Nanobubbles diffusion in metals: Theory and atomistic modelling

Stegailov V V[1,2,3,@] **and Antropov A S**[2,3]

[1] National Research University Higher School of Economics, Myasnitskaya 20, Moscow 101000, Russia
[2] Joint Institute for High Temperatures of the Russian Academy of Sciences, Izhorskaya 13 Bldg 2, Moscow 125412, Russia
[3] Moscow Institute of Physics and Technology, Institutskiy Pereulok 9, Dolgoprudny, Moscow Region 141701, Russia

[@] stegailov@gmail.com

Diffusion of gas bubbles in nuclear materials plays a significant role in their mechanical properties and in fission gas release processes from fuels. The presence of stable facets of nanobubbles in crystal lattice can significantly affect their diffusion coefficient [1], but the existing theory of this phenomenon is too general and cannot take into account atomistic structure of nanobubbles in a given material. Such a theory for the mechanisms of bubble motion in crystals can be extended and developed using methods of atomistic modelling [2]. In this work, we consider the movement of bubbles in the several bcc and fcc metals and report the analysis of possible mechanisms of diffusion for empty bubbles and for gas-filled bubbles [3, 4].

[1] Beere W 1972 *Journal of Nuclear Materials* **45** 91–95
[2] Veshchunov M, Boldyrev A, Kuznetsov A, Ozrin V, Seryi M, Shestak V, Tarasov V, Norman G, Kuksin A Y, Pisarev V *et al* 2015 *Nuclear Engineering and Design* **295** 116–126
[3] Antropov A and Stegailov V 2020 *Journal of Nuclear Materials* 152110
[4] Antropov A 2020 *JETP Letters* **112** 310–315