Molecular dynamics study of uranium-dioxide sintering process

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Uranium dioxide has received a lot of attention due to its unique nuclear properties and its various applications in nuclear industry Nowadays, there are many works devoted to sintering of uranium dioxide. However, the influence of crystalline misalignment between two nanoparticles on the process has not been sufficiently studied. In this work we study the process of sintering of UO_2, in particular, the influence of the grain boundary on the rate of this process, using the molecular dynamics method. Computations are performed on 2–4 cylindrical nanoparticles in the conditions of NVE ensemble, with the interatomic potential [1]. Periodic boundary conditions are used to avoid surface effects. Coefficients of grain-boundary and surface diffusion were obtained for four different misaligned angles. From the temperature dependence of the diffusion coefficients, the activation energy for each mechanism was calculated. Three theoretical models were used to obtain the total relative diffusion coefficient. The consistency of two-particle and many particles models has been investigated through the comparison of shrinkage and densification data, calculated using the first and the second model respectively. All computations were performed using LAMMPS package [2].

[1] Potashnikov S I, Boyarchenkov A S, Nekrasov K A and Kupryazhkin A Y 2007 *Al'ternativnaya Energetika Ekologiya* **8** 43–52
[2] Plimpton S 1995 *J. Comput. Phys.* **117** 1–19