First principles calculations of radiation defect properties in complex oxide crystals

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The radiation-resistant oxide insulators (Al_2O_3, $Y_3Al_5O_{12}$, $MgAl_2O_4$) are important materials for application in fusion reactors, e.g. as optical windows. For further prediction of the radiation stability of materials, it is necessary to determine main kinetic parameters - interstitial migration energy and diffusion pre-exponent.

The basic theory was presented in ref. [1,2]. It was showed that the correlation of diffusion parameters in strongly irradiated oxides satisfies the Meyer–Neldel rule (MNR) [2] observed earlier in glasses, liquids, and disordered materials.

We performed defect computer simulations combining the first principles calculation of the atomic, electronic, structure and optical properties of advanced defective oxides with the kinetics of defect recombination upon annealing. We performed large scale computer calculations of basic defects and analyzed available experimental kinetics of the F-type electronic and V-type hole center annealing for three different ionic solids: neutron/ion-irradiated Al_2O_3 (sapphire) [1-3], ion-irradiated $Y_3Al_5O_{12}$ (YAG) [4,5] and $MgAl_2O_4$ spinel [6], all three wide gap insulating materials but with different crystalline structures.

In sapphire upon an increase of radiation fluence, both the migration energy and pre-exponent are decreasing, irrespective of the type of irradiation. This is MNR with normal dose dependence. For YAG and spinel we have confirmed MNR, but the dose dependence is inverse. We discuss the cause of this phenomenon.

References

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