First principles Calculations of the Electronic and Magnetic properties for Defects in 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. It is very important to predict/simulate a long-time defect structure formation and evolution including thermal defect annealing after irradiation. For further prediction of the radiation stability of materials, it is also necessary to determine main kinetic parameters - interstitial migration energy E_a and diffusion pre-exponent D_0.

In this talk, we discuss the latest results of the defect computer simulations combining the first principles calculation of the atomic, electronic, magnetic structure and optical properties of advanced defective oxides with the kinetics of defect recombination upon annealing. Primary radiation defects in ionic solids consist of Frenkel defects—pairs of anion vacancies with trapped electrons (*F*-type centers) and interstitial ions. Many of these defects are paramagnetic and observed in ESR. Their thermal annealing is controlled by the interstitial ion migration, whose mobility is much higher than that of the *F* centers.

The basic theory (how to extract from experimental data the *migration energy* of interstitials and *pre-exponential factor* of diffusion) was developed and applied to irradiated insulators in our recent study [1,2]. It was showed that the correlation of these two parameters in strongly irradiated oxides satisfies the so-called *Meyer–Neldel rule* (MNR) [2] observed more than once earlier in glasses, liquids, and disordered materials**,** but not in radiation physics.

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. We demonstrated that in sapphire upon an increase of radiation fluence, *both* the migration energy and pre-exponent are *decreasin*g, 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.

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