MD simulation of melting and λ- transition in stoichiometric uranium dioxide

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New version of ionic model for stoichiometric uranium dioxide, reproducing the experimental density of solid stoichiometric UO_2 in a wide range of temperatures, is developed. Results of the high-temperature MD simulation on large cells, based on a novel fast method of computation of Coulomb forces, both in solid and liquid phases are presented and discussed. Properties of liquid UO_2, computed on the basis on the same potential model, are in good agreement with existing experimental data and predictions of other theoretical models. Simulation reveals characteristic features of a pre-melting λ-transition at a temperature near to that experimentally observed (T_λ=2670 K). A strong deviation from the Arrhenius behavior of the oxygen self-diffusion coefficient was found near the λ-transition point.