EXCITATION OF THE ELECTRONIC SYSTEM OF SUBSURFACE LAYERS OF TiO_2 IRRADIATED WITH SWIFT HEAVY IONS

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A swift heavy ion (SHI, *E*=1-10 MeV/nucl) penetrating through a solid deposits the largest part of its energy into the electronic subsystem of the target. Further kinetics of lattice excitation in the nanometric vicinity of the ion trajectory (ion track) depends crucially on achieved parameters of the disturbed electronic system.

Exchanging energy and particles with an environment, a subsurface layer of the target can react unusually to strong perturbation induced by an SHI, forming inhomogeneity in the parameters of excited electronic system along the ion trajectory.

Rutile (TiO_2) is an important material which has high chemical stability and radiation resistance and has been subjected to various applications using SHI beams. The most notable studies involved patterning of the TiO_2 surface using ion beam lithography which requires understanding of the SHI-surface interaction processes.

The developed Monte Carlo model (MC TREKIS [1,2]) is applied to describe such surface effects on the excitation kinetics of the electron subsystem of a TiO_2 film of 20 nm thickness irradiated with swift heavy ions. Complex dielectric function (CDF) formalism [3,4] is used to take into account the collective response of target electrons and the lattice to excitations when determining the cross sections of ion and electron scatterings in a target.

The MC model relies on the asymptotic trajectory method of the event-by-event simulation of individual particle propagation. Application of this MC model allows us to describe: (a) ionization of a target by a projectile resulting in appearance of primary fast electrons (δ- electrons), (b) scattering of these δ- electrons on lattice atoms and target electrons as well as the kinetics of all secondary generations of electrons arising during relaxation of the excited electron subsystem, and (c) Auger decay of deep shell holes, resulting also in the production of secondary electrons.

Results

Fig. 1 shows the dependence of the energy density of generated electrons in TiO_2 on the depth and on the distance from the Xe 167 MeV ion trajectory at 1 fs after the ion passage. Propagation of an excitation front is clearly demonstrated in this Figure. At these times the maximum of the excess energy of the electron subsystem is located at 1-3 Å from the ion trajectory and at ~15 nm in depth from the sample surface, which corresponds to the distance travelled by a Xe 167 MeV ion during 1 fs. (15,6 нм). The energy of electronic excitation at larger distances from the track axis dissipates fast due to spatial spreading of free electrons and their interaction with the electrons and lattice.

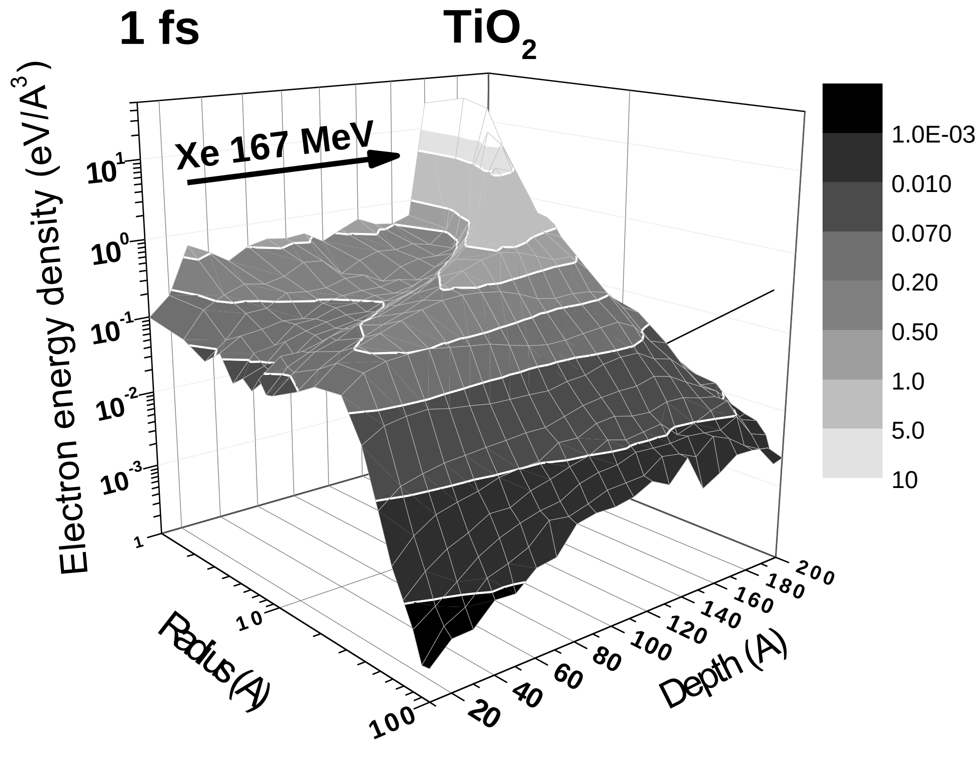

Figure 1. Energy density of delocalized electrons in track of Xe 167 MeV ion in TiO_2 at 1 fs after the projectile passage.

The distribution of the excess lattice energy density distribution on the distance from the ion trajectory and the depth is demonstrated in Figure 2. The excess energy accumulated in the lattice within the depth of 5-6 nm is lower by ~25% than that in the center of a layer due to emission of electrons from the surface and lower energy transfer to the ionic subsystem in this near-surface region.

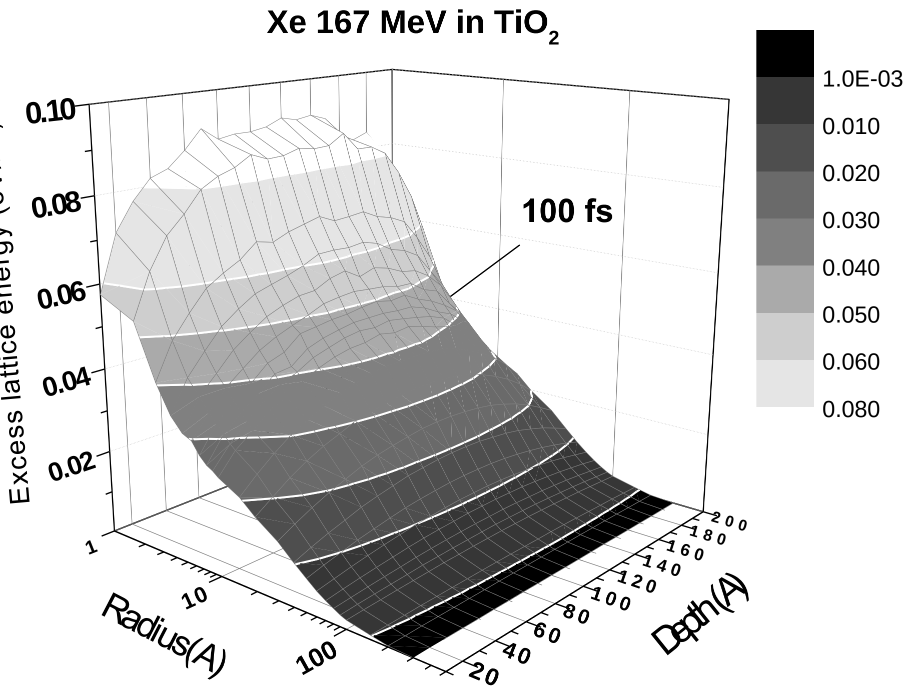

Figure 2. Lattice energy density in a track of Xe 167 MeV ion in TiO_2 at 100 fs.

Conclusions

We described the spatial and temporal dependencies of the kinetics of the electron ensemble energy and their density as well as the excess lattice energy distributions in a track of a swift heavy ion in titanium dioxide. The parameters of electron subsystem excitation dependence on the depth are determined. These distributions can serve initial conditions for further of electron-lattice energy exchange and structure transformations forming ion tracks, for instance, by means of the *ab initio* models, or molecular dynamics simulations.

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