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Submitted for publication in Physics Letters.

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Nonlinear elasticity is shown to produce a difference in the capture efficiencies of interstitial and vacancy type loops. Such a difference is a necessary, though not sufficient, prerequisite for the simultaneous formation of both types of loops during irradiation.

During irradiation of metals with energetic particles interstitials and vacancies are produced in equal numbers. They also recombine in equal numbers, and if it were not for the preferred capture of interstitials at dislocations an equal number of vacancies and interstitials would also be absorbed on the average at each of the sinks. If this were the case, such phenomena as void swelling and irradiation creep would hardly occur. However, due to the stronger interaction of the interstitial versus the vacancy with the stress field, the current of interstitials to a dislocation is somewhat larger than the current of vacancies, provided the vacancy excess not captured by the dislocation is absorbed at another sink with less or no preferred capture efficiency for interstitials. Hence, a net segregation of interstitials and vacancies requires the presence of at least two types of sinks with different capture efficiencies.

If well-annealed metals are irradiated at temperatures above the vacancy migration stage, dislocation loops are formed rapidly and abundantly. By virtue of their preferred capture for interstitials, the loops are commonly believed to be of the interstitial type. Although this has been confirmed experimentally [1], the simultaneous presence of both interstitial- and vacancy-types has also been reported [2-7]. Whereas the formation of vacancy-type loops appears to be restricted to temperatures close to the onset of vacancy migration and to low doses for most metals, exceptions are Ti [8], Zr [9] and its alloys [9,10]. Here, the formation of vacancy-type loops is profilic, but void formation is virtually absent.

The simultaneous growth of both loop types represents so far a paradox. If loops have a sufficiently large diameter, they may be viewed as curved edge dislocations, and therefore, the capture efficiencies of interstitial- and vacancy-type loops must be the same. Calculations by Wolfer and Ashkin [11] for infinitesimal loops have again revealed no difference in capture efficiencies. Up to now only the stress fields according to linear elasticity have been used in deriving capture efficiencies. In the present paper it is shown that a difference in the capture efficiencies between interstitial- and vacancy-type loops arises for small and medium loop sizes when second-order elasticity corrections are taken into account.

A rigorous demonstration of this fact would require the execution of three laborious tasks. First, the strain field of a dislocation loop would have to be computed according to non-linear elasticity theory. Second, with these finite strains one would have to derive the interaction energy with a point defect. Finally, the gradient of this interaction energy would enter as a drift term into the diffusion equation, which one would need to solve to obtain the point defect current to the dislocation loop. At the expense of mathematical rigor, we prefer a heuristic, but simple approach based on the following physical arguments.

The strain field of a prismatic dislocation loop as computed from linear elaticity is substantially in error close to the dislocation core. This means that a large discrepancy exists between the local Burgers vector (defined in the real lattice) and the ideal Burgers vector (defined in the perfect lattice) when the loop radius is small. Since the linear elastic strain field of the dislocation loop is proportional to the Burgers vector, we can simply account in an approximate manner for non-linear effects if we use some measure of the local Burgers vector in the strain field expressions obtained from linear elasticity. Such a measure, henceforth called the apparent Burgers vector, can be obtained in the following manner.

It is well known that second-order elasticity effects are the cause of density changes of crystals containing dislocations [12]. Seeger and Haasen [13] have shown that the volume expansion δV_d produced by edge dislocations is given by

$$\delta V_d = \frac{1}{3}\left[\frac{1-\nu-2\nu^2}{1-\nu}\,\frac{1}{K}\left(\frac{dK}{dp} - 1\right) + \frac{1-\nu+\nu^2}{1-\nu}\,\frac{2}{G}\left(\frac{dG}{dp} - \frac{G}{K}\right)\right] E_d \;, \qquad (1)$$

where ν is the Poisson's ratio, K and G the bulk and shear moduli, dK/dp and dG/dp their pressure derivatives, and E_d the strain energy associated with the edge dislocation as calculated from linear elasticity theory. Based on the arguments presented by Holder and Granato [14], Eq. (1) may also be used to compute the volume expansion δV_ℓ of a prismatic loop if we replace E_d by the strain energy of the loop,

$$E_\ell = \frac{G\, b_o^2}{2(1-\nu)}\, R\left[\ell n\, \frac{4R}{r_o} - 1\right] \;. \qquad (2)$$

Here, b_0 is the Burgers vector, r_0 the core radius, and R the loop radius. By the insertion or by the extraction of a circular platelet of atoms, the interstitial- or vacancy-type loop can be created, and the associated total volume change, called loop volume, is simply

$$V_\ell = \pm \pi R^2 b_0 + \delta V_\ell = \pm \pi R^2 b(R) \quad . \tag{3}$$

The plus (minus) sign holds for the interstitial- (vacancy-) type loop. Linear elasticity gives a loop volume equal to $\pm\pi R^2 b_0$. With second-order elasticity effects included, we may ascribe an apparent Burgers vector $\pm b(R)$ to the loop so as to reproduce the correct loop volume V_ℓ with the same expression. Since δV_ℓ is approximately proportional to R, the apparent Burgers vector b(R) approaches b_0 for large R. Equation (3) together with the Zener formula (1) predicts loop volumes in good agreement with computer simulation results reported by Dederichs et al. [15] for small interstitial-type loops in fcc metals.

The apparent Burgers vector b(R) can now be used instead of b_0 in previous expressions for the capture efficiency of loops [11,16]. These expressions as well as those for the capture efficiency of edge dislocations [17] have revealed that the capture efficiency (or bias factor) depends on the relaxation volume of the point defect and the Burgers vector b_0 of the dislocation or loop. Instead of using these previous expressions we employ here a simple interpolation formula for the capture efficiency which reproduces both results for the infinitesimal loop and the straight edge dislocation.

This formula is based on a recent result by Seeger and Goesele [18] for the point defect current to a circular loop,

$$J = \frac{4\pi^2 R}{\ln(8R/a)} D(C-C^o) \quad . \qquad (4)$$

Here, a is the dislocation pipe radius or the minor radius of the toroidal sink surface, D the diffusion coefficient, and C^o the concentration of point defects in local thermal equilibrium with the sink. Eq. (4) does not contain the effect of the long-range mechanical interaction on the current. However this effect can be modeled by replacing the pipe radius a by a capture radius c > a. Alternatively, we can define a capture efficiency or bias factor [16] by

$$Z = \ln(8R/a)/\ln(8R/c) \qquad (5)$$

with which we multiply the r.h.s. of Eq. (4). The radii a and c are determined by matching Eq. (5) to the results of the infinitesimal loop and of the edge dislocation. Two sets of values ($a_i = 8\ b_o$, $c_i = 20\ b_o$) and ($a_v = 2.7\ b_o$, $c_v = 3.5\ b_o$) are thereby obtained for the capture efficiencies Z_i and Z_v for interstitials and vacancies, respectively. When based on linear elasticity, the ratio Z_i/Z_v is the same for both loop types. It is shown as the dashed curve in Fig. 1.

Based on the arguments given above we can include second-order elasticity effects by replacing in the definition for the capture radius c the Burgers vector b_o by its apparent value b(R). In so doing, two different curves of Z_i/Z_v are obtained for the interstitial- and the

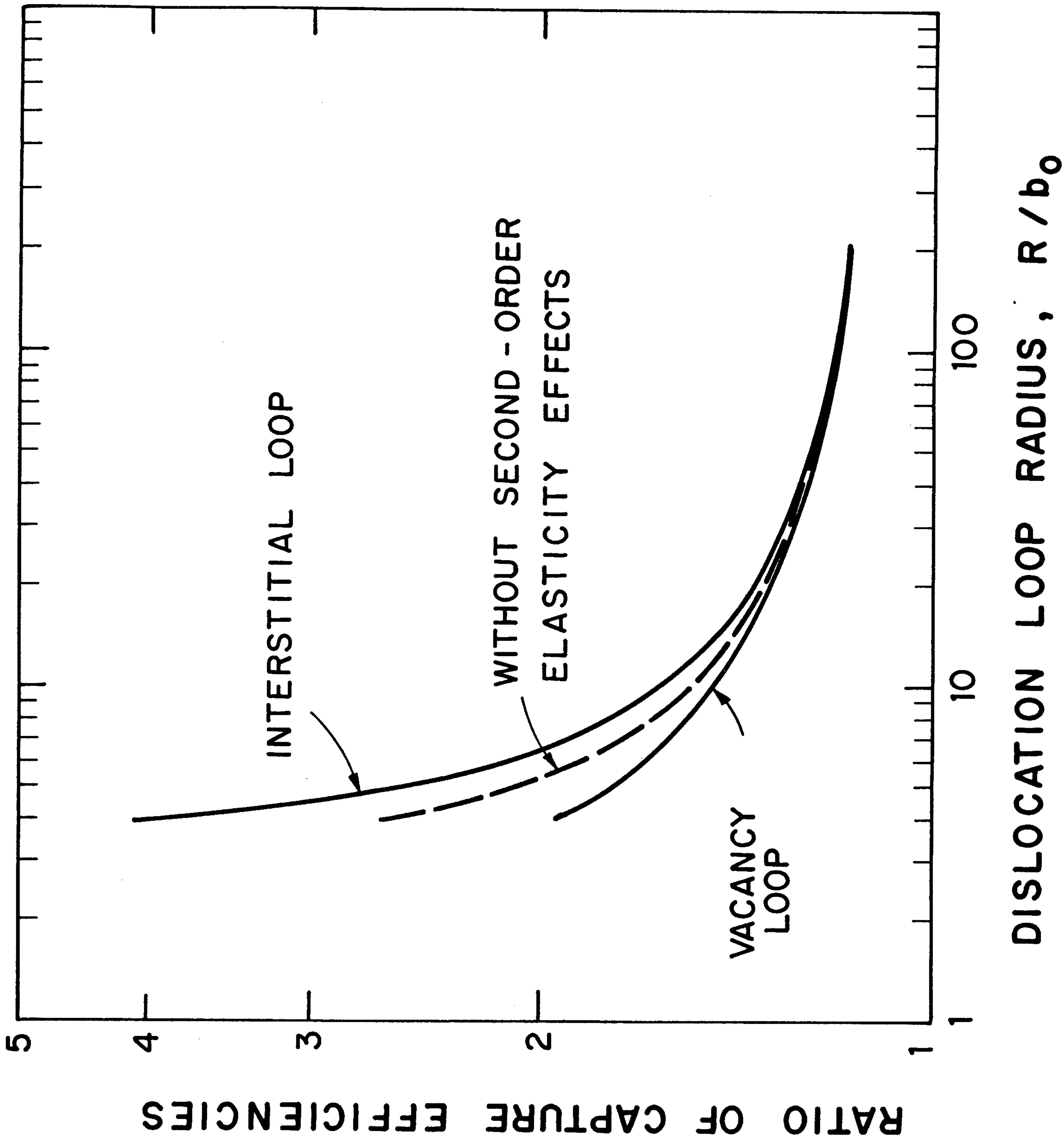

Fig. 1. The ratio of interstitial and vacancy capture efficiencies as a function of the dislocation loop radius.

vacancy-type loop. As seen from Fig. 1, however, the curves converge to one for large loop radii. The results given in Fig. 1 are for Ni and a temperature of 500°C. Similar results are obtained for other metals and temperatures.

Since there exists a bias difference between an interstitial- and a vacancy-type loop of equal radius, both types can indeed coexist, provided no other abundant sink is present whose capture ratio Z_i/Z_v falls below that of the vacancy-type loop. Such favorable conditions are expected to occur only in metals with a low line dislocation density and prior to the onset of void nucleation.

Acknowledgement

The support of this research by the U.S. Department of Energy under contract ER-78-S-02-4861 is gratefully acknowledged.

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