

## Bubble diffusivity in BCC metals: atomistic mechanisms and kinetic models

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Release of gas fission products in nuclear fuels is a practically important phenomenon based on the bubble diffusivity in crystal lattice. The bubble diffusion coefficient can be expressed through the volume and surface self-diffusion coefficients  $D_{vol}$  and  $D_{surf}$ . In the case of an empty bubble in a bcc lattice the corresponding expression is as follows (see [1]):

$$D_{bub}(R) = D_{vol} \frac{3\Omega}{2\pi R^3} + D_{surf} \frac{3\Omega^{\frac{4}{3}}}{4\pi R^4}, \quad (1)$$

where  $\Omega$  is an atomic volume and  $R$  is a radius of a bubble. The surface self-diffusion plays a significant role in the bubble motion in solids [2], but up to now the underlying mechanisms have not been studied well enough. In this work these mechanisms are studied via the classical molecular dynamic modelling in two representative metals: bcc U and bcc Mo.

We find the equilibrium facet shape of bubbles with different diffusion rates on different faces. We proposed the method of calculation of an average surface self-diffusion coefficient over all the bubble in [3]. The mean square displacement is found for the surface layer atoms that are identified by the Voronoi polyhedron method.

For the validation of formula (1) we calculate the bubble's diffusivities via the nonequilibrium molecular dynamics based on the Nernst-Einstein equation. On the example of a two-dimensional lattice it is shown that such a method gives correct results [4]. However in the case of facet bubbles the drift velocity can be not proportional to the applied force. It indicates a certain more complex mechanism of bubble movement. Our analysis shows that the velocity is determined by the rate of the nucleation of new steps at  $[110]$  faces (figure 1). The bubble diffusivities are obtained via the direct modelling and independently predicted by formula (1). The comparison between these results allows to correct the theory according to revealed mechanisms. Obtained results can be applied in kinetic models for computation of nuclear fuel properties. Work has been supported by the Russian Foundation for Basic Research (grant no. 18-08-01495), the grant of the President of Russian Federation for support of leading scientific schools grant NSh-5922.2018.8 and the program 5top100 of NRU MIPT.

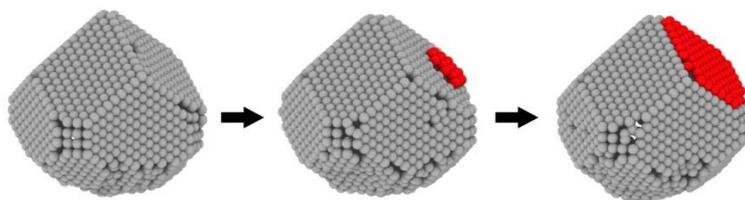


Figure 1: Surface atoms of the bubble in bcc U. The new emerging layer of the surface is shown as red atoms. Nucleation of such surface steps determines bubble mobility.

### References

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