POINT DEFECT INTERACTIONS AND GROWTH OF
DISLOCATION LOOPS*

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ABSTRACT

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A direct method of determining the effective measure of the interaction of point defects with dislocation loops is proposed. A system of partial differential rate equations for loop growth is formulated and is solved by a numerical method. An *in-situ* HVEM irradiation experiment was conducted to study growth kinetics of dislocation loops in Ni at 450°C. It is found from systematic variations of the vacancy migration energy, E_v^m , and the preference factor of dislocation loops for self-interstitials, δ_i , that $\delta_i = 0.06$ and $E_v^m = 1.2$ eV together yield reasonable agreement between the theoretical model and the experimental observations.

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Clustering of vacancies or self-interstitials into dislocation loops may occur when a super-saturation of point defects results from irradiation and also from quenching in the case of vacancies. Once formed, the subsequent growth or shrinkage of dislocation loops depends critically upon the interaction of point defects with dislocation loops. The effect of the elastic interaction on diffusion of the point defects to a dislocation loop has been analyzed recently by several investigators [1-6]. As discussed by the investigators and also by Balluffi in his review [7], such an analysis involves a number of approximations, the most difficult ones being the inner and outer boundary conditions. Additional difficulties also arise when taking into account the non-linear drift force terms in the diffusion equation. In the present paper, we propose a direct method of determining the overall effect of point defect - dislocation loop interaction on growth kinetics of dislocation loops that will circumvent most of the aforementioned difficulties.

First, a rate theory model for loop growth is developed. Since a number of material, defect, and experimental parameters are involved in the model, our second objective is to determine from an *in-situ* high-voltage electron microscope (HVEM) irradiation experiment sink strength constants and/or point defect migration energies based on other 'better known' parameters that enter into the model.

Rate Theory of Loop Growth

Consider a temperature region where the only important free defects are self-interstitials and vacancies and where only one type of dislocation loop, namely the interstitial type, evolves as internal sinks for point defects. Then, the growth rate of interstitial loops can be obtained from the following partial differential rate equations [8]:

$$\frac{\partial \rho}{\partial t} = \frac{2}{\rho b^3} \left[r_i D_i C_i - r_v D_v (C_v - \bar{C}) \right], \quad (1)$$

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$$\frac{\partial C_v}{\partial t} = \frac{\partial}{\partial x} \left(D_v \frac{\partial C_v}{\partial x} \right) + G - \alpha C_v C_i - K_v (C_v - C_v^e) , \quad (2)$$

$$\frac{\partial C_i}{\partial t} = \frac{\partial}{\partial x} \left(D_i \frac{\partial C_i}{\partial x} \right) + G - \alpha C_v C_i - K_i C_i , \quad (3)$$

where $\rho = \rho(x,t) = R(x,t)/b$ is the loop radius in units of Burgers vector, x the distance from a free surface, and t is the irradiation time. Subscripts v and i denote vacancies and interstitials, D 's are the diffusion coefficients, C 's the fractional point defect concentrations, r 's the effective capture radii of interstitial loop for point defects, K 's the reaction rate constants at internal sinks, G the defect generation rate, α the recombination rate, and $\bar{C}$ the thermal equilibrium concentration of vacancies at a faulted dislocation loop.

The reaction rate constants are related to the so-called 'sink strength constants' [9,10], $\beta_{v,i}$, by $K_{v,i} = D_{v,i} \beta_{v,i}$, and in turn $\beta_{v,i} = 4\pi N_\ell r_{v,i}$ and $r_{v,i} = r_c (1 + \delta_{v,i})$, where N_ℓ is the loop number density, r_c is the capture radius of the loop ignoring the defect-loop interaction, and $\delta_{v,i}$ are 'the preference factors' [10]. The toroidal volume of the dislocation loop core is replaced by an equivalent spherical volume using an analogy in electrostatic capacity [10]. Then, the expressions for the capture radius obtained previously for spherical sinks [5,9,10] apply for the present case. Physically, a non-zero preference factor indicates a measure of the strength of overall interaction between the point defects and the loops. The condition that $\delta_i > \delta_v$ is the primary cause of growth of interstitial loops during irradiation.

HVEM Irradiation Experiment

Foil specimen were thinned from a zone-refined nickel single crystal rod. The foil normal was near [001]; foil thickness was determined stereographically. Irradiations were performed at 723 K (450°C) using 650 KeV electrons. The progressive growth of the interstitial type Frank loops was measured from photographs taken as a function of irradiation time. Loop number density was essentially

constant during the time period examined at $N_L = 5 \times 10^{-20} \text{ m}^{-3}$. The defect generation rate $G = 6.4 \times 10^{-5} \text{ dpa} \cdot \text{sec}^{-1}$ was calculated from the measured flux $\phi = 3.8 \times 10^{23} \text{ cm}^{-2} \cdot \text{sec}^{-1}$ using a $\langle 100 \rangle$ threshold displacement energy of 36 eV [12,13] and a tabulated total displacement cross-section of 1.66 barns [14].

Results and Discussion

Diameters of 35 loops were measured at 11 irradiation times ranging from $t = 1$ to 62 minutes. The depth coordinate of each loop was determined by standard stereo microscopic technique, and the results are shown in Fig. 1. It is evident that the loops situated near the top and bottom surfaces were larger than those at the foil center, and also that the longer the irradiation time, the more pronounced this feature became. The mean values of the measured loop radii are plotted in Fig. 2. The time exponent for $(R/b) \propto t^n$ that best fits the measured data is found to be $n = 0.56$.

The system of rate equations [1-3] was solved by use of the method of lines and the stiff integrator package called GEAR-B [15]. The details of numerical calculations will be given elsewhere [8]. The defect parameters used for calculations were the vacancy formation enthalpy and entropy $E_V^f = 1.39 \text{ eV}$ and $S_V^f = 1.5 k$, and the defect migration energies and the pre-exponents of diffusivities $E_V^m = 1.0 \text{ eV}$, $D_V^0 = 0.19 \text{ cm}^2/\text{sec}$, $E_I^m = 0.15 \text{ eV}$, and $D_I^0 = 0.008 \text{ cm}^2/\text{sec}$. Since $D_I \gg D_V$ at $T = 450^\circ\text{C}$ and therefore D_V dictates the growth kinetics of interstitial loops [13,16], we chose to vary E_V^m and δ_I until a satisfactory self-consistency between the theory and the experiment is attained.

In the earlier calculations [2-4] the so-called 'bias factor' of an infinitesimal dislocation loop for point defects, $Z_{v,i} = 1 + \delta_{v,i}$, was found to depend on the loop size as $Z_{v,i} \propto (b/R)^2$. Such loop size dependent preference factors do not predict the observed loop growth. It is believed that the approximation of defect generation and recombination involved in the calculations is probably the reason for the disagreement. Assuming that $\delta_v = 0$, $\delta_I = 0.01 \sim 0.2$, and

$E_V^m = 0.6 \sim 1.4$ eV, we have tried a number of combinations of δ_i and E_V^m . As shown in Figs. 1 and 2, the set of $E_V^m = 1.2$ eV and $\delta_i = 0.06$ generates the curves which are in most reasonable agreement with the experimental data. Figure 2 shows that initial conditions do not affect the agreement significantly. The preference factor is independent of the character of a dislocation loop [5]. Therefore, the present results of $\delta_v = 0$ and $\delta_i = 0.06$ for Ni are the preference factors of both vacancy loops and interstitial loops for vacancies and interstitials, respectively.

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Fig. 1. Size and Depth Positions of Frank Loops.

Fig. 2. Growth Kinetics of Frank Loops.

Size and Depth Position of Frank Loops.

The Depth Positions Were Measured by Stereomicroscopy, and the Calculated Curves Were Obtained with $E_v^m = 1.2 \text{ eV}$, $\delta_1 = 0.06$.

Growth Kinetics of Frank Loops in Ni

Each Point is the Mean Value of 35 Loop Radii Measured, and the Curves Show the Average Loop Radius Predicted by the Model.

Fig. 2 Yoo and Stiegler