Effect of Stress Distribution on 1-D Motion of Radiation Defects

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1. Introduction

Irradiation induced mechanical property degradation of materials has been studied from several decades ago, but the mechanism is still in controversy. Two mechanisms have been proposed. One is the dispersed barrier hardening mechanism[1]. This explains defect clusters as barriers to the dislocation motion. And the other is the cascade induced source hardening mechanism[2], which places emphasis on a role of defects as Cottrell atmosphere to dislocation motions. However, the above mechanisms can be applied to only a part of experimental results. Any model has not given a solution to 1-D motion of defect clusters of size over 2 nm. 1-D motion of defects clusters has been observed by many researchers[3-8]. At first, Kroupa et al. proposed a conservative climb of dislocation loops by pipe diffusion[3]. Kiritani[4] tried to explain the driving force of motion with strain field. Some MD simulation results showed a kind of crowdion motion into close packed direction in a crystal[9,10]. But large clusters of more than a few hundred SIAs showed significantly reduced mobility. To know the effect of 1-D motion on radiation damage, it is important to clarify driving force of the motion. In this study, we tried to link an observation of the motion of loop to a stress field around loops calculated with the Peach-Koehler equation.

2. Methods and Results

2.1 Experimental

The starting material for this study was a binary Fe-Cu alloys made in our laboratory and Fe single crystal (99.98% Fe) supplied by Goodfellow. After Fe-Cu samples were solution-treated at 1,123K for 5 hrs in the vacuum condition, they were water-quenched. Samples were isothermally aged at 773K.

For examination in electron microscope, discs of diameter 3 mm were punched from aged samples. TEM samples were observed with 1.25 MeV HVEM in KBSI. The image of clusters formation was captured at a time interval of about 2 minutes. And the motion of clusters was recorded through CCD camera with a time interval of 1/30 s.

2.2 Calculation of Stress Field around a Loop

The Peach-Koehler equation for the self-stresses of any curved closed dislocation loop is given by the following line integral[11].

$$\begin{aligned}\sigma_{\alpha\beta} = &-\frac{G}{8\pi}\oint_C b_m \varepsilon_{im\alpha}\frac{\partial}{\partial x'_i}\nabla'^2 R\,dx'_\beta \\ &-\frac{G}{8\pi}\oint_C b_m \varepsilon_{im\beta}\frac{\partial}{\partial x'_i}\nabla'^2 R\,dx'_\alpha \\ &-\frac{G}{4\pi(1-\nu)}\oint_C b_m \varepsilon_{imk}\left(\frac{\partial^3 R}{\partial x'_i\,\partial x'_\alpha\,\partial x'_\beta}\right. \\ &\left.-\delta_{\alpha\beta}\frac{\partial}{\partial x'_i}\nabla'^2 R\right)dx'_k\,,\end{aligned} \tag{1}$$

where b_i is the Burgers vector, $\in$ is the permutation symbol, G is the shear modulus and ν is Poisson's ratio. The normal stress to loop plane, $\sigma_{z'z'}$ turns out to be

$$\begin{aligned}\sigma_{z'z'} = &-\frac{G}{4\pi(1-\nu}\left[b_{x'}\oint_C\left(\frac{\partial^3 R}{\partial z'^3}-2\frac{\partial R^{-1}}{\partial z'}\right)dy'\right. \\ &-b_{y'}\oint_C\left(\frac{\partial^3 R}{\partial z'^3}-2\frac{\partial R^{-1}}{\partial z'}\right)dx' \\ &+b_{z'}\oint_C\left(\frac{\partial^3 R}{\partial y'\partial z'^2}-2\frac{\partial R^{-1}}{\partial y'}\right)dx' \\ &\left.-b_{z'}\oint_C\left(\frac{\partial^3 R}{\partial x'\partial z'^2}-2\frac{\partial R^{-1}}{\partial x'}\right)dy'\right].\end{aligned} \tag{2}$$

where R is loop radius and z' is the normal direction of loop habit plane
The result for the above is given as following.

$$\begin{aligned}\sigma_{z'z'} = &-\frac{Gb_{x'}}{2\pi(1-\nu}\left[C_1E(k)+C_2K(k)\right] \\ &-\frac{Gb_{z'}}{2\pi(1-\nu}\left[C_3E(k)+C_4K(k)\right].\end{aligned} \tag{3}$$

where the coefficients C_1 to C_4 are given by Khraishi et al.[12]. K(k) and E(k) in equation (3) are complete elliptic integrals of the first and second kinds respectively.

2.3 Effect of Defect Density on 1-D motion

When the defect density was measured, 1-D motion in Fe-Cu and pure Fe samples started at 1.8×10^{21} /m^3

and 2.4x10^{21}/m^3. In pure Fe, the density was more than in Fe-Cu. But the difference was very small. When we assume the start density is 2.0x10^{21}/m^3, and the distribution of loops is uniform, the distance between loops is about 80 nm. The loop size was about 10 nm when the motion of loops started.

2.4 Stress Distribution around a Loop

The variation in σ_{zz} component along the loop diameter direction is shown at Figure 1, for the case when a loop is Frank type, the size of a loop is 10 nm and the distance from the normal direction of a loop is zero.

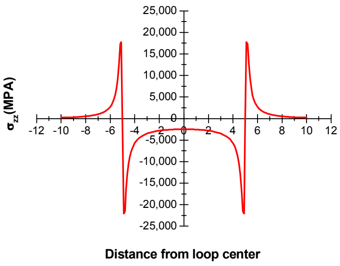

Fig. 1. σ_{zz} variation at z'=0 nm

At the edge of a loop, a change of stress is very high. On the loop, a compressive stress is applied. But at the outside of a loop, a tensile stress is applied.

At the position of 40 nm from loop habit plane, the stress distribution is shown At Figure 2.

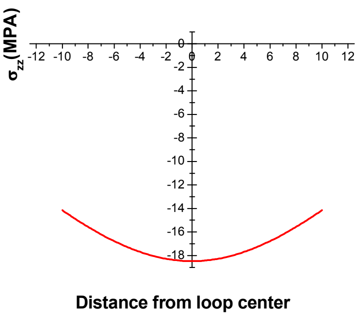

Fig. 2. σ_{zz} variation at z'=40 nm

All over a loop, a compressive stress is applied. But a maximum stress is about 18 MPa.

Fig. 3 shows the stress distribution at the center of a loop, when the distance from loop habit plane increases from 0 to 80 nm. At just above the habit plane, a larger compressive stress is applied than a stress on habit plane. At 80 nm, a applied stress is very small and can be disregarded. But these stresses are calculated by assuming there is no interaction between loops. At about 20 nm from loop habit plane, the stress change is very severe. Under HVEM condition, 1-D motion occurs without applied stress. Even though we cannot know a stress required for the 1-D motion until now, it can be known that 1-D motion occurs below the yield stress.

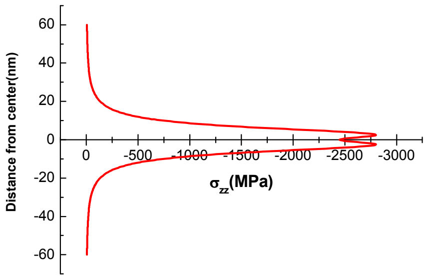

Fig. 3. σ_{zz} variation above the loop center.

3. Conclusion

The 1-D motion of radiation defects was observed. The motion occurred at the loop density of about 2.0x10^{21}/m^3. The stress variation around a interstitial loop was calculated with the Peach-Koehler equation. From the calculated stress distribution, a compressive stress is applied to normal direction of loop habit plane. Therefore the gradient of compression and expansion stress field is understood as a driving force of 1-D motion.. This work has been carried out as a part of Nuclear R&D program supported by Ministry of Science and Technology, Kore. And we thank the Korea basic Science Institute for the use of HVEM.

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