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Conservative climb motion of a cluster of self-interstitial atoms toward an edge dislocation in BCC-Fe

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ABSTRACT

We have developed a model for the conservative climb motion of a hexagonal self-interstitial atom (SIA) cluster that is under the influence of the stress field of a nearby dislocation. The parameters required for the calculations were derived by molecular simulations of body-centered-cubic Fe. Using these parameters, kinetic Monte Carlo simulations were conducted to simulate the absorption process of an SIA cluster through the conservative climb to an edge dislocation that has the parallel Burger vector. The velocity of the conservative climb was found to be proportional to the inverse square of the distance between the cluster and dislocation, which is the same dependency observed in a previous analysis. However, the absolute value of the velocity strongly depends on the number of extra atoms or vacant sites that inherently exist on the edges of the cluster, because they enhance the formation of another defect pair that will induce the conservative climb. The activation energy for the conservative climb is much higher than the activation energy for pipe-diffusion of an atom along the edge of the cluster, although the latter is an elementary process of the former. The velocity of the conservative climb is nearly proportional to the inverse eighth power of the cluster size. Both of these findings are significantly different from those of the elasticity analysis.

1. Introduction

One of the characteristic features of structural materials of nuclear power plants is that highly energetic neutrons produced by nuclear reactions cause damages through collision cascades. Molecular dynamics (MD) simulations have been used to clarify this process; so far, they have shown that clusters of self-interstitial atoms (SIAs), vacancy clusters, mono-SIAs, and mono-vacancies are formed within a few picoseconds during collision cascades [1]. The number of SIAs in these clusters varies from 2 to 10 or more, and the maximum size tends to increase with the energy of the primary knock-on atom (PKA) [2]. These clusters have a form that is best described as a small SIA dislocation loop [3], and some of them are the crowdion-type, i.e., the Burgers vector is represented by $\vec{b} = a_0/2\langle 111\rangle$, where a_0 is lattice constant for body-centered cubic (BCC) metals and $\vec{b} = a_0/2\langle 110\rangle$ for face-centered cubic metals [3]. Since the migration energy is very low and almost independent of the size, these clusters are highly one-dimensionally mobile along the direction of their Burgers vector [4]. They are energetically attracted to their stable positions through elastic interaction with internal stress originating mainly from a dislocation [5]. Indeed, it has been experimentally confirmed that small SIA clusters are accumulated in high density and trapped near dislocations with a very small separation as a result of collision cascades [6]. In the temperature range where swelling occurs significantly, these trapped SIA clusters are most likely absorbed in nearby dislocations. For the case of parallel Burgers vectors, in which the interaction is strongest and the probability of trapping is thus the highest, the absorption of these clusters requires a motion from their trapped position toward the core of the dislocation, the direction of which is different from their original glide direction. The critical feature is that the nature of this motion is size-dependent, i.e., the motion is completely different depending on cluster size. Previous studies showed that small clusters containing 2 to 3 SIAs [7], or up to 5 SIAs or less [8] for BCC-Fe, frequently change their

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glide direction. Hence, the motion of these small clusters toward the dislocation mainly involves the change in the Burgers vector to the non-parallel direction. However, Terentyev et al. showed that a cluster containing more than 5 SIAs does not change the direction at least within the MD time scale for BCC-Fe [8]. Unless the cluster makes a contact interaction with a dislocation, even the stress field originating from a dislocation does not induce a change in the Burgers vector in its vicinity [9,10]. More detailed calculations have been conducted by Gao and co-workers [11]. They showed that clusters containing more than 7 SIAs may not change the Burgers vector before they dissociate into small clusters, because the binding energy per SIA is smaller than the energy per SIA required for the directional change. The change in the Burgers vector would be a rare event, if any, for larger clusters containing more than 5 to 7 SIAs. The probability of the formation of these larger clusters during a collision cascade becomes higher with increasing PKA energy [12]. Obviously, the impact on swelling is greater with increasing size of the SIA cluster absorbed by a dislocation. To construct a predictive model for swelling, especially for structural materials of nuclear reactors that experience high PKA energy, it is therefore necessary to clarify and quantify the motion of larger SIA clusters toward the core of dislocations.

A conservative climb is a possible process for this motion. Often referred to as self-climb, it is the climb motion of a cluster during which its number of defects is preserved. There have been several experimental studies that confirm this motion of either SIA clusters or vacancy clusters, namely ion-irradiated UO_2 by annealing [13], neutron-irradiated Mo by annealing [14], quenched Al by annealing [15], and pure Fe during ion irradiation [16]. Theoretical studies have also been conducted. Kroupa and Price showed, for the first time, the possible mechanism for the conservative climb of a vacancy cluster toward an edge dislocation [17]. They showed that the gradient in the stress field inside the cluster originating from a dislocation causes a transfer of vacancies from one end of the cluster to the other by pipe-diffusion along the core of the cluster. Later, Kroupa and co-workers conducted another calculation for the conservative climb of a smaller cluster to a larger cluster by including cluster–cluster interactions and cluster–vacancy interactions [18]. Here, they simplified the calculations by two approximations: (i) the cluster was assumed to be a square shape, which simplified the relationship between the vacancy flux and the velocity of the conservative climb; (ii) an infinitesimally small cluster approximation was used, and it was assumed that the force on the cluster changed linearly from the nearest segment to the farthest segment. A few years later, Turnbull conducted more detailed calculations for the conservative climb of two circular clusters formed by ion-irradiated UO_2 [13]; however, the effect of dilatation caused by vacancies was not included because it is much smaller in ionically bound UO_2 than in metallic materials.

Here, we report the construction of a model that describes the conservative climb motion of an SIA cluster to an edge dislocation by incorporating atomistic behavior. The model is applied to the parallel Burgers vector case in BCC-Fe, where the parameters necessary for the calculation are obtained either by molecular statics (MS) or MD simulations. The rest of this paper is organized as follows. The calculation method for the conservative climb is described in the second section, and the procedures and results for MS/MD simulations are shown in the third section. Finally, the calculation results for the conservative climb and discussion are described in the fourth section, followed by the conclusions in the last section.

2. Calculation method

We begin with a hexagonal SIA cluster whose edge contains at least three atoms ($l \geq 3$), which consequently comprises 19 SIAs or more in total. The periphery of the cluster (denoted by the dotted line in Fig. 1(a)) is divided into segments with the length of one atomic diameter. Each segment is a possible location for a vacancy-like defect. We assume another hexagonal border lying one layer above the periphery (hereinafter, we refer to it as the "larger hexagonal border," denoted by the dashed line in Fig. 1(a)), which is divided in the same manner as that of the periphery. Each segment is a possible location for an SIA-like defect. We assume that a vacancy-like defect and an SIA-like defect can exist only on the periphery and larger hexagonal border, respectively.

An atom on the periphery occasionally jumps to one of the second-nearest segments on the larger hexagonal border, through which a pair of vacancy-like and SIA-like defects is generated on the periphery and larger hexagonal border, respectively (Fig. 1(b)) (see Footnote[1]). In some cases, we consider an irregular hexagonal cluster, where some extra atoms are initially placed on the larger hexagonal border, or some atoms on the periphery are initially removed; they are also treated as SIA-like defects or vacancy-like defects, respectively.

The pipe-diffusion of SIA-like defects begin along the larger hexagonal border with activation energy of E_m. In the meantime, vacancy-like defects also diffuse along the periphery. As we shall see in the next section, the activation energy for pipe-diffusion of a vacancy-like defect is essentially equal to that of an SIA-like defect. Hence, we treat the pipe-diffusion of a vacancy-like defect as the jump of an atom that exchanges its position with the vacancy-like defect in a direction opposite to that for the defect. Thereby, it is possible to treat the pipe-diffusion of both types of defects as the jump of atoms on the outermost layer.

There are two assumptions for jumps of an atom. The first one is that the outermost layer has to be either the periphery or the larger hexagonal border (Fig. 2(a)). An atom on the larger hexagonal border cannot jump to a position on top of another atom on the larger hexagonal border, because it would create an SIA-like defect above the larger hexagonal border (Fig. 2(a-2)). A jump of atoms located inside the periphery is also not permitted, because it would create a vacancy-like defect on the layer below the periphery (Fig. 2(a-3)). This assumption is set for the sake of simplicity. However, the results will show that owing to this assumption, there is a limit to the initial number of SIA-like defects ($N_{defect} > 0$) or vacancy-like defects ($N_{defect} < 0$) in our model. The second assumption is that all the atoms except those at the corners must

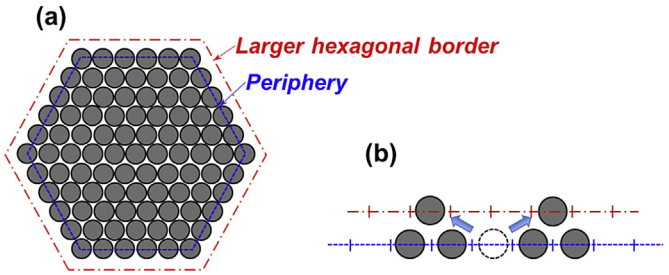

Fig. 1. (a) The periphery and larger hexagonal border of a hexagonal SIA cluster. (b) Formation of a defect pair.

[1] Through this process, an SIA-like defect is not formed at the first-nearest segments, but at one of the *second*-nearest segments. This happens because an SIA-like defect at the first-nearest segment would have only one adjacent inner atom, which is not permitted according to the second assumption for the jump process.