

Volume Swelling of UO₂ by Irradiation of Alpha Particles and Lattice Recovery by Molecular Dynamics Simulation

S. D. Günay^a and Ç. Taşseven

*Department of Physics, Faculty of Science, Yildiz Technical University,
Davutpaşa Campus, Esenler, 34210, Istanbul, Turkey
^asdgunay@gmail.com*

Abstract. Radiation damage in UO₂ crystal have great influence on reactor fuel performance. Heavy ions, fission products, especially alpha particles and neutrons are very effective for irradiation damage [1]. Experiments show that when an UO₂ crystal exposed to ~5 MeV alpha particles [2], Frenkel pairs came about in the direction of incoming one. Enlargement in the lattice parameter was observed which is related with the implemented dose [3]. In another experiment [4], they showed that as the temperature increased from ambient condition, recovery of lattice constant was observed. Based on this model, with molecular dynamic simulation technique, we generate frenkel pairs up to 30 frenkel pairs per 125 unit cells (~1.47 x 10²¹ pairs/cm³) and calculated the swelling of lattice. Then we anneal the crystal, which has defective structure, from 300 K up to 1000K. Recovery of crystal is similar to the previously reported results[3,4].

1. Hj. Matzke, *Radiation Effects*, **64**, 3-33 (1982).
2. W. J. Nellis, *Inorg. Nucl. Chem. Letters*, **13**, 393-398 (1977).
3. N. Nakae, T. Kirihara and S. Nasu, *Journal of Nuclear Materials*, **74**, 1-9 (1978).
4. N. Nakae, Y. Iwata and T. Kirihara, *Journal of Nuclear Materials*, **80**, 314-322 (1979).