Molecular dynamics simulations of primary radiation damage in Silicon Carbide

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Molecular dynamics (MD) simulations provide information on atomic displacement cascades on time dependence and account for the effects of crystal structure and temperature. MD can help to understand the material behaviour during ion irradiation, because it can capture details of radiation cascade in picoseconds or even femtoseconds scale. The classical molecular dynamic is a method that uses Newton's equation of motion. During passage through matter, ions lost their energy due to atomic collision and electronic excitation. In low energy regimes, elastic collisions are dominant and in many cases, electronic stopping is neglected. Here, MD simulations of 20 keV Argon irradiation are performed with and without adding the electronic stopping effects.

Methods

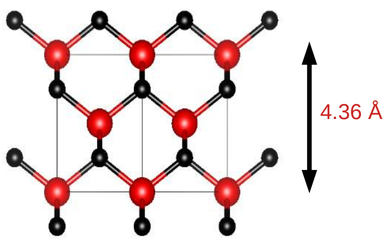
Simulations were performed with using LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) code. LAMMPS is a classical molecular dynamics simulation code that computes Newton's equation of motion for a system of particles [1].

$$m_i \frac{\partial v_i}{\partial t} = F_i(t)$$

To simulate electronic stopping effects, additional force was added to Newton equation to reduce ion velocity [2].

$$m_i \frac{\partial v_i}{\partial t} = F_i(t) - \frac{v_i}{|v_i|} \cdot S_e$$

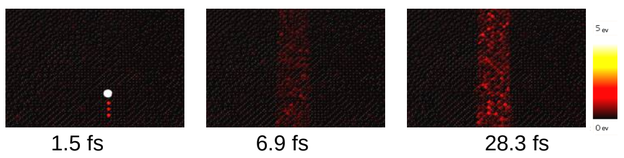
Electronic stopping power S_e was calculated by SRIM.
For interactions between Ar ion with SiC, Ziegler-Biersack-Littmark (ZBL) potential was used. For SiC - Tersoff/ZBL potential was employed. Sample was equilibrated with isothermal – isobaric ensemble. Ar ion irradiation were performed with the microcanonical ensemble. The cubic silicon carbide sample's size was 434 Å x 434 Å x 652 Å. Defects analysis was made in OVITO code with using Wigner Seitz analysis[3].



Cubic Silicon Carbide (3C-SiC)

Future Work

Energy deposited into the electron subsystem leads to lattice temperature increase (according to thermal spike model). In the two temperature model (ttm) in LAMMPS, the electronic subsystem is divided into a grid and treated as a background gas. The high-energy ions transfer energy to the electrons, and then the energy deposited in this electronic 'gas' is transferred to the atoms in the lattice [4][5].


1.5 fs 6.9 fs 28.3 fs

1 MeV Ar ion during passage through SiC deposited energy to electronic subsystem. This energy was transferred to the atomic lattice by electron phonon coupling.

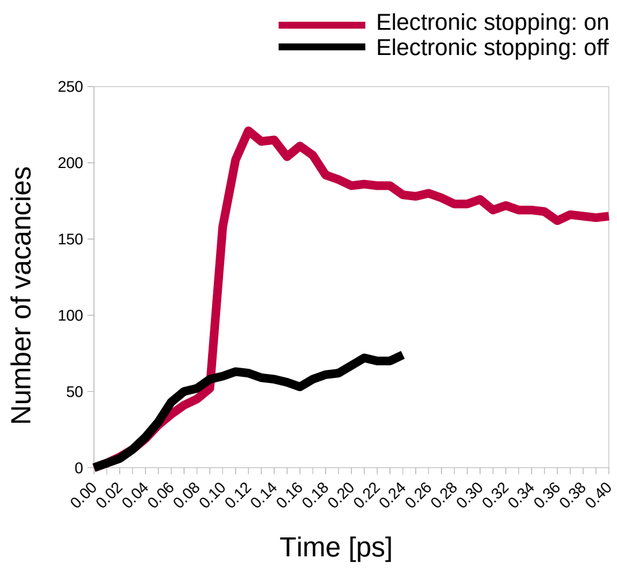
The heat diffusion in the electron and lattice subsystems can be described by two coupled differential equations

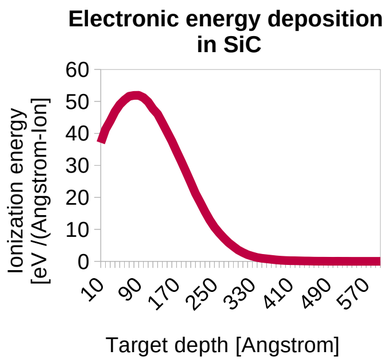
$$C_l \rho_l \frac{\partial T_l}{\partial t} = \nabla(\kappa_l \nabla T_l) + g_p(T_e - T_a)$$

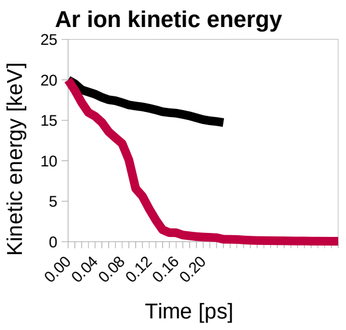
$$C_e \rho_e \frac{\partial T_e}{\partial t} = \nabla(\kappa_e \nabla T_e) - g_p(T_e - T_a) + g_s T'_a$$

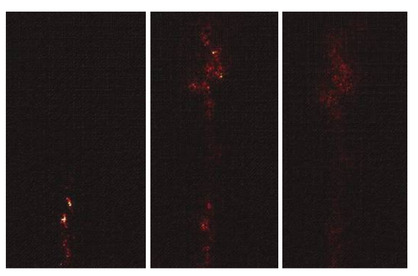
Results

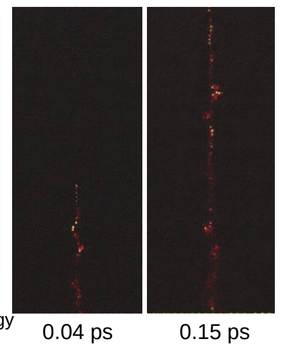
Number of vacancies in SiC:
results from 20 keV Ar ion irradiation simulation with and without electronic stopping

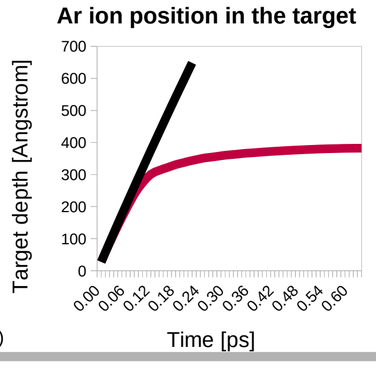







0.04 ps 0.15 ps 0.40 ps
Cascade after ion passage in SiC - kinetic energy (with electronic stopping)


0.04 ps 0.15 ps
Cascade after ion passage in SiC - kinetic energy (without electronic stopping)



Summary

In this work, the possibility of using MD to study primary radiation damage in SiC is presented. Simple calculations show that electronic stopping can affect the number of defects in 20 keV Ar ion irradiation cascade. Further investigation of the electronic stopping effects for primary radiation damage in SiC is needed.

References

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