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Atomistic simulations of swift heavy ion tracks in Al₂O₃

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The structure and formation threshold of swift heavy ion tracks in Al2O3 is studied using a combined modeling with original Monte-Carlo code TREKIS [1], describing the excitation of the electronic subsystem, and classical molecular dynamics of the lattice atoms. The advantages of developed approach are absence of free parameters and accounting for collective effects of solid state. The data obtained for Xe 167 MeV ion impact shows that the relaxation of the excess lattice energy results in the formation of a cylinder-like discontinued disordered region of about 2 nm in diameter, which is consistent with the recent transmission electron microscope observations. The estimation of SHI track formation threshold gives the value of ~7 keV/nm. The result of simulation of the x-ray diffraction pattrens of irradiated material demonstrates that Al atoms sublattice damaged stronger than the oxygen sublattice.

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