R4-O-028401

# SIMULATION OF ION TRACK FORMATION IN POLYETHYLENE

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Our model of polymer damaging by swift heavy ions (SHI) combines Monte-Carlo (MC) code TREKIS [1], describing electronic and lattice excitations, with all-atom reactive molecular dynamics (MD) for atomic response. The simulation traces structure transformations, chemical bond creation/rupture and new molecular species emergence in ion tracks. Polyethylene (PE) serves as a prototypical system for model validation.

Crystalline 20 nm × 20 nm × 5 nm PE supercell with ~3×106 atoms was created by Moltemplate tool [2] and modelled using AIREBO-M [3] force field in MD simulation. Crystalline sample was melted and treated by Charge-Implicit ReaxFF force field [4] to produce an amorphous supercell. All MD simulations were performed in LAMMPS package [5].

We apply MC code TREKIS to get an initial radial energy distribution in the atomic system. Then, this distribution is converted into velocities of atoms in cylindrical layers surrounding the ion trajectory. The Berendsen thermostat at 300 K was employed at the borders of the simulation box.

A comparison of the simulation results with experimental track shapes and diameters [6] shows a reasonable agreement. Elliptic shape of tracks stretching is observed in both, the simulation and an experiment. Evolution of chemical bonds in tracks are also tracked during the track kinetics. The simulation provides atomic resolution of track structure and traced chemical species emerging in PE targets irradiated with SHIs. The results can be used for development of track etching models.

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