Mechanisms of overpressurized xenon nanobubbles diffusion in UO_2

Antropov A S[1,2,@] and Stegailov V V[1,2]

[1] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[2] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

[@] antropov@phystech.edu

The diffusion of gas bubbles in nuclear fuels is an important topic for radiation materials science. The greatest attention is focused on the diffusion of xenon bubbles in uranium dioxide, as the most common nuclear fuel. The gas pressure is considered to be the key factor suppressing diffusion of nano-size bubbles [1, 2]. Verma estimates the diffusion coefficient of a bubble with a radius of 0.4–1 nm at a temperature of 1873 K: the magnitude of suppression is about 17 orders [3]. However this estimation lies far from experimental data [4]. In the present work, molecular dynamics modeling of xenon bubbles with a radius of 6–10 Å is carried out. Simulation made it possible to consider the kinetics of the diffusion process.

[1] Mikhlin E Y 1979 *Phys. Status Solidi A* **56** 763–768
[2] Veshchunov M S and Shestak V E 2008 *J. Nucl. Mater.* **376** 174–180
[3] Verma L, Noirot L and Maugis P 2020 *J. Nucl. Mater.* **528** 151874
[4] Baker C 1977 *J. Nucl. Mater.* **71** 117–123