Calculation of the vacancy diffusion rate: beyond the NEB precision

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Migration of point defects determines many microscopic processes in nuclear materials: climbing of dislocations, diffusion of fission products, formation of bubbles and swelling. Experimentally measured self-diffusion is a combination of effects of vacancies and interstitials, but in bcc metals the impact of vacancies is much higher. Calculation of the vacancy diffusion rate is important for building a mesoscale model of the evolution of fuel in reactor conditions. The generally accepted model for temperature dependence of diffusion of defects is the Arrhenius equation $D = D_0 \exp[-E_a/k_BT]$, where E_a is a free energy barrier and D_0 is a frequency factor, determining an effective frequency of jump attempts [1]. The most common method to obtain the energy barrier in molecular dynamic simulation is Nudged Elastic Band method [2]. However, the question of the accuracy of the NEB remains open. In particular, there is a question of delayed relaxation of the jumping atom environment, and consecutive effects on the mobility of vacancies [3]. This fact is considered as evidence that the NEB can give the reaction path different from the real one. The NEB method is also not applicable in cases when the lattice is unstable at zero temperature, e.g. bcc lattice of uranium [4].

This work shows that the molecular dynamic simulation of the motion of defects in bcc metals gives the result different from the NEB prediction. Temperature dependence of the migration energy is discussed, and the method for the accelerated calculation of this dependence is considered.

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