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Simulation of changes in thermal conductivity of aluminum oxide irradiated with swift heavy ions

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Thermal conductivity (TC) degradation of aluminum oxide induced by irradiation with swift heavy ions (SHI) at room temperature is studied and quantified with direct method of non-equilibrium molecular dynamics. The calculations were performed for an ideal crystal lattice, amorphous and irradiated states of aluminum oxide. Irradiated samples were described by the model of the track formation combining Monte-Carlo code TREKIS [1], describing the excitation of the electronic subsystem, with classical molecular dynamics of the lattice atoms [2]. Then these results were used as input data for simulation of thermal conductivity of irradiated state.

Simulation with direct method showed, that the obtained thermal conductivity of ideal alumina crystal is in good agreement with the experimental data from literature [3]. The calculated TC values for discontinuous crystalline tracks in irradiated alumina are also in good agreement with the experiment for low fluences (Time-Domain Thermal Reflectance method [3]). However, there are discrepancies between modeling and experiment in multiple track-overlapping regime. In order to solve this problem, Al2O3 was considered as layered system within multilayer thermal model including three regions: amorphous, near-surface damaged layer and discontinuous ion track region. This approach allowed us to describe the experimentally observed dependence of thermal conductivity of alumina on irradiation fluence. Obtained results reveal significant role of surface effects in Al2O3 in degradation of thermal properties under swift heavy ion irradiation.

References

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Primary author: AKZHUNUSSOV, Aidos (JINR)

Presenter: AKZHUNUSSOV, Aidos (JINR)

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