CIRCULAR EDGE DISLOCATION LOOP

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A solution of the stress, deformation and deformation energy is given for an edge dislocation with its dislocation line having the shape of a circle in an unlimited isotropic medium. The possibility of using this solution in studying the dislocation loop in a crystal is discussed.

КРУГОВАЯ ПЕТЛЯ ЛИНЕЙНОЙ ДИСЛОКАЦИИ

Дано решение напряжений, деформации и энергии деформации для линейной дислокации с линией дислокации в форме окружности в неограниченной изотропной среде. Дискутируется возможность использовать это решение при исследовании дислокационной петли в кристалле.

INTRODUCTION

Increased attention has recently been paid to the formation of small dislocation loops in crystals by the condensation of vacancies and the collapse of the surfaces of the flat cavity produced. It was found that such loops, produced particularly after quenching [1], can play an important part for example as slip nuclei [2], in the formation of dislocation networks [3], in the production of nuclei of a brittle fracture [4] etc. When considering these loops it is important to know the stresses, deformations and deformation energy caused by them.

In a crystal the plane of the loop is a certain important crystallographic plane and its dislocation line is formed from the straight section of important crystallographic directions. For the sake of simplicity, we shall consider the circular dislocation loop according to Fig. 1 in a continuous medium.

A related problem was dealt with by Franz and Kröner [5] when studying the stability of Guinier-Preston zones; using the method of continuous distribution of dislocations [6] they derived an approximate expression for the deformation energy of a circular dislocation loop.

It is stated in Kröner's book [6] that as yet unpublished papers by Pfleiderer and Keller also deal with the problems of dislocation loops from the point of view of continuous distribution of the dislocations. Questions of the interaction energy of circular dislocation loops are solved from the same aspect by de Wit [7]. A simplified expression for the energy of a circular dislocation loop is given in the book by Read [8]. In an earlier paper, Nabarro [9] studied the field of stresses of an infinitesimal dislocation loop for the different case of a Burgers vector lying in the plane of the loop.

When studying a circular dislocation loop it is not necessary to start out from the theory of the continuous distribution of dislocations but we can start from the classical theory of elasticity. For example, the general Burgers relation [10] can be used for a dislocation loop of arbitrary shape but the calculation is very complicated.

In the present paper we therefore use a different procedure for calculating the stresses, deformations and deformation energy of a circular dislocation loop, whereby we employ the symmetry of the whole problem with respect to the plane of the loop $z = 0$. Calculation is carried out for half-space $z > 0$ and the boundary condition on the plane $z = 0$ is chosen so that the solution corresponds to a circular dislocation loop located in unlimited space.

We shall then discuss the possibility of using the results, valid for a continuous medium on the assumptions of the classical theory of elasticity, for investigating dislocation loops in a crystal.

FORMULATION OF PROBLEM

We give the solution of the following problem of the classical mathematical theory of elasticity:

Problem 1: In an unlimited medium there is a Volterra edge dislocation with dislocation line having the shape of a circle and with Burgers vector normal to the plane of the circle. The components of the stress tensor, displacement vector and deformation energy, are to be determined.

The cylindrical coordinates are denoted by r, ϑ, z, and the dislocation line is chosen in the plane $z = 0$ as a circle with radius R, with the centre in the origin of the coordinates (Fig. 1). The Burgers vector has only one non-zero component in the direction of the z axis denoted by b. The components of the stress tensor in the cylindrical coordinates are further denoted by σ_r, σ_ϑ, σ_z, $\tau_{r\vartheta}$, τ_{rz}, $\tau_{\vartheta z}$, and the components of the displacement vector by u_r, u_ϑ, u_z. The medium is characterized by the shear modulus μ and by the Poisson constant σ.

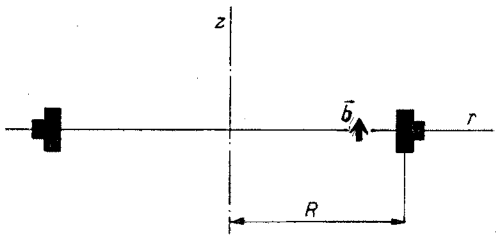

Fig. 1. Circular dislocation loop.

Since the problem is one with cylindrical symmetry, the solution does not depend on ϑ.

A circular dislocation loop as in Fig. 1 can be formed by taking out a thin circular plate of thickness b and radius R and then bringing together and joining the two circular bases of the cavity thus formed; the bases must be shifted in the z direction by $\frac{1}{2}b$ and $-\frac{1}{2}b$. We thus obtain continuous material in the $z = 0$ plane except for a singular dislocation line.

Due to the symmetry of the solution with respect to the plane $z = 0$, we can then carry out the solution only for the upper half-space with a boundary condition on the plane $z = 0$ for a displacement u_z; a supplementary condition must then ensure the symmetry and continuous transition of the solution into the lower half-space. The following problem is equivalent to problem 1.

Problem 2: To find a solution for the half-space $z > 0$ with the following mixed boundary condition:

$$(1) \qquad z = 0: \quad \text{for} \quad 0 \leqq r < R \ldots u_z(r, 0) = -\tfrac{1}{2}b\,, \qquad \text{for} \quad r > R \ldots u_z(r, 0) = 0\,;$$

$$(2) \qquad z = 0: \qquad \tau_{rz}(r, 0) = 0\,.$$

Condition (2) for a shear stress τ_{rz} ensures the required symmetry and continuous transition to the lower half-space. The solution of problem 2, for which the components of stress and displacement approach zero for $z \to \infty$ and $r \to \infty$, is the only one and is simultaneously the solution of problem 1.

CALCULATION OF STRESS AND DEFORMATION

The method of Hankel transformation, elaborated for cylindrically symmetrical problems of the theory of elasticity in Sneddon's book [11], is used to solve problem 2. Instead of the biharmonic stress function $\Phi(r, z)$, used earlier in solving cylindrically symmetrical problems, the stress function $G(\xi, z)$ is introduced as its Hankel transformation of zero order

$$G(\xi, z) = \int_0^\infty r\Phi(r, z)\, J_0(\xi, r)\, \mathrm{d}r\,, \tag{3}$$

where J_0 is the Bessel function of zero order. The stress and displacement components are expressed directly in [11] by means of the function G. It is thus possible to express the boundary conditions for the stress and displacement as conditions for the function $G(\xi, z)$.

It is further shown that the function $G(\xi, z)$ has the general form

$$G(\xi, z) = [A(\xi) + B(\xi)\, z]\, \mathrm{e}^{-\xi z} + [C(\xi) + D(\xi)\, z]\, \mathrm{e}^{\xi z} \tag{4}$$

where A, B, C and D are generally functions of the parameter ξ. The solution of the problem then becomes the determination of these four functions from the boundary conditions.

The following relations are obtained from the requirement of zero values of the stress and displacement for $z \to \infty$

$$C(\xi) = D(\xi) \equiv 0\,; \tag{5}$$

the boundary condition (2) for shear stress τ_{rz} gives the relation between $A(\xi)$ and $B(\xi)$ so that according to [11]

$$G(\xi, z) = \frac{B(\xi)}{\xi}\,(2\sigma + \xi z)\, \mathrm{e}^{-\xi z}\,. \tag{6}$$

The remaining unknown function $B(\xi)$ is determined from boundary condition (1) for displacement u_z. For this displacement it holds, according to [11], that

$$u_z(r, z) = \int_0^\infty \xi \left[\frac{\mathrm{d}^2 G}{\mathrm{d}z^2} - \frac{2(1-\sigma)}{1-2\sigma}\,\xi^2 G\right] J_0(\xi r)\, \mathrm{d}\xi\,. \tag{7}$$

By substituting this relation into boundary condition (1) and introducing the non-dimensional arguments

$$\varrho = \frac{r}{R}\,, \quad t = \xi R \tag{8}$$

and denoting

$$f(t) = B\left(\frac{t}{R}\right) t^2\,, \tag{9}$$

$$a = \frac{1-2\sigma}{4(1-\sigma)}\, R^3 b \tag{10}$$

we obtain the condition for the unknown function $f(t)$,

$$\int_0^\infty f(t)\, J_0(t\varrho)\, \mathrm{d}t = a \quad \text{for} \quad 0 \leqq \varrho < 1\,, \tag{11}$$

$$\int_0^\infty f(t)\, J_0(t\varrho)\, \mathrm{d}t = 0 \quad \text{for} \quad \varrho > 1\,.$$

By means of the inverse Hankel transformation we obtain (e.g. from the tables of Hankel transformations in [11])

$$f(t) = aJ_1(t)\,, \tag{12}$$

where J_1 is the Bessel function of the first order.

After substituting into relation (9) we can thus determine the sought function $B(\xi)$

$$B(\xi) = \frac{a}{\xi^2 R^2} J_1(\xi R)\,. \tag{13}$$

The stress function $G(\xi, z)$ is thus also determined according to Eq. (6) and the problem is solved.

By means of the general relations between the stress and displacement components and the stress function $G(\xi, z)$ given in [11] (one of them has already been used as Eq. (7)) we then calculate the required stress and displacement components if, for the sake of brevity, the following is introduced

$$I_m^n(\varrho, \zeta) = \int_0^\infty t^n J_m(t\varrho)\, J_1(t)\, \mathrm{e}^{-t\zeta}\, \mathrm{d}t\,, \qquad \zeta = z/R\,. \tag{14}$$

We then obtain for the stress components

$$\begin{aligned}
\sigma_z(\varrho, \zeta) &= \frac{b}{R}\frac{\mu}{2(1-\sigma)}\left[I_0^1 - \zeta I_0^2 - \frac{1-2\sigma}{\varrho} I_1^0 + \frac{\zeta}{\varrho} I_1^1\right],\\
\sigma_\vartheta(\varrho, \zeta) &= \frac{b}{R}\frac{\mu}{2(1-\sigma)}\left[\frac{1-2\sigma}{\varrho} I_1^0 - \frac{\zeta}{\varrho} I_1^1 + 2\sigma I_0^1\right],\\
\sigma_z(\varrho, \zeta) &= \frac{b}{R}\frac{\mu}{2(1-\sigma)}\left[I_0^1 + \zeta I_0^2\right],\\
\tau_{rz}(\varrho, \zeta) &= \frac{b}{R}\frac{\mu}{2(1-\sigma)}\,\zeta I_1^2\,,\\
\tau_{r\vartheta}(\varrho, \zeta) &= 0\,,\\
\tau_{\vartheta z}(\varrho, \zeta) &= 0
\end{aligned} \tag{15}$$

and for the displacement components

$$\begin{aligned}
u_r(\varrho, \zeta) &= \frac{b}{4(1-\sigma)}\left[(1-2\sigma)\, I_1^0 - \zeta I_1^1\right],\\
u_z(\varrho, \zeta) &= -\frac{b}{4(1-\sigma)}\left[2(1-\sigma)\, I_0^0 + \zeta I_0^1\right],\\
u_\vartheta(\varrho, \zeta) &= 0\,.
\end{aligned} \tag{16}$$

These components obviously satisfy the boundary condition for u_z and τ_{rz} and the conditions at infinity and are thus the only solution of our problem.

The stress and displacement components are expressed in Eqs. (15) and (16) by means of six integrals of the type (14) for $m = 0, 1$ and $n = 0, 1, 2$, which due to the term $\mathrm{e}^{-t\zeta}$ may be considered as Laplace transformations of the function $t^n J_m(t\varrho)\, J_1(t)$ with the variable t and parameter ϱ. In order to calculate the stresses numerically either numerical calculation of these integrals can be carried out or they can be expressed by means of hypergeometric functions, or by means of elliptic integrals. We carry out this calculation for two of the physically most interesting stress components, the shear stress on a slip cylinder $r = R$, i.e. for $\tau_{rz}(1, \zeta)$, and for normal stress on the plane of symmetry $z = 0$, i.e. for $\sigma_z(\varrho, 0)$. From Eqs. (15) we obtain after lengthy calculation using the relations for the integrals from the Bessel functions [12] and the relations for hypergeometric functions and their connection with complete elliptic integrals (given e.g. in [13]):

$$(17)\qquad \frac{\tau_{rz}(1, \zeta)}{\dfrac{b}{R}\dfrac{\mu}{2(1-\sigma)}} = \zeta \int_0^\infty t^2 J_1^2(t)\, e^{-\zeta t}\, dt =$$

$$= \frac{6}{\zeta^4}\left(\frac{\zeta^2}{\zeta^2+4}\right)^{3/2} {}_2F_1\left(\tfrac{3}{2}, -\tfrac{1}{2}, 2, \frac{4}{\zeta^2+4}\right) =$$

$$= \frac{k}{\pi\zeta}\,[(1-k^2)\,K(k) + (2k^2-1)\,E(k)]\,,$$

where

$$(18)\qquad k = \frac{2}{\sqrt{\zeta^2+4}}\,,$$

${}_2F_1$ is a hypergeometric function and E and K are complete elliptic integrals in the usual notation,

$$(19)\qquad \frac{\sigma_z(\varrho, 0)}{\dfrac{b}{R}\dfrac{\mu}{2(1-\sigma)}} = \lim_{\zeta\to 0} \int_0^\infty t J_0(t\varrho)\, J_1(t)\, e^{-\zeta t}\, dt\,,$$

for $0 \leqq \varrho < 1$

$$(20)\qquad \frac{\sigma_z(\varrho, 0)}{\dfrac{b}{R}\dfrac{\mu}{2(1-\sigma)}} = {}_2F_1(\tfrac{3}{2}, \tfrac{1}{2}, 1, \varrho^2) = \frac{2}{\pi}\,\frac{1}{1-\varrho^2}\,E(\varrho)\,,$$

for $\varrho > 1$

$$(21)\qquad \frac{\sigma_z(\varrho, 0)}{\dfrac{b}{R}\dfrac{\mu}{2(1-\sigma)}} = -\frac{1}{2\varrho^3}\,{}_2F_1(\tfrac{3}{2}, \tfrac{3}{2}, 2, 1/\varrho^2) =$$

$$= \frac{2}{\pi\varrho}\left[K(1/\varrho) - \frac{\varrho^2}{\varrho^2-1}\,E(1/\varrho)\right].$$

The tabulated values for complete elliptic integrals were used for the calculation. Relations (17), (20) and (21) are plotted in Figs. 2 and 3. The values for $\zeta < 0$, following from the condition of symmetry for a dislocation loop, are plotted for the function $\tau_{rz}(1, \zeta)$. Due to the symmetry the continuation into lower half-space for the solution of problem 1 is such that the displacements u_r and u_z are symmetrical with respect to the plane $z = 0$, i.e. u_r is an even and u_z an odd function of z. It then follows from Hooke's law that the normal stresses σ_r, σ_ϑ, σ_z are an even and the shear stress τ_{rz} an odd function of z.

DEFORMATION ENERGY

As is known, the deformation energy of a linear dislocation in an unlimited medium, calculated from the aspect of the classical theory of elasticity, is infinitely large for two reasons. The first is that the stresses in the immediate neighbourhood of the dislocation line are infinitely large. In a crystal, of course, the stresses are limited and when calculating the energy it is therefore best to cut off the immediate neighbourhood of the dislocation line — the dislocation centre — and estimate the energy of the centre from atomic considerations. The second reason for the infinite magnitude of the energy of a rectilinear dislocation is the slow decrease in stress with distance from the dislocation line; a limited body with dimensions equal in order of magnitude to the dimensions of crystals should therefore be considered instead of an unlimited medium.

The latter reason drops out for circular dislocation loops because, due to the interaction of the opposite parts of the dislocation, the stresses decrease rapidly with the distance, the energy is concentrated in the immediate neighbourhood of the loop and calculation can be carried out for an unlimited medium. The first reason remains, of course, since in the immediate neighbourhood of the dislocation line our solution has the same character at the limit as in the neighbourhood of a straight dislocation. When calculating the energy of a dislocation loop we therefore again cut off the centre of the dislocation and express the total energy of the loop W as a sum

$$W = W_1 + W_j\,, \tag{22}$$

where W_1 is the energy in an unlimited medium outside the dislocation centre and W_j is the energy of the centre.

The energy outside the centre is calculated as the work of external normal stresses in forming a dislocation

$$W_1 = 2\tfrac{1}{2}\int_0^{R-\varepsilon} [-\,\sigma_z(r, 0)]\,.\,(-\,\tfrac{1}{2}b)\,2\pi r\,\mathrm{d}r\,, \tag{23}$$

where ε is the radius of the centre, $0 < \varepsilon < R$ (for physical considerations as a rule $\varepsilon \ll R$).

After substituting from Eq. (19) into (23) using (8) and after one integration over r we obtain

$$\frac{W_1}{\dfrac{\mu b^2}{2(1-\sigma)}R} = \pi(R-\varepsilon)\int_0^\infty J_1[\xi(R-\varepsilon)]\,J_1(\xi R)\,\mathrm{d}\xi\,. \tag{24}$$

Further calculation, using [13], gives the final expressions

$$\frac{W_1}{\dfrac{\mu b^2}{2(1-\sigma)}R} = \frac{\pi}{2}\,\frac{(R-\varepsilon)^2}{R^2}\;{}_2F_1\left(\tfrac{3}{2}, \tfrac{1}{2}, 2, \frac{(R-\varepsilon)^2}{R^2}\right) = \tag{25}$$

$$= 2\left[K\left(\frac{R-\varepsilon}{R}\right) - E\left(\frac{R-\varepsilon}{R}\right)\right].$$

A quantity equal in order of magnitude to the Burgers vector [15], $\varepsilon \approx b$, is usually taken as the radius of the centre ε.

The estimate in [15], independent of the radius of the centre, is taken for unit length for the energy of the centre of an edge dislocation

$$w_j = \frac{\mu b^2}{4\pi(1 - \sigma)} .$$

We can with good approximation assume the same energy of the centre and unit length for our circular loop so that the energy of its centre is

$$W_j = \frac{\mu b^2}{2(1 - \sigma)} R . \tag{26}$$

The total energy of a circular dislocation loop is then given by the sum of the energy outside the centre and the energy of the centre, i.e. by Eqs. (22), (25) and (26).

For $\varepsilon \ll R$ we can use the limiting relations for complete elliptic integrals (see e.g. [14])

$$x \to 1 , \quad K(x) \to \ln \frac{4}{\sqrt{1 - x^2}} , \quad E(x) \to 1 ,$$

and we obtain the following approximate expression for the total energy

$$W \approx \frac{\mu b^2}{2(1 - \sigma)} R \left(\ln \frac{8R}{\varepsilon} - 1\right) , \tag{27}$$

which agrees with the expression given in [5].

DISCUSSION

Calculation was carried out for a circular dislocation loop such as would be formed in a crystal after the condensation of vacancies into a flat cavity and the approach of their surfaces. The solution for a circular loop with Burgers vector of opposite sign, corresponding on the contrary to a greater distance between the circular bases and the insertion of a thin circular plate — or in a crystal the assembly of interstitial or impurity atoms into a thin disc — is obtained from our relations by merely changing the sign at the Burgers vector $\boldsymbol{b}$.

The course of the stresses and displacements, as is shown by our Figs. 2 and 3, is very different from an edge dislocation with a straight dislocation line. The stresses decrease much more rapidly with distance, e.g. $\tau_{rz}(1, \zeta)$ as $1/\zeta^4$, $\sigma_z(\varrho, 0)$ as $1/\varrho^3$. From this follows small interaction of the dislocation loop with more distant defects in the crystal lattice.

The deformation energy of a dislocation loop is primarily concentrated in the immediate neighbourhood of the loop and the energy per unit length of the dislocation line is much smaller for a small radius of the loop than per unit length of a straight dislocation line. The energy of the centre is no longer negligible compared with the energy outside the centre; for example, for $\varepsilon/R = 10^{-2}$, $W_j/W_1 = 0{\cdot}22$.

For very small radii of the loop our solution no longer corresponds to the actual state in the crystal. As long as the flat cavity, produced by the condensation of vacancies, does not exceed the critical radius R_k, the bases of this cavity do not approach and the dislocation loop is not formed since the preservation of the cavity with free surfaces is more advantageous from the energy point of view. The condition of equality between the energy of the free surface of the cavity and the energy of the dislocation gives a rough estimate of the critical radius R_k

$$2\pi R_k^2 \gamma = W(\mu, \sigma, b, \varepsilon, R_k)$$

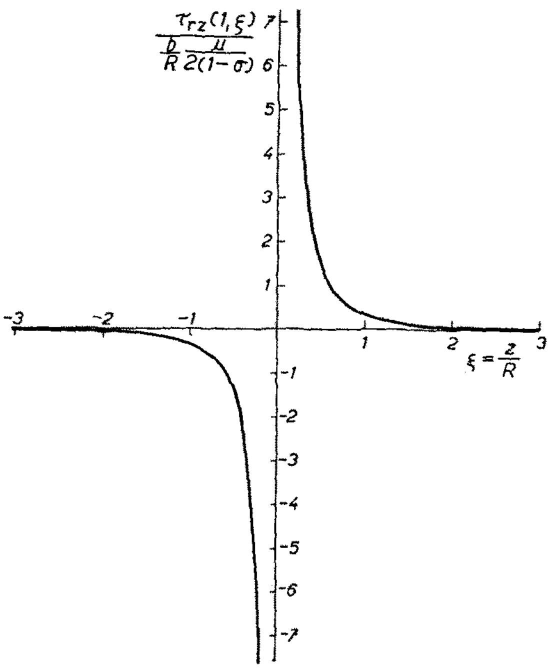

Fig. 2. Curve of shear stress τ_{rz} on slip cylinder $\varrho = r/R = 1$.

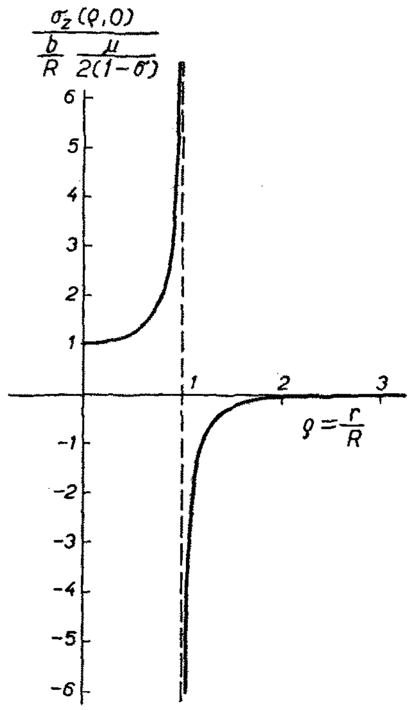

Fig. 3. Curve of normal stress σ_z in plane of loop $z = 0$.

where γ is the surface energy. For a cavity one atom thick, i.e. for a dislocation with minimum Burgers vector, the critical radius for metals is, however, very small, $R_k < 2b$.

Since the solution is carried out from the aspect of the classical theory of elasticity, the calculated values of the stresses and displacements in the neighbourhood of the dislocation approach infinity. The solution is not therefore valid in the centre of the dislocation. In order to calculate the stresses and displacements in the centre one must start out from other models, based on atomic concepts, or from the non-linear theory of elasticity. Our solution, however, holds well in a crystal outside the centre of the dislocation, where the atomic structure does not basically assert itself, and helps in solving a number of problems such as in studying the interaction of a loop with other defects.

A closer approximation of the actual conditions in a crystal would be obtained by a solution from the aspect of the anisotropic theory of elasticity and by considering a dislocation loop composed of straight sections instead of a circular loop, e.g. for the cubic crystal of a square or triangular loop (for loops in the (100) and (111) planes). Such a solution is, however, much more laborious.

The above solution may be the starting point for solving a circular dislocation loop from the aspect of the Peierls-Nabarro [16] model, which so far has only been elaborated for a rectilinear dislocation line in the same way as other models, e.g. the Yoffe model [17]. The basic Peierls-Nabarro integro-differential equation can be derived for the displacement $u_z(R, z)$ on a slip cylinder, analogously to Eshelby's procedure [18], as a condition for a continuous distribution of the dislocation loops on a cylindrical surface $r = R$ for which the shear stress $\tau_{rz}(R, z)$ is a periodic function of the mutual displacement of the atoms along both sides of the cylindrical surface in the direction of the z axis. For a shear stress τ_{rz} of the dislocation loop we can then use our expression (15). The Peierls-Nabarro equation is, however, very complicated and numerical methods should be used for its solution.

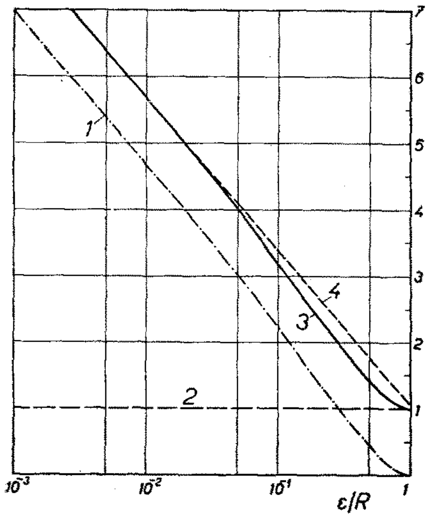

Fig. 4. Deformation energy of circular dislocation loop as a function of radius of centre ε.

curve 1 ... $\dfrac{W_1}{\dfrac{\mu b^2}{2(1-\sigma)} R}$,

curve 2 ... $\dfrac{W_j}{\dfrac{\mu b^2}{2(1-\sigma)} R}$,

curve *3* ... $\dfrac{W}{\dfrac{\mu b^2}{2(1-\sigma)} R}$,

curve *4* ... $\ln \dfrac{8R}{\varepsilon} - 1$.

CONCLUSIONS

An exact calculation is carried out of the stresses, displacements and energy of a circular dislocation loop, with Burgers vector normal to its plane, from the point of view of the classical isotropic theory of elasticity. The axial symmetry of the problem and the symmetry with respect to the plane $z = 0$ was made use of in the solution and the calculation was carried out by the method of Hankel transformation for half-space with corresponding boundary condition. The calculated stresses can be used with good accuracy for studying some of the properties of a dislocation loop formed in the crystal by the condensation of vacancies or interstitial atoms. Small interaction of the dislocation loop with more distant defects follows from the rapid decrease in stress with distance and the small deformation energy.

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