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Influence of Elastic Constants and Chemical Bonding on Radiation Stability of Silicates and Metal Oxides by Computer Simulations

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Vitrification, or immobilization of the nuclear waste in glass, has been and remains to be a popular way of its handling. But the operating period of glass matrix is about 40-50 years only. The effective alternative to vitrification has been immobilization of high-level waste in ceramic matrix and minerals. The central question is how effective a matrix will remain as a barrier over the required period of time (thousands years). In spite of considerable successes in radiative study of materials, the question of radiation stability of minerals is not studied enough.

The number of Frenkel pairs in periclase MgO, zircon $ZrSiO_4$ and quartz SiO_2 after propagation of thorium atom with a kinetic energy of 20 keV has been characterized by molecular dynamics method. Calculation of chemical bonds covalency degree in studied minerals has been performed using the Hartree-Fock. The results of researches show that the track length depends significantly on the elastic constants (especially C_{44} and C_{66}). It is also established that the minerals with higher energy increasing after oxygen atoms displacements more susceptible to radiation damage.

Results of this study can be used for solving fundamental and practice tasks connected with immobilization and disposal of a high-level waste.