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DETERMINATION OF THE PHENOMENOLOGICAL DISLOCATION THEORY PARAMETERS FOR ELASTIC TWINS IN CALCITE

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A method is proposed for determining from the strain diagram the phenomenological parameters of the dislocation theory of elastic twins, viz., the Peierls and surface-tension forces. For this purpose, the stressed state of a strip is calculated in the case of an antiplane deformation with boundary conditions realized in the experiment. The corresponding experiment has been performed. It has been possible for the first time to retain the twin in the crystal by means of a distributed load. The Peierls force was found to be 0.3–0.7 kg/cm^2 and the parameter M characteristic of the surface tension was 3 kg/cm$^{3/2}$. The surface energy of calcite can be estimated from these quantities as $\alpha \approx 10$ erg/cm^2.

INTRODUCTION

KOSEVICH and Pastur have developed a quantitative theory of thin elastic twins.[1,2] In this theory, in addition to the forces of elastic origin (proportional to the stress tensor), they considered also the Peierls lattice-resistance forces and the surface-tension forces. It is assumed in the theory that the effect of the surface-tension force is large only near the end of the twin, and it can be characterized by a certain constant quantity, similar to the "coupling modulus" at the ends of a crack, proposed by Barenblatt,[3] and also that the Peierls force is constant for all dislocations. The transcendental equation for the determination of the length of the twin consisting of screw dislocations in a strip[4] has in the case of interest to us the form

$$F(L) = \pi S_0 + \left[\frac{m}{2} \cot \frac{mL}{2}\right]^{1/2} M, \tag{1}$$

where

$$F(L) = \int_0^L \frac{m\sigma(\eta)\sin m\eta \, d\eta}{[(1-\cos m\eta)(\cos m\eta - \cos mL)]^{1/2}}, \quad m = \frac{\pi}{d}, \tag{1a}$$

$\sigma(\eta)$ is the component of the tensor of the stresses produced by the external load, L is the length of the twin, d is the width of the band, S_0 is a phenomenological dimension of the theory, characterizing the Peierls force, and M is a phenomenological parameter of the theory, characterizing the surface-tension force.

The quantities S_0 and M cannot be obtained within the framework of the theory itself, since they are governed by the atomic structure of the crystal, this being outside the sphere of applicability of the continual theory of dislocations. It is therefore of interest to determine S_0 and M, that is, the Peierls and the surface-tension forces, experimentally.

1. CALCULATION OF THE PEIERLS AND SURFACE-TENSION FORCES FROM THE STRAIN DIAGRAM

Relation (1) was used in [1,2] to determine the length of a twin for known F(L), S_0, and M. But it can also be regarded as an equation with which to determine S_0 and M for a known dependence of F(L) on the length of the twin. As seen from (1a), the function F(L) can be determined if one knows $\sigma(\eta)$—the stress due to the external forces on the twinning plane. In the case of loading as shown in Fig. 1b, it is possible to determine experimentally the dependence of the length on the load for a twin consisting of screw dislocations. The stressed state corresponds in this case to the case of antiplane deformation. By antiplane deformation is meant the deformation of a cylinder to whose surface are applied forces parallel to the generatrix and constant along the generatrix. In this case there is only one component of the displacement vector u_z. The displacement-balance equation in the absence of volume forces is

$$\Delta u_z = 0. \tag{2}$$

If we specify on the boundary the stresses

$$\sigma_{xz} = 2\mu \frac{\partial u_z}{\partial x}, \quad \sigma_{yz} = 2\mu \frac{\partial u_z}{\partial y}$$

(μ is the shear modulus), then we obtain for u_z a boundary-value problem similar to the planar problem of electrostatics.[5] Knowing the solution of this problem for one region, we can obtain it for another region by conformal mapping. For example, the solution of the problem for a strip with boundary conditions corresponding to Fig. 1b can be obtained by conformally mapping on the strip the solution for a half-plane loaded as shown in Fig. 1a.

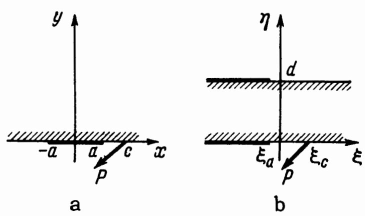

FIG. 1. Scheme of antiplane deformation: a – half-plane, b – strip.

The boundary conditions for the half-plane are as follows: a point force P is applied at the point c (c > 1) of the boundary and on the segment (−a, a) ($|a| < 1$) the displacements are equal to zero. We introduce the function

$$\Phi(z) = u_z + iv, \tag{3}$$

where v is a harmonic function conjugate to u_z. Then the tensor σ_{ik} is represented in the form of a vector in the complex plane

$$\sigma_{xz} + i\sigma_{yz} = 2\mu\bar{\Phi}'(z). \tag{4}$$

We can now solve this boundary-value problem for the half-plane with the aid of integrals of the Cauchy type,[6] and obtain for $\Phi'(z)$

$$\Phi'(z) = -\frac{1}{2\pi\mu}\int_{-\infty}^{\infty}\frac{f(x)\,dx}{x-z}, \tag{5}$$

where $f(x) \equiv \sigma_{yz}|_{y=0}$, and $\Phi(z)$ is the complex conjugate of $\bar{\Phi}(z)$.

Using a procedure frequently employed to solve the mixed problem of elasticity theory,[7] we find that no displacements are produced when the load density on the section (−a, a) satisfies the following integral equation

$$\int_{-a}^{a} p(x)\ln\frac{1}{|x'-x|}\,dx = P\ln\frac{1}{|x'-c|}. \tag{6}$$

The solution of this equation is (see [7])

$$p(x) = \frac{P}{\pi}\frac{(c^2-a^2)^{1/2}}{(a^2-x^2)^{1/2}(c-x)}. \tag{7}$$

Finally, for the antiplane deformation of the half-plane we obtain

$$\sigma_{xz} = \frac{P(c^2-a^2)^{1/2}}{2\pi}\left\{\frac{1}{(z^2-a^2)^{1/2}(z-c)} + \frac{1}{(\bar{z}^2-a^2)^{1/2}(\bar{z}-c)}\right\}$$

$$\sigma_{yz} = i\frac{P(c^2-a^2)^{1/2}}{2\pi}\left\{\frac{1}{(z^2-a^2)^{1/2}(z-c)} - \frac{1}{(\bar{z}^2-a^2)^{1/2}(\bar{z}-c)}\right\}. \tag{8}$$

After conformal mapping we obtain the stressed state of a strip with a force P applied on its boundary at the point ξ_c, and with the displacements equal to zero starting with the coordinate ξ_a on the upper and lower edges of the strip, up to $-\infty$. Finally, to components of the stress tensor as functions of η have for $\zeta = 0$ the form

$$\sigma_{\zeta\xi} = A\frac{e^{m\xi_c}\cos(m\eta-\varphi)-\cos\varphi}{(\operatorname{ch}2m\xi_a-\cos 2m\eta)^{1/4}(\operatorname{ch}m\xi_c-\cos m\eta)},$$

$$\sigma_{\zeta\eta} = A\frac{e^{m\xi_c}\sin(m\eta-\varphi)+\sin\varphi}{(\operatorname{ch}2m\xi_a-\cos 2m\eta)^{1/4}(\operatorname{ch}m\xi_c-\cos m\eta)},$$

$$\varphi = \frac{1}{2}\operatorname{arctg}\frac{\sin 2m\eta}{\cos 2m\eta-\exp(-2m|\xi_a|)},$$

$$A = \frac{P}{d}\frac{(\exp(2m\xi_c)\exp(2m|\xi_a|)-1)^{1/2}}{2^{5/4}\exp(m|\xi_a|/2)\exp(m\xi_c)}. \tag{9*}$$

2. EXPERIMENTAL PROCEDURE

To realize the loading scheme described above, it was necessary to produce first an elastic twin consisting of only screw dislocations, and then ensure its stability and development under the influence of the forces applied in the manner shown in Fig. 1b. Therefore prismatic samples of calcite, with prism axis perpendicular to the twinning plane and with one pair of faces aligned with the shear plane,[8] were glued into clamp 2 as shown in Fig. 2.[1)] A rod for transmission of the load was glued on at a small distance from the clamp.

*ch ≡ cosh, arctg ≡ $\tan^{-1}$.

[1)] When working with a real sample, it is never possible to satisfy the condition that the medium be infinite along the z axis (Fig. 1b.). We therefore carried out an analysis of the possible errors. The stressed state was regarded as a superposition of torsion, flexure, and an applied pointlike force. We calculated the stresses and the displacements for specified external force and sample dimensions. As a result we could verify that u_x and u_y are two order of magnitude smaller than u_z, and, what is more important, their derivatives with respect to the coordinates are very small. In addition, by a direct application of the theory of elasticity we established that u_z remains practically unchanged along the z axis. Therefore the scheme of Fig. 2 corresponds with sufficient accuracy to the conditions of antiplane deformation.

Before the experiment a concentrated load, sufficient for the formation of an elastic twinning layer consisting of screw dislocations only, was applied with the aid of a knife edge. It was uncertain at first whether it would be possible to maintain the produced twin in equilibrium after removal of the knife edge. It was known that an elastic twin could hitherto be observed only in the presence of a concentrated force applied directly to that part of the crystal where the twin layer emerged to the surface. It turned out that the elastic twin consisting only of screw dislocations does not need such a high stress concentration. This has made it possible to stabilize the produced twin after removal of the knife edge and using a suitable load P (Fig. 2). Further increase in P has made it possible to increase the length of the elastic twin. This has afforded an opportunity of comparing the length of the elastic twin with the value of the load P. The length of the twin was determined by an ocular micrometer accurate to ± 1%. The load was produced by direct application of a weight.

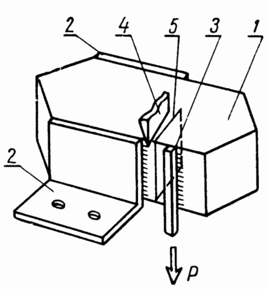

FIG. 2. Diagram showing loading and fastening of the crystal: 1 – calcite crystal 2 – clamps, 3 – rod, 4 – knife edge, 5 – twin.

All the measurements were made at room temperature. The rate of change of the load was not more than 2 g/sec at a total load on the order of 1 kilogram, so that the tests can be regarded as quasistatic. Since the twin layers were sufficiently thin, we were able to observe interference coloring. This increased the accuracy with which their dimensions and shapes were determined.

3. RESULTS AND DISCUSSION

To obtain F(L) it is necessary to substitute the obtained value of the stress component $\sigma_{\zeta\xi}$ (9) in expression (1a). After substituting the experimentally determined loads and the twin lengths corresponding to them, this integral was determined numerically by the trapezoid method. Since the integration interval was divided into a large number of sections, the accuracy of the numerical calculation could be improved to 1%. If we take into account the error in a measurement of the lengths of the twins and of the coordinates of the end of the twins (ξ_c and ξ_a), then the total error amounts to ~ 10%. The parameters S_0 and M were determined by the least squares method. The results of the calculations are listed in the table. The rms error does not exceed as a rule the experimental errors. Thus, the Peierls force is ~0.3–0.7 kg/cm^2, that is, ~10^{-6} μ, and M ~ 3 kg/cm$^{3/2}$. For a known value of M it is possible, in accord with [9], to estimate the surface energy. An estimate yields a value on the order of 10 erg/cm^2. A more accurate calculation is hardly of interest, since our entire calculation has been made in the isotropic approximation, and the estimate contains elastic moduli, so that we can be certain only of the order of magnitude.

Phenomenological parameters S_0 and M determined from data obtained by measuring the length of the twin and the corresponding value of the load.

Number of twin of crystal 1	S_0, kg/cm^2	M, kg/cm$^{3/2}$
1	0.45±0.005	3.368±0.04
2	0.46±0.003	3.18±0.019
3	0.5±0.003	2.56±0.015
4	0.56±0.01	3.035±0.055
5	0.52±0.006	2.76±0.032
6	0.3±0.006	3.681±0.074
7	0.74±0.007	2.47±0.025
Average for seven twins	0.5±0.049	3.1±0.39
Average for 18 twins	0.55±0.15	3±0.41
Twin in crystal 2	0.3±0.005	3.25±0.055

Let us compare the obtained values of the Peierls forces and of the surface tension with the results obtained earlier by others. The quantity S_0 should have as its upper limit the macroscopic yield point, determined by one of the authors of the present article[10] as being 9–11 kg/cm^2, and in individual cases 5–4 kg/cm^2.

An interesting method of measuring the starting stresses is contained in the paper by Bengus et al.[11] However, the starting stresses for twinning dislocations, in addition to the Peierls forces, include to some degree also the surface-tension force. Naturally, the starting stresses measured in [11] (8.7 kg/cm^2) turn out to be much higher than the Peierls stresses measured in the present paper. Starting from the assumption that essentially the entire work of twinning goes to produce the twin surfaces, Obreimov and Startsev[12] obtained for the surface energy in calcite values of the order of 10^3 erg/cm^2, which coincides in order of magnitude with the result obtained by Kaner[13] by a very approximate calculation. Obreimov and Startsev[12] note that the values they obtained for the surface energy are very large. At the same time, using the values of S_0 and M and assuming that the twinning work is consumed in the production of dislocations and in overcoming the forces of "dry friction" (Peierls) and the surface tension, we can obtain a value of the same order as the work necessary to overcome these resistance forces.

It is of interest to estimate the surface energy defined, according to Vladimirskiĭ,[14] as the work necessary to shift the interatomic planes. By estimating the theoretical strength as $^1/_{10}$–$^1/_{30}\,\mu$, we obtain a surface energy equal to (1.4–4.1) $\times 10^2$ erg/cm^2. Thus, the method of measuring the Peierls force and the surface-tension force, proposed and realized in this investigation, gives rather satisfactory results.

After determining the phenomenological parameters of the dislocation theory of elastic twins, we are able to use the quantitative character of this theory, namely, determine the length of the twin, its shape, etc. for a known load.

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