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

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

EXTENDED ABSTRACT - paper submitted to J. Nucl. Mater. after ICFRM-16.

Designing silicon carbide components for fusion reactor blankets requires a basic understanding of defect formation and evolution, and the associated property changes. Molecular dynamics irradiation cascade simulations were carried out in SiC at energies of 10 and 50 keV and a range of temperatures with the widely used Tersoff interatomic potential [1]. The radiation-induced point defects in SiC consist of interstitials (I) and vacancies (V) of both carbon and silicon, as well as antisite defects of C on a Si site and Si on a C site. The results indicated that in-cascade recombination was much lower than in metals. For example, the ratio of defects at the peak time to the number of stable defects at ~10 picoseconds is about 2 in SiC and more than 100 in metals such as iron. About half of the carbon V-I pairs are apparently separated by a distance less than a lattice parameter, and would normally be expected to recombine. 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). Both the Tersoff potential and an alternate modified embedded atom method potential reveal a barrier to recombination which is much higher than the DFT results (Figure 1). The barrier obtained with the newer Gao and Weber (GW) potential [2] is closer to the DFT result but the overall energy landscape is significantly different.

In order to demonstrate the sensitivity of cascade recombination to the value of barrier recombination additional cascade simulations have been done with the Gao-Weber potential. 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. In a contrast to Tersoff potential, the GW potential produces almost twice as many C vacancies and interstitials at the time of maximum disorder (~0.2 ps) but only about 25% more stable defects at the end of the simulation (Figure 2). The ratio of peak-to-stable defects is much higher for the GW potential. Only about 20% of the carbon defects produced with the Tersoff potential recombine during the in-cascade annealing phase, while about 50% recombine with the GW potential. Such a significant difference is caused by the fact that the energy barrier for carbon V-I recombination with the GW potential is much smaller than with the Tersoff potential barrier.

The number of defects at the end of cascade evolution is weakly temperature dependent for Tersoff potential but reduces with temperature for the GW potential. The difference is due to unphysically large migration barriers for Tersoff potential.

To conclude, GW gives a much more realistic description of cascade dynamics in SiC.

REFERENCES

1. J. Tersoff, *Phys. Rev. B* **39** (1989) 5566–5568 .
2. F. Gao and W. J. Weber, *Nucl. Instr. Methods Phys. Res. B* **191** (2002) 504-508.

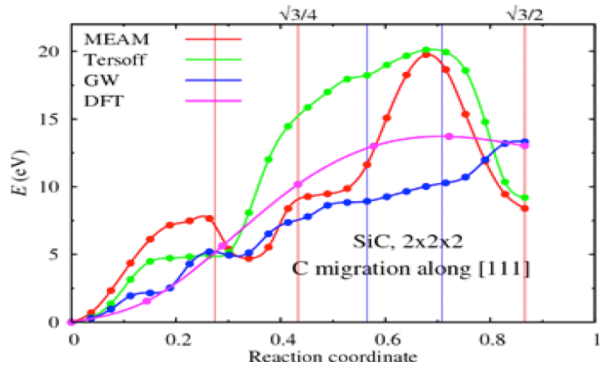

Figure 1. Energy of a carbon atom moved in the [111] direction.

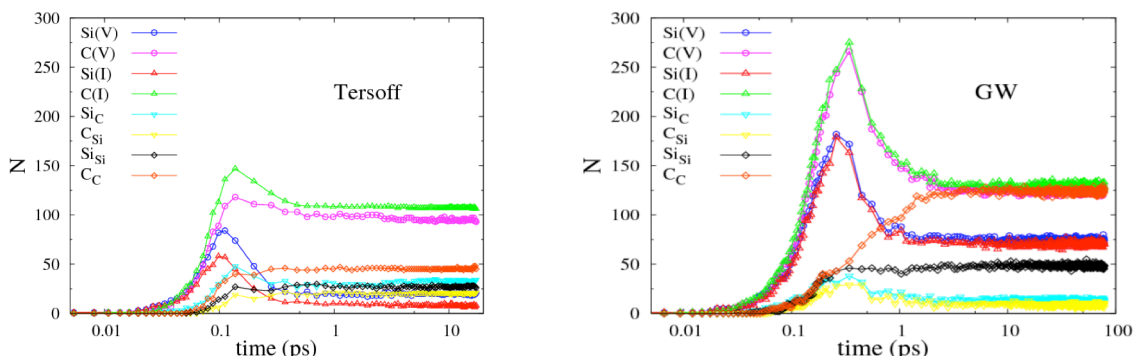

Figure 2. Time dependence of the number of point defects observed in MD displacement cascades.

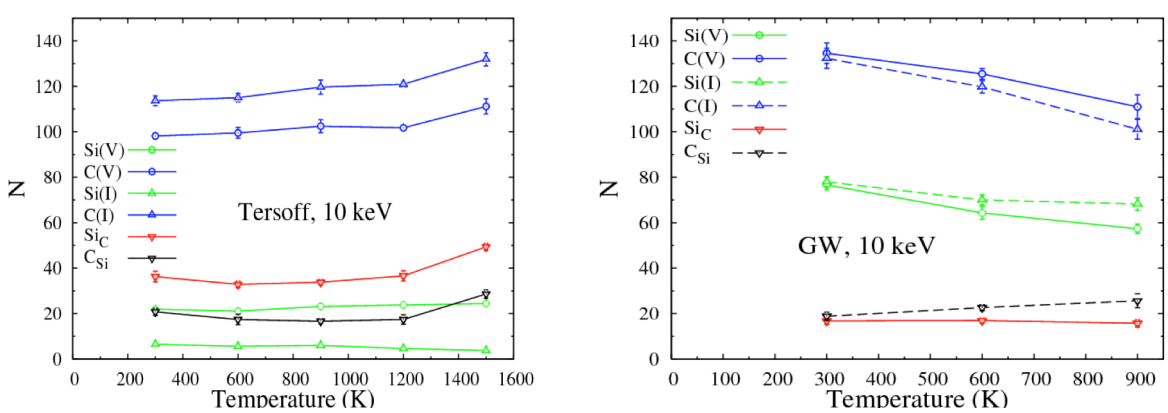

Figure 3. The number of defects at the end of cascade evolution.