

Ordered materials in nuclear engineering and radiation technology

Roman Voskoboinikov¹

NRC Kurchatov Institute, Kurchatov Square, 123182 Russia

Materials with ordered crystal structure are not just considered but have already been applied in a number of demanding nuclear power and radiation technology applications. For example, most existing research and test reactors are fueled with UAl_x or U_3Si_2 intermetallic fuel. Binary, ternary and quaternary intermetallic compounds of beryllium with Ti, V, Zr, Nb, Ta, Mo, W and/or Y are the main advanced breeder/multiplier candidates for use in blankets of future fusion reactors. γ' -Ni₃Al precipitates are a key strengthening component of the microstructure of Ni-based refractory alloys that affects their high temperature strength and creep resistance properties. Spinel ($MgAl_2O_4$) is a potential candidate for inert matrix fuels and a heterogeneous diluent of Pu and minor actinides (Am, Np and Cm) for subsequent transmutation/incineration in fast-neutron reactors. Complex oxides with perovskite and pyrochlore crystal structure are reckoned as promising ceramic hosts for immobilization of high-level nuclear waste.

All structural and functional materials with ordered crystal structure usually last longer and outperform their elemental constituents as well as disordered solid solutions with the same chemical composition under simultaneous impact of high operating temperature, applied loading, thermal flux, corrosive/ oxidation environment and fast particle irradiation. Despite a rich diversity of chemical compositions, crystal lattices, defect subsystems, operating conditions, service properties, *etc.*, ordered materials exposed to fast particle irradiation exhibit similar microstructural transformations. That provides an opportunity to gain a deeper insight into peculiarities of radiation effects in ordered solids by studying model materials with relatively simple microstructure and chemical composition. Afterwards, the obtained results can be extrapolated to the whole range of intermetallic alloys, spinels (AB_2O_4), perovskites (ABO_3), pyrochlores ($A_2B_2O_7$) and other complex oxides with fluorite-like crystal structures, *e.g.* δ -phases ($A_4B_3O_{12}$ and A_6BO_{12}).

A noticeable progress in the understanding of the governing mechanisms of radiation damage formation in ordered solids has been achieved by conducting molecular dynamics simulations of collision cascades in γ -TiAl, α_2 -Ti₃Al and γ' -Ni₃Al intermetallic compounds and the corresponding disordered solid solutions with the same chemical composition. All three intermetallics demonstrate a higher resistance against radiation damage formation comparing to their disordered counterparts.

A strong disproportion in the partition of interstitials that exceeds the stoichiometric composition has been observed in collision cascades in the three intermetallic compounds. In the case of the disordered solid solutions, the discrepancy is even more radical.

In irradiated intermetallic compounds, heavier projectiles generate more disorder, whereas lighter projectiles with the same energy produce more primary radiation damage. A simple quantitative correlation between the number of antisites and the number of Frenkel pairs created in collision cascades in intermetallic compounds has been revealed.

A significant fraction of the original radiation resistance of α_2 -Ti₃Al is retained even after complete disordering. In contrast to α_2 -Ti₃Al, disordered γ' -Ni₃Al intermetallics loses completely its initial radiation tolerance. It is highly likely that the short-range and long-range order contributions to the overall radiation tolerance are different in the two intermetallic compounds. A robust proof of the proposed hypothesis has yet to be accomplished.

¹ Email: roman.voskoboinikov@gmail.com