DEEP UNDERSTANDING AND PREDICTION OF ADVANCED MATERIALS FOR EXTREME RADIATION CONDITIONS

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Fusion reactors attract great interest as a potential source of environmentally clean energy. The radiation-resistant insulators (MgO, Al_2O_3, $MgAl_2O_4$, MgF_2, BeO, etc.) are of great importance for optical windows, diagnostic measurements, and other fusion reactor applications. From a practical point of view, it is very important to understand and predict their properties and functional characteristics in a very wide range of radiation doses under various radiation particle including a whole range of neutrons, protons, swift heavy and light ions as well as gamma radiation. Material properties are defined by radiation defects therein. Such accurate and objective predictions are especially important, since they are made for conditions that are difficult to verify experimentally and implement, due to both the high costs and the inaccessibility of the corresponding reactors.

This study was performed by the members of theoretical Laboratory of Kinetics in Self-organising Systems at the Institute of Solid State Physics, University of Latvia, and the experimental one at the Institute of Physics (Tartu University, Estonia). These activities were supported by the following projects and research programmes:

a) EUROfusion Enabling Research Programme (ENR-MFE19.ISSP-UL-02 "Advanced experimental and theoretical analysis of defect evolution and structural disordering in optical and dielectric materials for fusion application" (2019–2020), which our group received from EUROfusion as the only one among all the countries of Eastern Europe and the Baltic countries;

b) EUROfusion Functional Materials Programme (WP-15-PPPT-MAT, "Multiscale modelling of radiation effects in $MgAl_2O_4$ materials and general oxides", (2014–2020));

c) Latvian Council of Science Grant No. LZP-2018/1-0214 "Radiation damage studies in scintillator materials for high-energy physics and medical applications" (2018–2021)

In a series of papers, the radiation damage evolution and its subsequent thermal annealing was treated as the bimolecular process with equal concentrations of complementary point defects, such as anion vacancies of different charge states and appropriate interstitial defect, which was produced in pairs or cascades by different types of ionizing and particle irradiation – gamma, fast electron, protons, heavy ions or neutron irradiation. Knowledge of the mobility of produced radiation defects, the effect of incident radiation in the conditions of progressive radiation-induced material disordering are absolutely necessary for detailed description of radiation damage. The appropriate migration energies were obtained experimentally or derived from available thermal annealing kinetics for differently irradiated materials. The results obtained are compared with *ab initio* calculations of interstitial anion migration. Two kinds of primary radiation defects – neutral and charged oxygen interstitial atoms in corundum – were discovered and studied for the first time, both experimentally and theoretically.

The kinetics of thermal annealing of the basic electron and hole centres in stoichiometric corundum and spinel irradiated by fast neutrons and protons were analysed in terms of diffusion-controlled bimolecular reactions. Special attention was paid to:

(1) dose effects on *point defect* annealing;

(2) a detailed comparison of diffusion-controlled point defect thermal annealing in gamma, neutron, electron and heavy-ion irradiated oxides and halides;

(3) the point defect annealing and metal colloid formation in thermochemically reduced oxides and oxides and halides under irradiation.

Furthermore, properties of single crystals and optical polycrystalline spinel ceramics are compared. It is demonstrated that both transparent ceramics and single crystals, as well as different types of irradiation show qualitatively similar kinetics, but the effective migration energy and pre-exponent are strongly correlated. Such correlation is discussed in terms of the so-called Meyer-Neldel rule known in chemical kinetics of condensed matter. The unusual radiation damage accumulation kinetics under intensive irradiation of oxide materials related to this effect is predicted. This study allows us to prognosticate and control radiation and optical properties of advanced functional materials for fusion applications.

It is important to note that the results obtained turned out to be so interesting and promising for Eurofusion that our two new projects again received funding from EUROfusion Consortium in the framework of the Horizon 2020 research Programmes.

In particular, new projects are guided by a detailed analysis of the influence of structural and radiation defects in dielectric materials. Special attention will be devoted to the analysis of defects in large dielectric mirrors made of diamond with very large dimensions up to 20 cm in diameter. As before, this work is carried out in close collaboration with scientists from Karlsruhe Institute of Technology, Germany under the leadership of Prof. Dr. Theo Scherer. The main results are published in leading journals including *Scientific Reports*, *Journal of Chemical Physics*, *Nuclear Instruments and Methods*, etc. [1–12].

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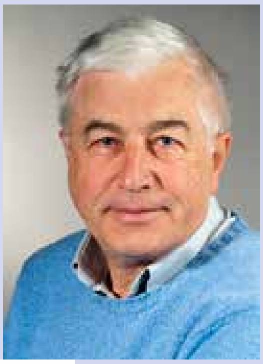

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