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Helium effects on microstructural change in RAFM steel under irradiation: Reaction rate theory modeling

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ABSTRACT

Reaction rate theory analysis has been conducted to investigate helium effects on the formation kinetics of interstitial type dislocation loops (I-loops) and helium bubbles in reduced-activation-ferritic/martensitic steel during irradiation, by focusing on the nucleation and growth processes of the defect clusters. The rate theory model employs the size and chemical composition dependence of thermal dissociation of point defects from defect clusters. In the calculations, the temperature and the production rate of Frenkel pairs are fixed to be $T = 723$ K and $P_V = 10^{-6}$ dpa/s, respectively. And then, only the production rate of helium atoms was changed into the following three cases: $P_{He} = 0$, 10^{-7} and 10^{-5} appm He/s. The calculation results show that helium effect on I-loop formation quite differs from that on bubble formation. As to I-loops, the loop formation hardly depends on the existence of helium, where the number density of I-loops is almost the same for the three cases of P_{He}. This is because helium atoms trapped in vacancies are easily emitted into the matrix due to the recombination between the vacancies and SIAs, which induces no pronounced increase or decrease of vacancies and SIAs in the matrix, leading to no remarkable impact on the I-loop nucleation. On the other hand, the bubble formation depends much on the existence of helium, in which the number density of bubbles for $P_{He} = 10^{-7}$ and 10^{-5} appm He/s is much higher than that for $P_{He} = 0$. This is because helium atoms trapped in a bubble increase the vacancy binding energy, and suppress the vacancy dissociation from the bubble, resulting in a promotion of the bubble nucleation. And then, the helium effect on the promotion of bubble nucleation is very strong, even the number of helium atoms in a bubble is not so large.

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1. Introduction

Reduced-activation-ferritic/martensitic (RAFM) steel is proposed as one of the candidates for blanket structural materials in a nuclear fusion reactor. Blanket structural materials suffer from 14 MeV high-energy-neutron bombardments, in which many types of point defect such as vacancies, self-interstitial atoms (SIAs) and helium gas atoms are produced by atomic displacement and nuclear transmutation. Those produced point defects thermally migrate and form defect clusters, e.g., interstitial type dislocation loops (I-loops), voids and helium bubbles. Such athermal lattice defects induce the microstructural change of a material, leading to the performance degradation and deformation. Especially, helium is known to enhance formation of voids, and promote void swelling and high temperature intergranular embrittlement;

therefore, detailed investigation of the helium effects is necessary for the study of nuclear fusion materials.

In the present study, helium effects on the formation kinetics of I-loops and helium bubbles in RAFM steel during irradiation was numerically investigated by means of reaction rate theory (mean field cluster dynamics modeling), with focusing on the nucleation and growth processes of the defect clusters.

2. Methods

2.1. Outline of rate theory model

The model assumptions employed here are as follows: at first, the target microstructure of RAFM steel in the present study is a lath martensite which consists of Fe–8Cr based matrix containing heterogeneous dislocations and several precipitates. For simplicity, the lath martensite is assumed to be a homogeneity field with a constant of dislocation density. In irradiation, Frenkel pairs of

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vacancies (V) and SIAs (I) are homogeneously produced by atomic displacement. The production rate of Frenkel pairs is P_V in the unit of dpa/s, where an effective production rate is described as $P_V(1 - \varepsilon_r)(1 - C_V^{eq})$ with the spontaneous recombination fraction ε_r and the thermal equilibrium vacancy concentration C_V^{eq}. Helium atoms (He) are also homogeneously produced, as interstitial helium atoms, by nuclear transmutation reaction. The production rate is P_{He} in the unit of appm He/s. Those produced point defects freely migrate depending on temperature. Dislocations play a role of main sink for migrating point defects with the dislocation bias $B_k = (Z_I - Z_k)/Z_I$, where Z_k is the capture efficiency of a point defect k (V, I and He) to a dislocation. Vacancies and SIAs interact with each other, and mutually annihilate (recombine). Helium atoms and SIAs do not interact with each other because both point defects have compressive fields around themselves. In contrast, helium atoms and vacancies interact with each other, in which vacancies occupied by helium atoms cannot move. Notice that the vacancies occupied by helium also can recombine easily with SIAs, emitting the helium atoms into the matrix. Namely, in the present study it is assumed that there is no difference between vacancies occupied by helium and vacancies with no helium in the recombination of SIAs. This is because the total formation energy becomes lower in the both reactions.

As to formation of defect clusters, SIAs interact with each other, and form SIA-clusters (I-loops). When I-loops interact with vacancies, they become shrunk. On the other hand, vacancies and helium atoms form helium-vacancy-clusters (helium bubbles). When helium bubbles interact with SIAs, the bubbles become shrunk. Notice that a helium bubble and an SIA can interact with each other, even the bubble has a relatively high internal pressure. This is because the strain field around such a bubble is not isotropic where the one side is compressive and the opposite side is dilative [1]. As to thermal stability of defect clusters, point defects are assumed to be emitted from I-loops and helium bubbles into the matrix, depending on binding energy and temperature.

2.2. Reaction model for the growth and shrinkage of defect clusters

At first, the shape of defect clusters in the present study is assumed to be spherical for helium bubbles and discoidal for I-loops. The growth or shrinkage of a defect cluster is determined by a balance between the influx and the outflux of point defects into/from the defect cluster. The influx and the outflux correspond to absorption rate and emission (thermal dissociation) rate of point defects, respectively.

Fig. 1(a) shows an illustration for reactions between a helium bubble B(n^{He}, n^V) and point defects k (V, I and He). B(n^{He}, n^V) denotes a helium bubble consisted of n^{He} helium atoms and n^V vacancies. In the present study, the size of a helium bubble is described by n^V. It is noted that B(1, 0), B(0, 1) and B(0, n^V) denote an interstitial helium atom, a single vacancy and an empty void with the size of n^V, respectively. Going back to B(n^{He}, n^V), the chemical composition ratio defined as n^{He}/n^V (the number of helium atoms per vacancy) is called the helium-to-vacancy ratio (He/V). In other words, this ratio is the helium density in a bubble and corresponds to the internal pressure of a bubble. The influx of point defects k into a bubble B(n^{He}, n^V) is described by $J_{k,B(n^{He},n^V)}^{IN} = 4\pi R_B D_k C_k/\Omega$ in the unit of s^{-1}, where D_k and C_k are the diffusion coefficient and concentration (atomic fraction) of point defects in the matrix. Ω is the atomic volume and R_B is the bubble radius with the relation for the volume $n^V\Omega = 4\pi R_B^3/3$. On the other hand, the outflux of point defects from a bubble is given by $J_{k,B(n^{He},n^V)}^{OUT} = 4\pi R_B D_k \exp(-E_{bind}^{k,B(n^{He},n^V)}/k_B T)/\Omega$ in the unit of s^{-1}, where $E_{bind}^{k,B(n^{He},n^V)}$ is the binding energy of a point defect k to a bubble
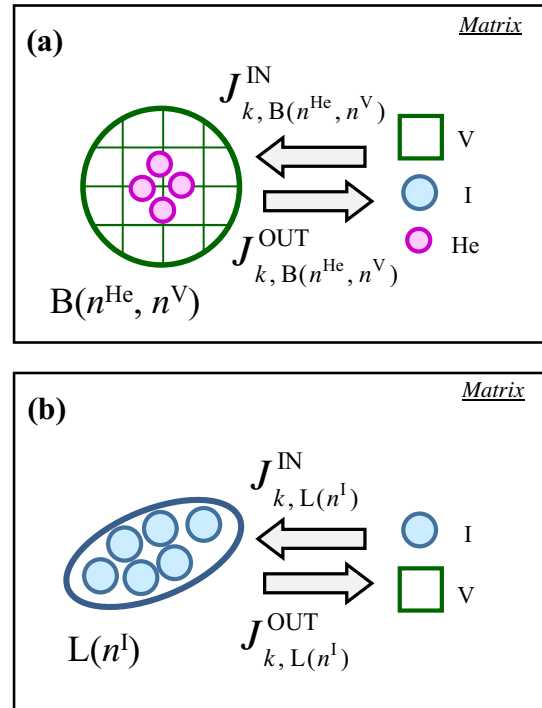

Fig. 1. Illustration for reactions between defect clusters and point defects: (a) for helium bubble B(n^{He}, n^V) and (b) for I-loop L(n^I).

B(n^{He}, n^V). Here, the binding energy is defined as energy required to remove a point defect from a defect cluster, and is corresponding to the thermal dissociation rate of point defects from a defect cluster; therefore, this energy is a very important parameter to evaluate the nucleation and growth processes of defect clusters. As for helium bubbles, the binding energy can be written by $E_{bind}^{k,B(n^{He},n^V)} = E_F^k - \mu^{k,B(n^{He},n^V)}$, where E_F^k is the formation energy of point defect k in the matrix and $\mu^{k,B(n^{He},n^V)}$ is the chemical potential of point defect k in a bubble B(n^{He}, n^V). Morishita et al. [2] derived the binding energy as a function of He/V, based on detailed molecular dynamics simulation results and continuum level equation. In the present work, the derived binding energy was employed to estimate the thermal dissociation rate of point defects from helium bubbles. Fig. 2 represents the binding energy of a point defect (V, I and He) to a bubble B(n^{He}, n^V) as a function of He/V. Notice that the area in shadow (He/V > 6) is beyond the application range of the continuum model description based on the linear elastic theory. As shown in the figure, with increasing the helium density in a
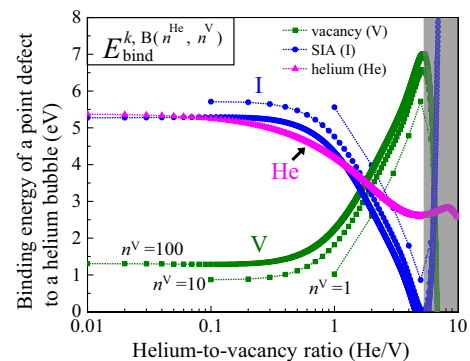

Fig. 2. Binding energy of a point defect k (V, I and He) to a helium bubble B(n^{He}, n^V) as a function of He/V.