DEFORMATION AND STABILITY LOSS OF A PART OF THE ATOMIC CHAIN AT THE TIP OF A CRACK

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Studying the fracture of solids caused by crack nucleation and growth requires a consideration of the processes taking place at the tip of a crack on the atomic level. Here, in spite of the recent development of the computer-aided engineering, the simplest atomistic models of cracks are still significant. Such a model permits a sophisticated analytical treatment while simultaneously it retains the main features of a real physical object, that is, a brittle crack in a solid.

One of such models is suggested by Hirth and is applied in [1] to the description of crack growth by kink propagation. The model is a linear tetratomic chain with an interaction of the nearest neighbors. The middle bond of the chain is located before the tip of the crack and breaks upon its advancement, while two extreme bonds simulate compliance of a crystal lattice. Markworth and Hirth [1] analyze the chain's behavior during quasi-static realization of a complete cycle: initial state—growth to an infinite length—return to the initial state. They obtained the results concerning breaking and rebounding of the middle atomic bond, the values of the energy barriers being overcome, and influence of the middle bond weakening. It was assumed that the chain retained symmetry at any degree of growth.

The problem of quasi-static growth of atomic chain located at the tip of a crack is considered analytically in the present paper: 1) in symmetrical statement, taking into account interaction of nonadjacent atoms, 2) without restriction on symmetry assuming the interaction of only nearest neighbors. The results are compared with that in [1] and some conclusions on the model's applicability are also made.

1. Statement of the Problem. Let us consider at 0 K a linear chain of a sufficiently large (no less than 6) number of single-type atoms with point masses, which permit displacement only along the chain line. The interaction between atoms will be assumed as a central paired one, so that the potential energy v of the interaction of two atoms is a function $v(r)$ of the distance r between them. In the initial state, under the absence of external forces, the distances between the atoms—nearest neighbors are some quantities which we consider to be equal and denote by r_0, neglecting a weak boundary effect.

We will grow the chain by external forces applied to extreme atoms which are equal in absolute value and opposite in direction. Then the distances between the atoms will change; it is assumed that these changes occur sufficiently slowly so that the chain (and of each atom singly) remains in the state of quasi-static equilibrium, i.e., of a minimum of potential energy.

We enumerate the atoms of the chain by integral numbers so that the atoms with numbers 1 and 2 fall in its center. Also, we will assume that upon growth the atoms with numbers ..., −1, 0, 3, 4,... always occupy the positions corresponding to an ideal structure of a grown chain:

$$\ldots = r_{-1,0} = (1/3) r_{0,3} = r_{3,4} = \ldots \tag{1.1}$$

($r_{i,j}$ is the distance between the atoms i and j).

Let the chain be grown to the state in which the bond lengths in (1.1) are equal to R. We fix all the atoms of the chain in ideal positions determined by the value of R, except for the atoms 1 and 2 which are unconstrained in displacements. Then the positions of unconstrained atoms depend totally on the lengths of their two bonds, for example, $r_{0,1}$ and $r_{2,3}$ (Fig. 1). Since $r_{0,3} = 3R$, we have

$$r_{1,2} = 3R - r_{0,1} - r_{2,3}. \tag{1.2}$$

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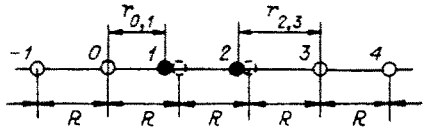

Fig. 1

Note that another appropriate selection of quantities, for example, $r_{0,1}$ and $r_{1,2}$ or $r_{0,2}$ and $r_{1,3}$, leaves the results unaffected.

Parameter R is a convenient characteristic of the chain growth, because it is connected with a deformation η of the atomic bond between the nearest neighbors by the relation $\eta = (R - r_0)/r_0$. A similar characteristic (the length of the tetratomic chain equal to 3R in our notation) appears in the Hirth model.

The total potential interaction energy W of the chain atoms can be presented in the form

$$W = W_c + W_d, \tag{1.3}$$

where $W_d \equiv W_d(r_{0,1};\ r_{2,3};\ R)$ is the interaction energy of the atoms 1 and 2 between themselves and with the neighbors and $W_c \equiv W_c(R)$ is the interaction energy of the remaining (constrained in displacements) atoms between themselves. It follows from (1.1) that W_c depends only on R. Thus, for a fixed value of R the total potential energy W and, consequently, the chain's equilibrium are determined by the quantity W_d.

Let us take the Morse function as a potential of interatomic interaction

$$v(r) = v_0\{\exp[-2\alpha(r - r_e)] - 2\exp[-\alpha(r - r_e)]\},\ v_0 > 0. \tag{1.4}$$

For a possibility and field of application of the Morse function to the strength analysis see, for example, [2].

Following the approach from [1], we introduce dimensionless variables

$$\xi_1 = \exp[\alpha(r_{0,1} - r_e)],\ \xi_2 = \exp[\alpha(r_{2,3} - r_e)],\ \rho = \exp[\alpha(R - r_e)]. \tag{1.5}$$

The last formulas established a one-to-one correspondence between the quantities ξ_1, ξ_2, ρ and $r_{0,1}$, $r_{2,3}$, R. Here ρ determines the chain growth and ξ_1 and ξ_2 determine its outline, i.e., the positions of two unconstrained atoms. With new variables (1.3) will have the following form

$$W(\xi_1, \xi_2, \rho) = W_c(\rho) + W_d(\xi_1, \xi_2, \rho), \tag{1.6}$$

where the function notations remain as before.

Investigating the equilibrium of the chain and determining its equilibrium configurations and their changes during the process of growth, we shall find an answer to the question of the chain's behavior upon quasi-static growth.

2. Interaction of Only Nearest Neighbors. With such a limitation the initial distance r_0 is equal to r_e. We introduce notations W^0, W_c^0, and W_d^0 for the functions W, W_c, and W_d, respectively. The quantity $W_d^0 \equiv W_d^0(r_{0,1};\ r_{2,3};\ R) = v(r_{0,1}) + v(r_{1,2}) + v(r_{2,3})$. Taking into account (1.2) and passing to variables (1.5), we have

$$W_d^0(\xi_1, \xi_2, \rho) = v_0\left(\xi_1^{-2} - 2\xi_1^{-1} + \xi_1^2\xi_2^2\rho^{-6} - 2\xi_1\xi_2\rho^{-3} + \xi_2^{-2} - 2\xi_2^{-1}\right). \tag{2.1}$$

Let us fix R and ρ corresponding to it, and thereby the positions of atoms of an "ideal" part of the chain. Then the chain's equilibrium configuration is determined by the equilibrium positions of the atoms 1 and 2, and W^0 depends only on ξ_1 and ξ_2 and is equal to W_d^0 + const. Therefore, the equilibrium equations for the chain $\partial W^0/\partial\xi_1 = 0$, $\partial W^0/\partial\xi_2 = 0$ take the form

$$\partial W_d^0(\xi_1, \xi_2, \rho)/\partial\xi_1 = 0,\quad \partial W_d^0(\xi_1, \xi_2, \rho)/\partial\xi_2 = 0, \tag{2.2}$$

coinciding with the equilibrium equations for the block of atoms 1 and 2.

Finding the derivatives

$$\partial W_d^0(\xi_1, \xi_2, \rho)/\partial\xi_1 = 2v_0\xi_1^{-3}\rho^{-6}\left(-\rho^6 + \xi_1\rho^6 + \xi_1^4\xi_2^2 - \xi_1^3\xi_2\rho^3\right),$$
$$\partial W_d^0(\xi_1, \xi_2, \rho)/\partial\xi_2 = 2v_0\xi_2^{-3}\rho^{-6}\left(-\rho^6 + \xi_2\rho^6 + \xi_1^2\xi_2^4 - \xi_1\xi_2^3\rho^3\right)$$

and factoring the expressions in parentheses, we see that system (2.2) is equivalent to a set of the following four systems of equations with the unknowns ξ_1, ξ_2 and parameter ρ:

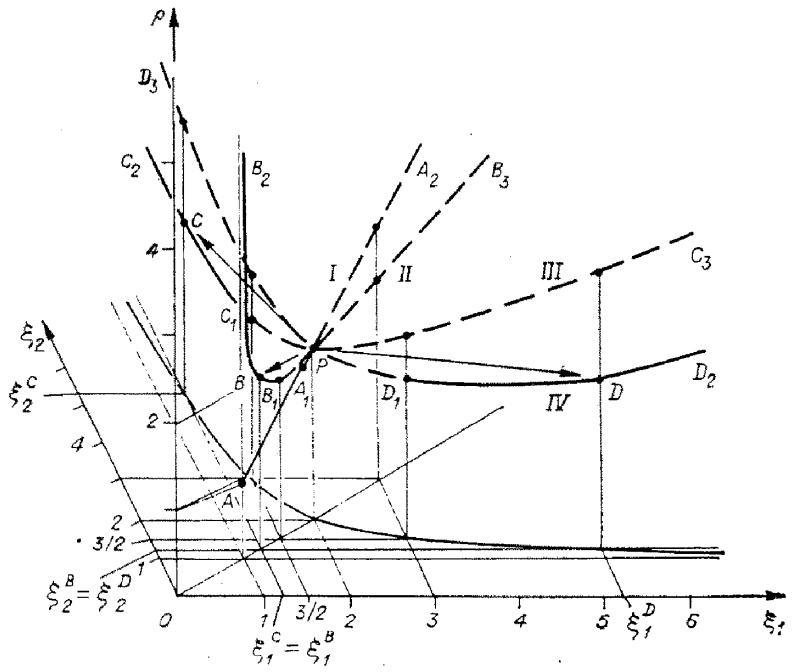

Fig. 2

$$\xi_1^2\xi_2 - \rho^3 = 0, \quad \xi_1\xi_2^2 - \rho^3 = 0; \tag{2.3a}$$

$$\xi_1^2\xi_2 + \rho^3 - \xi_1\rho^3 = 0, \quad \xi_1\xi_2^2 + \rho^3 - \xi_2\rho^3 = 0; \tag{2.3b}$$

$$\xi_1^2\xi_2 - \rho^3 = 0, \quad \xi_1\xi_2^2 + \rho^3 - \xi_2\rho^3 = 0; \tag{2.3c}$$

$$\xi_1^2\xi_2 + \rho^3 - \xi_1\rho^3 = 0, \quad \xi_1\xi_2^2 - \rho^3 = 0. \tag{2.3d}$$

Eliminating parameter ρ from each system separately shows that the solution of the first two of them must have the following property

$$\xi_1 = \xi_2, \tag{2.4}$$

and the solution of the last two systems must have the property

$$\xi_1\xi_2 = \xi_1 + \xi_2. \tag{2.5}$$

Systems (2.3) have one solution each, which, taking into account (2.4) and (2.5), can be written in the form

$$\{\xi_1 = \rho, \ \xi_2 = \rho\}; \tag{2.6a}$$

$$\{\xi_1^3(\xi_1 - 1)^{-1} = \rho^3, \quad \xi_2^3(\xi_2 - 1)^{-1} = \rho^3\}; \tag{2.6b}$$

$$\{\xi_1^3(\xi_1 - 1)^{-1} = \rho^3, \quad \xi_2^3(\xi_2 - 1)^{-2} = \rho^3\}; \tag{2.6c}$$

$$\{\xi_1^3(\xi_1 - 1)^{-2} = \rho^3, \quad \xi_2^3(\xi_2 - 1)^{-1} = \rho^3\}. \tag{2.6d}$$

We emphasize that Eqs. (2.6a)-(2.6d) are the solutions of systems (2.3) under conditions (2.4) and (2.5). Otherwise, certain extraneous values of ξ_1 and ξ_2, which are not the solutions of systems (2.3), satisfy these equations.

Relations (2.6) together with (2.4) and (2.5) determine in space $\{\xi_1, \xi_2, \rho\}$ four trajectories of the chain's equilibrium (see Fig. 2). The trajectories consist of stationary points of the potential energy function W_d^0 and are denoted by numbers I-IV according to (2.6a)-(2.6d). The function W_d^0 has no other stationary points. Equations of the trajectories, being given (explicitly or implicitly) in the form $\{\xi_i = \xi_i(\rho), \ i = 1, 2\}$, make it possible to find all possible equilibrium configurations of the chain for a fixed value of its growth.

The points of the straight line (2.6a) correspond to an "ideal" structure of the chain $r_{0,1} = r_{2,3} = R = r_e + \alpha^{-1}\ln\rho$ [from (1.5)], including the point A(1, 1, 1), which corresponds to the initial state; therefore, the equilibrium trajectory I will be called basic. Quasistatic growth of the chain from the initial state, i.e., growth ρ, corresponds to the motion along the basic trajectory from the point A in the direction of A_2, until the "ideal"

state of the chain becomes unstable. Then the chain will pass (smoothly or "crackwise"– is yet to be studied) into a stable "nonideal" state, determined by a point on one of the equilibrium trajectories II-IV, therefore called secondary ones. It follows from (2.6) that for the points of trajectory II "nonidealness" is characterized by the ratio between the lengths of the bonds $r_{0,1} = r_{2,3} \neq R$, for the points of trajectories III and IV $r_{0,1} \neq r_{2,3}$ and are not equal to R. An exclusion is the point

$$P(2, 2, 2) \tag{2.7}$$

common for all four trajectories, which is the only point of their intersection (see Fig. 2).

Let us consider a mutual arrangement of trajectories in space $\{\xi_1, \xi_2, \rho\}$ (Figs. 2, 3). From (2.4) and (2.5) it follows that trajectories I and II are located in the symmetry plane $\{\xi_1 = \xi_2\}$, while III and IV belong to a cylindrical surface, specified by Eq. (2.5), with generatrices parallel to the ρ axis, which intersects the plane $\{\xi_1 = \xi_2\}$ along the straight line $\{\xi_1 = \xi_2 = 2\}$. Further, ξ_1 and ρ in (2.6b) and (2.6c) are connected by the same relation

$$\xi_1^3(\xi_1 - 1)^{-1} = \rho^3, \tag{2.8}$$

Due to this trajectories II and III belong to the cylindrical surface, determined by Eq. (2.8), with generatrices parallel to the ξ_2 axis, and their projections on the plane $\{\xi_2 = \text{const}\}$ coincide. In the same manner trajectories II and IV belong to the cylindrical surface

$$\xi_2^3(\xi_2 - 1)^{-1} = \rho^3 \tag{2.9}$$

with generatrices parallel to the ξ_1 axis. In that case trajectory II is the intersection of surfaces (2.8), (2.9), and the symmetry plane $\{\xi_1 = \xi_2\}$.

Of two equations specifying each secondary trajectory, at least one has the form $x^3 - \rho^3 x + \rho^3 = 0$ (where ξ_1 or ξ_2 occupy the place of x). For $\rho \geq 3/\sqrt[3]{4}$ this equation has two real positive roots:

$$x_{(1)} = 2\sqrt{\rho^3/3}\cos(\varphi/3),\ x_{(2)} = 2\sqrt{\rho^3/3}\cos((\varphi + 4\pi)/3). \tag{2.10}$$

Here $\varphi = \arccos\left(-\left(\frac{27}{4\rho^3}\right)^{1/2}\right)$, moreover for $\rho = 3/\sqrt[3]{4}$ $x_{(1)} = x_{(2)} = 3/2$. For $\rho < 3/\sqrt[3]{4}$ the equation has no positive real roots. Therefore, at all the points of the secondary trajectories $\rho \geq 3/\sqrt[3]{4}$ and equality is attained at the "lowest" points

$$B_1(3/2, 3/2, 3/\sqrt[3]{4}),\ C_1(3/2, 3, 3/\sqrt[3]{4}),\ D_1(3, 3/2, 3/\sqrt[3]{4}) \tag{2.11}$$

of trajectories II-IV, respectively.

Points (2.11) divide "their own" trajectories into two infinite branches (depicted in Fig. 2 by solid and dashed lines). Specifying the value of ρ larger than $3/\sqrt[3]{4}$ determines exactly two points on each of the secondary trajectories [this follows from (2.5), (2.6), and (2.10)], which belongs to different branches, because one of the roots of (2.10) are then necessarily less than 3/2. In order to select one point out of two, it is required to additionally indicate the value of any coordinate, for example, ξ_1, thereby specifying a branch.

The points of curves I-IV, being a total set of stationary points of the potential energy function $W_d^0(\xi_1, \xi_2, \rho)$, determine all possible positions of the chain equilibrium. We verify the stability of each of them in the following way. For a fixed value of the variable ρ, the energy function $W_d^0(\xi_1, \xi_2, \rho)$ becomes the function of two variables ξ_1, ξ_2: $W_d^0|_{\rho=\text{const}} \equiv W_d^0(\xi_1, \xi_2)$. The extreme of the function $W_d^0(\xi_1, \xi_2)$ can be attained only at its stationary points, and existence and type of the extreme are determined by the signs of the expressions

$$(W_d^0)_{11}(W_d^0)_{22} - [(W_d^0)_{12}]^2 \text{ and } (W_d^0)_{11} \tag{2.12}$$

according to the known rules. Here

$$(W_d^0)_{11} \equiv \partial^2 W_d^0/\partial\xi_1^2 = 2v_0\xi_1^{-4}\rho^{-6}\left[(3 - 2\xi_1)\rho^6 + \xi_1^4\xi_2^2\right];$$
$$(W_d^0)_{22} \equiv \partial^2 W_d^0/\partial\xi_2^2 = 2v_0\xi_2^{-4}\rho^{-6}\left[(3 - 2\xi_2)\rho^6 + \xi_1^2\xi_2^4\right];$$
$$(W_d^0)_{12} \equiv \partial^2 W_d^0/\partial\xi_1\partial\xi_2 = \partial^2 W_d^0/\partial\xi_2\partial\xi_1 = 2v_0\rho^{-6}(2\xi_1\xi_2 - \rho^3).$$

Obviously, stationary points of the function $W_d^0(\xi_1, \xi_2)$ are the only points of intersection of trajectories I-IV with the corresponding plane $\{\rho = \text{const}\}$. Finding their coordinates from Eqs. (2.6) (which is possible, since ρ = const) and substituting them into the

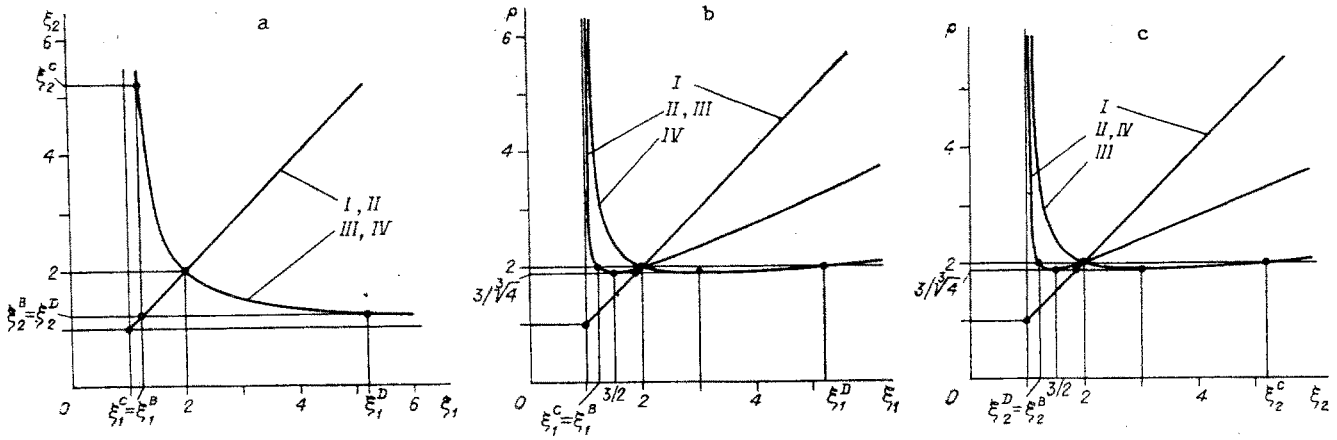

Fig. 3

second-order derivatives, we define the signs of (2.12). By making ρ vary, we obtain information on the existence and type of the extreme of the function $W_d^0(\xi_1, \xi_2, \rho)$ at each point of the equilibrium trajectories I-IV. This information is summarized in Table 1. A certain complexity lies in the fact that the correspondence between ρ and the points of secondary trajectories is not one-to-one. However, it will be such a correspondence for the points of the branches of these trajectories determined above. For this reason it was necessary to indicate in the table the values of ξ_1 together with ρ. Note that the analysis with the help of second-order derivatives does not give the answer to the question of whether the extreme exists at points P, B_1, C_1, and D_1. However, it is easy to make sure that there is no extreme of the function W_d^0 at these points, if we can find for each of them at least one curve passing through it and lying in the plane $\{\rho = \text{const}\}$, and such that upon motion along this curve the function W_d^0 has a bend at the point under consideration. For the points P and B_1 such a curve will be the straight line $\{\xi_1 = \xi_2\}$, and for the points C_1 and D_1, curve (2.5).

The data in Table 1 demonstrate that points of one of the two branches into which each secondary equilibrium trajectory is divided, correspond to minimums of W_d^0, while at points of the other branch, including the "division" point with index 1, the function W_d^0 has no extreme. Therefore, we will call the first of the indicated branches stable and the second, unstable. They are depicted in Fig. 2, as usual, by solid and dashed lines.

Remark. In what follows, we shall write, for short, "the equilibrium position (state) on the trajectory" instead of "equilibrium position (state), to which there corresponds a point on the trajectory."

Using the table data, we observe how the change of the extension parameter ρ affects the number and stability of the possible equilibrium positions of the chain. First of all let us note that for each value of ρ from the range $\rho \geq 1$ there exists an equilibrium position on the basic trajectory, which we will also call basic. It is stable if $1 \leq \rho < 2$ and unstable if $\rho \geq 2$. For $1 < \rho < 3/\sqrt[3]{4}$ the chain has no other equilibrium positions and for $\rho = 3/\sqrt[3]{4}$ there are three more unstable positions at points B_1, C_1, and D_1 of the secondary trajectories. If $3/\sqrt[3]{4} < \rho < 2$, there are seven possible equilibrium positions: the basic one and one per each of the six branches of three secondary trajectories. Since there are only three stable branches out of six, for $3/\sqrt[3]{4} < \rho < 2$ there exist four stable equilibrium positions and three unstable ones.

For $\rho = 2$ the pattern changes again. Three unstable equilibrium positions, located on the secondary trajectories, merge at point P with the basic position, forming unstable equilibrium positions on the basic trajectory. At the same time three unstable secondary positions hold: the points B(1.236; 1.236; 2), C(1.236; 5.236; 2), and D(5.236; 1.236; 2). Finally, for $\rho > 2$ there are again seven equilibrium positions: unstable basic position plus one stable and one unstable position on each of three secondary trajectories (according to stability of their branches).

Let us establish one more point concerning the behavior of the energy function W_d^0 at the points of the equilibrium trajectories (2.6). Let for a given value of $\rho = \rho_\Phi \geq 3/\sqrt[3]{4}$ the points $(\alpha_1, \alpha_2, \rho_\Phi)$, $(\beta_1, \beta_2, \rho_\Phi)$, $(\gamma_1, \gamma_2, \rho_\Phi)$ belong to stable branches of trajectories II-IV, respectively. Then from (2.5), (2.6), (2.8), and (2.9) it follows that $\alpha_1 = \alpha_2$, $\alpha_1 = \beta_1$, $\alpha_2 = \gamma_2$ and it is easy to show that the differences

TABLE 1

Trajectory	ρ	ξ_1	Part, branch of trajectory or point	Presence and type of extreme
I	$1 \leqslant \rho < 2$		From P in the direction of A_2	Minima
	2		P	No extreme
	$\rho > 2$		From P in the direction of A_2	Maxima
II	$3/\sqrt[3]{4}$	3/2	B_1	No extreme
	$\rho > 3/\sqrt[3]{4}$	$\xi_1 < 3/2$	B_1B_2	Minima
		$\xi_1 > 3/2$	B_1B_3	No extreme
III	$3/\sqrt[3]{4}$	3/2	C_1	» »
	$\rho > 3/\sqrt[3]{4}$	$\xi_1 < 3/2$	C_1C_2	Minima
		$\xi_1 > 3/2$	C_1C_3	No extreme
IV	$3/\sqrt[3]{4}$	3	D_1	» »
	$\rho > 3/\sqrt[3]{4}$	$\xi_1 < 3$	D_1D_3	» »
		$\xi_1 > 3$	D_1D_2	Minima

$$W_d^0(\beta_1, \beta_2, \rho_\Phi) - W_d^0(\alpha_1, \alpha_2, \rho_\Phi) \text{ and } W_d^0(\gamma_1, \gamma_2, \rho_\Phi) - W_d^0(\alpha_1, \alpha_2, \rho_\Phi)$$

are equal to zero, i.e., for a fixed ρ the values of W_d^0 (and W^0 as well) coincide at the corresponding points on stable branches of the secondary trajectories, in particular, $W_d^0|_B = W_d^0|_C = W_d^0|_D \approx -2.2725v_0$. The same is also valid for the points of unstable branches, as well as for points B_1, C_1, and D_1, where $W_d^0 = [2^{4/3}/3 - 2^{5/3}]v_0 \approx -2.3349v_0$. At point P $W_d^0|_P = -2.25v_0$.

We construct a general picture of the chain's response to growth. The degree of extension will be specified as before, i.e., with the help of parameter ρ.

1. $\rho = 1$. There is no action of external forces, the chain is at the initial state of stable equilibrium (point A) with equal bond lengths of the nearest neighbors: $r_{0,1} = r_{2,3} = R = r_0 = r_e$.

2. $1 < \rho < 3/\sqrt[3]{4}$. Under the influence of the applied load the chain grows, retaining an ideal structure due to uniqueness and stability of the basic equilibrium state. In space $\{\xi_1, \xi_2, \rho\}$ this corresponds to the motion along the basic trajectory from point A to point $A_1(3/\sqrt[3]{4}, 3/\sqrt[3]{4}, 3/\sqrt[3]{4})$.

3. $\rho = 3/\sqrt[3]{4}$. The chain is in a stable equilibrium state A_1, since the other three possible states B_1, C_1, and D_1 on the secondary trajectories are unstable.

4. $3/\sqrt[3]{4} < \rho < 2$. For each value of ρ in this range there are four different stable equilibrium configurations of the chain, in which the function W_d^0 has local minima.

However, if the energy barrier separating the "basic" minimum from the "secondary" ones is not overcome, the chain remains to be "ideal" up to the value $\rho = 2$, which corresponds to the motion from A_1 to P along the basic equilibrium trajectory.

5. $\rho = 2$. A critical moment of growth is the point P of stability loss of an "ideal" configuration of the chain. The function W_d^0 has a bend at the point P, while the barrier, which separated the "basic" equilibrium position from the "secondary" ones, is absent now and the chain, reducing the energy W_d^0 (and consequently W^0) by $0.0225v_0$, passes "crackwise" from an "ideal" configuration into one of three possible "nonideal" ones (the points B, C, and D on the secondary trajectories). Here the values of energy are equal (see above); therefore, it seems impossible within the present consideration to say definitely which configuration exactly will be acquired by the chain. This probably depends on some of its additional properties.

6. $\rho > 2$. Upon further growth the chain maintains a stable "nonideal" configuration, "selected" by it during the transition to one of the secondary trajectories, which corresponds

to the motion of a point over a stable branch of this trajectory in the direction of increasing ρ.

Let us assume that the chain configuration does not change by overcoming a certain energy barrier during the whole process of growth. Then there are three variants of the chain behavior at monotonic growth, determined by the following diagram:

$$\text{A} \xrightarrow[\text{Trajectory I}]{} \text{P} \xrightarrow{\text{crack}} \begin{cases} B \dashrightarrow B_2 \text{ and further} \\ \text{Along trajectory II} \quad \text{(V1)}, \\ \text{or} \\ C \dashrightarrow C_2 \text{ and further} \\ \text{along trajectory III} \quad \text{(V2)}, \\ \text{or} \\ D \dashrightarrow D_2 \text{ and further} \\ \text{along trajectory IV} \quad \text{(V3)}. \end{cases} \tag{2.13}$$

The dashed arrow in the diagram denotes a smooth transition from point to point along the indicated trajectory.

Let us trace the changes in the chain configuration upon following each of the variants (V1)-(V3). From Eqs. (1.1), (1.2), and (1.5) we have expressions of interatomic distances in the extended chain in terms of quantities ξ_1, ξ_2, ρ:

$$\begin{gathered} \ldots = r_{-1,0} = (1/3) r_{0,3} = r_{3,4} = \ldots = R = r_e + \alpha^{-1} \ln \rho, \\ r_{0,1} = r_e + \alpha^{-1} \ln \xi_1 = R + \alpha^{-1} \ln (\xi_1 \rho^{-1}), \\ r_{1,2} = r_e + \alpha^{-1} \ln \left(\xi_1^{-1} \xi_2^{-1} \rho^3\right) = R + \alpha^{-1} \ln \left(\xi_1^{-1} \xi_2^{-1} \rho^2\right), \\ r_{2,3} = r_e + \alpha^{-1} \ln \xi_2 = R + \alpha^{-1} \ln (\xi_2 \rho^{-1}). \end{gathered} \tag{2.14}$$

As follows from (2.13) and Eqs. (2.6) the bonds between the nearest neighbors at first extend equally: $\ldots = r_{-1,0} = r_{0,1} = r_{1,2} = r_{2,3} = r_{3,4} = \ldots = R$. It happens like this up to a critical moment of extension, when

$$\rho = \rho_* = 2, \quad R = R_* = r_e + \alpha^{-1} \ln \rho_* \approx r_e + 0{,}6931 \alpha^{-1}. \tag{2.15}$$

When it is attained the bond lengths $r_{0,1}$, $r_{1,2}$, $r_{2,3}$ of unconstrained atoms undergo sharp changes according to scheme (2.13). Using (2.14), the data of Table 1, and graphs of Fig. 2, 3, we consider in turn the variants given in the diagram.

Variant (V1). From (2.6b) follows

$$\begin{gathered} r_{0,1} = r_{2,3} = R + (1/3) \alpha^{-1} \ln (\xi_1 - 1) < R, \\ r_{1,2} = R - (2/3) \alpha^{-1} \ln (\xi_1 - 1) > R, \end{gathered} \tag{2.16}$$

since $\xi_1 < 3/2$. In particular, at point B

$$\begin{gathered} r_{0,1}^B = r_{2,3}^B \approx R_* - 0{,}4812 \alpha^{-1} \approx r_e + 0{,}2119 \alpha^{-1}, \\ r_{1,2}^B \approx R_* + 0{,}9624 \alpha^{-1} \approx r_e + 1{,}6556 \alpha^{-1}. \end{gathered}$$

As ρ increases the distance $r_{1,2}$ increases and the distances $r_{0,1} = r_{2,3}$ reduce, so that for $\rho \to \infty$ $r_{1,2} \to \infty$, $r_{0,1} = r_{2,3} \to r_e$.

Variant (V2). Combining (2.5) and (2.6c), we have

$$\begin{gathered} r_{0,1} = r_{1,2} = R + (1/3) \alpha^{-1} \ln (\xi_1 - 1) < R, \\ r_{2,3} = R - (2/3) \alpha^{-1} \ln (\xi_1 - 1) > R, \end{gathered} \tag{2.17}$$

since $\xi_1 < 3/2$. In particular, at point C

$$\begin{gathered} r_{0,1}^C = r_{1,2}^C \approx R_* - 0{,}4812 \alpha^{-1} \approx r_e + 0{,}2119 \alpha^{-1}, \\ r_{2,3}^C \approx R_* + 0{,}9624 \alpha^{-1} \approx r_e + 1{,}6556 \alpha^{-1}. \end{gathered}$$

As ρ increases the distance $r_{2,3}$ increases and the distances $r_{0,1} = r_{1,2}$ reduce so that for $\rho \to \infty$ $r_{2,3} \to \infty$, $r_{0,1} = r_{1,2} \to r_e$.

Variant (V3). Combining (2.5) and (2.6d), we have

$$r_{0,1} = R + (2/3) \alpha^{-1} \ln (\xi_1 - 1) > R,$$

$$r_{1,2} = r_{2,3} = R - (1/3)\alpha^{-1}\ln(\xi_1 - 1) < R, \tag{2.18}$$

since $\xi_1 > 3$. In particular, at point D

$$r^D_{0,1} \approx R_* + 0{,}9624\alpha^{-1} \approx r_e + 1{,}6556\alpha^{-1},$$
$$r^D_{1,2} = r^D_{2,3} \approx R_* - 0{,}4812\alpha^{-1} \approx r_e + 0{,}2119\alpha^{-1}.$$

As ρ increases the distance $r_{0,1}$ increases and the distances $r_{1,2} = r_{2,3}$ reduce, so that for $\rho \to \infty$ $r_{0,1} \to \infty$, $r_{1,2} = r_{2,3} \to r_e$.

The analysis carried out demonstrates that: a) a critical value of R* coincides with a critical bond length in an isolated biatomic molecule with an interaction according to (1.4) (the molecule is found from the maximum condition $d^2v/dr^2 = 0$ of the interaction force); b) when this critical value is attained, out of three interatomic bonds 0–1, 1–2, 2–3, which are "free" in selecting their lengths, two degrade and the third grows jumpwise to the length of a supercritical one, which under conditions of our problem can be interpreted as its breaking; c) new lengths of these three bonds do not depend in a quantitative sense on the variant of behavior selected by the chain [this follows from (2.16)-(2.18) and is well illustrated by the points B, C, and D]. Like the lengths of the remaining bonds, they are determined only by the degree of growth; and d) upon further monotonic growth of the chain there are no other qualitative changes in its state, similar to those described in item b.

3. Consideration of Interaction between Second Neighbors. In that case the term W_d in (1.3) will contain besides the energy W^0_d the sum $v(r_{-1,1}) + v(r_{1,3}) + v(r_{0,2}) + v(r_{2,4})$ of interaction contributions of atoms 1 and 2 with their second neighbors. From (1.1) and (1.2) it follows that $r_{-1,1} = R + r_{0,1}$, $r_{1,3} = 3R - r_{0,1}$, $r_{0,2} = 3R - r_{2,3}$, $r_{2,4} = R + r_{2,3}$. Passing to variables (1.5), we obtain

$$W_d(\xi_1, \xi_2, \rho) = W^0_d(\xi_1, \xi_2, \rho) + \varepsilon^2\xi_1^{-2}\rho^{-2} - 2\varepsilon\xi_1^{-1}\rho^{-1} + \varepsilon^2\xi_1^2\rho^{-6} -$$
$$- 2\varepsilon\xi_1\rho^{-3} + \varepsilon^2\xi_2^2\rho^{-6} - 2\varepsilon\xi_2\rho^{-3} + \varepsilon^2\xi_2^{-2}\rho^{-2} - 2\varepsilon\xi_2^{-1}\rho^{-1}, \tag{3.1}$$

where $W^0_d(\xi_1, \xi_2, \rho)$ is determined by (2.1) and

$$\varepsilon = \exp(-\alpha r_e) \tag{3.2}$$

is a dimensionless small quantity, which depends on the parameters of the Morse potential (for instance, for certain metals $1/88 < \varepsilon < 1/23$, according to [3]). Note that consideration of interaction between second neighbors leads to a change in the energy W_d by a small quantity of order ε: $W_d = W^0_d + \varepsilon O(W^0_d)$. Similarly, $W_c = W^0_c + \varepsilon O(W^0_c)$, due to which the chain's total potential energy $W = W^0 + \varepsilon O(W^0)$. In addition, Eq. (3.1) well illustrates that mutual repulsion of atoms, as compared to their attraction at great interatomic distances, may be neglected: the corresponding terms have different order with respect to ε.

In what follows we will neglect the terms containing ε to a power higher than the first. As in Sec. 2 we fix the value of ρ and, setting up equations for the chain equilibrium, we arrive at a system of equations with respect to ξ_1 and ξ_2:

$$-\rho^6 + \xi_1\rho^6 + \xi_1^4\xi_2^2 - \xi_1^3\xi_2\rho^3 + \varepsilon\xi_1\rho^5 - \varepsilon\xi_1^3\rho^3 = 0,$$
$$-\rho^6 + \xi_2\rho^6 + \xi_1^2\xi_2^4 - \xi_1\xi_2^3\rho^3 + \varepsilon\xi_2\rho^5 - \varepsilon\xi_2^3\rho^3 = 0.$$

We transform it to the form

$$(\xi_1^2\xi_2 - \rho^3)(\xi_1^2\xi_2 + \rho^3 - \xi_1\rho^3) - \varepsilon\xi_1\rho^3(\xi_1^2 - \rho^2) = 0,$$
$$(\xi_1\xi_2^2 - \rho^3)(\xi_1\xi_2^2 + \rho^3 - \xi_2\rho^3) - \varepsilon\xi_2\rho^3(\xi_2^2 - \rho^2) = 0. \tag{3.3}$$

Note that discarding the terms containing ε in the last system, we reduce it to the system ensemble (2.3), as would be expected.

One solution of (3.3) is obvious:

$$\{\xi_1 = \rho,\ \xi_2 = \rho\}; \tag{3.4}$$

however, to obtain the remaining solutions in the same way is impossible. Nonlinearity of the system's equations suggests that here the bifurcation theory methods for solving nonlinear equations can be applied [4]. Indeed, the analysis of interaction of the nearest neighbors has shown that the main point in studying the chain's equilibrium is the determination of the points and forms of stability loss of the basic equilibrium trajectory, i.e., the transition from a certain "basic" solution of equilibrium equations to "secondary" ones.

A general investigation, taking into account nonsymmetrical forms of the chain equilibrium ($r_{0,1} \neq r_{2,3}$), requires a solution of a complex problem of the bifurcation theory for the system of two equations in two unknowns ξ_1 and ξ_2, and two parameters ρ and ε; therefore, we consider below only a case of symmetry $r_{0,1} = r_{2,3}$.

Under such a condition $\xi_1 = \xi_2 = \xi$ and two equations of the chain equilibrium are reduced to one:

$$F(\xi, \varepsilon, \rho) = (\xi - 1)\rho^6 + \xi^6 - \xi^4\rho^3 + \varepsilon\xi\rho^5 - \varepsilon\xi^3\rho^3 = 0. \tag{3.5}$$

A real function F of real arguments is continuous and has continuous partial derivatives of any order with respect to all the arguments. Factoring the left-hand part of (3.5): $F(\xi, \varepsilon, \rho) = (\xi - \rho)F_1(\xi, \varepsilon, \rho)$, where

$$F_1(\xi, \varepsilon, \rho) = (\xi^2 + \xi\rho + \rho^2)(\xi^3 - \xi\rho^3 + \rho^3) - \varepsilon\xi\rho^3(\xi + \rho), \tag{3.6}$$

we have an apparent solution of (3.5)

$$\xi = \rho, \tag{3.7}$$

whose existence follows also from (3.4). Solution (3.7) corresponds to an "ideal" configuation of the chain and we will call it basic, as in Sec. 2. The point (ρ_b, ρ_b) will be a branch point of the basic solution (3.7), if there exists at least one solution

$$\xi = \xi(\varepsilon, \rho) \tag{3.8}$$

of the equation $F_1(\xi, \varepsilon, \rho) = 0$, satisfying the condition $\rho_b = \xi(\varepsilon, \rho_b)$ and defined in some neighborhood of the point (ρ_b, ρ_b). Geometrically this means that curves (3.7) and (3.8), lying in the plane (ξ, ρ), intersect at the point (ρ_b, ρ_b).

According to the general theory (see [4], pp. 13, 26), such points exist if the derivative $\partial F/\partial\xi$ is equal to zero at these points. Substituting the relation $\partial F(\xi, \varepsilon, \rho)/\partial\xi = 0$ into the equation $\xi = \rho$, we find the coordinates of the branch point (correct to the first-order magnitude with respect to ε)

$$\rho = 2 - (2/3)\varepsilon. \tag{3.9}$$

In order to find solutions (3.8), branching off from the basic solution at the point (ρ_b, ρ_b), we make a substitution $\xi = \zeta + \rho_b$, $\rho = \lambda + \rho_b$ in (3.6) and represent the expression $F_1(\zeta, \varepsilon, \lambda)$ in the form of a polynomial in the variables ζ and λ with coefficients depending on ε: $F_1(\xi, \varepsilon, \lambda) = \sum_{i,j} F_{ij}^1(\varepsilon)\zeta^i\lambda^j$. Applying the Newton's diagram method [4] to the equation $F_1(\zeta, \varepsilon, \lambda) = 0$, we obtain in the neighborhood of the point $(\zeta, \lambda) = (0, 0)$ its solution in the form of a convergent series in integral positive powers λ and coefficients depending on ε. According to the adopted simplification, we retain in these coefficients only the quantities of the order not higher than the first with respect to ε: $\zeta(\varepsilon, \lambda) = (3 - (4/3)\varepsilon)\lambda + o(\lambda)$. Making a reverse substitution, we find in the neighborhood of the point (ρ_b, ρ_b) the following solution

$$\xi(\varepsilon, \rho) = \rho_b + (3 - (4/3)\varepsilon)(\rho - \rho_b) + o(\rho - \rho_b) \tag{3.10}$$

of the equilibrium equation (3.5) branching off from the basic solution at the point (ρ_b, ρ_b) and presented in the form of a convergent series in integral positive powers $\rho - \rho_b$. Besides (3.7) and (3.10), Eq. (3.5) has no other solutions passing through the point (ρ_b, ρ_b).

It is easy to show that in space $\{\xi_1, \xi_2, \rho\}$ along the basic equilibrium trajectory of the chain $\{\xi_1 = \xi_2 = \rho\}$, determined by relation (3.4) [or (3.7)], the function W_d (without the terms with ε^2) has minima for $\rho < \rho_b$ and maxima for $\rho > \rho_b$. In addition, the function has a bend at the point (ρ_b, ρ_b, ρ_b), which is the point of stability loss of an "ideal" configuration of the chain and its transition to a "nonideal," but symmetrical (since $r_{0,1} = r_{2,3}$) configuration determined by (3.10) in the neighborhood of this point, taking into account that $\xi_1 = \xi_2 = \xi$.

We have obtained in Sec. 2 that upon interaction of the nearest neighbors symmetrical forms of the chain equilibrium are given by relations (2.6a) and (2.6b), while the coordinates of the branch point of the corresponding trajectories are given by Eq. (2.7). Using the Newton's diagram method we can represent the dependence (2.6b) in the neighborhood of point (2.7) in the form of the convergent series

$$\xi_1 = \xi_2 = 2 + 3(\rho - 2) + o(\rho - 2) \tag{3.11}$$

in integral positive powers $\rho - 2$.

Comparing (3.11) with (3.10) and (2.7) with (3.9), we arrive at a conclusion that in the symmetrical statement of the problem a consideration of interaction between the atoms—second neighbors leads to a change in the parameters being defined by a magnitude of the order ε.

4. Discussion. From the terms of the problem it is easily seen that it actually deals with a tetratomic chain with fixed terminal atoms 0 and 3, "inserted" into a rigidly fixed unidimensional atomic array. Such a statement is caused by the necessity to take into account the interaction between nonadjacent atoms and, generally speaking, in Sec. 2 it could be refused; the authors, however, did not do it for keeping the model's generality. Thus, the results obtained can be compared to the results from [1].

The comparison shows that removing the restriction on the symmetry, imposed on the chain in [1], results in the appearance of two nonsymmetrical forms of stability loss of its "ideal" configuration. Moreover, when the critical state (2.7) is attained, stability loss can take place both according to the symmetrical form analyzed in [1] and according to nonsymmetrical forms being revealed, and there is a coincidence of the corresponding characteristics of the chain (bond lengths and energy) in all the forms of secondary equilibrium. Probably, it should be expected that any imperfections in the chain's structure (for example, the presence of a substitutional atom) violate such an "equality" of forms. The authors of [1] analyzed one of such imperfections, namely, weakening of the chain's middle bond, but as applied to the calculation of energy barriers on the way of crack propagation and only on the assumption of the chain's symmetry.

Consideration of interaction between nonadjacent atoms, characterized by a change in the chain's potential energy by a magnitude of the order of a small parameter ε, does not introduce corrections into the qualitative behavior of the chain in a symmetrical statement of the problem, while quantitative changes in the parameters have the order of ε. In the general statement, however, even such a small variation can be of great importance, for example, in determining the form of the first stability loss of an "ideal" state of the chain.

If the Hirth model, due to symmetry, is applicable only to atomistically acute cracks, then the investigation results in Sec. 2 of a more general case of the chain growth can be used for modeling propagation of a crack blunted as a result of a shear and dislocation emission. Let atoms 0, 1, 2, 3 in Fig. 1 form the tip of the blunted crack, then application of the force that causes a critical chain growth results in breaking of one of 0—1, 1—2, 2—3 bonds. This can be considered as penetration of an acute crack from the tip of the blunted one.

The results of the work also relate to the problems of crack nucleation. Novozhilov [5] has formulated an approach to brittle cracks as nontrivial forms of equilibrium deformation of an elastic body on application of an extending load, illustrated by a simple example of stability loss of a medium atom in a triatomic chain. The above investigation into the equilibrium of a tetratomic chain with two free atoms confirms the concept proposed in [5].

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