CONFIGURATION OF THE ATOMIC PLANES BORDERING A CRACK IN THE MODIFIED PEIERLS-NABARRO MODEL

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A crack model similar to the Peierls-Nabarro model is used to investigate the dependence of the configuration of the atomic planes bordering a crack on the law of interplanar interaction. The maximum stress at the end of the crack is determined directly from the stress law, and the configuration of the crack is described by a smooth function satisfying nonlinear integro-differential singular equation (1.3). A semi-inverse method of solving this equation is proposed. The configurations of the atomic planes bordering the crack are constructed for a series of laws of interplanar interaction.

A fundamental problem of modern fracture mechanics is the analysis of the mechanisms of crack initiation and growth and the related problems of the interaction of cracks with dislocations, vacancies, and other structural defects. It is known that a crack is a powerful stress raiser; accordingly, in solving the above problems it is necessary to take into account the properties of the local elastic fields at the tip of the crack. The determination of these fields reduces to the problem of the shape of the crack tip.

At the microscopic level the question of crack shape is equivalent to the question of the configuration of the atomic planes bordering the crack [1]. A microscopic crack is usually defined as a segment on which the atomic planes are separated by a distance such that the interaction between them is essentially nonlinear. Moreover, a macroscopic crack is characterized by the presence of a segment on which this distance is so great that there is practically no interaction.

If the configuration of the atomic planes has been determined experimentally, then, employing the method used in [2], it is possible to solve the inverse problem, i.e., from the given configuration reconstruct the law of interaction of the atomic planes bordering the crack. Our intention is to investigate the direct problem, i.e., the problem of finding the configuration of the atomic planes bordering a crack from a given law of interplanar interaction.

The solution of this problem is complicated by the following factors: 1) geometric nonlinearity (finite strains), 2) nonlinearity of the stress law $\sigma_{ij} = \sigma_{ij}(\varepsilon_{kl})$, 3) the discreteness of real media.

In what follows we examine a certain special crack model [2] differing from that usually employed in the linear theory of elasticity.

1. If it is assumed that all the nonlinear effects are localized in a thin boundary layer surrounding the crack, then the body may be represented as two linear-elastic half-spaces separated in the equilibrium position by an interatomic distance a and interacting according to a certain nonlinear stress law $\sigma_1 = \sigma_1(u/a)$, where σ_1 is the normal component of the stress tensor, and u the relative normal displacement of the boundaries of the half-space.

Here the stress law is treated as the law of interaction of the atomic planes; accordingly, at small displacements Hooke's law must be satisfied, i.e.,

$$\left[\frac{d}{du}\sigma_1\left(\frac{u}{a}\right)\right]_{u=0} = \frac{E}{a} \qquad (E \text{ is Young's modulus}). \tag{1.1}$$

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The area bounded by the stress-law graph is numerically equal to the work done in separating the atomic planes, i.e., to twice the surface energy density γ; therefore the stress law should also satisfy the condition

$$\int_0^\infty \sigma_1(u/a)\,du = 2\gamma\,. \tag{1.2}$$

If the normal displacement $u_1(x)$, caused, for example, by internal stresses or the introduction of a wedge between the half-spaces, is given on part of the surface of the half-spaces, we can examine the problem of finding the displacements on the rest of the surface, i.e., the problem of the configuration of the crack tip.

The equilibrium equation of the crack has the form

$$D\mathbf{H}\frac{du}{dx} = \sigma\left(\frac{u(x)}{a}\right) \qquad \left(\mathbf{H}\varkappa(x) = \frac{1}{\pi}\int_{-\infty}^{\infty}\frac{\varkappa(\xi)\,d\xi}{\xi - x}\right). \tag{1.3}$$

Here H is the Hilbert transform operator, $D = {}^1\!/_4E$ for plane stress, $D = E/4(1-\nu^2)$ for plane strain, and ν is Poisson's ratio. By $\sigma(u(x)/a)$ we understand the total normal stress plotted as a function of $u(x)/a$.

Introducing the dimensionless stress g, we write Eq. (1.3) in the form:

$$\mathbf{H}\frac{du}{dx} = g\left(\frac{u(x)}{a}\right) \qquad \left(g\left(\frac{u(x)}{a}\right) = \frac{\sigma(u(x)/a)}{D}\right). \tag{1.4}$$

Entov and Saljanik [3], having examined the problem with a piecewise-linear stress law in a similar formulation, arrived at an analogous crack model.

2. The model in question is similar to that employed in Peierls-Nabarro dislocation theory [4]. We will consider a body containing an edge dislocation with Burgers vector $b_y = B$ (Fig. 1). According to Peierls, such a body may be represented in the form of two linear-elastic half-spaces, the interface coinciding with the plane $x = 0$. If one half-plane slips relative to the other, the shear stress τ at the edges of the half-spaces must be a periodic function in the tangential displacement of the half-spaces v.

In the Peierls-Nabarro model the equilibrium equation coincides (except for the coordinate notation) with Eq. (1.3) if σ on the right is replaced by τ and u in the integrand by v. As the stress law Peierls selected the function

$$\tau = -GD\sin(Rv) \qquad (G, R = \text{const}).$$

In this case the equilibrium equation admits the effective solution

$$v = \frac{2}{R}\,\mathrm{arc\,tg}\,(GRx).$$

The Peierls solution corresponds to very narrow dislocations; in order to simulate broader dislocations it is possible to employ the generalization of the Peierls solution proposed by Forman, Dzhesuon, and Wood [4]. The modified Peierls-Nabarro model can be used to analyze the shape of the atomic planes bordering the crack. In this case the cut must be taken along the plane $y = 0$ (Fig. 1) and the tangential, rather than the normal component of the stress tensor must be considered. The atomic planes m-m and n-n play the part of half-space boundaries. Thus, we arrive at the crack model considered above.

As may be seen from Fig. 1, the relative normal displacement of the half-space boundaries (i.e., the planes m-m and n-n) must satisfy the condition

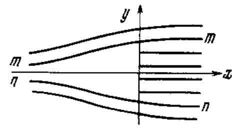

Fig. 1

$$u(-\infty) = 0, \qquad u(\infty) = B. \tag{2.1}$$

For the final formulation of the problem, apart from the law of interaction of of the half-spaces, we must specify the law of interaction between the half-spaces and the wedge.

However, it is easy to show that the surface energy of the crack, which can be written in the form

$$\Gamma = \int_{-\infty}^{\infty} \int_{0}^{u(x)} \sigma \, du \, dx$$

does not depend on the laws of interplanar interaction and interaction between the half-spaces and the wedge and is equal to $DB^2/2\pi$.

In order to solve the problem of the configuration of the tip of a macroscopic crack it is sufficient to approximate the stresses created by the wedge at the surface of the half-spaces, while satisfying the following conditions: the resultant force acting on the half-space must be equal to zero and, moreover, the effects associated with the interaction of the half-spaces with each other and with the wedge must be well separated, i.e., the configuration of the crack in the neighborhood of the wedge should not affect the configuration in the region of nonlinear interaction of the half-spaces. The second condition is characteristic of macroscopic cracks and is closely associated with the condition of autonomy of the crack tip [5]. From the second condition it follows that in the region of nonlinear interaction of the half-spaces the function $\sigma(u/a)$ coincides with the law of interplanar interaction $\sigma_1(u/a)$.

In particular, it may be assumed that the total stress $\sigma(x)$ (in what follows $\sigma(u(x)/a)$ and $\sigma(x)$, like $g(u(x)/a)$ and $g(x)$, are understood to represent the same function) is an odd function relative to the coordinate origin, which is so selected that $u(0) = \frac{1}{2}B$. (In this case the coordinate system in Fig. 1 must be shifted to the left.) Given this choice of $\sigma(x)$ the first condition is automatically satisfied; the satisfaction of the second condition will be verified after the solution has been found.

We could have tried to extend the analogy between the model in question and the Peierls-Nabarro model and use the solution of Forman, Dzhesuon, and Wood to analyze the configuration of the atomic planes bordering the crack. However, this solution does not possess the interval, characteristic of macrocracks, on which there are practically no stresses. Obtaining a series of solutions possessing such an interval is the principal mathematical difficulty of the problem in question.

3. In order to overcome this difficulty we will employ a semi-inverse method based on the integral representation of the solution of Eq. (1.4) for a right side of arbitrary form. As the basis of this solution we will take the linear-elastic solution of the crack problem.

In the approximation of the theory of elasticity the crack is regarded as a mathematical cut, whose edges are free of stresses. In what follows we shall require the solution of the problem of a crack generated by an edge dislocation with Burgers vector $b_y = B$, which is equivalent to the insertion of a semi-infinite wedge of width B. Let the crack be located in the plane $z = 0$ between the straight lines $x = -t$ and $x = t$. Then the equilibrium equation of the crack can be written in the form

$$\frac{1}{\pi} \int_{-t}^{t} \frac{du/d\xi}{\xi - x} d\xi = g(x). \tag{3.1}$$

Since the edges of the crack are free of stresses, on the right side of Eq. (3.1) we must set $g(x) = 0$ at $|x| < t$. The boundary conditions of Eq. (3.1) are

$$u(-t) = 0, \; u(t) = B. \tag{3.2}$$

The solution of homogeneous equation (3.1) with conditions (3.2) has the form [6]

$$\frac{du}{dx} = \mathrm{Re} \frac{B}{\pi \sqrt{t^2 - x^2}}, \qquad g(x) = -\mathrm{Re} \frac{B}{\pi \sqrt{x^2 - t^2}} \operatorname{sgn} x \tag{3.3}$$

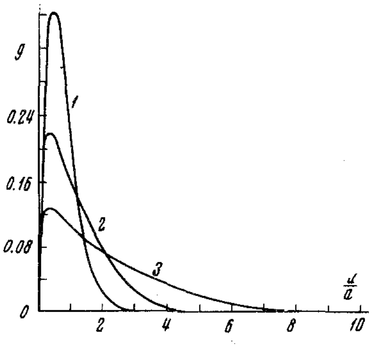

Fig. 2

where Re denotes the real part of the complex-valued function.

The length of the crack $L = 2t$ can be determined from energy considerations [7]:

$$L = \frac{DB^2}{4\pi\gamma} . \tag{3.4}$$

Equations (3.3) show that in the approximation of the theory of elasticity the tip of the crack acquires a parabolic shape, and the stresses in the neighborhood of the tip become infinite, which indicates the physical incorrectness of the linear-elastic approximation. Attempts to remove the singularity in the solution of the linear theory of elasticity have compelled a number of authors to take the forces of interaction between the crack edges into account [5, 8-10].

In the model considered the singularity problem is automatically eliminated: the atomic planes are always smoothly joined, the smoothness of the law of interplanar interaction ensuring the corresponding smoothness of the derivative of the displacement. It should be noted that in the electron micrograph of a dislocation crack in a sheet of copper phthalocyanin, presented in [2], the shape of the atomic planes differs strikingly from the shape expected on the basis of an analysis of solution (3.3): the tip of the crack is concave rather than convex, and, moreover, the atomic planes have positive curvature over almost the entire length of the crack, the sign of the curvature changing only near the wedge.

4. We now turn to the solution of Eq. (1.4). If we multiply the right side of the first of Eqs. (3.3) by some function f(t) and integrate with respect to t from |x| to t_1, the function obtained will also give the solution of the crack-equilibrium problem; however, the stress g(x) at the surface of the crack will, generally speaking, be nonzero. If $f(t) = 0$ on the interval $[0, l]$, $(l < t_1)$, then g(x) will also be equal to zero on that interval; if $f(t)$ is small on $[0, l]$, then g(x) will also be small. In the case in question $t_1 = \infty$ should be taken as the upper limit of integration.

Formally, we can proceed as follows. We introduce the complex-valued function of real argument

$$\Phi_f(x) = \varphi(x) + i\psi(x) \tag{4.1}$$

$$\varphi(x) = \int\limits_{|x|}^{\infty} \frac{f(t)\,dt}{\sqrt{t^2 - x^2}}, \quad \psi(x) = -\int\limits_{0}^{|x|} \frac{f(t)\,dt}{\sqrt{x^2 - t^2}} \operatorname{sgn} x . \tag{4.2}$$

The function $f(t)$ is assumed to be such that integrals (4.2) exist everywhere. Using (3.1) and (3.3), we can easily show that

$$\mathbf{H}\Phi_f(x) = -i\Phi_f(x) . \tag{4.3}$$

It can be shown that for any continuous function $\varkappa(x)$ decreasing at infinity not more slowly than $Nx^{-\alpha}$($\alpha > 0$), N is an arbitrary constant) there is a pair of functions $f^+(t)$ and $f^-(t)$ such that

$$\varkappa(x) = \varphi^+(x) + \psi^-(x) \quad (\varphi^\pm(x) + i\psi^\pm(x) = \Phi_f^\pm(x)) . \tag{4.4}$$

In fact, we treat expressions (4.2) as equations in the function $f(t)$. By virtue of the evenness and oddness of $\varphi(x)$ and $\psi(x)$, respectively, it is sufficient to obtain the solution at $x \geq 0$. By means of simple substitutions these equations are reduced to Abel integral equations [6], after which the solution is written in explicit form,

$$f(t) = -\frac{2t}{\pi} \int\limits_{t}^{\infty} \frac{d\varphi/dx}{\sqrt{x^2 - t^2}}\,dx, \quad f(t) = -\frac{2t}{\pi} \int\limits_{0}^{t} \frac{d\psi/dx}{\sqrt{t^2 - x^2}}\,dx . \tag{4.5}$$

We set

$$\varphi^+(x) = {}^1/_2\,[\varkappa(x) + \varkappa(-x)], \quad \psi^-(x) = {}^1/_2\,[\varkappa(x) - \varkappa(-x)] ; \tag{4.6}$$

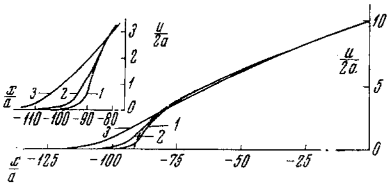

Fig. 3

now the unknown functions $f^+(t)$ and $f^-(t)$ are found from the first and second of Eqs. (4.5), respectively. [The proof is easily extended to the case of discontinuous $\varkappa(x)$].

We set

$$du / dx = \varphi^+(x) + \psi^-(x). \quad (4.7)$$

We can represent in this form an arbitrary function decreasing at infinity not more slowly than a power function with arbitrary negative exponent.

From (1.4) by virtue of (4.1) and (4.3) there follows

$$g(x) = \psi^+(x) - \varphi^-(x). \quad (4.8)$$

Thus, an arbitrary (in the above-mentioned class) solution of Eq. (1.4) can be represented in the form (4.7), (4.8). In what follows these equations are regarded as the parametric form of the stress law.

The above-mentioned Peierls solution is obtained from (4.7) and (4.8) with

$$f^+(t) = \frac{2G^3Rt}{(G^2R^2t^2+1)^{3/2}}, \quad f^-(t) = 0.$$

It is also easy to obtain the representation for the Forman, Dzhesuon, and Wood solution.

We now return to the problem in question. In order to obtain a solution containing only odd g(x), we set $f^-(t) = 0$. We transform the boundary conditions, assuming that $f^+(t)$ is integrable on the positive semi-axis. Condition (2.1) is written in the form

$$\int_0^\infty f^+(t)\,dt = \frac{B}{\pi}. \quad (4.9)$$

The analogous integral of $f^-(t)$ would vanish owing to the requirement that the resultant force acting on the body be zero.

It can be shown that in order to satisfy condition (1.1) it is sufficient that at large t

$$f^+(t) = \frac{BDa}{\pi E}\frac{1}{t^2} + o\left(\frac{1}{t^2}\right). \quad (4.10)$$

Condition (1.2) is written in the form

$$\int_0^1 K(k') \int_0^\infty f^+(t) f^+(kt)\,dt\,dk = \frac{2\gamma}{D} \quad (4.11)$$

where K(k) is a complete elliptic integral of the first kind, $k' = \sqrt{1-k^2}$ is the complementary modulus. Writing condition (1.2) in the form (4.11) is legitimate only for macroscopic cracks.

5. By assigning various functions $f^+(t)$, we can obtain a series of solutions of Eq. (1.4) corresponding to different stress laws. For the purpose of a specific calculation the following values of the parameters were selected:

$$D = E / 4(1-\nu^2), \quad \gamma = {}^1/_8\,\mu a, \quad B / a = 20, \quad \nu = 0{,}3$$

where μ is the shear modulus.

* With this choice of $f^+(t)$ a difficulty arises in connection with the fact that at zero $f^+(t)$ should vanish together with its derivative. If the parameter b is selected so that $\exp(-m^2b^2) \ll 1$, then from the function $f^+(t)$, almost without distorting its form, we can subtract a correction of the type $A_1/(t^3+1) + A_2t/(t^4+1)$, where A_1 and A_2 are selected so as to satisfy the condition $f^+(0) = 0$, $[f^+(t)]_{t=0} = 0$.

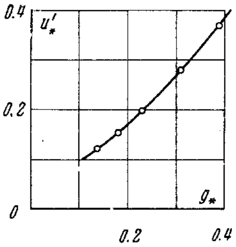

Fig. 4

The function $f^+(t)$ was taken in the form*

$$f^+(t) = \vartheta(b-t) A_0 \exp[-m^2(b-t)^2] + \vartheta(t-b)\frac{A_0 c^2}{(t-b)^2+c^2}$$

where $\vartheta(t)$ is the Heaviside unit function.

In this case conditions (4.9) and (4.10) are satisfied analytically, condition (4.11) was satisfied and integrals (4.2) evaluated numerically on a computer.

After conditions (4.9), (4.10), (4.11) have been satisfied, only the parameter b remains free. A series of configurations of the atomic planes bordering the crack corresponding to the stress laws plotted in Fig. 2 is presented in Fig. 3. The dashed line represents the configuration corresponding to $f^+(t) = S'\delta(t-s)$, ($\delta(t)$ is the Dirac delta function). The values of S and s were determined from conditions (1.2) and (2.1). Naturally, for this choice of $f^+(t)$ condition (1.1) cannot be satisfied.

We introduce the effective crack length L^*, that is, twice the distance from the coordinate origin to the point of inflection on the graph of the relative normal displacement u(x). It follows from Fig. 3 that L^* is almost independent of the form of the stress law and coincides with the equilibrium crack length L determined in the continuous linear-elastic approximation. This result is perfectly natural: the problem of determining the crack length is essentially a one-parameter problem (the single parameter is the surface energy density γ); therefore, when correctly defined, the equilibrium crack length should not depend on the model employed. It is also clear from Fig. 3 that the crack configurations corresponding to different stress laws do not differ significantly on a large part of the effective length, the principal difference being observed in the neighborhood of the point $x = -{}^1/_2 L^*$. This indicates that the specific form of the stress law is reflected only in the configuration of the tip of the macrocrack, which confirms the satisfaction of the condition of nondependence of the configuration of the tip of the macrocrack on the nature of the interaction in the neighborhood of the wedge.

As the inflection characteristic it is possible to select the maximum value of the derivative of the displacement u_*'. In Fig. 4 we have plotted the dependence of u_*' on the maximum value of the stress g^* for the given series of stress laws. As the piecewise-linear stress law is approached, u_*' may be expected to increase without bound, since in this case a logarithmic singularity should appear in u'(x).

In conclusion it should be noted that the representation of the solution of Eq. (1.3) can be used to analyze the shape of microscopic cracks and also to study the motion of broad dislocations.

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