Shape instability of dislocation line in a crystal supersaturated with point defects

L. A. Bol'shov, M. S. Veshchunov, and R. R. Galimov

Institute for Safe Development of Atomic Power
(Submitted 15 October 1991)
Zh. Eksp. Teor. Fiz. **101**, 1581–1598 (May 1992)

Instabilities of the dislocation shapes in crystals supersaturated with intrinsic point defects are theoretically investigated. It is shown that instabilities can develop via two different mechanisms, each of which having a threshold, i.e., they coexist only at sufficiently large supersaturation with point defects. The expressions obtained for the critical supersaturations and for the growth rates of instability developments lead to the conclusion that under the conditions of crystal irradiation the loss of stability of small-radius dislocation loops is substantially faster than that of infinite dislocations. This agrees with experimental observations of dislocations of unusual shape in a high-voltage electron microscope.

1. INTRODUCTION

The onset of inhomogeneous and periodic structures in various substances under nonequilibrium conditions is a well known phenomenon, most frequently observed when the system becomes supercooled. The cellular structure that develops on the phase-transition front of a solidifying alloy and the dendritic growth of crystals are well known examples of this behavior under conditions of sufficient supercooling (of the temperature of "concentration" type[1]). Spinodal decay is of frequently produced in rapidly quenched liquid alloys as a result of development of concentration waves in a crystal of homogeneous composition, and causes stratification of the material. When the cooling rate is increased the substance can go over into a metastable amorphous state.

Similar phenomena can be produced under nonequilibrium conditions by large fluxes of radiation or of particles. Thus, spinodal decay and stratification of alloys can be observed when a solid is irradiated by a sufficiently large neutron flux.[2,3] At very high irradiation the number of defects produced in the material can exceed a critical value and the substance becomes amorphous.[4] Another important phenomenon in irradiated materials is the appearance of periodic lattices of pores or gas bubbles, which can be quite naturally attributed to development of self-organization in a nonequilibrium dissipative system[5] and constitutes a crystal with nonequilibrium point-defect density.[6]

It appears that another example of such a behavior is the onset of dislocation loops of unusual shape in irradiated materials containing many nonequilibrium point defects. Thus, electron-microscope investigations reveal occasional appearance and growth loops in the form of "camomiles" or "rosettes" with "petal" dimensions much smaller than the loop radius.[7-9] Since such a shape is energywise unfavorable for a dislocation with isotropic linear tension, it is of interest to investigate the physical mechanism of its development. It is well known[10,11] that anisotropy of the elastic properties of a crystal can cause the dislocation line to be bent in a shape different from that typical of an isotropic crystal; this form, however, does not differ greatly from a "camomile" and furthermore the degree of anisotropy of the crystal decreases when it is irradiated, while "camomiles" are produced mainly under strong irradiation. In some cases the onset of loops of complicated shape may be due to blocking of the loop growth,[12,13] but no such blocking was observed in the cited experiments[7-9] and such a possibility can apparently be excluded.

In the present paper, in which our earlier results are generalized (see Refs. 14–16), the perturbation of the regular shape of a dislocation line is attributed to the onset of kinetic instability due to absorption of unequal numbers of excess vacancies (and interstitial atoms) by different sections of the dislocation line. In Sec. 2 we consider the case of an infinitely long open dislocation. Its instability has a threshold, i.e., sets in at point-defect densities exceeding a certain critical value. Numerical estimates of this threshold show that such densities can apparently not be reached under the experimental conditions of Refs. 7–9. In addition, we study the influence of the elastic interaction of the dislocation with point defects on the character of the instability of the dislocation shape. Allowance for this interaction decreases substantially the growth rate of the perturbation, while the threshold density of the point defects decreases by at least an order of magnitude.

In Sec. 3 we consider in this connection the influence of finite dimensions of a closed dislocation loop on the instability development mechanism. A new type of instability is produced in this case, and its influence on the shape of the dislocation decreases with increase of the radius of the latter, and vanishes completely in the limit of large dimensions. The threshold density for the development of the shape stability of such loops turns out here to be several orders smaller than in the previously investigated case, and reaches values of experimental order.

2. INSTABILITY OF LINEAR DISLOCATION

Consider a crystal of infinite size, containing straight-line edge dislocations. The vacancy density at the dislocation core is given, according to Ref. 17, by

$$c|_{r_n} = c_e \exp(-E_0/T),$$

where c_e is the thermodynamic-equilibrium density far from the dislocation, T is the temperature (in energy units), and E_0 is the energy of the elastic interaction of the vacancy with the dislocation. If, for one reason or another (quenching or irradiation of the crystal) the average vacancy c far from the dislocation exceeds c_e, the excess vacancies trickle down on the dislocations (one says that the latter serve as sinks for the former), and the result is creeping of the dislocations. It is obvious then that if, firstly, all the dislocations are parallel to

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each other (and to the x axis), secondly, the crystal contains no stoppers or microdefects with a geometry other than cylindrical (pores, dislocation loops, etc.), and thirdly, the vacancy density is independent of x, then we have a planar problem, and all the segments of the dislocation line climb at the same rate. On the other hand, if at least one of the foregoing conditions is violated, different segments of the dislocation line can climb at different rates, and the shape of the dislocation is altered as a result.

All the foregoing conditions are external for any fixed dislocation. The present study, however, just as in Refs. 14–16, deals with "internal" causes of the change of shape, connected with deviation of the initial form of the dislocation from ideal (straight line for an infinite dislocation or circular for a loop of finite size).

We introduce a Cartesian coordinate frame (x,y,z) such that the Burgers vector $\mathbf{b}$ of the dislocation is parallel to the y axis, the points of the dislocation line have at some initial instant of time t_0 the coordinates $Y=0$,

$$Z(t_0,X)=\sum_{n=1}^{\infty}[a_n(t_0)\sin(knX)+b_n(t_0)\cos(knX)]. \quad (1)$$

where a_n and b_n are functions of the time and must be determined, and k is the wave number. The shape of the dislocation is determined by the climb rate of the sections of the dislocation line

$$v(t,X)=v_0(t)+\sum_{n=1}^{\infty}[\dot{a}_n(t)\sin(knX)+\dot{b}_n(t)\cos(knX)]. \quad (2)$$

The vacant density at the core of the dislocation is[17]

$$c|_{r_n}=c_e\exp(-E/T)\exp[FK\Omega/(bT)], \quad (3)$$

where F is the energy of the elastic interaction of the vacancy with the considered dislocation, F and K are respectively the linear tension and the curvature of the dislocation line, Ω, is the atomic volume, and b is the modulus of the dislocation Burgers vector.

The main contribution to E is made by the so-called dimensional interaction, described by the expression[17,15]

$$E=\frac{1}{2}TL\int_{-\infty}^{\infty}\frac{(Z-z)-(X-x)dZ/dX}{[(X-x)^2+y^2+(Z-z)^2]^{3/2}}dX, \quad (4)$$

where

$$L=\frac{1+\nu}{1-\nu}\frac{\mu b\Delta\Omega}{3\pi T},$$

ν and μ are respectively the Poisson coefficient and the shear modulus of the crystal, and $\Delta\Omega$ is the dilatation volume of the vacancy. The integral in (4) can be determined analytically only under strong constraints on the amplitude of the harmonics, viz., a_n, $b_n \ll \rho$, where ρ is the radius of the dislocation core. Since ρ is of the order of (2–3)b, greater physical interest attaches to the opposite case a_n, $b_n > \rho$. We consider therefore first the sampler problem with $E=0$, which describes qualitatively correctly the behavior of the system, and take into account the influence of the elastic interaction of the defects later on.

a) Absence of elastic interaction

In this case Eq. (3) takes the form

$$c|_{r_n}=c_e\exp[FK\Omega/(bT)], \quad (5)$$

and the change of the vacancy density outside the dislocation core is described by the equation

$$\frac{\partial c}{\partial t}=D\Delta c, \quad (6)$$

where D is the vacancy-diffusion coefficient.

The characteristic dimension of the region from which the dislocation draws vacancies is $\tilde{Q}=2D/v_0$ (this will be seen from the solution of the diffusion equation, which has at $r/\tilde{Q}>1$ an exponentially decreasing asymptote). The dislocation velocity is ultimately determined self consistently with the degree of supersaturation $\Delta c=c-c_e$ of the crystal by vacancies:

$$v=\frac{1}{b}\int_s((D\nabla c+c\mathbf{v}),\mathbf{n})ds. \quad (7)$$

where $\mathbf{n}$ and ds are respectively the normal and the surface element ds of the core. Therefore at large supersaturation, when $\tilde{Q}\ll Q$ (where Q is of the order of half the average distance between the dislocations), the external conditions can be written in the form

$$c|_{r=\infty}=\bar{c}. \quad (8)$$

For the opposite case $\tilde{Q}\gg Q$ the external boundary conditions is specified on the surface of a cylinder of radius Q:

$$c|_{r=Q}=\bar{c}. \quad (9)$$

we assume hereafter that $\bar{c}$ is independent of time and consider, unless otherwise stipulated, a steady stage of the process with v_0 constant.

We change to a coordinate frame moving with velocity v_0:$z\to z-v_0t$. Obviously, we can regard the dislocation to be immobile in this system and solve instead of (6) the quasi-stationary continuity equation for the vacancy density

$$\Delta c+2\alpha\frac{\partial c}{\partial z}=0 \quad (10)$$

(where $\alpha=1/\tilde{Q}=v_0/2D$) under the condition that the characteristic time of change of the dislocation shape is much longer than the time of establishment of diffusion equilibrium on its core, i.e., that the following relations hold at $a_n\neq0$ and $b_n\neq0$:

$$\frac{a_n}{\dot{a}_n},\frac{b_n}{\dot{b}_n}\gg\frac{[2\pi/(kn)]^2}{D}. \quad (11)$$

Thus, to obtain the $a_n(t)$ and $b_n(t)$ dependences we must solve Eq. (10) with boundary conditions (5) on the dislocation core and (8) or (9) on the outer boundary of the region.

The curvature (1) of the dislocation line is equal to

$$K=-\sum_{n=1}^{\infty}[(kn)^2(a_n\sin(knX)+b_n\cos(knX))], \quad (12)$$

and the linear tension calculated using Blin's formula[18] can be written in the form

$$F=\frac{\mu b^2}{4\pi(1-\nu)}\ln\frac{H}{\rho}, \tag{13}$$

where H is determined by the ratios of a_n and b_n. We have thus $H\sim Q$ for an unperturbed dislocations and $H=2\pi/km$ for a dislocation with a perturbation wave vector km.

At not too low crystal temperatures and are not too high values of the amplitudes a_n and b_n we get the relation $FK\Omega/bT\ll 1$ and the boundary condition (5) can be written in the form

$$c|_{r_n}=c_e[1+FK\Omega/(bT)]. \tag{14}$$

It is easy to show that if the weak logarithmic dependence of F on a_n or b_n is neglected the diffusion problem formulated above is linear, i.e., all the quantities $\dot a_n$ and $\dot b_n$ are independent, and to determine them if suffices to solve the problem (10), (14), (8), or (9) for a dislocation line having the simple shape

$$Z(t_0, X)=a_n(t_0)\sin(knX), \tag{15}$$

which we shall indeed do, using for simplicity the transformations $kn\to k$ and $a_n\to a$.

At $a=0$ we have a straight dislocation for which the solutions of the sets (10), (14), (8), and (10), (14), (9) are respectively[19]

$$v_0=\frac{2\pi D/b}{\ln 1/\alpha\rho}\Delta c, \tag{16}$$

$$v_0=\frac{2\pi D/b}{\ln Q/\rho}\Delta c. \tag{17}$$

We consider now the case $\rho\ll\tilde Q\ll Q$, assuming $\rho\ll a\ll\lambda$, where $\lambda=2\pi/k$ is the length of the perturbation. Making in (10) the change of variables $\{x,y,z\}\to\{x,y,z-a\sin(kx)\}$ are retaining the terms linear in the parameter $ak\ll 1$, we obtain for the diffusion field the equation

$$\Delta c+2\alpha\frac{\partial c}{\partial z}-2ak\cos(kx)\frac{\partial^2 c}{\partial x\,\partial z}+ak^2\sin(kx)\frac{\partial c}{\partial z}=0. \tag{18}$$

the solution of which in polar coordinates ($r^2=y^2+z^2$, $\theta=\tan^{-1}(z/y)$) is[14]

$$\begin{aligned}
c=\bar c+\exp(-\alpha r\cos\theta)\Big\{&-\Delta c\Big[\frac{I_0(\alpha\rho)}{K_0(\alpha\rho)}K_0(\alpha r)\\
&+2\sum_{m=1}^{\infty}\frac{I_m(\alpha\rho)}{K_m(\alpha\rho)}K_m(\alpha r)\cos(m\theta)\Big]\\
&+ak\sin(kx)\Big\{\Big[c_e d_0 k\frac{I_0(\alpha\rho)}{K_0(\varkappa\rho)}K_0(\varkappa r)\\
&-3\Delta c\frac{\alpha}{k}\Big[\frac{I_0(\alpha\rho)}{K_0(\alpha\rho)}+\frac{I_1(\alpha\rho)}{K_1(\alpha\rho)}\Big]\Big[\frac{K_0(\alpha\rho)}{K_0(\varkappa\rho)}K_0(\varkappa r)-K_0(\alpha r)\Big]\Big]\\
&+\sum_{m=1}^{\infty}\cos(m\theta)\Big[2c_e d_0 k\frac{I_m(\alpha\rho)}{K_m(\varkappa\rho)}K_m(\varkappa r)-3\Delta c\frac{\alpha}{k}\Big[\frac{I_{m-1}(\alpha\rho)}{K_{m-1}(\alpha\rho)}\\
&+2\frac{I_m(\alpha\rho)}{K_m(\alpha\rho)}+\frac{I_{m+1}(\alpha\rho)}{K_{m+1}(\alpha\rho)}\Big]\Big[\frac{K_m(\alpha\rho)}{K_m(\varkappa\rho)}K_m(\varkappa r)-K_m(\alpha r)\Big]\Big]\Big\}\Big\},
\end{aligned} \tag{19}$$

where I_n and K_n are modified Bessel functions,[20] and $d_0=F\Omega/bT$. Substituting (19) in (7) and defining the growth rate ω of the perturbation in the linearized problem as usual by $\dot a/a$ (see, e.g., Ref. 21), we obtain it for the expression

$$\omega=\frac{2D}{\ln 1/\varkappa\rho}\Big[\alpha^2\ln\frac{\varkappa}{\alpha}-\frac{c_e}{4(1-\nu)}\frac{\mu\Omega}{T}k^2\ln\frac{2\pi}{k\rho}\Big], \tag{20}$$

where $\varkappa^2=k^2+\alpha^2$. Returning to the previous designation $k\to kn$, we see that the condition (11) is satisfied if k and n satisfy the relation $kn\gg 2\pi\alpha$, i.e., if the maximum wavelength of the perturbation does not exceed $\tilde Q$.

It follows from (20) that the change, influencing the instability development, of the vacancy flux into the dislocation core is determined by two competing factors. On the one hand, the asymmetry of the vacancy field ahead and behind the creeping dislocation leads to instability when the dislocation line is bent. On the other, the increase of the chemical potential of the vacancies located near the deformed section of the dislocation contributes to an increase of their equilibrium density and eliminates the instability.

It is easily seen that at high velocity, when $\tilde Q\ll Q$, the dislocation motion is always unstable to bending. To determine the threshold of this instability we must therefore consider the opposite case of slow motion ($\tilde Q>Q$). Solving the set (10), (14), and (9) we obtain in this case the following expression for the growth rate:[14]

$$\omega=\frac{2D}{\ln 1/\varkappa\rho}\Big[\alpha^2\ln\varkappa Q-\frac{c_e}{4(1-\nu)}\frac{\mu\Omega}{T}k^2\ln\frac{2\pi}{k\rho}\Big]. \tag{21}$$

It can be concluded from it that the critical supersaturation corresponding to $\omega=0$ is determined as the root of the equation

$$\Big(\frac{\pi\Delta c^*}{b\ln R/\rho}\Big)^2\ln\Big\{Q\Big[k^2+\Big(\frac{\pi\Delta c^*}{b\ln Q/\rho}\Big)^2\Big]^{1/2}\Big\}=\frac{c_e}{4(1-\nu)}\frac{\mu\Omega}{T}k^2\ln\frac{2\pi}{k\rho}.$$

Recognizing that the relation $\alpha\ll k$ holds for a slow dislocation, we get

$$\Delta c^*=\frac{bk}{\pi}\ln\frac{R}{\rho}\Big[\frac{c_e}{4(1-\nu)}\frac{\mu\Omega}{T}\frac{\ln 2\pi/k\rho}{\ln Qk}\Big]^{1/2}. \tag{22}$$

It is known that the diffusion coefficient D_d of the vacancies along a dislocation line is much larger in the immediate vicinity of the line than the vacancy diffusion coefficient D in the bulk of the crystal.[22] This produces a one-dimensional vacancy flux I proportional to the gradient of the chemical potential of the M vacancies located along the dislocation. Recognizing that

$$M(X)=T\ln\frac{c(X)}{c_e},$$

where $c(X)$ is given by Eq. (14), we have

$$I=\pi\rho^2\frac{D_d}{\Omega}\frac{dc(X)}{dX},$$

from which it follows that the diffusion along the dislocation tube becomes substantial for the elimination of the instability at

$$\lambda/\rho\ll 2\pi(D_d/D)^{1/2}.$$

The expression for the growth rate is then[14]

$$\omega = 2D\alpha^2 \frac{\ln \varkappa/\alpha}{\ln 1/\varkappa\rho} - D_d \frac{c_e}{4(1-\nu)} \frac{\mu\Omega}{T} \ln \frac{\lambda}{\rho} k^4\rho^2. \quad (23)$$

We consider now the stability of the system to a perturbation produced by the deviation of v_0 from the stationary state described by Eq. (17). The difference from the earlier treatment is that account must be taken in the computations of the time dependence of the perturbed density field. In the case $\alpha Q \ll 1$ the root of the obtained dispersion relation is $\tilde{\omega} \approx -D\alpha^2$, i.e., the motion of a dislocation having a stationary v_0 is stable. In the second limiting case, $\alpha Q \gg 1$ there exists, alongside the root $\tilde{\omega} \approx -D\alpha^2$, a positive growth rate $\tilde{\omega} \approx D\alpha^2\rho\alpha$. However, by virtue of the condition $\alpha\rho \ll 1$ the instability corresponding to this solution evolves within a time

$$t_1 = \frac{1}{\tilde{\omega}} = \frac{\tilde{Q}^2/D}{\alpha\rho},$$

which is much longer than the characteristic diffusion time $t_2 = \tilde{Q}^2/D$, as does also (under the condition $\lambda \ll 2\pi\tilde{Q}$) the evolution time of the instability to dislocation-line bending, given by the Eq. (20):

$$t_3 = \frac{1}{\omega} = \frac{\tilde{Q}^2}{D} \frac{\ln 1/\varkappa\rho}{\ln \varkappa/\alpha}.$$

The dislocation motion is thus stable to changes of the steady-state velocity v_0.

b) Allowance for elastic interaction

If the perturbation of the dislocation shape is small (if the condition $|Z(X)| \ll \rho$ satisfied in a coordinate frame moving with the dislocation) the right-hand side of (4) can be integrated for any point located in the region $\mathbf{r} \gg \rho$. In this region the expression for the energy of interaction between a vacancy and a dislocation takes the form

$$E = E_0 + \frac{1}{2} TL \sum_{n=1}^{\infty} \{ (kn)^2 [a_n \sin(knx) + b_n \cos(knx)] \times [-K_0(knr) + K_2(knr)\cos(2\theta)] \}, \quad (24)$$

where $E_0 = TL \cos\theta / r$.

Let us write down a continuity equation for the vacancy density in a coordinate frame moving with velocity v_0 (the values of v_0 and $\{\dot{a}_n, \dot{b}_n\}$ can differ in the presence of elastic interaction from those corresponding to the case $E = 0$; our problem is to determine them):

$$\Delta c + 2\alpha \frac{\partial c}{\partial z} + \nabla c \nabla E = 0. \quad (25)$$

It follows from (25), (3), (24), and (8) or (9) that under the condition $(E - E_0) \ll T$ we have again a linear problem, so that the values of $\dot{a}$ and $\dot{b}$ can be determined separately for each fixed n by considering the problem (15) for a dislocation line of simple form.

We make, as before, the notation changes $kn \to k$ and $a_n \to a$ and determine

$$E_1 = E - E_0 = {}^1/_2 TLk^2 a \sin(kx) [-K_0(kr) + K_2(kr)\cos(2\theta)].$$

We write the expression for the density in the form $c = c_0 + c_1$, where c_0 is the solution of the two-dimensional problem for a straight dislocation:

$$\Delta c_0 + \nabla c_0 \nabla E_0 + 2\alpha \frac{\partial c_0}{\partial z} = 0, \quad (26)$$

$$c_0(\rho, \theta) = c_e \exp(-E_0)|_{(\rho,\theta)}, \quad (27)$$

$$c_0(Q, \theta) = \bar{c}, \quad (28)$$

and c_1 is the solution of the three-dimensional problem

$$\Delta c_1 + \nabla c_1 \nabla E_0 + 2\alpha \frac{\partial c_1}{\partial z} = -\nabla c_0 \nabla E_1, \quad (29)$$

$$c_1|_{r_n} = c|_{r_n} - c_0|_{r_n}, \quad (30)$$

$$c_1(x, Q, \theta) = 0. \quad (31)$$

Solving (26)–(28) (see Ref. 23) and (29)–(31) (see Ref. 15) we obtain for the density an equation of the form

$$c = \bar{c} + \exp\left[-\frac{1}{2}\left(\frac{L}{r} + 2\alpha r\right)\cos\theta\right] \times \sum_{m=0}^{\infty} \{ce_m(\theta, q)[\alpha_m Ce_m(\tau, -q) + \beta_m Fek_m(\tau, -q) + ak \sin(kx)\psi_m(r)]\}, \quad (32)$$

where $ce_m(\theta,q)$, $Ce_m(\tau - q)$, and $Fek_m(\tau, -q)$ are regular and modified Mathieu functions,[24] $q = -\alpha L/2$, α_m and β_m are constants determined from the boundary conditions (27) and (28), and $\psi_m(r)$ is the solution of the one-dimensional problem

$$\psi_m'' + \frac{1}{r}\psi_m' - \psi_m\left[\varkappa^2 + \frac{\mathbf{a}_m}{r^2} + \left(\frac{L}{2r^2}\right)^2\right] = \Phi_m(r), \quad (33)$$

$$\psi_m(\rho) = \psi_{m0}, \quad (34)$$

$$\psi_m(Q) = 0, \quad (35)$$

where $\mathbf{a}_m$ is an eigenvalue of the function $ce_m(\theta,q)$, while $\Phi_m(r)\ \psi_{m0} - m$ are the mth terms of the expansions of

$$-[ak\sin(kx)]^{-1}\exp\left[\frac{1}{2}\left(\frac{L}{r} + 2\alpha r\right)\cos\theta\right]\nabla c_0 \nabla E_1$$

and

$$[ak\sin(kx)]^{-1}\exp\left[\frac{1}{2}\left(\frac{L}{\rho} + 2\alpha\rho\right)\cos\theta\right]c_1|_{r_n}$$

in terms of $ce_m(\theta,q)$, respectively.

The rate of creeping of a section of the dislocation line in the presence of elastic interaction with vacancies is determined self-consistently by the expression

$$v = \frac{1}{b}\int_s \left(\left(D\nabla c + Dc\nabla\frac{E}{T} + c\mathbf{v}\right), \mathbf{n}\right) ds. \quad (36)$$

Substituting (32) in (36) and integrating,[15] we readily obtain an equation for the growth rate (it is too complicated to write out here), in which the only known quantity is the derivative $\psi_m'(\rho)$. To determine this derivative, Eq. (33) was solved numerically[15] using boundary conditions (34) and (35).

Figures 1–4 show the dependences of the growth rate on the physical parameters. It was assumed in all computations that $Q = 100b$, corresponding to a dislocation density on the order of $3 \cdot 10^{10}$ cm^{-2}, which is established in metals during the stationary irradiation stage. The characteristic values of the parameters L, c_e, and d_0 were chosen to correspond to

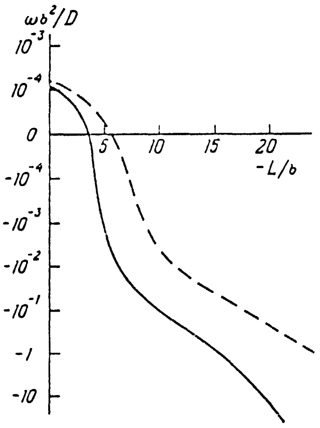

FIG. 1. Growth rate vs intensity of elastic vacancy—dislocation interaction at $\alpha b = 5 \cdot 10^{-3}$ and $\lambda / b = 25$. Solid line—$\rho / b = 2$, dashed $\rho / b = 3$.

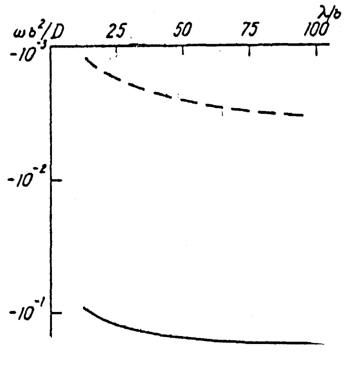

FIG. 3. Growth rate vs wavelength of dislocation line at $\alpha b = 5 \cdot 10^{-3}$ and $\rho = 2b$. Solid line—$L / b = -10$, dashed—$L / b = -5$.

metals in the temperature interval $0.3\, T_m < T < 0.6 T_m$ (T_m is the melting temperature), where the recombination of vacancies and interstitial atoms can be neglected and where radiation-stimulated processes prevail over thermal ones.[26] Figures 1, 3, and 4 correspond to the value $\alpha = 5 \cdot 10^{-3}/b$ deduced from the following considerations: Firstly, it is seen from Fig. 2 that the growth rate becomes positive (meaning instability) only at sufficiently dislocation climb rates (values of α). Secondly, according to (16) the relation between the effective supersaturation of the point defects and α is

$$\Delta c = \alpha b \ln (Q / \rho) / \pi,$$

so that substitution of $Q = 100\rho$ and $\alpha = 5 \cdot 10^{-3}/b$ yields $\Delta c \approx 5 \cdot 10^{-3}$, i.e., very large vacancy supersaturation attainable only at high irradiation intensities.

The computation results can be readily explained qualitatively. The increase of the growth rate with increase of α is an already known phenomenon, due to asymmetry of the field ahead ($z > 0$) and behind ($z < 0$) the vacancy field; this asymmetry is larger the higher the velocity. The decrease of ω with increase of the elastic interaction is made clear by analysis of the character of the vacancy field around an immobile ($\alpha = 0$) linear vacancy.[27] Indeed, it follows from the results of Ref. 27 that the difference between the vacancy flux densities at equal distances in front of and behind the dislocation is negative, and its modulus is larger the larger $|L|$. Thus, the forward segments of the perturbed dislocation line absorb fewer vacancies than the rear ones, bringing them closer together, i.e., decreasing the amplitude of the perturbation. On the other hand, the growth rate increases the core radius because the absolute value of the interaction energy decreases rapidly with increase of the distance from the dislocation line. It can be seen from Fig. 3 that the dependence of the growth rate on the perturbation wavelength is quite weak.

As follows from the figures, elastic interaction between vacancies and an infinite dislocation increases the instability of the latter. Recognizing that a typical value of L of a metal at a temperature $\sim 0.5 T_m$ is 10 b, it is easily seen that the growth rate can become positive only at very high supersaturation, $\Delta c > 10^{-2}$ vacancies per atom, close to the threshold of amorphization of the material by irradiation. In addition, it will be shown in Sec. 3 that allowance for the presence of interstitial atoms in the irradiated material lowers the growth rate further.

It can thus be concluded from the foregoing that the shape of a straight dislocation is stable under the experimental conditions of Refs. 7–9, so that the finite dimensions of the dislocations must be taken into account.

3. INSTABILITY OF A DISLOCATION LOOP

It was noted above that there exist at least two types of "internal" instability produced when the form of the dislocation line deviates from ideal. The first, due to motion of the

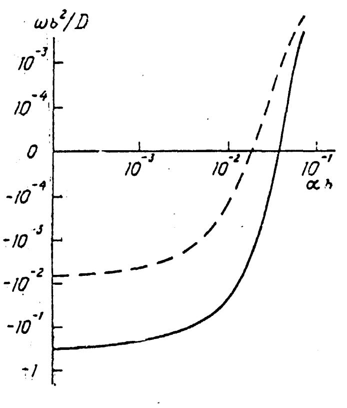

FIG. 2. Growth rate vs dislocation velocity at $\rho / b = 2$ and $\lambda / b = 25$. Solid line—$L / b = -10$, dashed—$L / b = -5$.

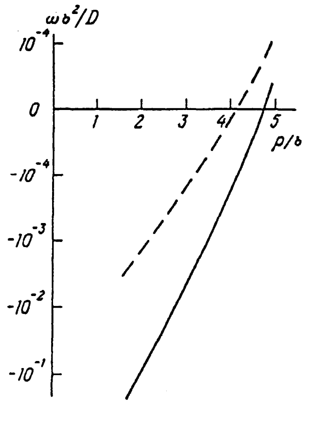

FIG. 4. Growth rate vs dislocation-core radius at $\alpha b = 5 \cdot 10^{-3}$ and $\lambda / b = 25$. Solid line—$L / b = -10$, dashed—$L / b = -5$.

dislocation as a whole ($v_0 \neq 0$) was investigated in the preceding section. We shall find it convenient to study the second using the example of prismatic dislocation loops. Recognizing that the influence of the elastic interaction decreases with the loop radius[28] (owing to the overlap of elastic fields of opposite sign from different dislocation segments), we assume hereafter $E = 0$.

Consider a dislocation loop of the vacancy type (interstitial loops will be discussed at the end of the section) with the Burgers vector perpendicular to the plane of the loop and with a distance from the points of the axis at the initial instant of time to the center of the loop

$$P(t_0, \varphi) = R(t_0) + \sum_{n=1}^{\infty} (a_n(t_0)\sin(n\varphi) + b_n(t_0)\cos(n\varphi)), \quad (37)$$

where R is the radius of the loop and φ is the polar angle. We assume that $a_n(t_0)$ and $b_n(t_0)$ for all n are such that in the considered time interval we have the following relations:

$$na_n,\ nb_n \ll R. \quad (38)$$

The dislocation climb rate is

$$v(t, \varphi) = v_0(t) + \sum_{n=1}^{\infty} (\dot{a}_n(t)\sin(n\varphi) + \dot{b}_n(t)\cos(n\varphi)). \quad (39)$$

The vacancy density at the points of the loop core is specified by expression (14), with the curvature and linear tension defined, accurate to terms of second order of smallness, by

$$K = \frac{1}{R}\left\{1 + \frac{1}{R}\sum_{n=1}^{\infty} [(n^2-1)(a_n \sin(n\varphi) + b_n \cos(n\varphi))]\right\}. \quad (40)$$

$$F = \frac{\mu b^2}{4\pi(1-\nu)} \ln\frac{4R}{\rho}. \quad (41)$$

Note that (41) was obtained under the assumption that the relations

$$\dot{a}_n/a_n,\ \dot{b}_n/b_n \ll v_0/R.$$

hold for all $a_n \neq 0$ and $b_n \neq 0$. It will be clear from the solution of the problem that these conditions are violated at sufficiently high supersaturation of the crystal by vacancies. However, as in the case of a straight-line dislocation [see Eq. (16)], this leads only to a very insignificant change (decrease) of F, with practically no effect on the final results.

Let us carry out the calculation for the largest loop growth rates, when the time to establish a quasistationary vacancy density is much shorter than the characteristic time of change of the loop's geometric parameters. In this approximation, which will be corroborated below, the vacancy distribution is described by the Laplace equation

$$\Delta c = 0. \quad (42)$$

In view of the obvious linearity of the formulated problem, we shall investigate below the solution for a loop of simple shape

$$P(t_0, \varphi) = R(t_0) + a_n(t_0)\sin(n\varphi), \quad (43)$$

where the number of lobes obeys relations (38) and

$$n \ll R/\rho. \quad (44)$$

The external boundary condition is chosen initially in the form (8).

Let the z axis of the Cartesian frame (x,y,z) (at the center of the loop) be perpendicular to the plane of the loop. We introduce a curvilinear coordinate system (φ,ξ,γ) such that

$$x = [R + a_n \sin(n\varphi) + \xi\cos\gamma]\cos\varphi,$$
$$y = [R + a_n \sin(n\varphi) + \xi\cos\gamma]\sin\varphi, \quad z = \xi\sin\gamma. \quad (45)$$

The coordinates of the core points are here (φ,ρ,γ).

We solve the system (42), (14), and (8) by the potential method,[29] placing a filament with a "charge" density

$$q_n(\varphi) = A_0 + A_n \sin n\varphi$$

along the loop axis ($\xi = 0$). The vacancy density at any point (x,y,z) outside the core is equal, accurate to a constant $\bar{c}$, to the potential produced by the filament at this point: $c = \bar{c} + V$, where

$$V = \int_0^{2\pi} \frac{(A_0 + A_n \sin n\psi)\, d\psi}{\{[x - (R + a_n \sin n\psi)\cos\psi]^2 + [y - (R + a_n \sin n\psi)\sin\psi]^2 + z^2\}^{1/2}}. \quad (46)$$

The constants A_0 and A_n are determined from the boundary condition (14). In particular, at $a_n = 0$ (i.e., in the case of an undeformed loop), we get

$$A_n = 0, \quad A_0 = (c_R - \bar{c})\frac{R}{2}\ln\frac{8R}{\rho},$$

and obtain the known relation[30]

$$c = \bar{c} - \frac{\bar{c} - c_R}{\ln 8R/\rho}\frac{2R}{r_1}K(k),$$

where

$$c_R = c_e\left(1 + \frac{d_0}{R}\right), \quad d_0 = \frac{F\Omega}{bT}, \quad k^2 = \frac{r_1^2 - r_2^2}{r_1^2},$$

r_1 and r_2 are the longest and shortest distances from the observation point to the loop axis, and $K(k)$ is a complete elliptic integral.[13]

Substituting in (46) expressions (45) for x, y, and z, expanding (46) in a series of elliptic integrals, and using the expressions[20] for the limits of the latter as $k \to 1$, we find from the boundary condition (14) that the expression given above is valid for A_0, and that A_n is given by

$$A_n = -\frac{(\bar{c} - c_R)\ln(R/\rho n^{1/2})/\ln(8R/\rho) - (n^2-1)(d_0/R)c_e}{2\ln R/n\rho}. \quad (47)$$

Substituting this solution in (7), we obtain finally the following expressions for the rate of change of the average loop radius and for the growth rate $\omega_n = \dot{a}_n/a_n$ of the perturbation:

$$v_0 = \frac{2\pi D/b}{\ln 8R/\rho}(\bar{c}-c_R). \tag{48}$$

$$\omega_n = \frac{2\pi D/b}{\ln 8R/\rho}\frac{\bar{c}-c_R}{R}(\tau_n-\eta_n). \tag{49}$$

where

$$\tau_n = \frac{\ln n}{2\ln R/n\rho}, \qquad \eta_n=(n^2-1)\frac{d_0}{R}\frac{\ln 8R/\rho}{\ln R/n\rho}\frac{c_e}{\bar{c}-c_R}. \tag{50}$$

Expression (48) confirms the validity of using in (42) a quasistationary approximation for loops that are not too large. In fact, it follows from (48) that the characteristic diffusion time $(2R)^2/D$ is much shorter than the time R/v_0 necessary for a noticeable increase of the loop radius, for arbitrary vacancy-supersaturation levels satisfying the condition $\Delta c \ll b/(8\pi R)$. Thus, if the loop radius is $R \leqslant 100\, b$, Eq. (42) is valid for $\Delta c \leqslant 10^{-4}$ vacancies per atom. Furthermore, comparing the growth rates (49) and (20) corresponding to like values of λ, it is easily seen that at a loop radius $R \leqslant 10^2\, b$ and for crystal supersaturation by vacancies $\Delta c \leqslant 10^{-3}$ the amplitude of the perturbation increases considerably faster than in the case of infinite dislocations. This means that practically under all irradiation conditions, allowance for the climb of a small loop in the diffusion equation for point defects can lead only to an insignificant increase of the growth rate (49).

It follows from (49) that the direction of the development of the dislocation-loop shape is determined by the ratio of τ_n and η_n. The second of these quantities can be easily seen from (50) to be governed by linear tension and to make a negative contribution to the growth rate. The first term τ_n, however, is positive for any number $n \geqslant 2$ of lobes satisfying the conditions (38) and (44). The nature of this term is governed by the asymmetry of the geometric locations of the "convex" and "concave" sections of the deformed dislocation loop. Roughly speaking, loop sections closer to the center are located in a region with a high density of drains (if drains are taken to mean sections of the dislocation loop), and those farther from the center are in regions with lower drain density. The effect of absorption of a large number of point defects by drains in "rarefied" regions compared with drains in "dense regions" is well known (see, e.g, Refs. 19 and 31 for ensembles of straight parallel dislocations).

From (48) and (49) follow expressions for the relative growth rates of the geometric parameters of the loop:

$$\frac{\partial a_n}{\partial R} = \frac{a_n}{R}(\tau_n-\eta_n), \tag{51}$$

$$\frac{\partial (a_n/R)}{\partial R} = \frac{a_n}{R^2}(\tau_n-1-\eta_n), \tag{52}$$

from which it can be seen that an instability called absolute[32] (the perturbation amplitude increases when the loop grows) is present when $\tau_n > \eta_n$, as against a relative instability (the amplitude increases faster than the radius) is present at $\tau_n > (1+\eta_n)$.

The critical supersaturation Δc_n^* corresponding to a growth rate $\omega_n = 0$, is equal to

$$\Delta c_n^* = \frac{n^2-1}{\ln n}\frac{2d_0 \ln 8R/\rho}{R}c_e. \tag{53}$$

It is independent of the perturbation amplitude, decreases slowly with increase of the loop radius, and increases with increase of the number of lobes [but is never very large by virtue of Eqs. (38) and (44)]. The condition under which ω_n is positive is $\Delta c > \Delta c_n^*$. When the crystal is irradiated, the harmonic numbered $n=2$ is the first to develop in the dislocation loop, and this takes place when the supersaturation

$$\Delta c^* = \frac{3}{\ln 2}\frac{2d_0 \ln 8R/\rho}{R}c_e. \tag{54}$$

is exceeded.

The loop critical radius R_n^*, such that at $R > R_n^*$ the amplitude a_n increases, is given by

$$\frac{R_n^*}{\ln(4R_n^*/\rho)\ln(8R_n^*/\rho)} = \frac{b}{2\pi(1-\nu)}\frac{\mu\Omega}{T}\frac{n^2-1}{\ln n}\frac{c_e}{\Delta c}. \tag{55}$$

R_n^* increases rapidly with increase of the number of the harmonic, and decreases slowly with increase of the supersaturation of the crystal by vacancies. Recall that according to Ref. 30 the critical radius of a growing loop (which is not deformed) is given by

$$\frac{R_{cr}}{\ln 4R_{cr}/\rho} = \frac{b}{4\pi(1-\nu)}\frac{\mu\Omega}{T}\frac{c_e}{\Delta c}.$$

Comparison of the last equation with (55) shows readily that the relation $R_n^* > R_{cr}$ is valid for any number of lobes $n \geqslant 2$, i.e., growth of the loop radius is a necessary but not sufficient condition for stability of its shape. The minimum loop dimension at which the amplitude of at least one harmonic is increased is determined from the equality

$$\frac{R}{\ln(4R^*/\rho)\ln(8R^*/\rho)} = \frac{b}{2\pi(1-\nu)}\frac{\mu\Omega}{T}\frac{3}{\ln 2}\frac{c_e}{\Delta c}. \tag{56}$$

We consider now the case of large supersaturation of a crystal by vacancies

$$\Delta c \gg (n^2-1)\frac{d_0}{R}\frac{2\ln 8R/\rho}{\ln n}c_e, \tag{57}$$

when one can neglect the terms η_n in the equation for the growth rate and write it in the form

$$\omega_n = \frac{2\pi D/b}{\ln 8R/\rho}\frac{\tau_n}{R}\Delta c. \tag{58}$$

It follows from (58) that at sufficient supersaturation the growth rate is independent of either the linear tension or the character of the dislocation density distribution on the core of the dislocation loop.

For those supersaturations at which (57) is valid one can neglect the terms η_n also in Eqs. (51) and (52); it follows hence that satisfaction of the relations (38), (44), and (57) always leads to absolute instability, as well as a relative instability if the inequality $\tau_n > 1$ holds. When (57) is satisfied, the perturbation amplitude takes as a function of the loop size the simple form

$$a_n = a_n(t_0)\left[\frac{\ln R/n\rho}{\ln R(t_0)/n\rho}\right]^{1/2\ln n}, \tag{59}$$

from which it follows that for loops of equal radius the amplitude increases monotonically with increase of the number of lobes. According to (38) and (44), however, the number of lobes cannot be too large (for otherwise the solution of the problem changes). It can therefore be assumed that to each value of R there corresponds a definite quite large but finite "optimal" number of lobes. It follows from (59) that when the crystal is highly supersaturated with vacancies the perturbation amplitude corresponding to some limiting dimension R of the growing loop does not depend on the supersaturation and is determined, given the initial values of $R(t_0)$ and $a_n(t_0)$, only by the dimension ρ of the loop core and by the number n of lobes.

By way of example let us find the perturbation-amplitude change corresponding to a fivefold increase of the loop radius $[R = 5R(t_0)]$, at the parameter values $\rho = 3b$, $n = 15$, $R(t_0) = 100\,b$ satisfying (38) and (44) and corresponding approximately to see the experiments of Refs. 7–9. Substitution of these values in (59) yields $a_n/a_n(t_0) = 4.5$, i.e., the amplitude is increased by approximately the same factor as the radius. An estimate according to (57) shows that to satisfy the validity of the obtained value of $[a_n/a_n(t_0)]$ at a temperature equal to half the melting temperature of the crystal the supersaturation should be not less than $\Delta c \sim 300\, c_e$, which for metals is of the order of 10^{-6} vacancies per atom. This supersaturation level was certainly achieved in the cited experiments. Note that the conditions (38) and (44) prevent us from considering large values of $a_n(t_0)$, but even at $a_n(t_0) = 3b$ we obtain $a_n = 14\,b$, i.e., a value fully sufficient to observe a perturbation of the loop shape in an electron microscope.

When account is taken of the presence in the crystal of other drains (besides the considered loop) via replacing the boundary condition (8) by (9) (where Q is the sphere radius), and if the relation $Q \gg R$ is valid, the field of vacancy density near the loop (at $r \leqslant R$), as well as the rate of increase of its radius and the growth rate, are determined (accurate to second-order terms) by the earlier equations in which we substitute $\bar{c}$ defined as

$$\bar{c} = \tilde{c} + (\tilde{c} - c_R)\frac{\pi R/Q}{\ln 8R/\rho - \pi R/Q}, \tag{60}$$

where $\tilde{c}$ is determined from the vacancy-balance equation.[33]

Obviously, for an interstitial dislocation loop in a crystal supersaturated with vacancies, the earlier expression (49) for the growth rate remains valid if the sign of τ_n is reversed, that is to say, the loop is stable. The same stability conclusion is valid for a vacancy loop in a crystal supersaturated with interstices, even if one disregards the strong elastic interaction of the loop with the interstitial atoms (approximately double the interaction with the vacancies). However, for an interstitial loop in a crystal supersaturated with interstitial atoms the signs of its growth rate will coincide with signs in Eq. (49). Moreover, by virtue of the exceedingly small thermodynamic-equilibrium interstice density c_e (Ref. 19) we can neglect the term η_n, and the growth rate might seem to be positive for any supersaturation. In fact, however, the high energy of the elastic interaction with the interstices causes the growth rate of an interstice loop in a crystal supersaturated with interstitial atoms to be smaller [at like values of $D\Delta c$] of the growth rate of a vacancy loop in a crystal supersaturated with vacancies. Note that crystals supersaturated simultaneously by vacancies and interstices have not been considered in the present section. This situation is discussed in Sec. 3.

It follows from the very nature of the instability due to asymmetry of the geometric arrangement of the various segments of the dislocation line that the line should be so widespread rather than a distinguishing feature of closed loops of simple form; in particular, instability can set in on individual segments of dislocations having a sufficiently large local curvature. This instability can result in an increase of the dislocation density due to dislocation-line bending.

4. ALLOWANCE FOR INTERSTITIAL ATOMS

Up to now we have dealt mainly with an idealized situation with only vacancies as the point defects in the crystal and with no interstitial atoms. Usually (e.g., following irradiation), however, excess vacancies as well as excess interstices are produced in a crystal. In this case both the average climb rate of the dislocation-line segments and the average instability growth rate increase. This has in general two causes: first, the mutual recombination lowers the supersaturation levels of both types of point defect, and second, the absorption of interstitial atoms by a segment of a dislocation line produces a climb in a direction opposite to that corresponding to vacancy absorption. As noted above, at temperatures $T > 0.3T_m$ (which are typical for materials in the active zone of a reactor) the recombination can be neglected. The continuity equations for the vacancy and interstice densities are therefore independent and linear. For simplicity, we disregard here in the calculation of the growth rates the elastic interaction of the point defects with the dislocations.

We denote the relative difference between the average dislocation and interstitial-atom fluxes (called "preference") to a dislocation (infinite of closed) by $B = (J_v - J_1)/J_v$. It is easily seen that the average climb rate of the dislocation-line sections, for both slow and fast motion, is given with good accuracy by

$$v_0 = Bv_{0v}, \tag{61}$$

where v_{0v} is the climb rate in the absence of interstitial atoms.

The expression for the growth rate of a fast infinite dislocation is

$$\omega = 2\pi\Bigg\{\frac{v_0}{2b}\Bigg[(\bar{c}_v - c_{rv})\frac{\ln \varkappa_v/\alpha_v}{\ln(1/\rho\varkappa_v)\ln(1/\rho\alpha_v)} - \bar{c}_i\frac{\ln \varkappa_i R}{\ln(1/\rho\varkappa_i)\ln(1/\rho\alpha_i)}\Bigg] - \frac{1}{4\pi(1-\nu)}\frac{\mu\Omega}{T}k^2\ln\frac{2\pi}{k\rho}\frac{D_v c_{rv}}{\ln 1/\rho\varkappa_v}\Bigg\}, \tag{62}$$

where

$$\alpha_{v,i} = \frac{v_0}{2D_{v,i}}, \qquad \varkappa_{v,i}^2 = k^2 + \alpha_{v,i}^2.$$

It is taken into account in (62) that, firstly, the equilibrium density of the interstitial atoms is negligibly small and, secondly, that under real conditions the relation $v_0 \gg 2D_i/Q$ is never satisfied. Taking into account (62) and the fact that we always have $\Delta c_v \gg \Delta c_i$, we can write

$$\omega = B\omega_v, \tag{63}$$

where ω_v corresponds to absence of interstitial atoms. Since the dislocation preference can reach an order of 10%,[33] expression (63) can serve as an additional confirmation of the validity of the conclusion drawn in Sec. 2, that the shape of a linear dislocation is stable.

Using Eqs. (48)–(50), we can readily show that if the preference of a finite-radius dislocation loop amounts to

$$B \gg 2(n^2-1)\frac{\ln 8R/\rho}{\ln n}\frac{d_0}{R}\frac{c_{rv}}{\bar{c}_v-c_{R\tau}}, \qquad (64)$$

then allowance for the presence of excess interstitial atoms in the crystal leads to an expression similar to (63) for the growth rate:

$$\omega_n = B\omega_{nv}, \qquad (65)$$

where ω_{nv} corresponds to the absence of interstices. The earlier dependence (59) of the amplitude on the loop radius remains therefore in force.

Assume a number of lobes $n\sim 10$, a radius $R\sim 100/b$, and a loop preference $B\sim 10\%$. It is easily seen then from (64) that expression (59) remains in force only at a sufficient supersaturation $\Delta c_v > 10^4\, c_{rv}$ of the crystal by vacancies. However, to satisfy the less stringent condition $\omega_h > 0$ at the same values of the problem parameters it suffices to have a supersaturation lower by at least an order of magnitude. Thus, the presence of interstitial atoms in the crystal raises somewhat the threshold vacancy density corresponding to the onset of the instability of the dislocation-loop shape.

5. CONCLUSION

We investigated the conditions for the development of shape instability of dislocation lines in crystals supersaturated with point defects; two different mechanisms of the development of this instability were studied.

We have shown that the first mechanism, which ensures a change of the shape of a linear dislocation, is connected with absorption of unequal amounts of excess vacancies by different segments of a dislocation climbing with sufficient speed.

The action of the second mechanism, present in loops of finite radius, is also connected with nonuniform absorption of point defects by different sections of a dislocation line. Compared with the first, however, this mechanism ensures an onset of instability at substantially lower climb rates and is determined by the asymmetry of the point-defect density fields inside and outside the dislocation loop.

We have shown that both types of instability have thresholds, i.e., are produced only when definite critical values of the supersaturation of the crystal by point defects and (or) of the loop radius. The critical supersaturation for loops decreases slowly with increase of their radius and increases rapidly with the number of the harmonic (the number n of the lobes), whereas the critical radius decreases slowly with increase of the supersaturation and increases rapidly with increase of n. The expressions obtained for the critical supersaturation agree with the experimental data on the observation of "camomile" loops.

The results have been generalized to allow for the influence of factors such as the presence of elastic interaction with point defects, tubular diffusion along a dislocation, preference (i.e., preferred absorption of one type of point defect over others) and the presence of many extended defects in the crystal.

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Translated by J. G. Adashko