as antisite defects of C on an Si site (C_{Si}) and Si on a C site (Si_C). The carbon defects predominate as shown by the green and purple symbols in Fig. 1a. Half of these V-I pairs are separated by a distance less than lattice parameter, and would normally be expected to

recombine. Examples of these close-pair C(V)-C(I) are shown in Fig. 2 as large (I) and small (V) green spheres.

In order to understand this lack of recombination, the energy landscape in the region of a carbon interstitial was analyzed using the interatomic potential employed in these MD simulations and compared with first principles calculations using density functional theory (DFT). Some of the results are shown in Fig. 3, which plots the energy of a carbon atom moving in the [111] direction. Both the Tersoff potential used in this work and an alternate modified embedded atom method (MEAM) potential reveal a barrier to recombination which is much higher than the DFT results. The barrier obtained with a newer potential by Gao and Weber (GW) is closer to the DFT result but the overall energy landscape is significantly different.

These results suggest that essentially all of the cascade simulations that have been carried out previously for SiC are not representative of how the material will respond to irradiation. A new potential needs to be created using the whole set of defect properties obtained by DFT.

FUTURE WORK

In the next three months we are planning to simulate the cascades in SiC with GW potential in order to further assess the impact of the recombination barrier on stable defect formation. This will provide further insight that can be used to correct the current generation of interatomic potentials for SiC.

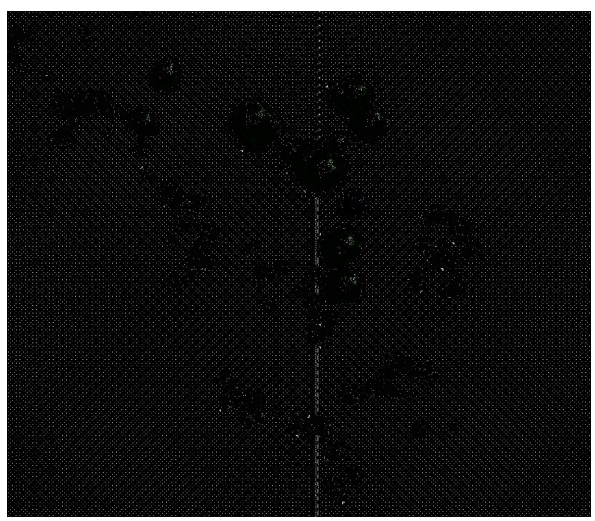

Fig. 2. Carbon (green) and silicon (red) interstitials (large spheres) and vacancies (small spheres) at the end of 50 keV Si recoil event in SiC. Blue and purples spheres correspond to Si_C and C_{Si} antisites, respectively.

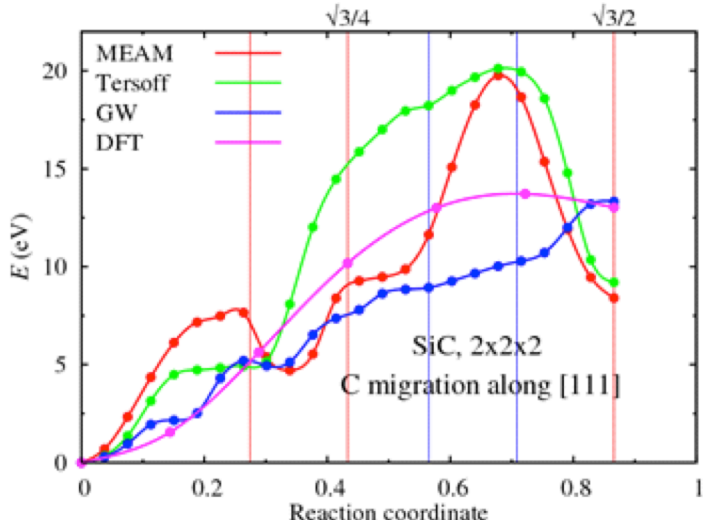

Figure 3. Carbon atom migration barrier in [111] direction.