

The equation has two limiting cases at $\sigma = \sigma_c$ and at $\sigma = \infty$, where

$$\dot{a} = \dot{a}_{max} \left(1 - \frac{a_0}{a}\right), \quad \dot{a} = \dot{a}_{max} \sqrt{1 - \frac{a_0}{a}},$$

respectively. Various empirical estimates give

$$\dot{a}_{max} = \sqrt{\pi/\kappa} c_t \cong 0.6 - 0.9 c_t.$$

Problem of a crack tip. Griffith not only had inset into engineering mechanics the physical quantity, surface energy, but tried to introduce an idea of the molecular structure of a material [5]. “Molecular attraction in a crack is small everywhere excluding the immediate vicinity of its ends. On this base, the crack can be considered as a free of tensile stresses surface, therefore the mathematical theory of elasticity must give right stresses in the all points of a body excluding the points in the vicinity of crack ends. Here two surfaces of the crack are very near to each other, and so in this region there are large forces of molecular attraction of order of theoretical strength.” Griffith gave evidence in favor of his assumption with a very original way. He made a ring which opening was adjusted to a steel ball for bearings. The ball passed through the ring easily, but if to wet the ring, the ball gets stuck. Water molecules of the thin film showed huge forces of cohesion with each other.

As the character of molecule attraction in a crack tip was unknown, Griffith used energy approach and took a crack in the form of an oblate ellipse. The approximation of a crack with an ellipse is a postulate. As any postulate, it can be accepted or not be accepted. Later there appeared other models of cracks [8]: a notch crack with a tip converging to an interatomic distance (P.A. Rebinder, 1936), a beak-shaped crack that contains interatomic bonds at different stages of tension (H.A. Elliott, 1947), etc. Having no direct evidence on the character of cohesion forces and their distribution on a crack surface, any mechanician is compelled to introduce hypotheses in order to construct a mathematical theory of cracks.

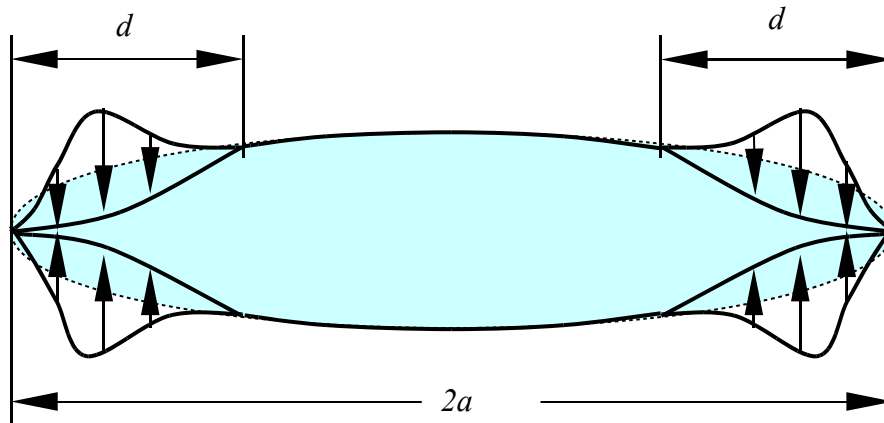


Fig. 8. Form of a crack and distribution of cohesion forces according to Barenblatt.

Among them one of the most popular models that even was incorporated into the seven-volume encyclopedic handbook “Fracture” [2] and the well-known Course of Theoretical Physics by Landau and Lifshits [9] is due to G.I. Barenblatt (1959). Here the crack surface is divided into two parts (Fig. 8): in the internal part of a crack the opposite crack faces are far off from each other, their interaction is small and the crack surface is considered to be free of stress. In the vicinity of crack ends there are large forces of cohesion. To make calculation, two postulates are introduced:

- The size of crack-tip regions is small in comparison to the size of all crack,
- The form of crack-tip regions, and therefore the local distribution of cohesion forces, do not depend on applied forces and is one and the same for a given material at given conditions (temperature, pressure and so on).

Taking into account that “molecular attraction in a crack tip” is a crucial point of any mathematical theory, one can see that the postulates accepted are changing as times goes by. According to J.N. Goodier [2] “the mathematical theory of cracks is an attempt to characterize quantitatively processes in some idealized medium that has the properties so simplified that it is possible to make mathematical study. At the same time the medium must have similarity with real materials to ensure practical value. The use of continuum models is a commonly accepted approach to avoid mathematical difficulties, but for study of cracks microstructure is very essential. At the atomic level crack propagation is the process of separating one atom from the neighboring one by the plane of a crack. Relation between a separation force and a separation of atomic planes is not known exactly, but it is essentially a *nonlinear relation*. The mathematical theory of crack propagation is not developed to such extent that it is possible introducing a concept of this interaction as a commonly accepted postulate. The main issue is how to embody large strains and fracture in a small region near a crack tip.”

3. Molecular dynamics

3.1. Crystalline materials

Beginning. The radically new impetus was given to a study of cracks by transition from continuum models to discrete ones, especially by using molecular dynamics. That approach had performed a key role because it gave possibility observing microscopic mechanisms of fracture without introducing various postulates, and what is more, to verify the grounds on which the continuum models were based. The first investigations were made under undue influence of fracture mechanics and were devoted to a study of *crack propagation* [10]. A crack was introduced into a crystal rather artificially by cutting up a part of interatomic bonds between two adjacent atomic planes or by removing a part of an atomic layer out of a closed packed plane. The main idea of such investigation was to determine a crack type, i.e. to find out whether a crack will cleave, emit dislocations or blunt. Besides, it was assumed that molecular dynamics could be used to verify the assumptions and analytical solutions of fracture mechanics and dislocation theory, to establish relations between fracture toughness and a crystal structure, and to clear up the influence of a temperature on fracture in a straightforward way. That pragmatic approach was based on the conviction that if one knew crack behavior, one would be able to make conclusions about ductility and brittleness of technologically important materials. A series of molecular dynamics studies for α -iron demonstrated cleavage crack extension of a pre-existing crack as well as dislocation generation at a crack tip [13, 14]. However, because of a limited number of atoms (~1700) the question had remained opened: whether it was possible to transfer the fracture mechanism found to real large crystals. Another question concerned the validity of the empirical interatomic potential constructed by R.A. Johnson for studying point defects in α -iron.

Crack nucleation. Almost simultaneously with the above-mentioned mechanical approach, a physical approach to the crack problem was developed [15, 16]. The method is based on the molecular dynamics simulations of two-dimensional systems. In that approach, deformation and fracture is modeled as a whole instead of studying an individual crack in a particular material. Such approach is of basic importance because it allows abandon Procrustean bed of fracture mechanics with its criteria and postulates, sometimes rather artificial. Moreover it is not connected a priori with two basic structure elements of continuum theories of deformation and fracture, dislocations and cracks, and can be used for investigation of

crack nucleation in perfect and imperfect crystals that have no pre-existing cracks or dislocations. Besides the approach allows study general features of fracture of discrete media.

Molecular dynamics simulations of two-dimensional systems have revealed that a crack can be nucleated as follows:

- At a void surface [15],
- By fracture of a low-strength inclusion [17, 18],
- At the boundary of a high-strength inclusion and surrounding crystalline material [18, 19],
- Due to hindered slip of the dislocations of intersecting slip planes and following dislocation reactions [20],
- Due to twinning under conditions of constrained strain [21],
- By cleavage of a sessile dislocation core [22-26],
- By rupture of weak and strong bonds in a chain crystal [27].

Comparison with dislocation models. It is worth noting that some of the revealed mechanisms of crack nucleation were suggested earlier in the framework of the theory of dislocations [7, 8]. For example, at the first stage crack nucleation due to the hindered slip of dislocations moving on two intersecting slip planes resembles the dislocation mechanism suggested by A.H. Cottrell (1958) for b.c.c. metals. According to Cottrell, dislocations of two intersecting slip systems $\langle 111 \rangle$, having the Burgers vector $\frac{1}{2} \langle 111 \rangle$, react and transform into sessile dislocations with the Burgers vector $\langle 100 \rangle$. Combining, they create a crack nucleus. Just the same, at the first stage crack nucleation, due to twinning under conditions of constrained strain, resembles the dislocation mechanism suggested independently by V.N. Rozhanskij (1958) and J.J. Gilman (1958). According to the authors, the slip planes are bending as a result of dislocation passing. Then in the bent slip band, a crack is opened under the action of normal stresses. However it is necessary to stress that both dislocation mechanism suggested operate only at the first stage of fracture. After that the fracture develops in a more complicated way than it was predicted. But what is more essential, molecular dynamics did not confirm a lot of dislocation mechanisms suggested for crack nucleation on purely geometrical reasoning without taking into consideration the influence of temperature.

Crack propagation. The analysis of molecular dynamics experiments shows that all diversity of space-time fracture of homogeneous and heterogeneous crystals can be reduced to two mechanisms [7, 28]:

- Successive rupture of interatomic bonds in the tip of a growing crack, i.e. the brittle fracture in a pure form (*brittle crack*).
- Many-stage process which incorporates at first either rupture of interatomic bonds in front of a growing crack or dislocation emission from a crack tip and rupture of interatomic bonds in cores of the emitted dislocations; both processes lead to nucleation of new cracks. Then the new cracks grow and coalesce with the initial main crack (*ductile crack*).

It must be emphasized that the type of a crack and details of fracture depend on several factors. They are: temperature, strain state, and crystallography. Consider some examples for 2D copper crystals described by the Morse pair potential.

Zero temperature. If the crack in 2D crystal is orientated along the closed packed direction that is normal to tensile strain and the initial tensile strain is 7%, what corresponds to the Griffith stress, we have a brittle crack [22]. If the strain is 10%, i.e. half again as many, the brittle crack transforms into ductile and blunts. If a crack is introduced at an acute angle to this direction, it propagates as a ductile in a zigzag way, but does not blunt [22].

Low temperatures. At 100 K the general picture is the same as described above. However the temperature decreases both critical strains. The strain of opening a crack becomes

6%; the strain of the brittle-to-ductile transition reduces to 7% [7, 24]. In the interval between two critical strains, the crack propagates as a brittle and grows throughout the entire length of the crystal.

The increase of temperature to 200 K changes the character of fracture [7, 23]. Here the rupture of interatomic bonds not lying on the crack propagation line in front of the growing crack leads to crack blunting. As a result, the loose amorphous pre-fracture zone is formed in front of the blunted crack facilitating its expansion; the zone consisting of vacancies and defects that are characteristic for two dimensional crystals. The defects are known as pentagonal defects or nuclei of sessile dislocations. Further fracture proceeds due to rupture of interatomic bonds in front of the crack in the loose zone and the crack propagates slowly.

High temperatures. At 350 K the crack begins to emit Frenkel-Kontorova dislocations [7, 29] from its tip. These dislocations transform into Melker-Govorov dislocations [7, 30] which in their turn into sessile dislocations and at last into voids. In parallel with this mechanism the other process is observed. With increasing temperature the free length of dislocations emitted by the crack decreases according to [31]

$$\lambda(T) = \frac{2\lambda}{1 + 9T/\theta_D}$$

Here λ is the free length, T is the temperature, θ_D is the Debye temperature. For copper $\theta_D = 339$ K, therefore the free length of dislocations at 350 K decreases more than five times. As a result, the crack grows emitting and absorbing continuously its own dislocations. If to observe the crack at large intervals, one can come to the conclusion that the crack grows, as in the case of brittle cleavage at low temperatures, due to successive rupture of interatomic bonds at its tip without crystal relaxation. In reality, the growth is a complex process. It is connected with emitting Frenkel-Kontorova dislocations, but these dislocations have no time to go away from the crack and so under the action of tensile stress they transform into Melker-Govorov dislocations, and the latter into sessile dislocations which are absorbed by the crack. As a result, the crack changes the direction of growth many times propagating along different slip lines by jumps, so that the fracture surface has numerous small jogs. At the macro level it corresponds to ductile fracture. If to introduce the vector of crack propagation that passes from the end of notch crack to its tip, then it turns out that the angle between this vector and the initial orientation of the crack is close to 20° . It is interesting to note that fracture mechanics predicts just the same value for local fracture in the form of generalized normal fracture [3]. At that, the minimum fracture load is attained that is equal to the 0.97 Griffith load. Apparently at high temperatures and large strains the crystalline structure (discreteness of a model) does not influence on the direction of the vector of crack propagation.

We have considered some typical results of molecular dynamics simulations. The main merit of molecular dynamics lies in the fact that it introduces temperature into consideration and thereby allows go beyond the scope of mechanics. As a consequence, we can pass from the macroscopic notion of brittle and ductile materials to the notion of brittle and ductile fracture associating the mechanism of these processes with the type of a growing crack. As a result, we are led to the following notions: brittle and ductile crack. This provides a possibility of separating crack dynamics and nature of a material.

Problem of potentials. This problem is tight connected with the problem of a crack tip. Really, as pointed out above, the first molecular dynamics investigations of cracks were made under undue influence of fracture mechanics; see e.g. the reviews [34, 35]. At that time the main efforts went into solving the problem of crack tip. The investigators introduced various nonlinear atomic forces not thinking out their physical basis. Transition from three-dimensional systems to two-dimensional ones had allowed increase a size of crystals and study crack cleavage and dislocation emission at a larger scale [34, 35]. The progress in computer

facilities made it possible to return to three-dimensional crystals [36, 37]. Those simulations had revealed suddenly an entirely new aspect of simulation problem. Whereas the Johnson α iron exhibited brittle cleavage, the Morse α iron showed spontaneous dislocation emission and twin nucleation at a crack tip leading to crack blunting observed experimentally.

Two important conclusions followed from these earlier simulations:

- The results of molecular dynamics simulations depend on the interatomic potential used,
- The long-range potential is more suitable for α iron and probably for other transition metals.

That discovery gave impetus to develop new interatomic potentials for transition metals. The new potentials took into considerations not only pairwise interaction, but also many-body interactions [38]. Those potentials became very popular, for example, the embedded atom method (EAM) [39]. The results obtained in this work were quite fantastic. The simulation had shown that in nickel a crack, created by removing a part of an atomic layer, behaved in such a way as if nickel were an inherent brittle metal that contradicts to all experimental data. What is the reason? One of the reasons is that the construction of the embedded atom potential is based on the same principles as the construction of their predecessors, empirical pair potentials [40], so that the new potential incorporated the drawbacks of their predecessors. The crucial drawback is that they are short-range functions of an interatomic distance [41, 42]. As a result, the size of crack-tip region d (Fig. 8) is implicitly reduced to zero that in its turn reduces to zero all the efforts of the specialists in fracture mechanics.

Another drawback of short-range potentials lies in the fact that, in spite of adding the multi-body terms, they do not allow describe the difference between individual metals [43]. The clearest evidence was given by the large-scale simulations of brittle and ductile failure in f.c.c. crystals [44]. In spite of the number of atoms in a three-dimensional slab amounted to 100 million, the authors were unable to discover the difference in behaviour of the Lennard-Jones nickel, the Morse nickel, and the EAM nickel. The authors came to the following conclusion: “We should state our concern that using any potential for a real metal through the entire range of strain to failure is highly questionable and should be scrutinized by doing first principle calculations”.

Really, the intrinsic property of metals is a long-range interaction between ions [45-47]. In due time, we have developed the long-range potentials for nickel [48] and α iron [49] derived from the pseudopotential theory. These potentials were used with success for modeling large clusters of vacancies in nickel and α iron that led to explaining the nature of swelling of these metals [50, 51]. The long-range interatomic potential, based on physical grounds and obtained by quantum mechanics methods using the pseudopotential theory, demonstrated its effectiveness for studying crack nucleation and growth in three-dimensional crystalline aluminum [52].

3.2. Noncrystalline materials

Here and below we restrict ourselves to a recital of established computer simulation results because a theory of these phenomena in the most cases is absent.

Amorphous materials. Molecular dynamics simulations of two-dimensional systems have revealed that a crack can be nucleated inside of a torn boundary of disorientation of two adjacent crystalline regions of amorphous material [53, 54]. The cracks propagate mainly along these boundaries.

Polymers. Molecular dynamics simulations of polyethylene tension [55] have shown that at first an initial globule was transforming into an oriented polymer. After that fracture was similar to that of a chain crystal [27], i.e. extension was going due to rupture of covalent C–C bonds. At that, cracks propagated parallel to tensile force.

3.3. Carbon nanotubes

Tension of achiral single wall nanotubes. At low temperatures (100 K) the fracture of an achiral single wall nanotube develops in a plane normal to a tensile force and has brittle character [56]. At high temperatures (1300 K) the fracture embraces a larger area and proceeds at an angle to a tensile force as if shear stress were acting. At that, the stress-strain curve normal to the tensile force has oscillations. This indicates that a crack propagates by jumps. The structure snaps testify that we have a ductile crack.

Tension of chiral single wall nanotubes. At low temperatures (100 K) the fracture develops through rupture of interatomic bonds independently in two nonadjacent regions and is accompanied by local compression of the damage regions [57, 58]. The structural changes are similar to those of achiral nanotubes at high temperatures. At middle temperatures (500 K) the fracture does not differ significantly from that of at low temperatures. At high temperatures (1100 K) the fracture character is very similar to that of a chain crystal that models a highly oriented polymer [27]. At the macroscopic level it corresponds to polymer splitting along a tensile force. Just the same process occurs in a carbon nanotube at the nanoscopic level.

Compression of achiral single wall nanotubes [59]. At low temperatures (100 K) the fracture develops through rupture of interatomic bonds in the middle region of a tube and is accompanied by extrusion of the damaged region. At middle temperatures (500 K) intrusion is added to extrusion. At high temperatures (900 K) both processes proceed to a larger extent. The structure of the fracture zone consists of a set of various conformations that were observed in fullerenes. In all cases fracture develops at an angle of 45° to the nanotube (compression) axis.

Torsion of achiral single wall nanotubes [60, 61]. At low temperatures (100 K) the fracture develops mainly in a narrow band normal to the nanotube axis. It has a brittle character. However, at first all hexagonal cells of the fracture band deform as in the case of shear, so the fracture band behaves itself as a shear band. At that, the anomalously stretched covalent bonds appear, and then they break. At room temperature (300 K) the fracture has a brittle character and is accompanied by extrusion of the damaged region. Qualitatively it resembles the compression fracture at low temperatures. At high temperatures (1200 K) the ductile failure occurs. Here a crack propagates at an angle of $\sim 25^\circ$ to the nanotube axis. Unusual fracture takes place at intermediate temperatures (600 K). Here at first compression occurs and only then fracture. Qualitatively the structure resembles that of forming under tension at the same temperature interval. In the region bordering the crack there form anomalously stretched covalent bonds.

Models of fracture and cracks. The analysis of molecular dynamics experiments shows that the fracture of carbon nanotubes in some respects resembles the fracture of crystals and in others that of polymers. In [57-61] we have suggested some models that allow characterize the fracture quantitatively. However the models have a phenomenological character, so we will not consider them.

4. Solitonic theory of brittle crack motion

Potential relief. Consider the quantitative physical model of brittle propagation of a crack. The mathematical analysis always has to deal with idealization. The problem lays in the fact that it necessary to find the best idealization and here the right setting up a problem is of greater importance than simply solution. The most important part of a crack is its tip. Here the rupture of an interatomic bond leads to the transition of its atoms from a volume to a surface (Fig. 8). As a consequence, the crack grows and propagates.

Imagine the crack growth as the motion of atoms of a bond being ruptured in a phase space, i.e. as the motion on a certain energy surface (Fig. 9). The surface has two minima; the left minimum corresponds to the atoms in the volume of a material and the right one does to the same atoms on a crack surface in the state of equilibrium (D. Stuart, O. Andersen, 1953; G.M. Bartenev, 1954) [28, 62].

Therefore the first step is to calculate a realistic potential relief. That can be done as follows. Within the nearest neighbor approximation, the problem appears at first glance to be equivalent to that of the potential of an atom which is the middle one of a three-atom chain being stretched.

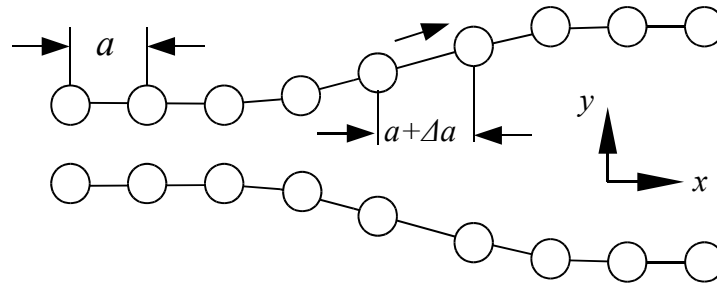


Fig. 8. Propagation of a crack as the motion of atoms from a volume to a surface, caused by the rupture of interatomic bonds.

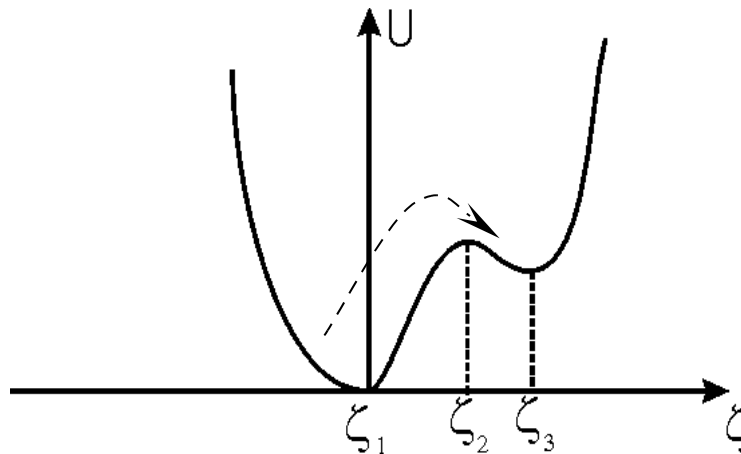


Fig. 9. Motion of rupturing bond atoms on an energy surface during crack propagation (a dotted line). Here U is the potential energy, ζ is the strain of an interatomic bond being stretched (scheme).

The quantitative distinction of the chain from a crystal consists in the following. In the crystal the left minimum is z_V times deeper, and the right one in z_S times deeper; z_V , z_S being the coordination number in a volume and on a surface, respectively. Beginning with some strain (bifurcation point), a single-well potential of the inner atom (Fig. 10a) transforms into a double-well potential (Fig. 10b). As a result, the internal atom finds itself in an unstable state at the top of the barrier that separates two wells of the symmetric double-well potential and so beyond the bifurcation point this atom falls into one of the wells (Ya.I. Frenkel, 1935). For the Morse potential, the formulas describing such quasi-static process are given in [7, 63]. However the three-atom-chain model has an essential drawback: one of two atoms of the stretched bond belongs always to one of two grips, although a crack usually nucleates far away a grip.

In reality, the process is more complex and the more realistic is a four-atom-chain model [7, 64]. According to the molecular dynamics simulations, the atoms of a bond being ruptured

are moving [7, 64] (Fig. 10c), which the main minimum is below than that of for the quasi-static deforming (Fig. 10b). For the Morse potential, the formulas describing such dynamic process are given in [7, 64]. It might be well to point out that the calculated potential closely resembles the imaginary one (Fig. 9).

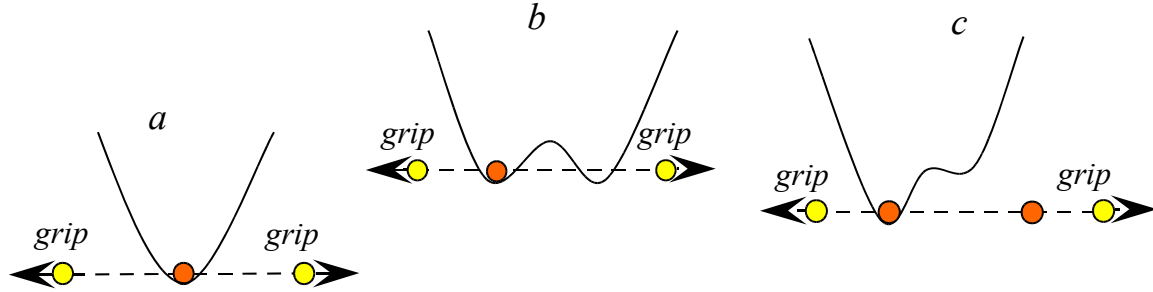


Fig. 10. Potential of an internal atom versus strain: a) under a bifurcation point, b) beyond a bifurcation point, c) a four-atom model; potential is shown only for one of internal atoms.

Equation of a moving crack. The potential relief obtained helps to explain some results of molecular dynamics simulations but does not solve the main problem describing the dynamics of brittle crack growth. Consider a two-dimensional square lattice of atoms in which a crack of normal fracture propagates. Let in the rectangular system of coordinates xy the tensile load σ is applied along the axis y normal to the line of crack propagation (Fig. 8). Assume that the crack is moving in the direction of the negative axis x . Single out one of the chains of atoms confining the crack and consider, for example, the upper one. Denote by u_n , v_n respectively the longitudinal (along the axis x) and the transverse (along the axis y) displacement of atom n from its equilibrium position in the volume of a material. The length change of the bond being ruptured can be written as

$$\Delta a_n = \sqrt{(a + u_n - u_{n-1})^2 + (v_n - v_{n-1})^2} - a,$$

where a is the lattice parameter. With crack growth the longitudinal displacement remains limited but the transverse one can be very large, so passing from the discrete argument n to the continuous coordinate $x=na$, restrict ourselves by the following terms

$$u_{n-1} = u_n - a u_x, \quad v_{n-1} = v_n - a v_x + \frac{a^2}{2} v_{xx}.$$

Here the low index denotes the differentiation with respect to x . From this it follows

$$(a + u_n - u_{n-1})^2 = a^2 (1 + 2u_x),$$

$$(v_n - v_{n-1})^2 = a^2 \left(v_x^2 - a v_x v_{xx} + \frac{a^2}{4} v_{xx}^2 \right),$$

$$\Delta a(x) = a \sqrt{1 + 2u_x + v_x^2 - a v_x v_{xx} + \frac{a^2}{4} v_{xx}^2} - a = \frac{a}{2} \left(2u_x + v_x^2 - a v_x v_{xx} + \frac{a^2}{4} v_{xx}^2 \right).$$

The work of strain forces per one interatomic bond is defined by the expression

$$\varphi(x) = \frac{k}{2} [\Delta a(x)]^2,$$

and for the whole chain, if only the nearest neighbors interact, by the expression

$$U = \frac{k}{2} \int_0^l [\Delta a(x)]^2 \frac{dx}{a}$$

Holding in the expansion of the function $[\Delta a(x)]^2$ the terms of the fourth order with respect to v_x , one obtains

$$[\Delta a(x)]^2 = a^2 \left(u_x + \frac{1}{2} v_x^2 - \frac{a}{2} v_x v_{xx} + \frac{a^2}{8} v_{xx}^2 \right)^2 = a^2 \left[u_x^2 + u_x \left(v_x^2 - a v_x v_{xx} + \frac{a^2}{4} v_{xx}^2 \right) + \frac{1}{4} v_x^4 \right]$$

The kinetic energy of the chain is equal to

$$E_{kin} = \frac{m}{2} \int_0^l (u_t^2 + v_t^2) \frac{dx}{a}$$

where m is the mass of an atom.

In order to find the equation of motion, one can use the variational principles of mechanics [7]. They separate real motion from other possible. The real motion of a mechanical system is such for which the physical value having the dimension of the product of energy by time t has the minimum value. If to take the Lagrange function $L = E_{kin} - U$ and to write down the integral

$$S = \int_{t_0}^t L dt = \min$$

we obtain the Hamiltonian action function (W.R. Hamilton, 1835). This functional is the mathematical expression of the least action principle which can be written also in the form

$$\delta S = 0$$

Here δ is the symbol of the isochronous (incomplete) variation for which the time is not varied. In our case the Hamiltonian action function has the form of the double integral

$$S = \int_{t_0}^t (E_{kin} - U) dt = \frac{1}{2} \int_{t_0}^t \int_0^l \left\{ m (u_t^2 + v_t^2) - k [\Delta a(x)]^2 \right\} dx dt$$

The extremum conditions for a double integral can be written as the system of partial derivative equations [65] obtained by M.V. Ostrogradskij (1855). Since the subintegral function does not depend explicitly on the functions $u(x, t)$ and $v(x, t)$, Ostrogradskij's equations have a simpler form [7]

$$\frac{\partial}{\partial t} \left(\frac{\partial E_{kin}}{\partial u_t} \right) - \frac{\partial}{\partial x} \left(\frac{\partial U}{\partial u_x} \right) = 0$$

$$\frac{\partial}{\partial t} \left(\frac{\partial E_{kin}}{\partial v_t} \right) - \frac{\partial}{\partial x} \left(\frac{\partial U}{\partial v_x} \right) + \frac{\partial^2}{\partial x^2} \left(\frac{\partial U}{\partial v_{xx}} \right) = 0$$

For small longitudinal displacements Ostrogradskij's equation transforms into the common equation for string vibrations

$$\ddot{u} - c^2 u'' = 0$$

Here $u'' = u_{xx}$, $c = a(k/m)^{1/2}$ is the velocity of longitudinal waves. The equation has the solution in the form of a monochromatic wave

$$u = u_0 \exp [i(qx - \omega t)]$$

where q is the wave vector directed along the axis x , $\omega=cq$ is the frequency.

For large transversal displacements we leave, as before, the terms of the fourth order derivatives with respect to v . Then we obtain in series

$$\begin{aligned} \frac{\partial U}{\partial v_x} &\sim u_x(2v_x - av_{xx}) + v_x^3, & -\frac{\partial}{\partial x}\left(\frac{\partial U}{\partial v_x}\right) &\sim -u_x(2v_{xx} - av_{3x}) - 3v_x^2v_{xx} \\ \frac{\partial U}{\partial v_{xx}} &\sim u_x\left(-av_x + \frac{a^2}{2}v_{xx}\right), & \frac{\partial^2}{\partial x^2}\left(\frac{\partial U}{\partial v_{xx}}\right) &\sim u_x\left(-av_{3x} + \frac{a^2}{2}v_{4x}\right), \\ -\frac{\partial}{\partial x}\left(\frac{\partial U}{\partial v_x}\right) + \frac{\partial^2}{\partial x^2}\left(\frac{\partial U}{\partial v_{xx}}\right) &\sim u_x\left(-2v_{xx} + \frac{a^2}{2}v_{4x}\right) - 3v_x^2v_{xx} = \frac{a^2}{2}u_xv_{4x} - v_{xx}(3v_x^2 + 2u_x) \end{aligned}$$

and the equation of motion takes the form

$$\frac{1}{c^2}\ddot{v} + \frac{a^2}{4}u'v^{IV} - \left[\frac{3}{2}(v')^2 + u'\right]v'' = 0$$

where the character strokes denote the differentiation with respect to x .

We seek the solution in the wave form

$$v(x, t) = v(x - Vt)$$

Such waves travel at the constant velocity V and satisfy to the linear wave equation

$$\ddot{v} - V^2v'' = 0$$

At that, the differential equation with partial derivatives transforms into the ordinary differential equation

$$\frac{a^2}{4}u'v^{IV} + \left(\frac{V^2}{c^2} + u'\right)v'' - \frac{3}{2}(v')^2v'' = 0$$

Denote $v'=\chi$, where χ is the tangent of shear angle induced by the large transversal displacements of atoms. Then the equation takes the form

$$\frac{a^2u'}{4}\chi''' + \left(\frac{V^2}{c^2} + u'\right)\chi' - \frac{3}{2}\chi^2\chi' = 0$$

Sharp notch. The solution can be obtained by the method of successive approximations. Setting in the first approximation $u'=0$, we obtain

$$\chi = \sqrt{2/3}\frac{V}{c}$$

or

$$v = \sqrt{2/3}\frac{V}{c}x + const$$

By virtue of the boundary condition $v|_{x=0}=0$, const is equal to zero, so that

$$v = 0.82\frac{V}{c}(x - Vt)$$

This solution describes a brittle crack in the form of a triangular sharp notch. The velocity of crack propagation does not depend on a crack length and applied stress, but depends, through

the velocity of longitudinal waves, on an elastic modulus and a material density. In our model the shear angle corresponds to the angle of crack opening φ , i.e.

$$\chi = \tan \varphi$$

or

$$\varphi = \arctan 0.82 \frac{V}{c}$$

Therefore, the more is the velocity of crack propagation, the larger is the angle of crack opening. Notice that the angle of crack opening is a more convenient characteristic than simply opening.

Crack as a soliton. In the second approximation we take into consideration a local stress field in the vicinity of a crack tip. We average the local stress putting $u' = -\langle \varepsilon \rangle$. Then the equation takes the form

$$\frac{\langle \varepsilon \rangle a^2}{4} \chi''' - \left(\frac{V^2}{c^2} - \langle \varepsilon \rangle \right) \chi' + \frac{3}{2} \chi^2 \chi' = 0$$

Upon integrating with respect to x , we obtain

$$\frac{\langle \varepsilon \rangle a^2}{4} \chi'' - \left(\frac{V^2}{c^2} - \langle \varepsilon \rangle \right) \chi + \frac{1}{2} \chi^3 = \text{const}$$

Let us multiply the equation by χ' and integrate once more with respect to x . This leads to the equation

$$\langle \varepsilon \rangle a^2 (\chi')^2 - 4 \left(\frac{V^2}{c^2} - \langle \varepsilon \rangle \right) \chi^2 + \chi^4 + f \chi = E$$

where f, E are constants. Rewrite the equation in the form

$$\langle \varepsilon \rangle a^2 (\chi')^2 + U(\chi; V, \langle \varepsilon \rangle) = E$$

The equation can thus be interpreted as the energy conservation law for a non-linear oscillator if we take x be the time, χ is the dimensionless coordinate of a fictitious particle having the mass $2\langle \varepsilon \rangle a^2$, and E its total energy. The particle moves in the field of the potential energy

$$U(\chi; V, \langle \varepsilon \rangle) = \chi^4 - 4 \left(\frac{V^2}{c^2} - \langle \varepsilon \rangle \right) \chi^2 + f \chi$$

Let us discuss the form of the potential energy. The constant f is the force of an external homogenous field in which the chain of atoms is enclosed after the crack nucleation. The sole external force that is acting on the chain is the compression force that displaces the atoms out of the equilibrium positions at the distance $(-\nu \varepsilon_0 a)$. Here ν is Poisson's ratio, ε_0 is the tensile strain along the axis y normal to the growth direction of the crack. The force can be taken into consideration if to replace c and $\langle \varepsilon \rangle$ with $c(\varepsilon_0)$ and $\langle \varepsilon(\varepsilon_0) \rangle$, respectively, but these corrections are small.

Putting $f=0$, we obtain

$$U(\chi; V, \langle \varepsilon \rangle) = \chi^4 - A \chi^2,$$

where

$$A = 4 \left(V^2 / c^2 - \langle \varepsilon \rangle \right).$$

The extremum condition leads to the equation

$$\chi (\chi^2 - A) = 0.$$

In general, this equation has three real roots. The first root, $\chi=0$, exists always, two others are defined by the expression

$$\chi = \pm \sqrt{A} = \pm 2 \sqrt{(V/c)^2 - \langle \varepsilon \rangle}.$$

Thus we have a single-well potential at $A < 0$ (Fig. 10a), and a double-well one at $A > 0$ (Fig. 10b). As a consequence, in the general case we have anharmonic vibrations, but in a particular case solitary waves can occur at the definite values of E , V , $\langle \varepsilon \rangle$ [7].

From the energy conservation law follows that

$$\frac{d\chi}{dx} = \pm \frac{1}{a} \sqrt{\frac{E - U(\chi; V, \langle \varepsilon \rangle)}{\langle \varepsilon \rangle}}.$$

Introduce the dimensionless coordinate

$$\xi = x / (a \sqrt{\langle \varepsilon \rangle}).$$

Taking into account

$$dx = a \sqrt{\langle \varepsilon \rangle} d\xi$$

write down in the implicit form the tangent of shear angle χ

$$\pm \xi = \int_0^\chi \frac{d\chi}{\sqrt{E - U(\chi; V, \langle \varepsilon \rangle)}}.$$

Consider the particular cases. At $E=0$ we have

$$\begin{aligned} \pm \xi &= \int_0^\chi \frac{d\chi}{\sqrt{A\chi^2 - \chi^4}} = \int_0^\chi \frac{d\chi}{\chi^2 \sqrt{A\chi^{-2} - 1}} = - \int_0^\chi \frac{d\chi^{-1}}{\sqrt{A\chi^{-2} - 1}} = - \frac{1}{\sqrt{A}} \int_0^\chi \frac{d\sqrt{A}\chi^{-1}}{\sqrt{A\chi^{-2} - 1}} \\ &= - \frac{1}{\sqrt{A}} \text{Arch} \sqrt{A}\chi^{-1} \pm \xi_0 \end{aligned}$$

where ξ_0 is a constant. Consequently

$$\pm \sqrt{A} (\xi_0 - \xi) = \text{Arch} \sqrt{A}\chi^{-1}, \quad \sqrt{A}\chi^{-1} = \text{ch} \sqrt{A} (\xi - \xi_0),$$

and we obtain the soliton

$$\chi = \sqrt{A} \text{sech} \sqrt{A} (\xi - \xi_0).$$

Setting

$$\xi_0 = -Vt / (a \sqrt{\langle \varepsilon \rangle})$$

for the wave running in the negative direction of the axis x (Fig. 8), write the soliton solution in the canonical form

$$\chi = \chi_0 \text{sech} \left(\frac{x + Vt}{\Delta} \right).$$

Here

$$\chi_0 = \sqrt{A} = 2 \sqrt{V^2 / c^2 - \langle \varepsilon \rangle}$$

is the soliton amplitude,

$$\Delta = \frac{a \sqrt{\langle \varepsilon \rangle}}{2 \sqrt{V^2 / c^2 - \langle \varepsilon \rangle}}$$

is its width. At that

$$\chi_0 \Delta = a \sqrt{\langle \varepsilon \rangle} = \text{const}$$

Accordingly the angle of crack opening is

$$\varphi = \arctan \left[\chi_0 \operatorname{sch} \left(\frac{x + V t}{\Delta} \right) \right]$$

Find the displacement along the axis y

$$v = \int \chi dx = a \sqrt{\langle \varepsilon \rangle} \int \operatorname{sch} \sqrt{A} (\xi - \xi_0) \sqrt{A} d\xi$$

The integrals of trigonometric functions can be reduced to the integrals of rational functions with the help of substitutions. For an even integrand the substitution

$$t = \operatorname{sh} \sqrt{A} (\xi - \xi_0)$$

gives

$$\sqrt{A} (\xi - \xi_0) = \operatorname{Arsh} t, \quad \sqrt{A} d\xi = dt / \sqrt{1+t^2}, \quad \operatorname{ch} \sqrt{A} (\xi - \xi_0) = \sqrt{1+t^2},$$

and the integral takes the form

$$\frac{v}{a \sqrt{\langle \varepsilon \rangle}} = \int \frac{dt}{1+t^2} = \arctan t + \text{const} = \arctan \operatorname{sh} \sqrt{A} (\xi - \xi_0) + \text{const}$$

The constant of integration can be found from the boundary condition

$$v|_{x \rightarrow -\infty} = 0$$

With $\xi \rightarrow -\infty$, we obtain $\arctan t \rightarrow -\pi/2$, so $\text{const} = \pi/2$. Therefore

$$v = a \sqrt{\langle \varepsilon \rangle} \left[\frac{\pi}{2} + \arctan \operatorname{sh} \left(\frac{x + V t}{\Delta} \right) \right]$$

The solution has the form of a shock wave propagating in the negative direction of the axis x . At that, the vertical displacement produced by the crack is equal to

$$\pi a \sqrt{\langle \varepsilon \rangle}$$

Consequences. Consider the main consequences that follow from the formulas obtained.

1. There is the minimum velocity of brittle crack propagation

$$V_{\min} = \sqrt{\langle \varepsilon \rangle} c,$$

that enlarges with the increase of a load applied to a body.

2. The crack-tip length can be uniquely determined as the half-width of shock wave

$$d = \frac{a \sqrt{\langle \varepsilon \rangle}}{4 \sqrt{V^2 / c^2 - \langle \varepsilon \rangle}},$$

instead of very various static estimates [2, 9, 66]. Besides, this formula shows that the crack-tip length decreases with the rate increase of crack growth.

3. The analysis of the molecular dynamics experiments described above shows that for formation of a stable crack in the triangular lattice, it is necessary to have the displacement along the axis y larger than the half of breaking length of an interatomic bond multiplied by $\cos 30^\circ$. Therefore

$$\pi a \sqrt{\langle \varepsilon \rangle} > a \varepsilon_m \sqrt{3} / 4,$$

where ε_m is the strain corresponding to the breaking length. Supposing that $\langle \varepsilon \rangle = \nu \varepsilon$, where ε is the tensile strain, ν is Poisson's ratio, and setting $\nu = 1/3$, we obtain the criterion of crack propagation

$$\varepsilon > \frac{3}{16 \pi^2 \nu} \varepsilon_m^2 \cong 0.06 \varepsilon_m^2$$

Contrary to the Griffith criterion, this criterion does not contain such a difficulty defined value as the surface energy [66]. If the interatomic interaction is described by the Morse potential, then $\varepsilon_m = 5.77 \varepsilon_c$, where ε_c is the strain corresponding to the ultimate stress limit of the interatomic bond [7]. Usually $\varepsilon_c \sim 0.18$, so $\varepsilon_m \approx 1.04$. Consequently the strain above which the crack does not collapse equals $\varepsilon \sim 6.5\%$. This value is practically coincides with the value 6% obtained in molecular dynamics simulations at 100K.

4. The criterion of brittle crack propagation in essence is the estimate of real rupture strength. For the plane strain state it can be written as

$$\sigma_c = \frac{3 \varepsilon_m^2}{16 \pi^2 \nu (1 - \nu^2)} E$$

For the coefficients accepted, we obtain

$$\sigma_c \cong 0.067 E$$

5. Conclusion

We have analyzed the main ideas and principles lying at the basis of mechanical models of cracks. We considered advantages and drawbacks of these models. It is widely believed that fracture mechanics rests on two foundations: some unified integral criterion that can be applied for studying quasi-static and dynamic crack propagation in all elastic and inelastic materials and relevant computer simulations [67, 68]. We have tried to shake up that point of view. In our opinion two pioneering works had changed engineering fracture mechanics, namely, the paper "The phenomena of rupture and flow in solids" (1920) by A.A. Griffith, and to a lesser degree the paper "Fracture of metals: some theoretical consideration" (1948) by N.F. Mott. Griffith introduced into engineering mechanics the physical quantity – surface energy of a crack and gave a criterion of failure. Mott added another physical quantity – kinetic energy into Griffith's criterion.

The next substantial contribution was done by a large group of researchers who applied a rather new computational physical method – molecular dynamics for studying the problems of fracture. This approach revealed some features of crack behavior that one cannot imagine on the basis of speculative knowledge.

And at last, we have tried to attract attention to the modern tendency in physics, using the theory of solitons [69–74]. Strictly speaking, the nonlinear waves, now known also as solitons, were already applied with success in the theory of dislocations [75–78]. The nonlinear equation for a moving dislocation was formulated in the paper “On the theory of plastic deformation and twinning” (1938) by T.A. Kontorova and Ya.I. Frenkel long before the term ‘soliton’ was invented in 1965. The continuum approximation of their equation, under the name sine-Gordon equation (1970), is widely used in different fields of physics [74]. Later in the paper “Dislocations in two-dimensional crystals” (1988) by A.I. Melker and S.V. Govorov, the generalization of the Frenkel-Kontorova equation was suggested to describe dislocation behavior in molecular dynamics experiments [78].

The solitonic approach was also applied for studying fracture of one-dimensional systems in the paper “Rupture-inducing fluctuations and solitary waves” by A.I. Melker [79]. Almost simultaneously the paper “Solitonic model of brittle growth of a crack” (1987) was sent into the journal “Fizika Tverdogo Tela”, but was rejected. The short note was published in 2002 [28], and the full version in Russian only in 2004 [7]. This example as well as a lot of others [74, 80] shows once more: “In spite of all its revolutions, science remains conservative” (Robert Oppenheimer).

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