Temperature dependence of the kinetics of structural changes in swift heavy ion tracks in silicon carbide

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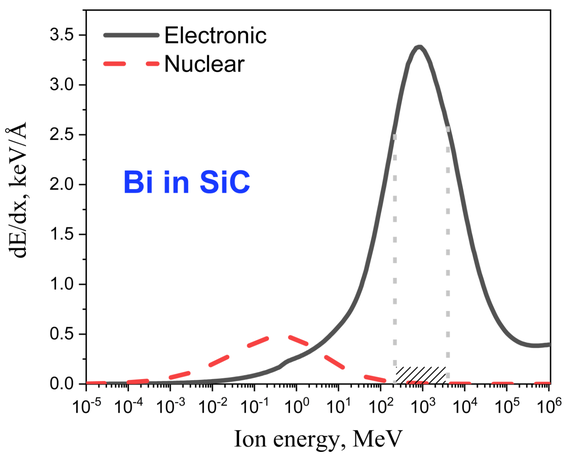
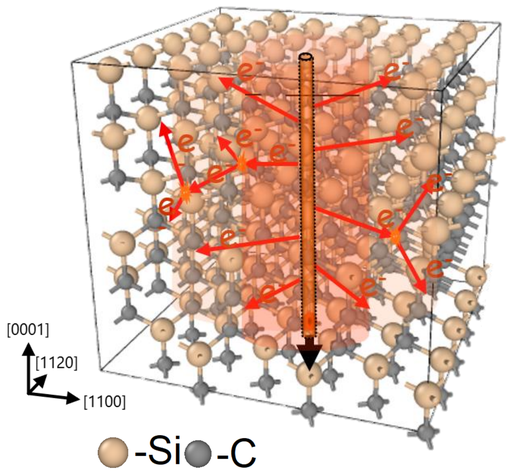
1. Introduction



Energy loss of Bi ion 710 MeV

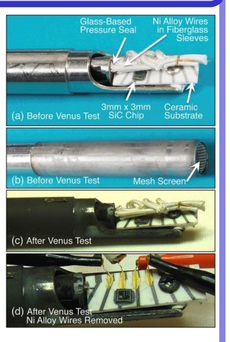
E_{ion} = 1–10 MeV/nucl and M_{ion} > 10 m_p



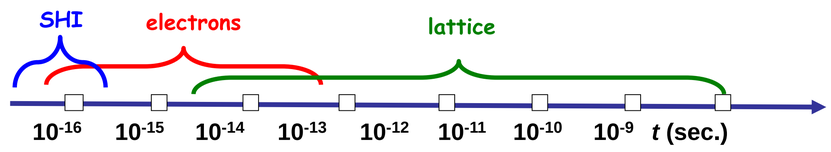
Schematic representation of ion passage through the 6H-SiC lattice

He R., et al., Journal of Advanced Ceramics 10 (2021) 4014502104

https://doi.org/10.48550/arXiv.2209.10270



SiC applications



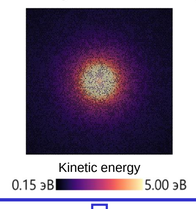
Characteristic scales of processes in the SHI track

2. Model

Monte-Carlo code **TREKIS-3** [1].

Description of electron excitation and energy transfer to the lattice.

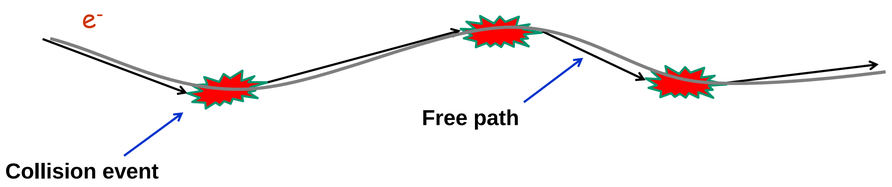
Generate initial atomic velocities for Molecular Dynamics (MD) [2].



LAMMPS package [3].

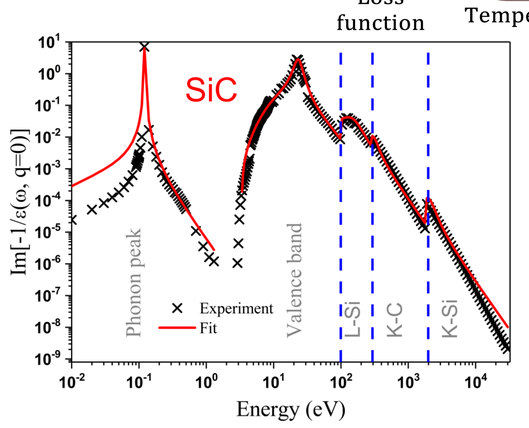
Simulation of the evolution of the excited atomic subsystem by methods of classical MD.

MC simulation



Differential scattering cross section on a system of interacting particles [4]:

$$\frac{d^2\sigma}{d(\hbar\omega)d(\hbar q)} = \frac{2\left[Z_{eff}(v,q)\right]^2 e^2}{n_{sc}\hbar^2\pi v^2}\frac{1}{\hbar q}\underbrace{Im\left[\frac{-1}{\varepsilon(q,\omega)}\right]}_{\text{Loss function}}\underbrace{\frac{1}{\left(1-e^{-\frac{\hbar\omega}{k_b T}}\right)}}_{\text{Temperature factor}}$$

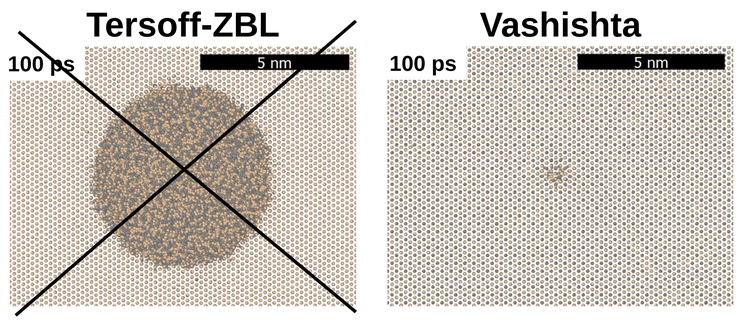


Complex dielectric function from optical experiments

MD simulation

Bi 710 MeV

No tracks were experimentally observed at 300 K [5]!



Vashishta's potential is used in the calculations [6]

The trajectories of the particles in MD are found by the Verlet algorithm:

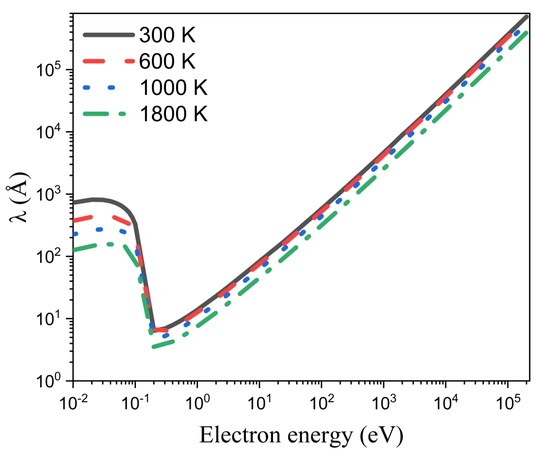
$$\vec{r}(t+\Delta t) = \vec{r}(t) + \vec{v}(t)\Delta t + \frac{\vec{f}(t)}{2m}\Delta t^2$$

$$\vec{v}(t+\Delta t) = \vec{v}(t) + \frac{\vec{f}(t+\Delta t)+\vec{f}(t)}{2m}\Delta t$$

$$\vec{f}(t) = \frac{\partial}{\partial \vec{r}}U(\{\vec{r}_i(t)\})$$

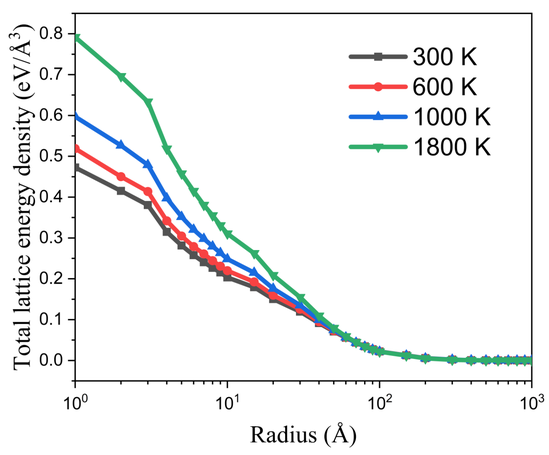
3. Simulation results

Bi 710 MeV (34 keV/nm)



Mean free path length of electrons before scattering on the lattice

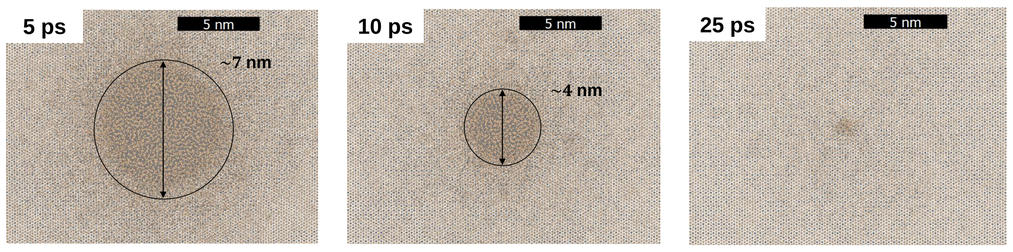
Scattering cross section increases with lattice temperature



Energy density transferred from electron excitation to the lattice

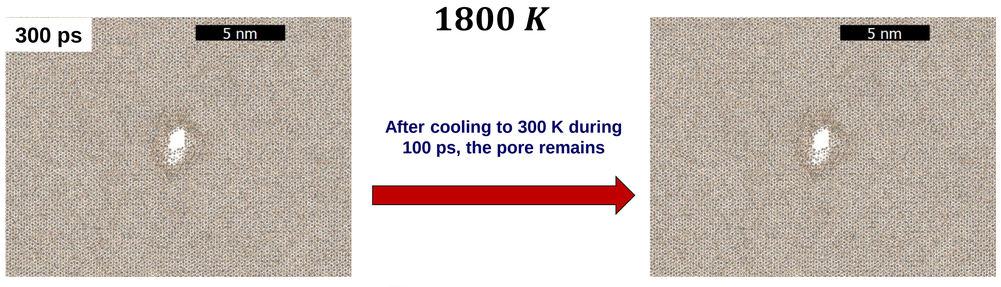
Energy density also increases with lattice temperature

300 K



Recrystallization of primary damage during ~25 ps

1800 K



Void formation in the central region of the track

After cooling to 300 K during 100 ps, the pore remains

The elongated part of the pore ~3nm is directed along the [0001] axis

Conclusion: Predicted formation of radiation damage in SiC at high irradiation temperatures

[1] N.A. Medvedev, R.A. Rymzhanov, A.E. Volkov, J. Phys. D. Appl. Phys. 48 (2015).

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