Contribution ID: **20** Type: **not specified**

Model of swift heavy ion tracks excitation

Wednesday, June 21, 2017 4:00 PM (1h 45m)

This report presents theoretical study of swift heavy ion (SHI, M > 20 amu., E > 1 MeV/nucl) tracks formation kinetics depending on the initial state of an irradiated material. This research is stimulated by so far an open question how the lattice structure or temperature affect material excitation process. To investigate this problem, we apply a new version of TREKIS code [1,2] for description of excitation of alumina in the nanometric vicinity of trajectories of SHIs decelerated in the electronic stopping regime.
TREKIS code is based on a Monte-Carlo algorithm describing kinetics of fast electrons and valence holes, which appear due to material ionization, as well as their interaction with the lattice up to ~100 fs after the projectile passage. Building cross sections within the dynamic structure factor/complex dielectric function (DSF-CDF) formalism [3], this model takes into account collective response of the electronic and ionic subsystems to excitation which can be of principal importance for realization of unusual pathways of the extreme track kinetics.
To describe interaction of excited electronic subsystem with the lattice, the presented upgraded version of TREKIS uses cross sections based on the DSF of the lattice, calculated with an in-house molecular dynamic code. The DSF of Al2O3 lattice was calculated for the wide range of temperatures (80-1000 K), that enables to investigate effects of initial states of this target on the SHI track kinetics. In particular, a sharp increase of mean free paths of electron scattering on the lattice is found in simulations when the temperature of Al2O3 crystals is below 200 K.

References

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Session Classification: Poster Session with Coffee break