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Temperature dependence of dislocation bias factors in metals

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ABSTRACT

Recently, it has been shown that edge dislocations are not stable sinks for vacancies. Trapping and detrapping of vacancies occur as a thermally-activated process. In this paper, the temperature dependence of vacancy absorption coefficient of edge dislocations under irradiation was calculated by using rate equations in Fe and Ni. The temperature dependence was almost the same in both Fe and Ni and did not depend on the damage rate between 10^{-10} dpa/s and 10^{-6} dpa/s. At low temperatures such as room temperature, the coefficient was low and with increasing irradiation temperatures, it had a peak (500 K) and decreased.

1. Introduction

In metals under high-energy particle irradiation, equal numbers of vacancies and interstitials are formed. Most of these are annihilated at sinks, of which edge dislocations are one of the most important. It has been a commonly-held belief that point defects near edge dislocations are absorbed easily, which allows dislocation climb by the formation and movement of jogs. In the dislocation bias model [1,2], a small unbalanced reaction between point defects and edge dislocations, the preferential diffusion of self-interstitials relative to the diffusion of vacancies to dislocations, causes void swelling. The model is based on the idea that edge dislocations are perfect sinks for point defects. However, ample evidence has been obtained that indicates the existence of vacancies trapped on edge dislocations [3–6].

In this paper, we demonstrate that edge dislocations are not perfect sinks for vacancies, and a temperature dependence of the vacancy absorption coefficient is presented. In Section 2, the interaction between vacancies and edge dislocations developed by Heald [7], based on elastic theory, is explained. In Section 3, recent experimental results which indicate the existence of trapped vacancies and their behavior are introduced [3–6]. In Sections 4 and 5, the temperature dependence of the vacancy absorption coefficient is presented, based on reaction kinetic analysis.

2. Elastic interaction between vacancies and edge dislocations

Dislocation bias factors are essential for the calculation of nucleation and growth of voids by the dislocation bias model. For the determination of the factor, only the elastic interaction between point defects and edge dislocations has been considered. Heald [7] has given the expression to obtain a bias factor B as follows:

$$B = (Z_i - Z_v)/Z_v, \tag{1}$$

where

$$Z_\alpha = 2\pi I_0(L_\alpha/2r_0)/(K_0(L_\alpha/2R)\cdot I_0(L_\alpha/2r_0) - (K_0(L_\alpha/2r_0)\cdot I_0(L_\alpha/2R)) \tag{2}$$

and

$$L_\alpha = (1+\nu)\mu\Delta V_\alpha b/(3(1-\nu)kT\pi). \tag{3}$$

The subscript α denotes the type of point defects, i (interstitial) and v (vacancy), respectively. $K_0(z)$ and $I_0(z)$ are the modified Bessel functions of zero order. ν, μ, ΔV, and b are Poisson's ratio, the shear modulus, the local volume change, and the Burgers vector of the dislocation, respectively. Although the effect of temperature is included in Eq. (3), the temperature dependence of the bias factor is weak. Even if the temperature changes by a factor of 400, the bias factor changes by only 3 times in Heald's calculations [7].

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3. Trapped vacancies on edge dislocations

There have been reports that indicate the existence of isolated vacancies on edge dislocations. Häkkinen et al. first indicated the existence of vacancies associated with the dislocation line [3,4]. They calculated positron lifetimes of edge dislocations and vacancies on edge dislocation lines in Al and Cu. Kamimura et al. also calculated the positron lifetimes in Fe [5], where the obtained values were 117 ps for edge dislocations and 140 ps for vacancies on edge dislocation lines.

We have reported vacancy trapping and detrapping behavior on dislocations [6], which was different from the formation and absorption of point defects by jogs. The existence of vacancies trapped on dislocations and their detrapping behavior during isochronal annealing were experimentally demonstrated in deformed Fe and Ni. Fig. 1 shows the isochronal annealing behavior of the positron annihilation lifetime in pure Fe for high-speed deformation using an impact deformation apparatus [8]. The long lifetime of 197 ps at 300 K was attributed to a combining lifetime of monovacancies (180 ps [9]), vacancy clusters (2–3 vacancies), and vacancies on the edge dislocation line. After annealing at 473 K, the long lifetime was shorter than that of vacancies in the matrix. A number of vacancies in the matrix were considered to have migrated to the dislocation line without annihilation, because the intensity of the long lifetime did not change. Their lifetime change was from 180 ps to 140 ps. The lifetime of the jogs of edge dislocations is 117 ps [5], exactly equal to that of edge dislocations and too short to allow separation of the lifetime component from the matrix component (104 ps [9]). If vacancies were annihilated at jogs in the edge dislocations, the long lifetime would further decrease. After annealing at 573 K, the long lifetime and mean lifetime both increased. In particular, the intensity of 35% was constant during annealing between 373 K and 673 K. Most vacancy clusters were not annihilated and grew by means of vacancy absorption. For vacancy clusters to grow without a change in concentration caused by isochronal annealing, vacancies must have been formed somewhere at 573 K. However, a large number of vacancies could not have been generated from grain boundaries or jogs in the edge dislocations at thermal equilibrium at 573 K or 673 K. The only possible source of vacancies was the release of trapped vacancies from edge dislocations. Vacancies were detrapped from edge dislocations, aggregated in the matrix, and formed large vacancy clusters at 573 K.

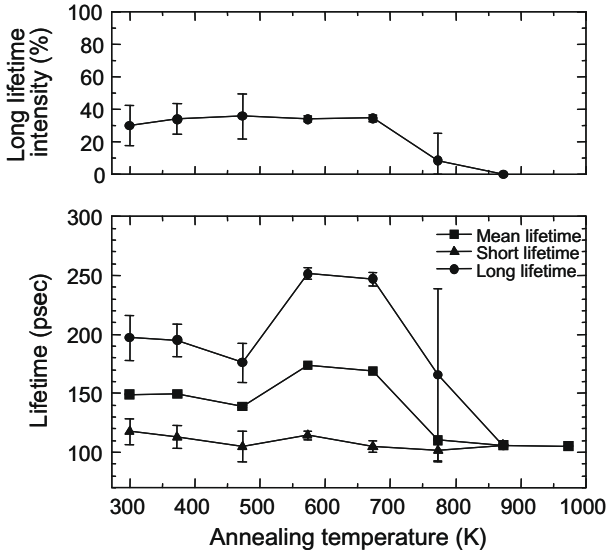

Fig. 1. Isochronal annealing behavior of positron annihilation lifetime and long lifetime intensity in Fe for high speed deformation (strain rate, 4.3×10^5/s; annealing time, 10 h).

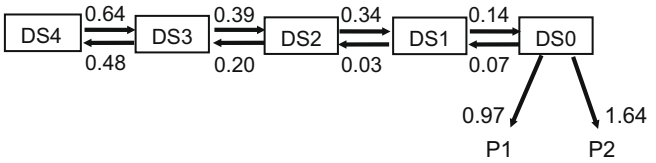

Fig. 2. Vacancy migration energy near an edge dislocation in Fe obtained by computer simulation [6].

The migration energy of vacancies near perfect edge dislocations in Fe and extended dislocations in Ni was calculated employing the *N*-body potential, and an energy calculation for the model lattice was performed employing the static method [10,11]. Results obtained with these calculations are shown in Fig. 2 for Fe and Fig. 3 for Ni [6]. In both figures, "DS0" is the dislocation core and "DSn" ($n = 1,...4$) is on the slip plane of dislocation. "P1" and "P2" are vacancy migration along dislocation core (pipe diffusion). "SFn" ($n = 1,2...$) in Fig. 3 is on the staking fault. "SFC" denotes the center of the stacking fault ribbon. A vacancy was introduced at each position and the vacancy migration energy between two positions was calculated.

These results indicate that the absorption of vacancies by edge dislocations is a thermally-activated process and consequently dislocation bias factors are temperature-dependent, but do not exhibit the same temperature dependence as L_α, which is shown in Eq. (3). In the next section, the temperature dependence of the absorption of vacancies by edge dislocations is estimated. The same temperature dependence of sink efficiency exists in self-interstitials. The trapping energy of self-interstitials on dislocations is, however, large enough that detrapping is not expected.

4. Reaction kinetic analysis

The equilibrium vacancy concentration C_v in the matrix was estimated, based on the steady state rate equations:

$$dC_v/dt = P - Z_{iv}(M_i + M_v)C_iC_v) - C_sM_vC_v = 0, \quad (4)$$

$$dC_i/dt = P - Z_{iv}(M_i + M_v)C_iC_v - C_sM_iC_i = 0, \quad (5)$$

where C_i is the self-interstitial concentration, P is the point defect production rate, Z_{iv} is the geometrical factor of mutual annihilation, M is the mobility of point defects, and C_s is the sink efficiency. Interstitial mobility M_i and that of vacancies M_v are expressed as follows:

$$M_i = \upsilon_0 \exp(-E_{mi}/kT), \quad (6)$$

$$M_v = \upsilon_0 \exp(-E_{mv}/kT), \quad (7)$$

where υ_0 is frequency of lattice vibration, 10^{13}/s. $E_{m\alpha}$ is migration energy of point defects in the matrix, 0.78 eV for Fe and 1.17 eV for Ni [6], k is the Boltzmann constant, and T is absolute temperature.

An analysis using a rate equation was performed in Fe. The vacancy concentrations at "DS4", "DS3", "DS2", "DS1" and "DS0" are expressed as C_0, C_1, C_2, C_3 and C_4, respectively. The vacancy concentration along dislocation core is $C_n (n \geqslant 4)$. The vacancy concentration C_0 was assumed to not be influenced by the dislocations or constant. So $C_0 = C_v$. The variations of the above parameters at time t are

$$dC_0/dt = 0, \quad (8)$$

$$dC_1/dt = -M_{10}C_1(1 - C_0) - M_{12}C_1(1 - C_2) + M_{01}C_0(1 - C_1) + M_{21}C_2(1 - C_1), \quad (9)$$

$$dC_2/dt = -M_{21}C_2(1 - C_1) - M_{23}C_2(1 - C_3) + M_{12}C_1(1 - C_2) + M_{32}C_3(1 - C_2), \quad (10)$$

$$dC_3/dt = -M_{32}C_3(1 - C_2) - M_{34}C_3(1 - C_4) + M_{23}C_2(1 - C_3) + M_{43}C_4(1 - C_3), \quad (11)$$

$$dC_4/dt = -2M_{43}C_4(1 - C_3) - M_{45}C_4(1 - C_5) + 2M_{34}C_3(1 - C_4) + M_{54}C_5(1 - C_4), \quad (12)$$

...

$$dC_n/dt = M_{n-1n}C_{n-1}, \quad (13)$$