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LOSS OF STABILITY OF ON ATOMIC CHAIN REGION IN THE PRESENCE OF IMPURITY. STRENGTH REDUCTION OF CRACKED BRITTLE SOLIDS

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1. Introduction. "The applied significance of fracture mechanics is due to the possibility (under various real conditions) of decreasing considerably the critical levels of stresses and fracture energy compared with those measured in standard tests of material. This possibility arises under the action of defects and surface-active media" [1, p. 97]. Impurities are among to the most important and common defects of the crystal structure of actual solids [2, chaps. 5 and 8; 3]. "The available theories of solids can neither take into account nor explain many factors that are known to metallurgists as those determining the structure and various properties of solid solutions. Some factors such as, e.g., chemical affinity or the difference in atomic sizes, are considered only semiempirically" [2, p. 489]. In atomistic models of fracture, the influence of an impurity is considered semiempirically using the main factors (dimension or energy) that determine the behavior of impurities in solid solutions. The dimensional factor is given in the form

$$\delta = (r_Q - r_M)/r_M, \tag{1.1}$$

where r_M and r_Q are the shortest interatomic spacings in the lattices of solvent M and dissolved element Q, respectively [2, p. 503]. For nonzero δ at the atomic scale, the atoms of the solvent and the dissolved element are shifted from their mid-positions in the crystal lattice and thus are in an elastically stressed state of constant static shift [2, p. 500; 4]. Thus, the key parameter in the numerical experiments of [5, 6] is the difference in atomic size between the crystallite and the thin film (of one or a few atomic layers) that covers the crack surface. In addition, if the sizes of the film atoms are smaller than those of the crystallite, brittle fracture is observed throughout the plastic crystallite. The energy factor is ignored.

This paper, using a one-dimensional atomic model as an example, shows the possibility of strength reduction of a solid whose atomic lattice contains impurities. Particular examples that have a physical meaning are given. In principle, the decrease in strength can reach one or two orders of magnitude and is determined by differences in atomic interaction. Under the model conditions, this decrease can be calculated from the given formulas using numerical values of the parameters of the known potential function of the interaction between the main and impurity atoms. In this case, allowance for both dimensional and energy factors is required.

2. Atomic Model of Brittle Fracture in the Presence of Impurity. The general statement of problem formulated in [7] remains unchanged. The triatomic chain studied is built into an infinite chain of fixed atoms, but one atom of the chain is considered an impurity atom (substitution atom). Accordingly, the interaction of this atom with its neighbors and, hence, the potential function parameters are changed.

Triatomic chains with an impurity atom which is either central or at the end are considered. The equilibrium patterns and the relation $t = P_*/p_*$ between the critical values of the force P that extends a chain with an impurity atom and the critical value of the force p that extends an "ideal" chain are determined. This

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relation depends on the difference in the atomic interaction parameters. In this case, both the dimensional and energy factors are taken into account. As an interatomic potential we take the Morse potential

$$v(r) = D(\exp(-2\alpha(r - r_e)) - 2\exp(-\alpha(r - r_e))). \tag{2.1}$$

Since, in the general case, there are two sets of potential parameters D, α, and r_e, the analysis can be simplified by assuming interaction only between the nearest neighbors. The impurity atom is denoted by Q and the other atoms are denoted by M. The M–Q interaction is described by the Morse function

$$v_{MQ}(r) = D_{MQ}(\exp(-2\alpha_{MQ}(r - r_e^{MQ})) - 2\exp(-\alpha_{MQ}(r - r_e^{MQ}))). \tag{2.2}$$

For M–M interaction, the previous notation of (2.1) without subscripts and superscripts is retained. We now consider a set of real positive dimensionless quantities:

$$k = D_{MQ}/D; \tag{2.3}$$

$$\mu = \alpha_{MQ}/\alpha; \tag{2.4}$$

$$æ = \exp(\alpha(r_e^{MQ} - r_e)). \tag{2.5}$$

The first two quantities reflect the influence of the energy factor, and the latter reflects the influence of the dimensional factor under the assumption that this factor is determined by the difference in the parameters r_e and r_e^{MQ} of potentials (2.1) and (2.2), respectively.

We denote an arbitrary atom of the chain by 0. The remaining atoms are denoted by integers (Fig. 1). We assume that under extension atoms with subscripts $\ldots, -3, -2, -1, 1, 2, 3, \ldots$ always occupy positions that correspond to the ideal structure of the extended chain, i.e.,

$$\ldots = r_{-3,-2} = r_{-2,-1} = 0.5\, r_{-1,1} = r_{1,2} = r_{2,3} = \ldots\,. \tag{2.6}$$

Let the chain be extended by a force P to the state in which the bond lengths in (2.6) are equal to a certain value d. We fix all atoms of the chain, except for the "zeroth" atom, in their "ideal" positions. In this case, the position of the "zeroth" atom is fully determined by one of the quantities $r_{-1,0}$ or $r_{0,1}$, i.e., by the distances to its nearest neighbors (Fig. 1). We assume that the quantity $r_{-1,0}$ is the determining one. Since $r_{-1,1} = 2d$, we have

$$r_{0,1} = 2d - r_{-1,0}. \tag{2.7}$$

Let us describe the behavior of the given "zeroth" atom as a function of both the degree of extension of the chain and the presence of an impurity. The degree of extension is defined by the parameter d, which is related to the deformation η of the atomic bond of the nearest neighbor by $\eta = (d - d_0)/d_0$. We consider the case of interaction between the nearest neighbors only. Long-range action has been considered in [7]. By condition, relation (2.6) remains valid in the presence of an impurity, i.e., all atoms of the chain, except for the free atom, are fixed rigidly in accordance with the value of P (value of d), including the initial moment when $P = 0$. Thus, for a nonzero dimensional factor δ, the given triatomic part of the chain is in a stressed state of either compression or extension, and the atomic bonds in it are subject to deformation. This is in agreement with the above-mentioned influence of the dimensional factor. However, atomic relaxation is ignored. To take it into account, one must change accordingly the length of the triatomic chain compared with d.

Let us introduce the dimensionless variables

$$\xi = \exp(\alpha(r_{-1,0} - r_e)), \qquad \rho = \exp(\alpha(d - r_e)). \tag{2.8}$$

Note that ξ and ρ are always positive. Moreover, since extension is considered, we have $r_{-1,0} \geqslant r_e$ and $d \geqslant r_e$, and, hence, $\xi \geqslant 1$ and $\rho \geqslant 1$. Formulas (2.8) give a one-to-one correspondence between sets of the quantities ξ and ρ or $r_{-1,0}$ and d, and the problem can be solved for the variables ξ and ρ. In this case, ρ determines chain extension, and ξ, the position of atom 0.

In [7], the force p that extends an "ideal" infinite chain is calculated by the formula $p = p(\rho) = (2D\alpha/\rho^2)(\rho - 1)$, and the critical force p_* (for $\rho = \rho_* = 2$), by the formula $p_* = p(\rho_*) = D\alpha/2$, i.e., p_* equals p_m (the theoretical tensile strength of the atomic bond).

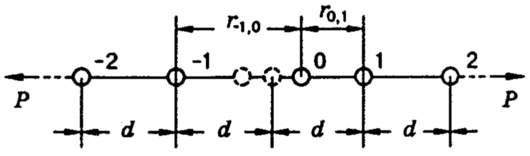

Fig. 1

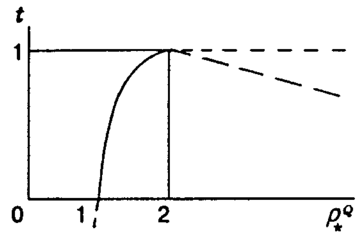

Fig. 2

TABLE 1

M	Q	α	α_{MQ}	D	D_{MQ}	r_e	r_e^{MQ}
Cu	Gd	1.355	0.775	0.338	0.310	2.871	4.058
Gd	Cu	0.763	0.775	0.302	0.310	4.469	4.058
Al	Gd	1.052	0.810	0.274	0.339	3.400	4.097
Gd	Al	0.763	0.810	0.302	0.339	4.469	4.097
Fe	Al	1.358	0.972	0.418	0.373	2.871	3.378
Al	Fe	1.052	0.972	0.274	0.373	3.400	3.378
Cu	Au	1.283	1.315	0.579	0.623	2.811	2.937
Au	Cu	1.403	1.315	0.725	0.623	3.048	2.937
Ni	Fe	1.366	1.419	0.754	0.645	2.720	2.755
Fe	Ni	1.893	1.419	0.727	0.645	2.820	2.755

Model conditions and the derivation of this formula by limit passage allow this formula to be applied to the impurity-containing chain. Hence,

$$t = P_*/p_* = 4(\rho_*^Q)^{-2}(\rho_*^Q - 1), \qquad (2.9)$$

where $P_* = p(\rho_*^Q)$; ρ_*^Q is the critical parameter of chain extension with an impurity.

Remark. The discrete criterion of Novozhilov's brittle strength [8, 9] is directly related to the use of the estimated theoretical strength of an atomic structure at the crack tip. The theoretical strength in the presence of impurity can sharply decrease.

The curve of $t(\rho_*^Q)$ is plotted in Fig. 2. The case of $\rho_*^Q < 1$ is of no interest, because then $t < 0$ and $P_* < 0$, which indicates rupture of the chain before application of an extending force. In turn, the inequality $\rho_*^Q > 2$ means that both bonds of the free atom are "stronger" than the bonds of atoms of the constrained parts of the chain for which $\rho_* = 2$; this case is excluded by the statement of the problem. Only the part of the graph shown by the solid curve, which corresponds to the intercept $1 \leqslant \rho_*^Q \leqslant 2$, has a real meaning. This case is interesting from the standpoint of the decrease in critical forces and only this case will be considered below.

Note that the tensile strength of the chain can decrease considerably. Thus, $t < 0.2$ for $1 \leqslant \rho_*^Q < 1.056$; $t < 0.1$ for $1 \leqslant \rho_*^Q < 1.026$, and even $t < 0.01$ for $1 \leqslant \rho_*^Q < 1.0025$. Being situated at the tip of a brittle crack, this chain can cause crack propagation under loads that are 1–2 orders of magnitude smaller than the theoretical material strength. As will be shown, ρ_*^Q and, hence, t are determined from relations (2.3)–(2.5) between the parameters of the potential functions. The body of data on the parameters of Morse's potential function of the atomic interaction in two-component systems are rather limited. Table 1 summarizes the parameters of Morse's potential functions calculated for Cu_3Au and Ni_3Fe alloys [4] and for GdAl, GdCu, and Fe_3Al alloys [10], i.e., for ten M–Q pairs. These data were used in the calculations for each model case.

3. Chain Extension with a Free Impurity Atom. We now consider the problem of the stability of an atomic chain under extension. In this case, the free atom 0 is a Q-type impurity atom. The asymmetric equilibrium position of this atom is shown by either hatching or filling in Fig. 3. Thus, we have a (-1)–0–1

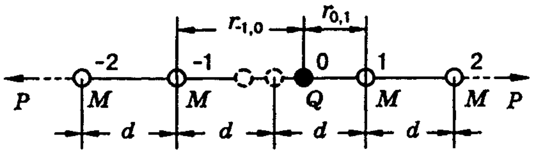

Fig. 3

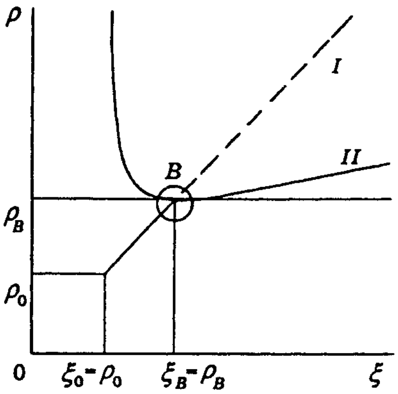

Fig. 4

triatomic chain that consists of two M–Q bonds inserted in the "middle" of an infinite chain of M–M bonds. We determine the portion V_0 of the total potential energy of atomic interaction that falls on the "zero" atom

$$V_0 \equiv V_0(r_{-1,0}, d) = v_{MQ}(r_{-1,0}) + v_{MQ}(2d - r_{-1,0}). \tag{3.1}$$

Introducing dimensionless variables ζ and λ [see (2.8)],

$$\zeta = \exp(\alpha_{MQ}(r_{-1,0} - r_e^{MQ})), \qquad \lambda = \exp(\alpha_{MQ}(d - r_e^{MQ})), \tag{3.2}$$

we completely extend the solution for $\varepsilon \equiv 0$ from [7] to the given case by replacing D by D_{MQ}, x by ζ, and y by λ. The results obtained are quite similar to those in [7]. As λ increases from the initial value λ_0 [see formula (3.4)], which corresponds to the absence of external action on the chain $P = 0$, the impurity atom 0 is in a stable equilibrium state, which is symmetric to the nearest neighbors -1 and 1. This holds up to $\lambda = \lambda_B = 2$, inclusively. The value of λ_B corresponds to the branch point $B(\lambda_B, \lambda_B)$ of the basic equilibrium trajectory $\{\zeta = \lambda\}$ of atom 0 in space $O\zeta\lambda$. As the critical value $\lambda_B = 2$ is exceeded, the impurity atom 0 occupies one of two stable asymmetric (relative to its neighbors) positions, which are characterized by the relation $\zeta^2 - \lambda^2\zeta + \lambda^2 = 0$. These secondary positions of the impurity atom can be shown to be mutually symmetric about the center of symmetry of the (-1)–0–1 triatomic chain. One of the (-1)–0 and 0–1 bonds has a supercritical length for M–Q interaction, which is identical to its rupture. The pattern of equilibrium states of the chain in space $O\xi\rho$ is the same as in the "ideal" case [7] and is given in Fig. 4, in which curves I and II describe the basic and secondary equilibrium trajectories, and B is the branch point. In the interaction of only the nearest neighbors, the critical value is $\lambda_* = \lambda_B = 2$ and the force is $P_* = P(\lambda_*) = P_B$. To determine P_* and t (2.9), we express the variable ρ from (2.8) in terms of the variable λ. We have $\lambda = \exp(\alpha_{MQ}(d - r_e^{MQ})) = (\exp(\alpha(d - r_e))\exp(-\alpha(r_e^{MQ} - r_e)))^\mu = (\rho/æ)^\mu$, i.e.,

$$\rho = æ\lambda^{1/\mu}, \tag{3.3}$$

where μ and $æ$ are given by (2.4) and (2.5). Since the initial value is $\rho = \rho_0 = 1$, we have

$$\lambda_0 = (\rho_0/æ)^\mu = æ^{-\mu} = \exp(\alpha_{MQ}(r_e - r_e^{MQ})), \tag{3.4}$$

i.e., the initial length of the bond is $d_0 = r_e$.

If we express the variable ζ in (2.8) in terms of ξ, we can construct a diagram for the equilibrium states of the chain in space $O\xi\rho$ and compare it with the diagram for the "ideal" case. As follows from Fig. 5 (curve 1 is an "ideal" chain and curve 2 is a chain with a free impurity atom Q), this pattern does not change quantitatively with impurity introduction. However, branching of the basic equilibrium trajectory I occurs at point B_Q, when, by virtue of (3.3),

$$\rho_*^Q = æ\lambda_*^{1/\mu} = 2^{1/\mu}æ. \tag{3.5}$$

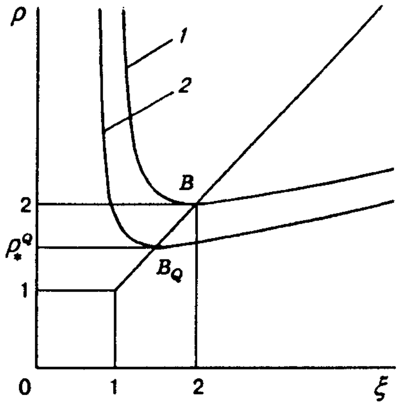

Fig. 5

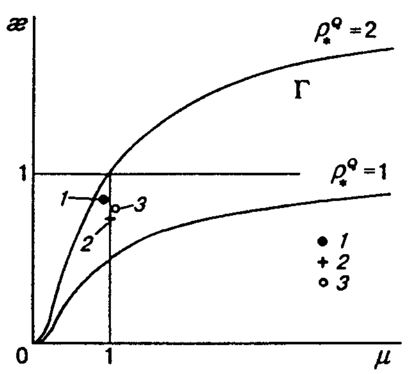

Fig. 6

TABLE 2

M	Q	ρ_*^Q	t
Au	Cu	1.793	0.987
Gd	Cu	1.445	0.8528
Gd	Al	1.446	0.8535

Substituting (3.5) into (2.9), we obtain the dependence of t on two quantities: μ and æ. The former means that the possibility of decreasing the level of critical forces is influenced by the shape of the curve of the potential function, which is determined by the quantity α. The possibility is the greater, the steeper the walls of the potential "hole" of the M–Q impurity bond [function (2.2)]. The second quantity represents the influence of the dimensional factor (1.1). The shorter the equilibrium length r_e^{MQ} of the M–Q bond compared with r_e, the more this bond is deformed in the chain and the smaller the effort required for its rupture. P_* and t decrease if the joint action of these factors leads to a decrease in the critical length of the M–Q bond,

$$r_m^{MQ} = r_e^{MQ} + \alpha_{MQ}^{-1} \ln 2, \tag{3.6}$$

compared with r_m. Note that the quantity k is does not enter into formula (3.5) and, hence, the relation between the depths of the potential "holes" on curves of v_{MQ} and v is of no importance. Thus, in our case, the influence of the energy factor on chain rupture is generally limited.

Two limiting cases can occur where $\rho_*^Q = 2$ and $t = 1$ and where $\rho_*^Q = 1$ and $t = 0$. In the former case, $æ = 2^{1-1/\mu}$ and in the latter, $æ = 2^{-1/\mu}$. These dependences are plotted in Fig. 6. It is readily seen that values $0 < t < 1$, i.e., a decrease in the tensile strength of the triatomic chain with a central impurity atom, correspond to points $(\mu, æ)$ in region Γ. In this case, if the point $(\mu, æ) \in \Gamma$ is closer to the curve of $æ = 2^{-1/\mu}$, the value of t is smaller. In Fig. 6, (1) is a point of the region that corresponds to a Cu impurity in Au, (2) corresponds to a Cu impurity in Gd, and (3), to an Al impurity in Gd. Calculations using the data from Table 1 show that a decrease in the critical force for three M–Q pairs. The calculated results are given in Table 2.

4. Extension of a Triatomic Chain with an End Impurity Atom. Let one of the two nearest neighbors of the free atom of the chain be an impurity atom and be located at, e.g., site 1 (in Fig. 7, it is darkened). Thus, the (−1)-0-1 triatomic part of the chain is of the form M–M–Q and the energy of the "zeroth" atom is

$$V_0 \equiv V_0(r_{-1,0}; d) = v(r_{-1,0}) + v_{MQ}(2d - r_{-1,0}). \tag{4.1}$$

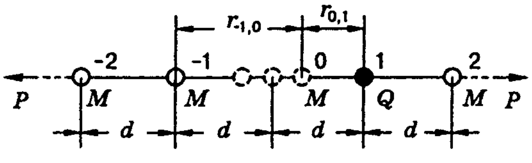

Fig. 7

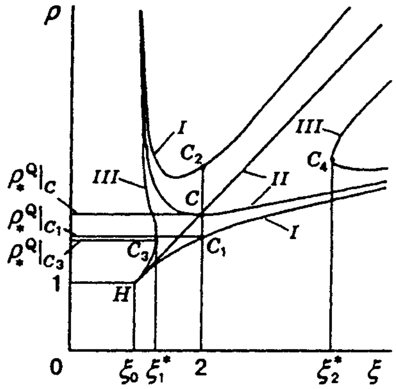

Fig. 8

Transforming to the variables ξ and ρ using formulas (2.8), we have $V_0 \equiv V_0(\xi, \rho)$ and, hence,

$$\left(\frac{2}{D}\right)V_0 = \frac{1}{\xi^2} - \frac{2}{\xi} + k\left(\frac{\xi^2 æ^2}{\rho^4}\right)^\mu - 2k\left(\frac{\xi æ}{\rho^2}\right)^\mu. \tag{4.2}$$

Thus, the equilibrium equation for the "zeroth" atom $\partial V_0/\partial\xi = 0$ is equivalent to the equation

$$(\xi - 1)\rho^{4\mu} - k\mu æ^\mu \xi^{\mu+2}\rho^{2\mu} + k\mu æ^{2\mu}\xi^{2\mu+2} = 0 \tag{4.3}$$

(the parameters k, μ, and $æ$ are considered fixed).

Finding solutions of equilibrium equation (4.2) and their study using analytical methods is a much more complex problem than in the case of an "ideal" chain. Thus, in the general case, it is impossible to write a solution of Eq. (4.3) in the form $\xi = \xi(\rho)$. We solve this equation for ρ:

$$\rho_{(1),(2)} = \left(\frac{k\mu æ^\mu \xi^{\mu+2}}{2(\xi - 1)}\left(1 \mp \left(1 - \frac{4(\xi - 1)}{k\mu\xi^2}\right)^{1/2}\right)\right)^{1/2\mu}. \tag{4.4}$$

Here the plus sign refers to $\rho_{(2)}$. The real solutions of Eq. (4.4) exhibit the property that

$$\rho_{(1)}(\xi) \leqslant \rho_{(2)}(\xi) \tag{4.5}$$

for a given ξ and exist on the condition that $k\mu\xi^2 - 4\xi + 4 \geqslant 0$. We introduce the notation

$$\varphi = k\mu. \tag{4.6}$$

Obviously, the quantity φ is positive [see expressions (2.3) and (2.4) reflecting the influence of the energy factor]. We rewrite the latter inequality as

$$\varphi\xi^2 - 4\xi + 4 \geqslant 0. \tag{4.7}$$

Its solution depends on φ. For $\varphi > 1$, inequality (4.7) is rigorous and holds for all ξ, so that inequality (4.5) is also rigorous.

Before considering the case of $0 < \varphi \leqslant 1$, we must solve the equation

$$\varphi\xi^2 - 4\xi + 4 = 0. \tag{4.8}$$

It can be solved in real numbers for $\varphi \leqslant 1$. Its roots are

$$\xi_{1,2}^* = \frac{2}{\varphi}(1 \mp \sqrt{1 - \varphi}), \tag{4.9}$$

where the plus sign refers to ξ_2^*. For $\varphi = 1$, the roots coincide, i.e., $\xi_1^* = \xi_2^* = 2$. Thus, for $0 < \varphi \leqslant 1$, condition (4.7) is satisfied and solutions (4.4) hold for either $\xi \leqslant \xi_1^*$ or $\xi \geqslant \xi_2^*$. In this case, $\rho_{(1)}(\xi) = \rho_{(2)}(\xi)$ if and only if $\xi = \xi_{1,2}^*$.

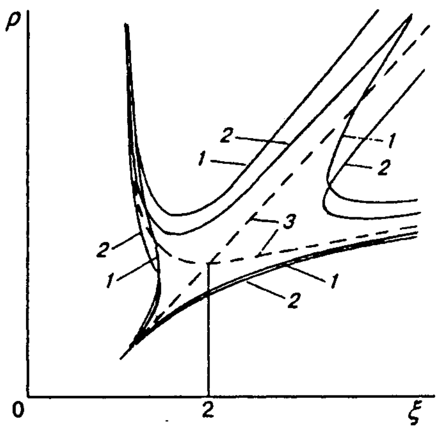

Fig. 9

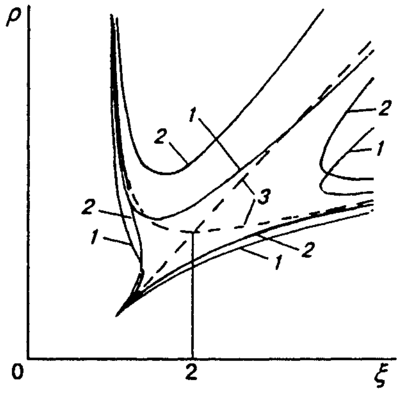

Fig. 10

Equations (4.4) relate the chain extension parameter ρ to the configuration parameter ξ for the equilibrium states of the chain. These relations are shown schematically by curves in plane $O\xi\rho$. Each point corresponds to a definite equilibrium state. Figure 8 shows the characteristic position of these curves for $\varphi > 1$, $\varphi = 1$, and $\varphi < 1$ for the same constant value of æ (curves I–III).

The influence of changes in the parameters k, μ, and æ on the shape of curves (4.4) can be seen in Figs. 9–11, in which curves 3 are the equilibrium trajectories in the "ideal" case for $k = \mu = æ = 1$. In Fig. 9, curves 1 and 2 correspond to $k = 1.1$ and 0.9 for $æ = 1$, $\varphi = 0.855$ and 1.125. Curves 1 and 2 in Fig. 10 correspond to $\mu = 1.25$ and 0.9 for $æ = 1$, $\varphi = 0.81$ and 1.2. In Fig. 11, curves 1 and 2 correspond to $æ = 0.75$ and 1.25 for $\mu = 1$, $\varphi = 0.8$ and 1.2.

Since the solutions of (4.4) have the form $\rho = \rho(\xi)$, it is impossible to study the entire behavior of the chain under extension, i.e., to determine ρ from ξ. Thus, we shall examine only some characteristic equilibrium states of the chain and try to describe qualitatively the changes in the chain under extension.

First, we consider the initial equilibrium state of the chain (point H in Fig. 8) for $P = 0$, $\rho = \rho_0 = 1$, and $d = d_0 = r_e$. Substituting $\rho = 1$ into Eq. (4.3) and taking into account (4.6), we obtain an equation for the corresponding value of ξ_0:

$$\varphi æ^{2\mu}\xi_0^{2\mu+2} - \varphi æ^{\mu}\xi_0^{\mu+2} + \xi_0 - 1 = 0. \tag{4.10}$$

We write Eq. (4.10) as $\varphi æ^{\mu}\xi_0^{\mu+2}(æ^{\mu}\xi_0^{\mu} - 1) + (\xi_0 - 1) = 0$ and assume that $æ < 1$. Obviously, $\xi_0 > 1$; otherwise the left-hand side of the equality would have been negative. Therefore, we have $æ^{\mu}\xi_0^{\mu} - 1 < 0$, i.e., $\xi_0 < 1/æ$. Hence,

$$1 < \xi_0 < 1/æ \quad \text{at} \quad æ < 1. \tag{4.11}$$

Similarly,

$$1/æ < \xi_0 < 1 \qquad \text{at} \quad æ > 1; \tag{4.12}$$

$$\xi_0 = 1 \qquad \text{at} \quad æ = 1. \tag{4.13}$$

Thus, for a zero dimensional factor ($æ \neq 1$), the (-1)–0 and 0–1 bonds are deformed even in the initial state. For the given k, μ, and æ, the lengths of these bonds are determined via ξ_0. In particular, both bonds are extended for $æ < 1$.

We now determine the values of ξ and ρ in the critical states of each of the (-1)–0 and 0–1 bonds.

According to (3.6), the critical length of the 0–1 impurity bond is

$$r^*_{0,1} = r_e^{MQ} + \frac{\ln 2}{\alpha_{MQ}}. \tag{4.14}$$

If we denote [cf. (3.2)]

$$\zeta = \exp(\alpha_{MQ}(r_{0,1} - r_e^{MQ})), \tag{4.15}$$

$r_{0,1}^*$ corresponds to $\zeta_* = 2$. Using Eqs. (2.4), (2.7), and (2.8), we determine the relation between the parameters ρ, ξ, and ζ:

$$\rho^2 = \zeta^{1/\mu} æ \xi. \tag{4.16}$$

Substituting $\zeta_* = 2$ into this formula, we obtain

$$\rho_*^Q = (2^{1/\mu} æ \xi^*)^{1/2}. \tag{4.17}$$

Here ξ^* corresponds to $\zeta_* = 2$ in an equilibrium state of the chain. To find ξ^*, we substitute (4.17) into Eq. (4.3) and exclude ρ. After simplification we obtain $\varphi(\xi^*)^2 - 4\xi^* + 4 = 0$. This means that ξ^* is a root of Eq. (4.8) that exists only for $\varphi \leqslant 1$ [see (4.9)].

Thus, there are not more than two equilibrium states of the chain with critical length (4.14) of the 0–1 impurity bond, provided that $0 < \varphi \leqslant 1$. The values of ρ_*^Q are determined by substituting (4.9) into (4.17).

The following two cases are possible.

(1) If $\varphi = 1$, then $\xi_1^* = \xi_2^* = 2$, and the critical states studied coincide (the intersection point C of curves II in Fig. 8). In state C of the chain, the (−1)–0 bond is also extended to the critical length

$$r_{-1,0}^* = r_e + \alpha^{-1} \ln 2. \tag{4.18}$$

At point C,

$$\rho_*^Q\Big|_C = (2^{1+1/\mu} æ)^{1/2}. \tag{4.19}$$

This case is similar to the case in Section 3. The critical force P_* for the impurity-containing chain is smaller than that for the "ideal" chain if $1 \leqslant \rho_*^Q < 2$. This inequality, together with (4.19), is used to determine a set of pairs of the parameters μ and $æ$ for which the tensile strength of the chain decreases in the presence of an impurity. This set corresponds to points of region Γ in Fig. 12 ($\varphi = 1$).

(2) If $0 < \varphi < 1$, it can be easily shown that

$$1 < \xi_1^* < 2 < \xi_2^*. \tag{4.20}$$

Indeed, let us assume the opposite, e.g., $\xi^* > 2$. Then, $1 - \varphi \geqslant \sqrt{1 - \varphi}$, which is impossible for $0 < \varphi < 1$. Similarly, we prove (by contradiction) the remaining parts of the inequality. For $0 < \varphi < 1$, there are two different equilibrium states of the chain in which the 0–1 impurity bond is extended to the critical length (4.14). In Fig. 8, these are designated by C_3 and C_4. These points are the "sewing" points of the branches of curves (4.4), because for $\xi = \xi_{1,2}^*$ inequality (4.5) becomes an equality. The values of ρ_*^Q at these points are found by substituting (4.9) into (4.17). Note that $\rho_*^Q(\xi_1^*) < \rho_*^Q(\xi_2^*)$ by virtue of (4.20), and, hence, for quasistatic extension of the chain with a gradually increasing force P and length d, state C_3 is reached first at $\rho = \rho_*^Q(\xi_1^*)$. The point that characterizes the chain moves therewith from the initial state H to C_3 along the left equilibrium trajectory III in Fig. 8. Since relations (4.2)–(4.4) are rather complex, the changes in chain configuration with passage through point C_3 can be examined only qualitatively. The graph shows [allowing for condition (4.7) and inequality (4.20)] that at point C_3 the quantity ξ reaches the largest value ($\xi_1^* < 2$) on the "left" branch, and, hence, the largest length $r_{-1,0}$ of the (−1)–0 bond is shorter than the critical length (4.18). Further quasistatic extension [$\rho > \rho_*^Q(\xi_1^*)$] leads to a decrease in ξ and an increase in ζ.

Since ξ is a limited quantity, according to (4.16), $\zeta \to \infty$ as $\rho \to \infty$. This implies that $r_{-1,0} \to \infty$, i.e., the 0–1 impurity bond is broken. To prove a decrease in ξ, we express ξ in terms of ρ and ζ using formula (4.16) in the form

$$\xi = \zeta^{-1/\mu} æ \rho^2 \tag{4.21}$$

and substitute the result into Eq. (4.3). We obtain a representation of ρ^2 via ζ:

$$\rho^2 = \frac{\zeta^{2+1/\mu} æ}{2\varphi(\zeta - 1)} \left(1 \mp \left(1 - \frac{4\varphi(\zeta - 1)}{\zeta^2}\right)^{1/2}\right). \tag{4.22}$$

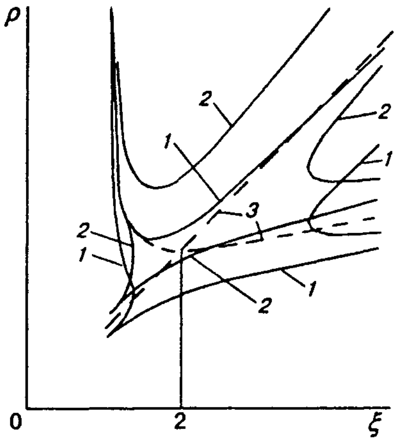

Fig. 11

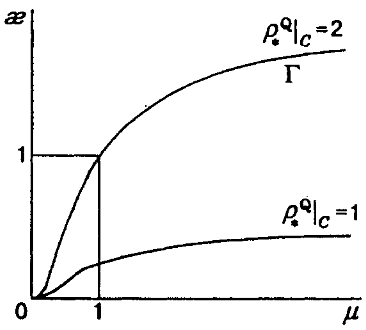

Fig. 12

Formulas (4.21) and (4.22) are used to determine the relation between ξ and ζ at points of the equilibrium trajectory for $0 < \varphi < 1$, i.e., along curves III in Fig. 8. In particular, at points of the upper part of the "left" trajectories [i.e., for $\rho > \rho_*^Q(\xi_1^*)$], we have

$$\xi = \frac{\zeta^2}{2\varphi(\zeta - 1)} \left(1 - \left(1 - \frac{4\varphi(\zeta - 1)}{\zeta^2}\right)^{1/2}\right).$$

Passing to the limit $\zeta \to \infty$ in the latter equality, we obtain $\xi \to 1 + 0$. Thus, $r_{-1,0} \to r_e$.

For $\varphi > 1$, as was mentioned above, no equilibrium states of the chain with the critical length of the 0–1 bond exist. To clarify the behavior of the chain, we consider the behavior of the chain under (−1)–0 bond extension. Its critical length is given by formula (4.18) and is reached for $\xi = \xi_* = 2$. A comparison of these values of ξ with condition (4.7) shows that the equilibrium states of the chain with the critical length of the (−1)–0 bond are possible only for $\varphi \geqslant 1$.

We assume that $\varphi > 1$ (the case of $\varphi = 1$ was considered above [point C in Fig. 8)]. Let ζ^* be a value of the parameter ζ that corresponds to $\xi_* = 2$ in an equilibrium state. The relation between ρ, ξ, and ζ [see (4.16)] for $\xi = \xi_* = 2$ yields

$$\rho_*^Q = (2æ(\zeta^*)^{1/\mu})^{1/2}. \tag{4.23}$$

Substituting (4.23) and $\xi = 2$ into Eq. (4.3), we obtain

$$(\zeta^*)^2 - 4\varphi\zeta^* + 4\varphi = 0, \tag{4.24}$$

and find two values of ζ^*

$$\zeta_{1,2}^* = 2\varphi\left(1 \mp \sqrt{1 - \frac{1}{\varphi}}\right), \tag{4.25}$$

which can exist in real numbers only for $\varphi \geqslant 1$. The plus sign corresponds to ζ_2^*. Thus, we obtained another proof that for $\varphi < 1$ there are no equilibrium states of the chain with the critical length of the (−1)–0 bond.

We now consider other corollaries of formula (4.25). Employing arguments used to prove inequality (4.20), we have

$$1 < \zeta_1^* < 2 < \zeta_2^*, \tag{4.26}$$

i.e., for $\varphi > 1$ there are two different equilibrium states of the chain in which the (−1)–0 bond is extended to the critical length (4.18). In Fig. 8, these states are designated by C_1 and C_2, respectively. The value of ρ_*^Q at these points is determined by substituting (4.25) into (4.26). In this case, $\rho_*^Q(\zeta_1^*) < \rho_*^Q(\zeta_2^*)$ by virtue of

(4.26), and, hence, in the quasistatic extension of the chain, state C_1 is the first to be attained at $\rho = \rho_*^Q(\zeta_1^*)$. Figure 8 shows that the point that characterizes the chain moves from the initial point H to C_1 along the "lower" of two equilibrium trajectories I, which is determined by $\rho_{(1)}(\xi)$ in (4.4).

To study the supercritical behavior of the chain, we find a representation of ζ via ξ at points of the "lower" trajectory and exclude ρ from (4.16) by means of (4.4). We obtain an expression similar to (4.23):

$$\zeta = \frac{\varphi\xi^2}{2(\xi - 1)}\left(1 - \left(1 - \frac{4(\xi - 1)}{\varphi\xi^2}\right)^{1/2}\right). \tag{4.27}$$

It can be readily shown that for $\varphi > 1$ the value of ζ in (4.27) always exceeds unity. A test of function (4.27) for monotony and extremum shows that, with increasing ξ, $\zeta(\xi)$ increases to the largest value $\zeta_1^* < 2$ at the critical point C_1 on the "lower" trajectory. Then it decreases so that $\zeta \to 1 + 0$ as $\xi \to \infty$. Thus, within the entire range of ξ variations along the "lower" trajectory the quantity ζ is limited. Relation (4.16) shows that ρ and ξ tend to infinity. Thus, for $\varphi > 1$, the (-1)–0 bond is broken; its length $r_{-1,0} \to \infty$ as $\rho \to \infty$, while the 0–1 impurity bond, without reaching the critical length (4.14), begins to reduce so that $r_{0,1} \to r_e^{MQ}$ as $\rho \to \infty$.

Note that the above consideration of the behavior of the chain is valid under the assumption that there is no possibility of overcoming the energy barrier separating the stable equilibrium states of the chain. Chain equilibrium stability along both the "left" equilibrium trajectory III and the "lower" trajectory I is proved by studying the signs of the second derivative $\partial^2 V_0/\partial\xi^2$ along these branches.

We consider the decrease in the tensile strength of the chain under the action of an impurity. The critical value ρ_*^Q is determined by the dimensionless positive parameters φ, μ, and æ for $0 < \varphi < 1$ from formulas (4.17) and (4.9),

$$\rho_*^Q = \rho\Big|_{C_1} = \left(2^{1+1/\mu}\text{\ae}\frac{1}{\varphi}(1 - \sqrt{1 - \varphi})\right)^{1/2}; \tag{4.28}$$

for $\varphi > 1$, from formulas (4.23) and (4.25),

$$\rho_*^Q = \rho\Big|_{C_3} = \left(2^{1+1/\mu}\text{\ae}\left(\varphi\left(1 - \sqrt{\frac{1}{\varphi}}\right)\right)^{1/\mu}\right)^{1/2}; \tag{4.29}$$

and for $\varphi = 1$, from formula (4.19). The latter case can be added to one of the above.

The physical meaning of the parameter φ is

$$\varphi = k\mu = \frac{D_{MQ}\alpha_{MQ}}{D\alpha} = \frac{p_m^{MQ}}{p_m},$$

i.e., φ is the measure of the ratio of the theoretical tensile strengths of the atomic M–Q and M–M bonds. Thus, the point of rupture of the chain in the model studied is determined mainly by the energy factor, i.e., by the ratio of bond strengths. The weaker bond is broken (an obvious result at first glance). However, the absence of an effect of the dimensional factor is interesting. This is apparently due to the constraint on the atoms in the model ("triatomic chain with one free atom"). The effect of both factors (dimensional and energy) on chain strength is manifested quantitatively in the value of ρ_*^Q. It was shown in Section 2 that the chain strength decreases in the presence of an impurity if $1 \leqslant \rho_*^Q < 2$, where ρ_*^Q is calculated from formulas (4.28) and (4.29) according to φ. The data in Table 1 show that, in seven of ten M–Q pairs, the strength P_* of a chain consisting of atoms of type M with impurity Q is smaller than the strength p_* of an "ideal" M chain. For three pairs, a decrease in strength is also observed in the problem of Section 3.

The calculation results are given in Table 3. The absence of a dependence of the results on each of the quantities k, μ, æ, and φ (and also of ξ_0, r_m, and r_m^{MQ}) is of interest. Thus, in two of the above-mentioned seven cases, æ exceeds unity and in five cases it is smaller. In four cases, φ exceeds unity, while in three other cases it is smaller. Moreover, no regularity is observed in the joint influence of two quantities, e.g., φ and æ, or k and æ.

The above analysis suggests that all factors that can have an effect on strength should be taken into

TABLE 3

M	Q	k	μ	æ	φ	ρ_*^Q	t
Gd	Cu	1.027	1.016	0.731	1.044	1.551	0.916
Gd	Al	1.124	1.062	0.753	1.193	1.450	0.856
Al	Fe	1.361	0.924	0.977	1.258	1.661	0.958
Cu	Au	1.077	1.026	1.176	1.104	1.887	0.996
Au	Cu	0.859	0.937	0.856	0.805	1.578	0.928
Ni	Fe	0.856	1.039	1.050	0.889	1.751	0.980
Fe	Ni	0.887	0.749	0.884	0.665	1.680	0.964

account within the framework of the model. Ignoring one of the factors [see (2.3)–(2.5)] can change the result significantly. Of course, as the number of parameters increases, the solution of the problem becomes complicated. Sometimes, the problem can be solved by analytical methods.

5. Conclusions. Using a one-dimensional model of brittle fracture as an example, we showed the possibility of strength reduction of solids whose atomic lattice contains impurities. The reduction can reach one or two orders of magnitude and is determined by differences in atomic interaction. Under the model conditions, the strength decrease can be calculated from the resulting formulas using numerical values of the parameters of the potential interaction function.

A decrease in the tensile strength of an atomic chain with an impurity located at the tip of a brittle crack [7–9] can decrease sharply the local resistance to fracture and lead to crack propagation under loads that are substantially smaller than the strength of the materials containing no impurities.

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