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MODELING OF AN EDGE DISLOCATION AND ESTIMATE OF THE DISLOCATION CORE FOR A CLOSE-PACKED ATOMIC LAYER

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A model description of narrow dislocation cores is obtained. The discrete structure of the dislocation core is revealed in the Frenkel'–Kontorova and Peierls models. A model of the dislocation core is proposed that agrees well with the concepts of solid mechanics.

Introduction. It is well known that the stress–strain state caused by dislocations cannot be described by one-dimensional models. The stress, displacement, and strain fields are described adequately by the theory of elasticity [1, 2] only at a considerable distance from the dislocation center. In the polar coordinates (r, θ) [2], the elastic stress field of an edge dislocation is given by

$$\sigma_{rr} = \sigma_{\theta\theta} = -\frac{D\sin\theta}{r}, \quad \sigma_{r\theta} = \frac{D\cos\theta}{r}, \quad D = \frac{\mu b}{2\pi(1-\nu)}. \tag{1}$$

Here the origin of the polar coordinates (r, θ) coincides with the center of the edge dislocation, μ is the shear modulus, ν is Poisson's ratio, and b is the magnitude of the Burgers vector for the edge dislocation. The stress field (1) has the form $f(\theta)/r$ and does not possess radial symmetry.

To describe the stress–strain state of the dislocation core, it is necessary to use a discrete model that takes into account the structure of a crystal lattice. Moreover, in specific calculations, one should use the interatomic-interaction potentials that have a clear physical meaning and employ computational techniques for solving problems with strong physical and geometrical nonlinearities.

Predvoditelev et al. [1, p. 184] pointed out that "most specific features of the behavior of dislocations that are responsible for the mechanical properties of crystals ... depend strongly on the structure of the dislocation core." At the present time, the commonly accepted concept of the plastic-deformation mechanism in the presence of a dislocation is the following [1, 2]: the larger the dislocation core, the more readily plastic slipping occurs in a crystal with the dislocation.

Discrete Model of a Dislocation Core. It is rather difficult to study the stress–strain state of an edge dislocation in full measure; moreover, certain difficulties arise in the interpretation of numerical results obtained. Therefore, we will consider the simplest two-dimensional dislocation models proposed by Frenkel' and Kontorova [3] and Peierls [4].

Frankel'–Kontorova Model. The interaction between two rows of atoms in a close-packed lattice is considered. The lower row consists of motionless atoms fixed at the lattice nodes and generates a periodic force field. The upper row is a chain of atoms which can be displaced in the horizontal direction. We first examine the case where the atoms in the lower and upper rows form perfect three-atomic cells. Then, a single atom is introduced normally to the upper row, leading to displacement of the atoms of the upper row and formation of a dislocation (Fig. 1).

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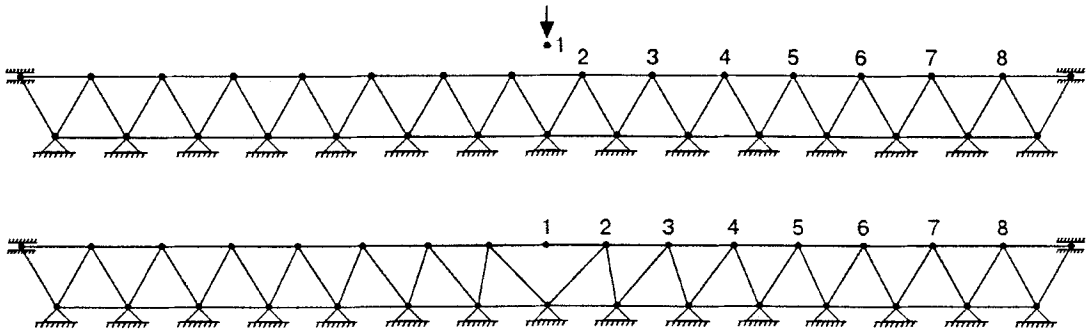

Fig. 1

The action of interatomic forces is assumed to be central with the Morse interaction potential [5]

$$U(r) = D[\mathrm{e}^{-2\alpha(r-r_e)} - 2\,\mathrm{e}^{-\alpha(r-r_e)}], \tag{2}$$

where r is the distance between the atoms, r_e is the equilibrium position, and D and α are constants. For $r = r_e$ (equilibrium state), the central interaction force is equal to zero, for $r < r_e$, the force is repulsive (negative), and for $r > r_e$, the force is attractive (positive), which attains a maximum f_m at a certain distance r_m. With further increase in the distance between the atoms, the central force of their interaction decreases, and at a distance $2r_e$, it is an order of magnitude smaller than its maximum value. The first derivative of potential (2) yields the following expression for the central force

$$f(r) = \frac{\partial U(r)}{\partial r} = 2D\alpha[\mathrm{e}^{-\alpha(r-r_e)} - \mathrm{e}^{-2\alpha(r-r_e)}],$$

whence $r_m = r_e + \ln(2/\alpha)$ and $f_m = D\alpha/2$. Calculations were performed for the following dimensionless constants: $D = 3$, $\alpha = 1.4$, and $r_e = 1$.

Numerical Analysis of Deformation of an Atomic Lattice. The nonlinear problem of atomic lattice deformation is solved by the finite-element method [6]. Since the finite-element size agrees with the atomic lattice constant, we arrive at the problem of the mechanics of deformable solids with a structure where the interaction of the structural elements is determined by the acting physical potentials. The deformation of the atomic lattice is similar in character to that of a bar structure (truss): the lattice atoms and the segments connecting the atoms can be treated as nodes of a truss and nonlinear bars, respectively (Fig. 1). Each atom in the lattice is acted upon by external forces and the forces exerted by the neighboring atoms. The equations of motion of the atomic lattice are obtained from the virtual work principle: the virtual work of internal forces is equal to the virtual work of external and inertial forces. For the moment t, this equality is written in the form

$$\sum_{k=1}^{n} f_k(t)\delta r_k(t) = R(t),$$

where $f_k(t)$ is the central force of interaction of the atoms in the kth atomic pair, $r_k(t)$ is the distance between the atoms in the kth atomic pair, $R(t)$ is the virtual work of external forces, and n is the number of atoms in the atomic lattice. To integrate the equations of motion, we use the stepwise procedure proposed in [6]: at the moment t, the equilibrium configuration and internal forces of the atomic lattice are assumed to be known, and the equilibrium configuration and internal forces corresponding to the moment $t+\Delta t$ are determined. For a rather small integration step Δt, the solution of the nonlinear system of equations reduces to the solution of a linearized system of equations. At each time step, this solution is refined by the Newton–Raphson iterative procedure. Then, the procedure is repeated for the next step.

Korobeinikov [7] obtained the matrices and vectors of the finite element for an atomic pair and used the virtual-work principle to derive the following linearized equations of atomic lattice motion:

$$M\ddot{\boldsymbol{U}}(t+\Delta t) + K(t)\boldsymbol{U} = \boldsymbol{R}(t+\Delta t) - \boldsymbol{F}(t),$$

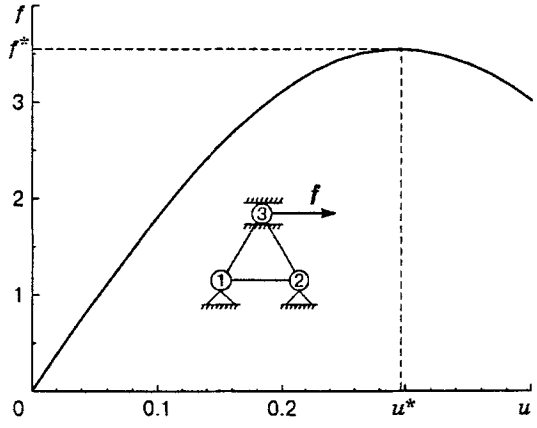

Fig. 2

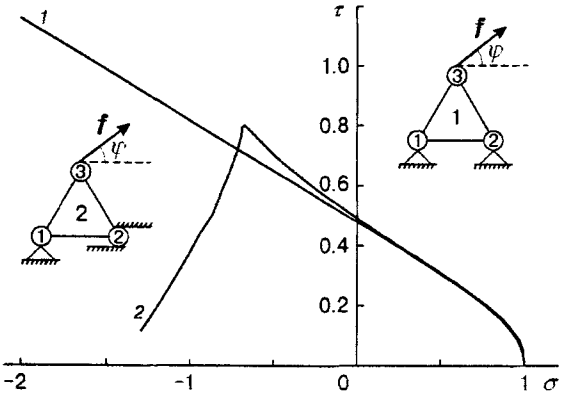

Fig. 3

where M is the diagonal mass matrix of the atomic lattice, $\boldsymbol{U} = \boldsymbol{U}(t+\Delta t) - \boldsymbol{U}(t)$ is the vector of increments in atom displacements, K is the tangent stiffness matrix, $\boldsymbol{R}$ is the vector of the external forces acting on the atoms, and $\boldsymbol{F}$ is the internal-force vector. For quasistatic deformation, the inertia terms are ignored. The resulting equations

$$K(t)\boldsymbol{U} = \boldsymbol{R}(t+\Delta t) - \boldsymbol{F}(t) \tag{3}$$

are called the linearized equations of equilibrium of an atomic lattice.

Deformation of a Three-Atomic Cell. An ideal three-atomic cell is an elementary object from which a plane close-packed crystal lattice is constructed (Fig. 2). Figure 2 shows the external force $\boldsymbol{f}$ as a function of the displacement of the third atom. When the force reaches a maximum value, the cell loses stability and further deformation occurs with decrease in the external force. The maximum load corresponds to the local maximum on the load–displacement curve. At the point of local maximum, we have $\det|K(t)| = 0$. This deformed state of the atomic lattice is called the eigenstate [7].

Because of large displacements and rotations, the physically nonlinear problem of atomic lattice deformation becomes geometrically nonlinear. Solutions of these problems contain eigenstates of the maximum-load type. The principal difficulty arising in solving these problems is that the external force that acts on the atomic lattice cannot be chosen as a monotonically increasing deformation parameter. In addition, the solution becomes more complicated since the tangent stiffness matrix degenerates when the maximum load is reached. In this case, the Newton–Raphson iterative procedure does not converge. To overcome the indicated difficulties, according to [7], the external-force parameter is introduced as an unknown and system (3) is supplemented with the equation of the arc length in the $(\boldsymbol{U}(t), \lambda)$ space [$\boldsymbol{U}(t)$ is the displacement vector and λ is the external-force parameter].

Kornev and Kurguzov [8] studied the behavior a three-atomic cell for different variants of fixing and for a slope of the external loading to the horizontal axis φ varying from $-\pi/2$ to $\pi/2$. Figure 3 shows diagrams of the limit relations $\tau - \sigma$ for the complex stress state ($\boldsymbol{f} = \sigma\boldsymbol{i} + \tau\boldsymbol{j}$). Curves 1 and 2 correspond to the deformation schemes 1 and 2 (in scheme No. 1, atom 2 is fixed and in scheme No. 2, its horizontal displacement is allowed for). These curves describe the theoretical strength of a solid for various loading paths and covers the entire fracture range from brittle and quasibrittle fracture ($\sigma > 0$) to plastic fracture ($\sigma < 0$). In Fig. 3, the abrupt decline of curve 2 (it becomes downward convex) on the left of the corner point indicates the superhigh sensitivity of the atomic lattice to occurrence of vacancies.

We consider the following scheme of a dislocation core, which agrees well with the concepts of solid mechanics. Outside the dislocation core, the displacements do not exceed values that correspond to the local theoretical shear strength of the atomic lattice: $u < u^*$. This estimate of the dislocation core size differs from the commonly accepted estimate (in solid-state physics) obtained from given displacements in the dislocation

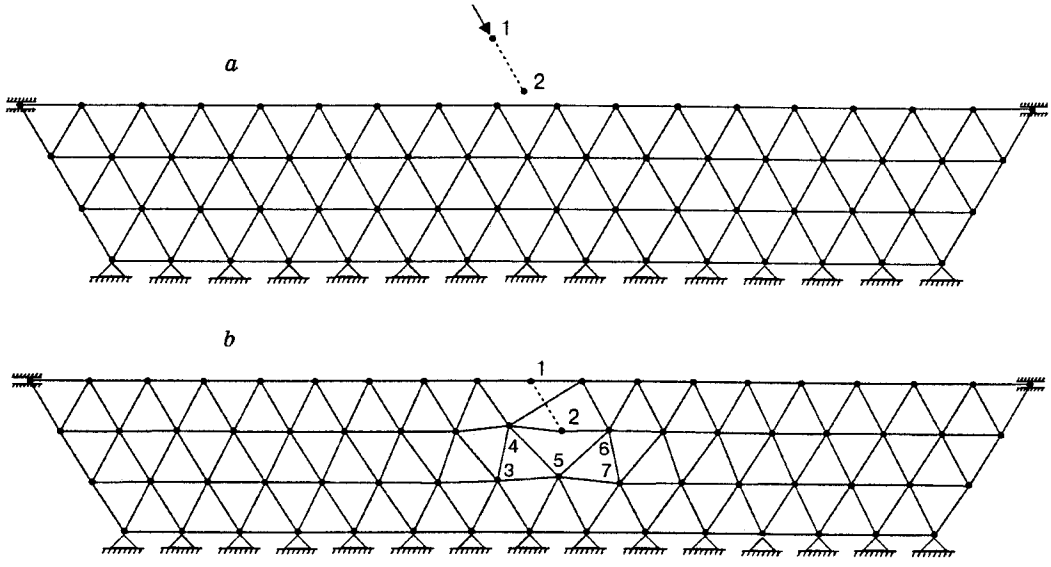

Fig. 4

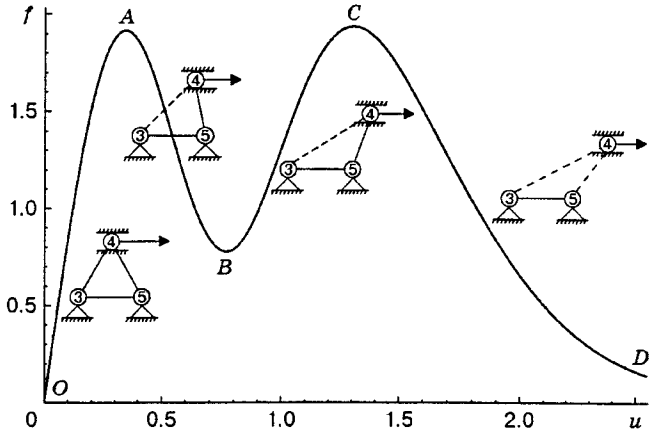

Fig. 5

core $u < b/8$ [2]. In the continual approach, a dislocation core can exist only because the external part of the atomic lattice of a solid is in the state of subcritical deformation. In the discrete approach, the three-atomic lattices in a dislocation core are in a postcritical state, and their turning over is prevented by the counteraction of three-atomic cells outside the dislocation core, which are in the subcritical state.

To determine the width of the dislocation core, we solved the problem of the instability of a three-atomic cell in shear (see Fig. 2). The critical displacement for which instability occurs was found to be $u^* = 0.296$. For the upper-row atoms denoted by numerals 2–8 in Fig. 1, the following displacements were obtained: $u_2 = 0.347$, $u_3 = 0.225$, $u_4 = 0.136$, $u_5 = 0.078$, $u_6 = 0.042$, $u_7 = 0.023$, and $u_8 = 0.014$. Thus, only the displacement of node 2 exceeded the critical value. For a close-packed crystal lattice, the dislocation core was found to be rather narrow (two interatomic distances). This is attributed to the fact that before the instability, a three-atomic cell is rather stiff, in other words, its compliance is small for subcritical loading.

Thus, the Frenkel'–Kontorova model [3] describes the dislocation core in a rough approximation.

The Peierls Model [4]. The interaction of four atomic rows in a plane close-packed crystal lattice is considered. The lower row consists of motionless atoms fixed at the lattice nodes. The upper row is a chain of atoms which can be displaced in the horizontal direction. The atoms in the second and third rows are

allowed to be displaced in an arbitrary direction (Fig. 4a). Two rigidly bonded atoms are introduced into the upper row at an angle of 60°. This leads to displacements of the atoms in the second and third rows and the formation of a dislocation (Fig. 4b). In contrast to the one-dimensional Frenkel'–Kontorova model, the Peierls model is substantially two-dimensional.

To determine the width of the dislocation core, we analyzed the instability of a cell 3–4–5, which is deformed under conditions of the generalized stress state. Figure 5 shows the external force versus the displacement of atom 4. A specific feature of this curve is the presence of two maxima. In the interval OA, the cell is in a subcritical state; in the interval AB, the 3–4 bond is in a postcritical state, and a repulsive force acts between atoms 5 and 4 (the distance between atoms 5 and 4 is smaller than r_e); in the interval BC, the 3–4 bond breaks and the 5–4 bond is in a subcritical state; in the interval CD, the 3–4 bond and the 5–4 bond are broken. We assume that the value $u^* = 0.342$, which corresponds to the first maximum in Fig. 5, is the critical displacement u^* for which instability occurs. For a four-layer atomic structure (see Fig. 4b), the displacement of the atom No. 4 exceeds the critical value: $u_4 = 0.365$. The instability of the 5–6–7 cell is analyzed in a similar manner. In the remaining cells, the displacements of the atoms are smaller than the critical values. Consequently, for the Peierls model, the width of the dislocation core is also approximately equal to two interatomic distances.

Conclusions. The numerical experiment has shown that it is possible to develop a simple model that describes crack propagation under shear for the case where the part of the crystal structure in the neighborhood of the crack tip is in a subcritical state. According to the ideas of Leonov and Panasyuk [9] and Novozhilov [10], in formulating a sufficient criterion of quasibrittle strength for crystals, it is assumed that the crack tip falls in the first three-atomic cell which is in a subcritical state, and the postcritical behavior of the crystal structure inside the crack is modeled by the corresponding loading of the crack edges.

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