ULTRAFAST NONTHERMAL PHASE TRANSITIONS IN COMPOUND INSULATORS BY EXTREME ELECTRONIC EXCITATIONS

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Irradiation of solids with swift heavy ions (SHI) or free-electron laser beams (FEL) highly excites the electronic system of a target. Subsequent energy transfer to the target lattice may lead to structural changes in the irradiated solid. However, electron density modifications induce changes in the interatomic potential even at subpicosecond timescales, before the cooling of the electronic system. With a sufficient level of excitation, various kinds of responses can occur in the crystal structure of the material, including the so-called nonthermal melting of its lattice (ultrafast disordering without a significant increase of the ionic temperature [1]) as well as changes in the band structure.

We apply the density functional theory-based molecular dynamics (DFT-MD) to study an effect of the modified interatomic potential caused by extreme excitation of the electronic system (T_e ~ 1-10 eV) on nonthermal instability in various insulators and semiconductors. We demonstrate a creation of a superionic state in Al_2O_3 – an exotic state with a coexistence of nonthermaly melted oxygen sublattice and a crystalline aluminum one [2].

In Y_2O_3 and NaCl nonthermal amorphization occurs, whereas in TiO_2 a transition into a new crystalline phase is predicted.

We also show that instability of the band gap depends on a level of the bond ionicity of a material [3]. In covalent and mixed-bonded materials, the band gap significantly shrinks or even collapses within characteristic times of the electronic system cooling after an SHI irradiation. Although nonthermal melting is highly improbable to occur in a single SHI track [4], even slight atomic displacements contribute to overall lattice damage and cause significant electronic structure changes (e.g., the band gap shrinkage) affecting electron-lattice coupling in SHI track. Considering that described effects are even more important at high intensity beams expected at GSI-FAIR facilities, we conclude that nonthermal changes should be taken into account in theoretical models of SHI tracks formation.

REFERENCES

[1] N. Medvedev, V. Tkachenko, V. Lipp, Z. Li, and B. Ziaja, 4open 1, 3 (2018).
[2] R. A. Voronkov, N. Medvedev, and A. E. Volkov, Phys. Status Solidi - Rapid Res. Lett. 14, 1900641 (2020).
[3] R. A. Voronkov, N. Medvedev, and A. E. Volkov, Sci. Reports 2020 101 10, 1 (2020).
[4] R. A. Voronkov, N. Medvedev, R. A. Rymzhanov, and A. E. Volkov, Nucl. Instruments Methods Phys. Res. Sect. B Beam Interact. with Mater. Atoms 435, 87 (2018).