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X-ray diffraction study and modeling of damaged layers in Y3Al5O12 ceramics after swift heavy ions irradiation.

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Ceramics based on mineral-like structures (garnets, scheelites, monazites) are being studied as promising matrices for the immobilization of radioactive waste. This paper presents an investigation of polycrystalline ceramic samples of Y2.5Nd0.5Al5O12 (YAG:Nd) obtained by spark plasma sintering. During the operation of such materials, the matrix structure undergoes intense radiation impact caused by its own residual radioactivity. To test the behavior of materials in such conditions, external irradiation with swift heavy ions (SHI) is used. Therefore, the purpose of this work is to study the effect of SHI irradiation (Xe+, 160 MeV, fluence 10^12 –10^13 cm^-2) on the structure of the near surface layers of ceramics based on YAG.

The study of structural changes in such ceramics has been carried out both theoretically and experimentally. The method of X-ray diffractometry (XRD) was used in the Bragg-Brentano and grazing incidence geometries [1]. Mathematical modeling of the interaction of SHI with the YAG matrix was carried out using Monte Carlo methods (MC, TREKIS) [2] and molecular dynamics (MD, LAMMPS) [3].

During the XRD experiments, the formation of an amorphous and deformed YAG phase in the disturbed near surface layer was detected. The study of changes in microstructure parameters (degree of crystallinity, crystallite sizes, deformation) from ion fluence was carried out, and the thickness of the disturbed layer was estimated.

To verify the correctness of the results of XRD experiments, MC&MD modeling of the interaction of SHI with YAG was performed. The simulation results qualitatively and quantitatively confirmed the experimental results and made it possible to illustrate the mechanisms of defect formation at the atomic level.

Primary authors: NAZAROV, Artem (IPM RAS); Mr YUNIN, Pavel (IPM RAS)

Co-authors: Dr NOKHRIN, Aleksey (UNN); Mrs ALEKSEEVA, Liudmila (UNN)

Presenter: NAZAROV, Artem (IPM RAS)

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