8.1 MOLECULAR DYNAMICS MODELING OF 10 AND 50 keV 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 under fusion irradiation conditions and describe microscopic origin of such experimentally observed phenomena as amorphization [1-6] and swelling [7-9].

SUMMARY

Molecular dynamics (MD) simulations of atomic displacement cascades in 3C-SiC were carried out at a range of temperatures and two energies. A new code for post processing the MD results was developed to analyze the results. We simulated cascades produced by 10 and 50 keV primary knock-on atoms (PKA) at temperatures of 300, 600, 900, 1200 and 1500 K. Similar to previous results [10, 11] it was observed that the main defects produced in 3C-SiC are carbon interstitials (C(I)) and carbon vacancies (C(V)). The temperature dependence of number of defects is weak. 30 % of defects are accumulated into clusters of size ~20 defects, which are often, interpreted [11] as amorphous domains. Many pair clusters of C(I)-C(V) were observed. The stability of these objects is a result of specific crystal structure of 3C-SiC. The 3C-SiC lattice has “empty space” in the unit cell positions (3/4, 3/4, 3/4) and (1/2, 1/2, 1/2).

PROGRESS AND STATUS

Introduction

3C-SiC subjected to fusion conditions is changing their microstructure and hence mechanical properties. Understanding the details of this process is necessary for predicting changes, estimation of material lifetime. Experimental studies have demonstrated that depending on the structural material composition and particular conditions such phenomena as amortization [1-6], swelling [7-9] were observed.

Formalism

The LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator, see http://lammps.sandia.gov) code was used for atomistic molecular dynamics simulations [12]. The interactions between atoms were described by a hybrid Tersoff/ZBL potential [13-15]. The simulation cell contains from 80x80x80 unit cells (409600 atoms) for 10 keV the PKA kinetic energy, 100x100x100 unit cells (8000000 atoms) for 50 keV PKA kinetic energy at temperature 600 K and 120x120x120 unit cells (13824000 atoms) for 50 keV PKA kinetic energy at temperature 1200 K. The initial system was equilibrated for 2 picoseconds with time step 0.1 femtosecond. Each cascade was initiated by giving a Si atom kinetic energy of 10 or 50 keV keeping zero total momentum. The cascade evolves for ~20 ps and the time step is modified such that the distance covered by the fastest particle in the system is less than 0.014 A. We apply constant volume through the iteration and the lattice parameter is chosen from the condition of zero pressure of system in equilibrium at particular temperature. The Wigner-Seitz cell analysis method was used to determine defects in the modeling system. The defects separated by distance less than a lattice parameter are interpreted as a defect clusters.

RESULTS

The number of point defects as a function of time for different temperatures and 10 or 50 keV PKA kinetic energy are presented in Figures 1-7. On this figures the notations Si(V) and C(V) correspond to silicon/carbon vacancies, Si(I) and C(I) – interstitials, Si_C and C_{Si} – aniticites and Si_{Si} and C_C – replacement atoms (Si atoms in Si lattice site came from other position).

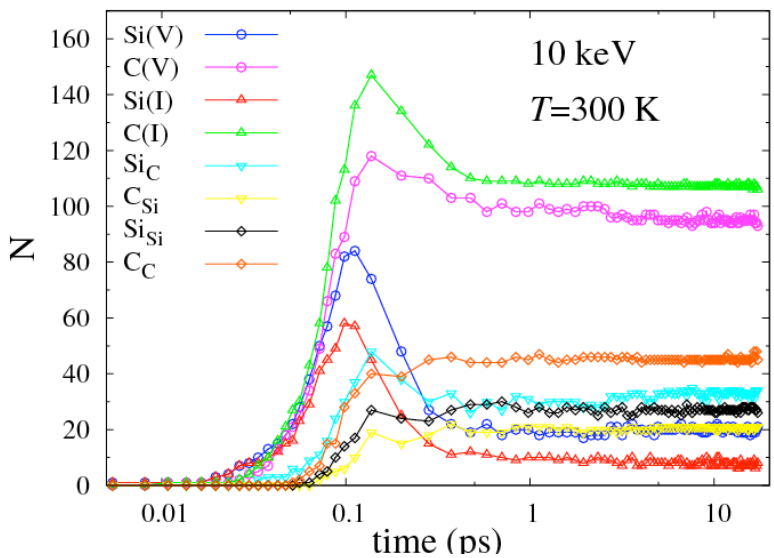

Figure 1. Plot of defect count for 300 K and 10 keV Si displacement cascade.

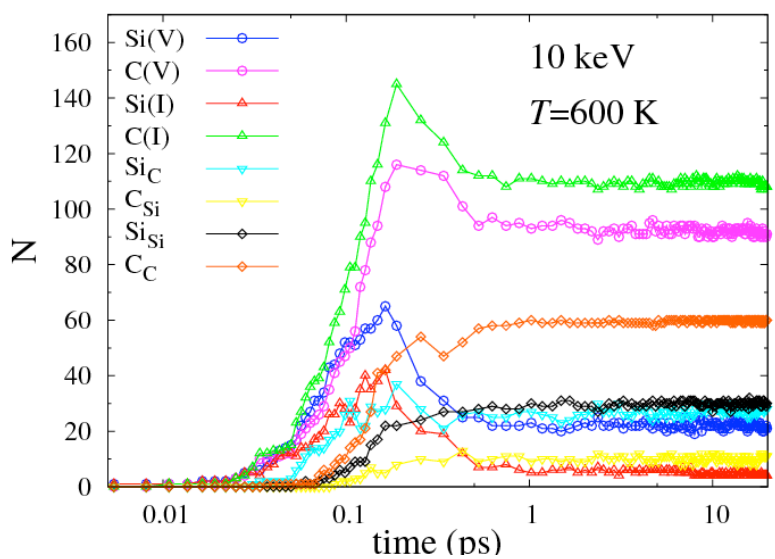

Figure 2. Plot of defect count for 600 K and 10 keV Si displacement cascade.

Analysis of cascade evolution in SiC indicates that by 0.2 picoseconds the PKA has lost most of its kinetic energy and by 1 picosecond its kinetic energy is close to background energy. After this time the velocity of cascade evolution is significantly reduced. The number of defects doesn't demonstrate significant dependency of the temperature. Carbon vacancies and interstitials are the main type of defects observed. They number 2.5 times more than Si defects. At ~1.5 picosecond the number of defects reaches a maximum value and is reduced by ~30% for carbon vacancies/interstitials and by 60 % for silicon defects. The time evolution of carbon (C_{Si}) and replacement atoms does not exhibit this maximum. The number of these type of defects monotonically increases with time until it reaches saturation at a time of ~2 picoseconds. This difference in the behavior could be related to the fact that formation energy for replacement atoms is equal to zero and is very low for C_{Si} defects. The largest formation energy corresponds to Si(I) and Si(V) defects and this fact reflects the larger (3 times increase at 1.5 picoseconds) spike in time dependence.

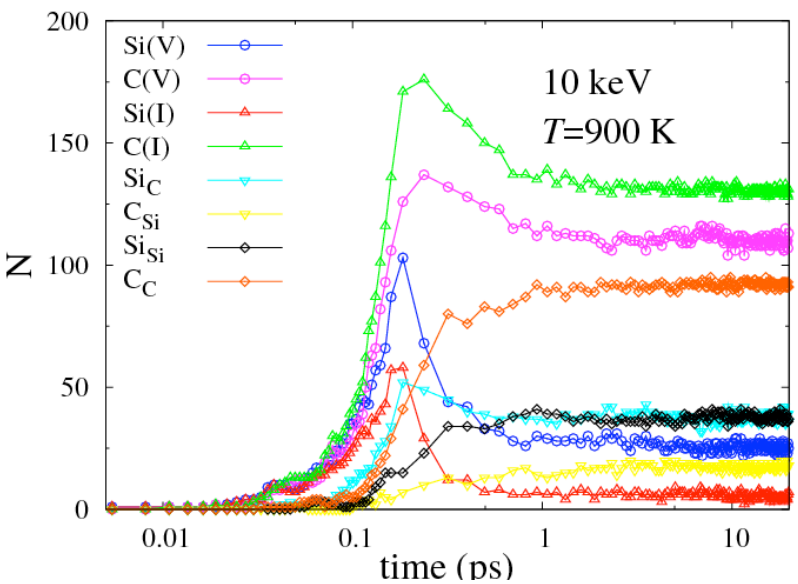

Figure 3. Plot of defect count for 900 K and 10 keV Si displacement cascade.

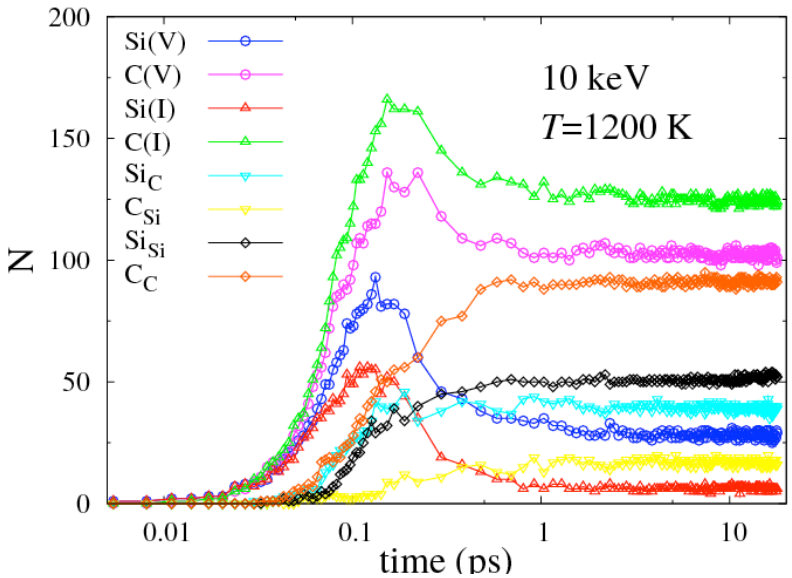

Figure 4. Plot of defect count for 900 K and 10 keV Si displacement cascade.

The defects cluster distribution calculated from the 10 keV PKA cascade at temperature 300K and time 20 picoseconds is presented in Figure 8. Single point defects comprise 15 % of the surviving defects. Almost the same fraction of defects is contained in clusters of size two. Most of these size two clusters consist of C(I)-C(V) defects. The stability of these objects is a result of low formation energy caused by specific crystal structure of 3C-SiC. The 3C-SiC lattice has an “empty space” in relative position (3/4, 3/4, 3/4) and (1/2, 1/2, 1/2). The energy to shift a C atom from its “perfect” position to the “empty space” is comparable to formation energy of single C defects. The three clusters of size ~20 defects can be interpreted as amorphous domains.

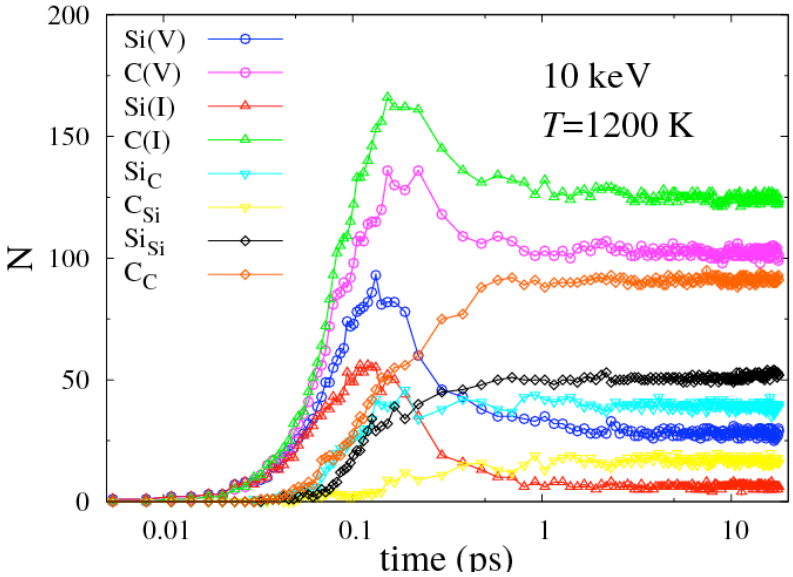

Figure 5. Plot of defect count for 1200 K and 10 keV Si displacement cascade.

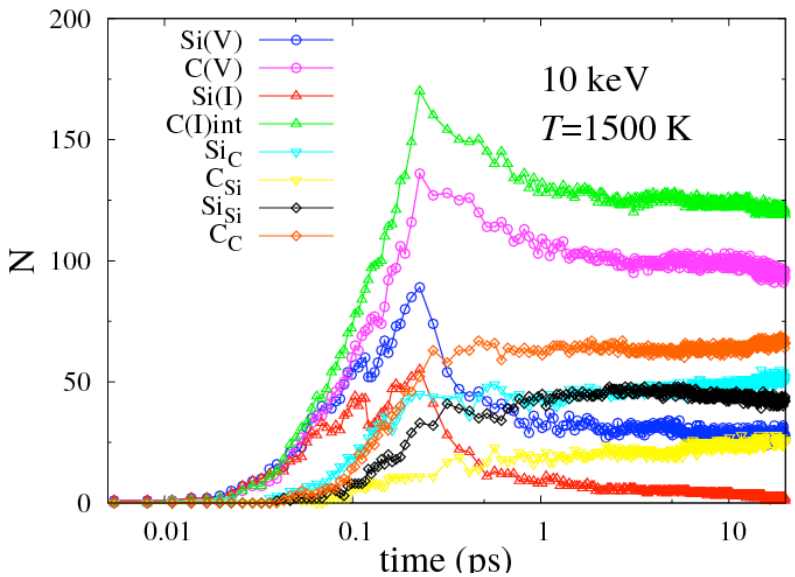

Figure 6. Plot of defect count for 1500 K and 10 keV Si displacement cascade.

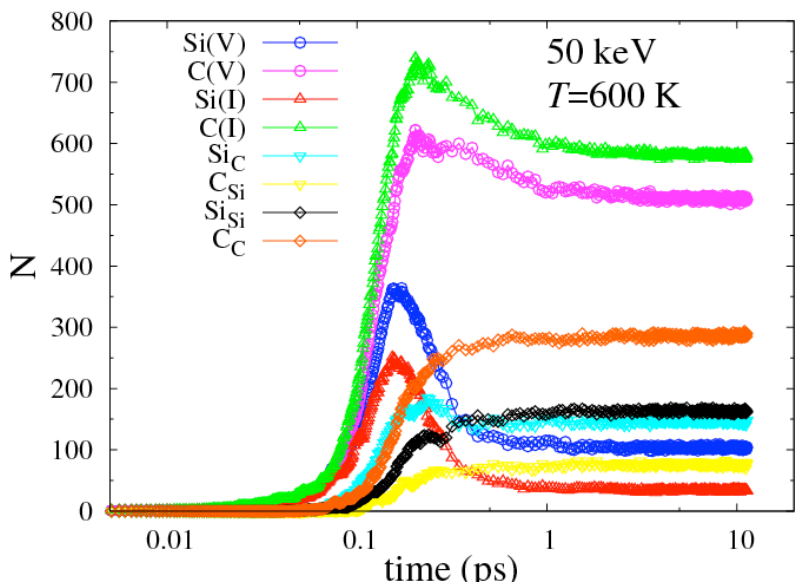

Figure 7. Plot of defect count for 1200 K and 50 keV Si displacement cascade.

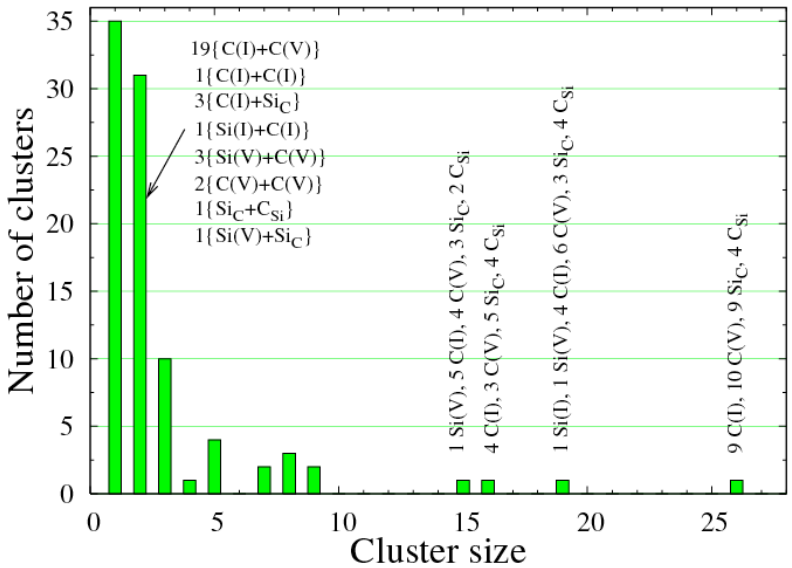

Figure 8. Defect cluster distribution in 10 keV cascade after 20 ps at temperature 300 K.

FUTURE WORK

Simulations are underway at additional temperatures at 50 keV to provide direct comparisons with the 10 keV results. Additional simulations will also provide further information on statistical variations. More detailed analysis of the structure of defect clusters is planned to determine whether or not they are consistent with an amorphous structure. Finally, MD simulations of defect mobility are underway to characterize diffusion in SiC.

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