# ATOMISTIC SIMULATION OF PHASE TRANSITIONS AND STRUCTURE TRANSITIONS UNDER IRRADIATION IN U-MO ALLOYS

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Uranium is the main component of nuclear fuel. Due to high values of thermal conductivity and density, a metal nuclear fuel based on uranium alloys is the promising fuel for generation IV reactors. In addition, U-Mo fuels has high thermal conductivity, low thermal expansion, and high melting point.

The investigation found that structure of $\gamma^0$-lattice is similar to body-centered tetragonal (bct) lattice with a displacement of central atom at basic cell into [001] direction. The lattice parameters fulfil the following condition: $a = b > c$. Moreover, high temperature $\gamma$-phase of uranium and uranium alloys has quasi-bcc lattice. At such state, local positions of atoms correspond to bcc lattice with displaced central atoms in basic cell. Also, the various mechanisms of structure changes in irradiation are examined. In particular, the simulation results indicate that the defects formation may be produced without melting and subsequent crystallization. Threshold stopping power of swift ions for the defects formation in irradiation in the various conditions are calculated.