§18. Multiscale Modeling of Radiation Damage Processes in Fusion Materials

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Significant efforts toward modelling the nucleation and growth of helium bubbles in irradiated metals were made a few decades ago. Katz and Wiedersich, Russell, and Mansur and Coghlan [1)] separately used the classical nucleation theory to provide the nucleation rate of helium bubbles. Their efforts succeeded to explain experimental observations such as the bimodal size distribution of helium bubbles and the shift of temperatures at which void swelling occurs. This model is well established and can still be applied enough to bubble formation, where helium is created by (n, α) nuclear transmutation reactions in metals and hence the concentration of helium in the matrix is relatively low. On the other hand, the theoretical treatment of the nucleation and growth of highly-pressurized helium bubbles has been developed separately by Trinkaus and by Greenwood, Foreman and Rimmer, and by Glasgow and Wolfer.

Recently, we performed both atomistic calculations using empirical interatomic potentials and analytical evaluation based on the continuum model approach with the linear elasticity theory and the equation of states (EOS) for helium, to evaluate the formation and binding energies of helium bubbles in iron.[2)] It was found that the binding energy significantly depends on the helium density of bubbles rather than bubble size. When the helium density increases, both the binding energies of an SIA and an SIA loop to a helium bubble significantly decrease to very low positive values. This fact practically indicates that an SIA and an SIA loop have enough possibilities to be emitted *thermally* from a highly-pressurized helium bubble at finite temperatures, before the athermal mechanisms mentioned above begin to work.

In the present study [3)], the SIA emission was treated as a thermal process, similar to the vacancy emission. And unified formalization was constructed for description of the nucleation and growth of helium bubbles, available for both the regimes of high and low helium pressures. This treatment is quite reasonable when one considers the symmetric behaviour of interactions in metals between vacancies and SIAs. Based on such formalization, the nucleation path of helium bubbles in bcc iron during irradiation was investigated by the kinetic Monte-Carlo simulation technique for a wide range of concentrations of helium in the matrix.

The nucleation and growth process of an isolated single helium bubble in bcc iron was investigated by the kinetic Monte-Carlo (KMC) simulation technique. Events employed in the simulation were the absorption and emission of a vacancy, an SIA and interstitial helium by a single helium bubble, while an event associated with SIA loops or substitutional helium was neglected here for simplicity.

The occurrence probability of the events for absorption and emission was respectively given by equations (1) and (2) that were given in the unit of per second:

$$J_k^{\mathrm{in}} = \frac{4\pi R Z_k D_k}{\Omega} C_k^{\mathrm{matrix}}(\infty), \qquad (1)$$

$$J_k^{\mathrm{out}} = \frac{4\pi R Z_k D_k}{\Omega} \exp\left(-\frac{G_k^{\mathrm{bind}}}{k_{\mathrm{B}} T}\right). \qquad (2)$$

Here, $G_k^{\mathrm{bind}} = E_k^{\mathrm{F}} - \mu_k^{\mathrm{bubble}}$ is the binding free energy of the type *k* mobile defect to a helium bubble.

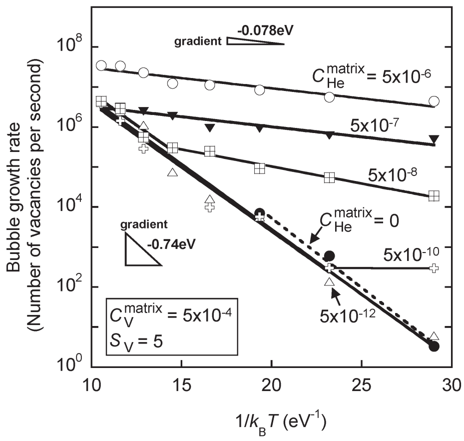

Fig. 1 The Arrhenius plot of growth rates of He bubbles in Fe.

Fig. 1 shows the Arrhenius plot of the bubble growth rates as a function the concentration of helium in the matrix. This indicates that there are two different mechanisms for bubble growth: one is controlled by vacancy diffusion and another is controlled by interstitial helium diffusion. The interstitial helium diffusion controlled growth is associated with the SIA emission, where the formation of helium bubbles is almost independent on temperatures and helium bubbles can form even at low temperatures where vacancies cannot migrate. The former mechanism can operate frequently in the fusion first wall materials where helium is created by (n, α) nuclear transmutation reactions. The latter mechanism can often operate in the fusion divertor materials where helium is directly implanted. These two different mechanisms can explain a qualitative difference in the temperature dependence of bubble formation observed by experiments. These modeling efforts shown here will be available to establish more realistic simulation studies to predict microstructural changes in materials during irradiation.

Reference

1) L.K. Mansur *et al*., J. Nucl. Mater., **119** (1983) 1.
2) K. Morishita, *et al*., J. Nucl. Mater., **353** (2006) 52.
3) K. Morishita, Phil. Mag., 87 (2007) 1139.