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Multiscale modelling of AIN irradiation by swift heavy ions

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This work is devoted to the modelling of radiation effects of swift heavy ions in AlN. This material was chosen because it is promising for using in nuclear reactors. The multiscale model was employed. To describe the ions impact and further electron kinetics we use the TREKIS model based on MC-methods. After this, on atomic dynamic stage, MD-methods were applied to trace the atoms movement.

The first step was modelling of ionic impact on material and further electron kinetics of AlN. As the irradiating particles we used ions of Ar, Xe and Bi with energies 100, 158 and 700 MeV respectively. The study shows that electron excitation in the damaged area is faded out to 100 fs after ion impact. The second step of the study was the modelling of ionic subsystem relaxation with molecular dynamics both in the bulk and at the surface. It was found out that in the bulk ion tracks are not formed because of strong recrystallization ability of AlN, only few point defects along the ion trajectory are observed. In contrary, the presence of an open surface allows atoms to go away from the damaged volume including emission of atoms and forming hillocks. As the result, deficiency of the mass in subsurface area, on the one hand, suppresses the processes of recrystallization producing conical hillocks, on the other hand, leads to formation of small cavities. The modelling results are in reasonable agreement with experimental data from the literature.

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