Diffusion-controlled kinetics of metallic colloid formation in irradiated Al_2O_3, MgO and NaCl crystals

V.N. Kuzovkov[1]*, E.A. Kotomin[1], A.I. Popov[1], R. Vila[2]

[1]Institute of Solid State Physics, Riga, Latvia
[2]CIEMAT, Madrid, Spain
*kuzovkov@latnet.lv

Radiation resistant Al_2O_3 (corundum) is a promising material for fusion reactors, e.g. for construction components of the diagnostic systems. This is very important to predict/simulate the kinetics of diffusion-controlled defect accumulation under neutron irradiation as well as long-time defect structure evolution. There are numerous experimental measurements of the primary defect kinetics (first of all, *F* color centers—oxygen vacancy Vo with two trapped electrons) as a function of dose rate and temperature and references therein). It is well known also that at high irradiation doses and/or high temperatures the primary defects become mobile and aggregate, giving rise to metallic colloids. Another way to produce colloids is additive coloration of corundum crystals by heating at 2000°C under strongly reducing conditions. A study of metallic colloids in corundum is also important since they are related to reactor material degradation. Metal colloids are observed also in heavily irradiated NaCl-type ionic solids which are very sensitive to the radiation.

One of the main theoretical approaches to the kinetics of radiation damage is based on the rate equations which take into account defect production and recombination but neglect similar defect aggregation and spatial inhomogeneities in defect distribution. In particular, such approach cannot study the kinetics of colloid formation. Its another disadvantage is use of many phenomenological parameters—reaction rates—which should be estimated from experiments or theoretical calculations. We developed and applied here the alternative approach based on the formalism of the correlation functions [1-3] describing spatial distribution of similar (F-F centers) and dissimilar (Frenkel pair of defects: F center – interstitial O(Cl) ions) which is much better suited for the study of defect kinetics and aggregation. Based on our calculations, we estimate the migration energy of the F centers, interstitial defects and their interaction energy and estimate colloid size. Theoretical results are compared with experimental data.

References

[1] E.A. Kotomin and V.N. Kuzovkov: *Modern Aspects of Diffusion-Controlled Reactions: Cooperative Phenomena in Bimolecular Processes*, Vol. **34** of *Comprehensive Chemical Kinetics* (Elsevier, North Holland, Amsterdam, 1-612, 1996).

[2] V.N. Kuzovkov, E.A. Kotomin, and W. von Niessen: *Discrete-lattice theory for Frenkel-defect aggregation in irradiated ionic solids.* Phys. Rev. B **58**, 8454-8463 (1998).

[3] V.N. Kuzovkov, A.I. Popov, E.A. Kotomin, M.A. Monge, R. González, Y. Chen: *Kinetics of nanocavity formation based on F-center aggregation in thermochemically reduced MgO single crystals.* Phys. Rev. B, **64**, 064102-5 (2001).