Energetics of formation process of a <001> prismatic dislocation loop via the collision between two 1/2<111> loops in α-iron

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Abstract. It has been proposed by Marian et al. [1] that a [001] interstitial-type dislocation loop can be formed in body-centered cubic iron via the collision between a 1/2[111] loop and 1/2[〈111〉] loop, which undergo one-dimensional glide diffusion, and the subsequent shear reaction. However, the formation of [001] loops through this reaction has not been reproduced by other works even though the two 1/2<111> loops collided with each other. In the present paper, the origin of the difficulty in this reaction is discussed within the framework of isotropic elasticity theory. The sign of the driving force for the reaction is heavily dependent on the reaction path. The two 1/2<111> loops colliding to form a [110] junction can transform to a single [001] loop when a shear loop generated within the 1/2[111] loop propagates in sync with the other shear loop within the 1/2[〈111〉] loop. However, unsynchronized motion of the two shear loops significantly suppresses the propagation of the shear loops, which might be caused by the thermal fluctuation at finite temperatures. This will be one of the origins of the difficulty in the formation of [001] loops through the collision between the two 1/2<111> loops.

1. Introduction

Body-centered cubic (bcc) iron-based steels are major candidate materials for the future nuclear-fission and nuclear-fusion reactors. It is known that prismatic perfect dislocation loops—agglomerations of self-interstitial atoms—with the Burgers vector, $\mathbf{b}$, of <001> are formed in bcc iron upon high-energy particle irradiation at elevated temperatures, as well as dislocation loops with $\mathbf{b}=1/2<111>$ [2, 3].

The detailed process of the formation of <001> loops, however, has not been fully understood. Eyre and Bullough [3] proposed that an extremely small 1/2[011] imperfect dislocation loop with a stacking fault, which is the agglomeration of [011] dumbbells on the (011) plane, is unfaulted and changes into a 1/2[111] loop or [001] loop through the following shear reactions on the loop plane, when it grows:

\[
\frac{1}{2}[011]+\frac{1}{2}[100] \rightarrow \frac{1}{2}[111] \quad (1)
\]

\[
\frac{1}{2}[011]+\frac{1}{2}[0\overline{1}1] \rightarrow [001]. \quad (2)
\]
In accordance with the result obtained by Dudarev et al. [4], the latter reaction is expected to more frequently occur than the former reaction at high temperatures; this will yield the formation of $<001>$ loops.

On the other hand, Masters [2] proposed that the coalescence between a $1/2[111]$ loop and $1/2[\overline{1}T1]$ loop leads to the formation of a single $[001]$ loop, via the following reaction:

$$\frac{1}{2}[111] + \frac{1}{2}[\overline{1}T1] \rightarrow [001].$$

This kind of loop-loop interaction as well as the behavior of individual loops must be influential in the microstructural evolution under irradiation. In 2002, Marian et al. [1] showed a picture of the process expressed by equation (3), based on the idea that $1/2<111>$ loops can undergo one-dimensional glide diffusion in their $b$ direction [1, 5, 6]. They confirmed by using molecular dynamics calculations that when a $1/2[111]$ loop lying on a $\{01\overline{1}\}$ plane (loop A) accidentally collides with a $1/2[\overline{1}T1]$ loop lying on another $\{01\overline{1}\}$ plane (loop B) side by side via their one-dimensional motion, a $[001]$ junction can be formed. They proposed that when the sizes of the two loops are comparable and the loop A plane involves the $b$ of loop B and the loop B plane involves the $b$ of loop A, propagation of a shear loop within loop A generated due to a shear stress applied by loop B and that within loop B generated by loop A expand the $[001]$ junction and finally form a single $[001]$ loop. In contrast, other molecular dynamics calculations conducted by Osetsky et al. [7] and Dmitry et al. [8] have not reproduced the formation of a $[001]$ loop even when loop A collided with loop B. In addition, in a recent experiment by using in-situ transmission electron microscopy [9], the formation of a $[001]$ loop was not observed even when the collision occurred, and rather it was observed that a larger loop absorbed smaller one after the collision. It should be noted that these results do not necessarily mean that the formation of a $[001]$ loop via the mechanism proposed by Marian et al. [1] can not be realized. However, these results seem to imply that the Marian’s mechanism [1] rarely works if any. In the present paper, the origin of the difficulty in the formation of $[001]$ loops via Marian’s mechanism [1] will be touched on, by evaluating the sign of the driving force for the reaction based on non-singular isotropic elasticity theory [10].

2. Verification of the Marian’s mechanism [1]

When loop A collides with loop B side by side, there are two manners of the collision between the two loops, depending on the spatial configuration of them. A $[001]$ junction is formed in one case, and a $[110]$ junction is formed in the other case. The necessary condition for the formation of the $[001]$ loop via the shear reaction is not the formation of the $[001]$ junction, as claimed by Marian et al. [1], but that of the $[110]$ junction via the collision between loop A and loop B, if we adopt the traditional terminology in dislocation theory. Hereafter, the loop shape approximates the rectangular, for simplicity.

2.1. Driving force for the formation of the $[001]$ loop

In order to examine whether the driving force for the $[001]$ loop formation is positive or negative and to clarify the origin of the promotion or suppression of the reaction, we evaluate the driving force for the propagation of the shear loops for $[011]$ junction case [9] and extract the origin of the sign of the driving force. Figure 1 shows the dislocation structure for the calculation. Here, the dislocation directions point into the paper or the right. The loop A plane is $(01\overline{1})$, and the loop B plane is $(0\overline{1}1)$. We assumed that the segments transformed to $[00\pm 1]$ ones could immediately glide and cancel the 90-degree bend to reduce the total energy, as shown by the segment named $\eta$ and $\zeta$. The total elastic energy, $W$, is calculated by the summation of the self-energies of all the segments and the interaction energies between all different segments. The self- and interaction energies were calculated within the framework of nonsingular isotropic elasticity theory, proposed by Cai et al. [10]. The total driving force for the $[001]$ loop formation, $F$, was evaluated by the following equation:
\[ F = -\frac{\partial W}{\partial (d_{AS} + d_{BS})}. \]  

(4)

Figure 2 shows one of examples for the calculated results of the driving force for the [001] loop formation as a function of \(d_{AS}+d_{BS}\). Initially, the shape of loop A and loop B was square, and all the side length values were 10 nm. The length \(d_{AS}\) and \(d_{BS}\) were alternately incremented by a length of \(a/3\), where \(a\) is the lattice constant (\(= 0.28665\) nm). In this figure, in addition to the driving force calculated from the total energy, the components originated from the typical interaction energies and the total self-energies are shown. From this figure, it is clarified that the driving force is always positive mainly due to the repulsive interaction between \(\beta\) and \(\delta\) and the attractive interaction between \(\delta\) and \(\epsilon\) and that of \(\alpha\) and \(\beta\) when the distances between the noted pair of segments are short, although the driving force from the total self-energies becomes negative after the reaction progresses to some extent. Thus, if a shear loop propagates in sync with the other shear loop, the [001] loop can be easily formed.

Figure 3 shows another example of the calculated result of the driving force. In this case, only \(d_{BS}\) was firstly increased from \(a\) to \(6a\) while \(d_{AS}\) was fixed. After it, \(d_{AS}\) was increased while \(d_{BS}\) was fixed. As shown in this figure, while \(\delta\) progresses after \(\beta\) precedes, it undergoes significant attractive force from \(\beta\) and it yields the negative driving force. The origin of this attractive force only locally appearing is due to the spatial variation in the sign of the shear stress around edge dislocations [11]. Thus, unsynchronized propagation of the two shear loops suppresses the formation of the [001] loop. At finite temperatures, the thermal fluctuation will enhance this kind of unsynchronized motion of the
shear dislocations. This will be one of the origins of the difficulty in the formation of [001] loops via the shear reaction following the collision between loop A and loop B.

3. Concluding remarks
A 1/2[111] loop (loop A) and a 1/2[111] loop (loop B) must collide with each other so that they form a [110] junction to form a single [001] loop through the shear reaction following the collision. By the calculations based on isotropic elasticity theory, we have found that the driving force for the shear loop propagation within loop A and loop B (a [001] loop formation) after the [110] junction formation is heavily dependent on the reaction path. Synchronized propagation of the two shear loops within loop A and loop B yielded the promoted formation of the [001] loop; whilst, unsynchronized propagation of the two shear loops significantly suppressed the [001] loop formation. At finite temperatures, such an unsynchronized motion of the shear dislocations will be enhanced due to the thermal fluctuation; it will be one of origins of the difficulty in the formation of [001] loops via the shear reaction following the collision between loop A and loop B.

Acknowledgements
This work was financially supported by Priority Assistance for the Formation of Worldwide Renowned Centers of Research—The Global COE Program (Project: Center of Excellence for Advanced Structural and Functional Materials Design) from the Ministry of Education, Culture, Sports, Science and Technology (MEXT), Japan.

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