

## SHEAR STRAIN EFFECTS ON THE THEORETICAL STRENGTH OF AN ATOMIC LATTICE

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*A four-atomic unit cell corresponding to a close-packed layer of atoms is considered. It is shown that with occurrence of a shear the system prematurely loses stability. It is concluded that in Novozhilov-type integral criteria for brittle strength, it is reasonable to take into account shear strains.*

Modified Novozhilov's discrete criteria of brittle strength [1] use the theoretical strength of crystals, which is commonly estimated ignoring shear strains. The shear strains occurring when an ideal crystal is stretched along the symmetry axis of the atomic lattice results in a premature shear deformation [2, 3]. Macmillan and Kelly [4] performed a statistical analysis of the stability of an ideal crystal using the Newtonian approach and described the interatomic interaction by semiempirical potentials such as the Lennard-Jones and Born-Mayer potentials. In this case, in studies of the effects of external conservative forces on the mechanical behavior of crystals, the sum of the force potential and effective energy of interatomic interactions is chosen as a function of the total potential energy of the system. As noted in [3], such an approach often provides appropriate information for description of the macroscopic mechanical properties of a solid.

In the present work, a four-atomic unit cell corresponding to a close-packed layer of atoms is considered. The shear strain effects on the stability of a rhombic four-atomic cell stretched along the diagonal under homogeneous deformation is studied within the framework of the approach described in [3, 5]. Interatomic interaction is taken into account by the Morse potential [6, 7]. Although for almost all metals, the interatomic forces are not central even approximately, most of the energy change due to changes in the atomic configuration at constant atomic volume can be described in terms of the central interaction [6-8]. Therefore, even if noncentral interactions make a substantial contribution to the energy of the atomic lattice, it is still possible to obtain satisfactory estimates of some properties using a simple model of pair central interactions [1, 7, 9].

The system studied exhibits unstable supercritical behavior. It is found that with occurrence of a shear, the system prematurely loses stability and the critical point on the strain line is determined by the parameters of the Morse potential function. Therefore, in Novozhilov's integral criteria of brittle strength, it is reasonable to use a refined estimate of the theoretical strength of crystals taking into account shear strains.

**Formulation of the Problem.** Let us assume that the potential energy of interaction between any two atoms is a function  $w(s)$ , which is a spherically symmetric two-body interaction potential for which the force of interaction is directed along the line connecting their centers ( $s$  is the distance between the centers). Below, we confine ourselves to considering the interaction of only the two nearest atoms since we cannot state for sure that the Morse potential adequately describes the atomic field at distances exceeding several distances between the nearest neighboring atoms [6]. In this case, it is assumed that only planar, kinematically admissible displacement fields with homogeneous deformations and only two degrees of freedom can occur in crystals. We study the stability in tension of a planar four-atomic cell corresponding to a close-packed layer of atoms. In particular, we consider the case of tension in the direction perpendicular to the close-packing where

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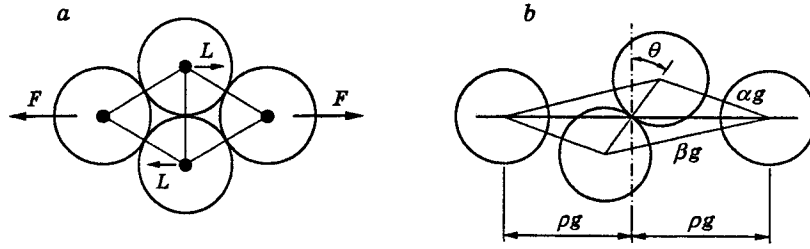


Fig. 1

the stress applied to the layer tends to separate the close-packed chains of atoms with probable rotation of them but with no change in the chain length.

Since for an unloaded crystal, the total force acting on each atom is equal to zero, the crystal can be regarded as a close-packed lattice of spheres with diameter  $g$ , where  $\left. \frac{dw}{ds} \right|_{s=g} = 0$ . As  $w(s)$ , we take the Morse potential [1, 6, 7]

$$w(s) = D[\exp(-2a(s-g)) - 2\exp(-a(s-g))].$$

Assuming that  $\gamma = s/g$  ( $\gamma$  is the dimensionless translation),  $b = ag$  and  $2D = Ag^{-6}$ , we obtain

$$v(\gamma) = w(\gamma g) = Ag^{-6} \left[ \frac{1}{2} \exp(-2b(\gamma-1)) - \exp(-b(\gamma-1)) \right]. \quad (1)$$

Here  $D$ ,  $a$ , and  $g$ , and, hence,  $A$  and  $b$  are parameters determined by the type of atoms. The force of interaction  $T$  between two atoms is given by the equality

$$T = \frac{dw}{ds} = -Abg^{-7} [\exp(-2b(\gamma-1)) - \exp(-b(\gamma-1))], \quad (2)$$

and for  $\gamma = \gamma_* = 1 + \ln 2/b$ , it reaches the maximum  $T_2 = Ab/(4g^7)$  or, in dimensionless form,

$$T_* = \frac{T_2 g^7}{Ab} = \frac{1}{4}. \quad (3)$$

When some assumptions [3] are satisfied, the total potential energy of an infinite planar layer is proportional to the energy  $V(\theta, \rho)$  of a unit cell consisting of four atoms. Figure 1a shows an unstrained cell and Fig. 1b (taken from [3, Fig. 69]) shows a rhombic cell stretched along the diagonal.

The strain of the unit cell can be determined using the independent generalized coordinates  $\theta$  and  $\rho$ ;  $\theta = 0$  for an ideal system (ignoring shear). We introduce two independent variables  $\alpha$  and  $\beta$  (Fig. 1b):

$$\alpha^2 = 1/4 + \rho^2 - \rho \sin \theta, \quad \beta^2 = 1/4 + \rho^2 + \rho \sin \theta. \quad (4)$$

Let us consider the deformation of the system under the action of the forces  $F$  and  $L$  (Fig. 1a). The function of the total potential energy of the unit cell can be written in the form [3]

$$V(\theta, \rho, F, M) = 2v(\alpha(\theta, \rho)) + 2v(\beta(\theta, \rho)) - 2F\rho g - M\theta,$$

where  $M = Lg$  is the moment of the force  $L$ . The partial first-order derivatives of the function  $V$  with respect to  $\theta$  and  $\rho$  are  $V_\theta = 2v_\alpha \alpha_\theta + 2v_\beta \beta_\theta - M$  and  $V_\rho = 2v_\alpha \alpha_\rho + 2v_\beta \beta_\rho - 2Fg$ , respectively. Here  $v_\alpha$  and  $v_\beta$  are the derivatives of function (1) with respect to  $\gamma$ :

$$v_\gamma = -Abg^{-6} [\exp(-2b(\gamma-1)) - \exp(-b(\gamma-1))]. \quad (5)$$

The partial derivatives of the functions  $\alpha(\theta, \rho)$  and  $\beta(\theta, \rho)$  are obtained from relations (4) as derivatives of the implicit functions. For an ideal system with no shear, we have  $M = 0$ . Then, from the equations of equilibrium  $V_\theta = 0$  and  $V_\rho = 0$ , we can find the basic solution with  $\theta = 0$ . It is determined from the equation

$$2v_\gamma \gamma_\rho = Fg, \quad (6)$$

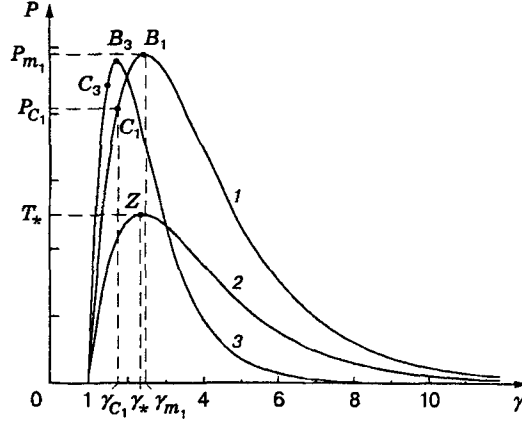


Fig. 2

where  $\gamma$  is replaced by  $\alpha$  or  $\beta$ . We note that for  $\theta = 0$ , we have  $\alpha = \beta$ ,  $\alpha_\rho = \beta_\rho$  and

$$\alpha\alpha_\rho = \beta\beta_\rho = \rho = \sqrt{\gamma^2 - 1/4}.$$

**Discussion of Results.** Using (5) and (6), for the dependence of the force  $P$  on the strain  $\gamma$  of a four-atomic cell we finally obtain

$$P = P(\gamma) = \frac{Fg^7}{Ab} = \frac{2v_\gamma\gamma_\rho g^6}{Ab} = \sqrt{4\gamma^2 - 1}[\exp(-b(\gamma - 1)) - \exp(-2b(\gamma - 1))]/\gamma. \quad (7)$$

The force as a function of strain is shown in Fig. 2. Curves 1 and 3 correspond to a four-atomic cell with  $b = 0.5$  and 1 [see relation (7)], and curve 2 refers to a pair of atoms with  $b = 0.5$  [see relation (2)]. The extrema on curves 1 and 3 are denoted by the points  $B_1$  and  $B_3$ , to which the strain parameters  $\gamma_{m_1}$  and  $\gamma_{m_3}$  and the forces  $P_{m_1}$  and  $P_{m_3}$  correspond; the points  $C_1$  and  $C_3$  correspond to the critical strain parameters  $\gamma_{C_1}$  and  $\gamma_{C_3}$  and critical forces  $P_{C_1}$  and  $P_{C_3}$  at which the system loses shear stability. The critical strain parameter  $\gamma_*$  and the force  $T_* = 1/4$  [see relation (3)] correspond to the maximum point  $z$  on curve 2. Because of the symmetry of the system, the derivative  $V_{\theta\rho}$  is equal to zero for each value of  $b$  on the main equilibrium trajectory. Therefore, the stability of the equilibrium trajectory is determined by two stability coefficients  $V_{\theta\theta}$  and  $V_{\rho\rho}$  [3]. At the maximum point  $B(\gamma_m, P_m)$  on the equilibrium trajectory (the points  $B_1$  and  $B_3$  in Fig. 2), the coefficient  $V_{\rho\rho}$  vanishes. Because on the main equilibrium trajectory,  $\theta = 0$  and, hence,  $\alpha_{\rho\rho} = \beta_{\rho\rho}$ , the condition  $V_{\rho\rho} = 0$  leads to the equality

$$V_{\rho\rho} = 4(v_{\gamma\gamma}\gamma_\rho^2 + v_{\gamma\rho\rho}) = 4\{Ab^2g^{-6}[2\exp(-2b(\gamma - 1)) - \exp(-b(\gamma - 1))](\rho/\gamma)^2 - Abg^{-6}[\exp(-2b(\gamma - 1)) - \exp(-b(\gamma - 1))](\gamma^2 - \rho^2)/\gamma^2\} = 0.$$

Hence, since  $\gamma^2 = 1/4 + \rho^2$  at  $\theta = 0$ , for the coordinate  $\gamma = \gamma_m$  of the maximum point  $B(\gamma_m, P_m)$  of the equilibrium trajectory we obtain the equation

$$\exp(-b(\gamma_m - 1)) = \frac{b\gamma_m(4\gamma_m^2 - 1) - 1}{2b\gamma_m(4\gamma_m^2 - 1) - 1}. \quad (8)$$

We note that the coordinate  $\gamma = \gamma_m$  of the critical point  $B(\gamma_m, P_m)$  can be found using expression (7) and the condition that the derivative of the function  $P(\gamma)$  with respect to  $\gamma$  is equal to zero. The point  $C(\gamma_C, P_C)$  at which the coefficient  $V_{\theta\theta}$  turns to zero is a bifurcation point (the points  $C_1$  and  $C_3$  in Fig. 2), at which shear strains with nonzero values of  $\theta$  can develop. The dimensionless displacement  $\gamma_C$ , whose value depends on the parameters of the potential function, corresponds to this second critical point. Setting  $V_{\theta\theta} = 0$ , we obtain the corresponding critical value  $\gamma = \gamma_C$  from the equation  $v_{\gamma\gamma} - v_\gamma/\gamma = 0$  or, after some obvious

TABLE 1

$b$	$\gamma_m$	$\gamma_*$	$\gamma_C$	$P_m$	$P_C$	$\Delta P/P_m, \%$
0.5	2.424	2.386	1.770	0.489	0.417	14.7
1	1.721	1.693	1.467	0.478	0.440	7.9
2.076	1.348	1.334	1.262	0.464	0.447	3.7
4	1.179	1.173	1.150	0.453	0.446	1.5
6	1.119	1.116	1.104	0.447	0.443	0.9
8.46	1.084	1.082	1.076	0.444	0.442	0.4

transformations, from the equation

$$\exp(-b(\gamma_C - 1)) = \frac{b\gamma_C + 1}{2b\gamma_C + 1}, \quad (9)$$

which depends on the parameter  $b$ , which characterizes the type of atoms.

Let us show that the bifurcation point  $C$ , which corresponds to occurrence of shear strains, appears before the main equilibrium trajectory reaches the maximum point  $B$ . To this end, we first prove that for any  $b > 0$ , the value of  $\gamma_C$  determined from Eq. (9) is smaller than  $\gamma_* = 1 + \ln 2/b$ , at which the force of interaction  $T(\gamma)$  of two atoms reaches a maximum. A plot (curve 2) of the function  $T(\gamma)g^7/(Ab)$  for  $b = 0.5$  is shown in Fig. 2, where the maximum point  $Z(\gamma_*, T_*) = Z(\gamma_*, 1/4)$  is denoted according to Eq. (3). We note that the function  $f(\gamma) = \exp(-b(\gamma - 1))$  is decreasing for  $b > 0$ . Since for  $\gamma_C > 0$ , the inequality

$$\exp(-b(\gamma_C - 1)) = \frac{b\gamma_C + 1}{2b\gamma_C + 1} = \frac{1}{2} + \frac{1}{2(2b\gamma_C + 1)} > \frac{1}{2} = \exp(-b(\gamma_* - 1))$$

is valid, we obtain  $\gamma_C < \gamma_*$ . We then show that for  $b > 1/6$ , the inequality  $\gamma_* < \gamma_m$  is valid. Since  $\gamma \geq 1$  from physical considerations, we have  $2b\gamma(4\gamma^2 - 1) - 1 > 0$  for  $b > 1/6$ . Therefore, using Eq. (8) we have

$$\exp(-b(\gamma_m - 1)) = \frac{b\gamma_m(4\gamma_m^2 - 1) - 1}{2b\gamma_m(4\gamma_m^2 - 1) - 1} = \frac{1}{2} - \frac{b\gamma_m(4\gamma_m^2 - 1)}{2(2b\gamma_m(4\gamma_m^2 - 1) - 1)} < \frac{1}{2} = \exp(-b(\gamma_* - 1))$$

and taking into account that the function  $f(\gamma) = \exp(-b(\gamma - 1))$  decreases for  $b > 0$ , we obtain  $\gamma_* < \gamma_m$ . Thus, for  $b > 1/6$ , the chain of inequalities  $\gamma_C < \gamma_* < \gamma_m$  is proved analytically, i.e., it is shown that with occurrence of a shear, the system prematurely loses stability and the corresponding critical point  $\gamma = \gamma_C$  on the strain curve is determined by the parameters of the potential function chosen. Thus, if the Morse potential is chosen,  $\gamma_m$  and  $\gamma_C$  are determined from relations (8) and (9), respectively, and they depend on the parameter  $b$ , which characterizes the type of atom. However, for the Lennard-Jones potential, we have  $\gamma_C = (7/4)^{1/6} < (13/7)^{1/6} = \gamma_m$  irrespective of the type of atoms in the lattice [3]. We note that in this case the value of  $((P_m - P_C)/P_m) \cdot 100\% \approx 0.73\%$  is constant, does not depend on the type of atom, and can be substantially smaller than that for the Morse potential, for example, for  $b < 4$ .

For  $A = 1$ ,  $g = 1$ , and various  $b$  ( $0.5 \leq b \leq 8.46$ ), the values of  $\gamma_m$  and  $\gamma_C$  and the corresponding loads  $P_m$  and  $P_C$  determined from formula (7) are given in Table 1. The values of  $\gamma_* = 1 + \ln 2/b$  are also given here; the value  $T_* = 1/4$  which, according to (3), corresponds to them for any  $b$  is omitted. We note that for any  $b$ , the data in Table 1 satisfy the inequality  $P_m < 2P_*$ , which can be easily explained by the physical meaning of the initial model. The values of the parameter  $b$  are borrowed from various papers on solid-state physics (see [9] and the references in it). In [9], these data were used to analyze the influence of impurity atoms on the reduction in the strength of stretched atomic chains. In the last column, the relative deviation of the load  $P_C$  from  $P_m$  in percent is given:  $((P_m - P_C)/P_m) \cdot 100\%$ . The data of Table 1 show that for  $b \approx 2$ , the force  $P_C$  has an extremum. In this case, the four-atomic cell is most stable against shear when the interatomic interaction is described by the Morse potential.

**Conclusions.** The load  $P_C$  at which shear strain occurs can be 7.9% smaller than the load  $P_m$  at which the ideal system begins to fail. The loads  $P_C$  and  $P_m$  correspond to the physical parameter  $b = 1$ . We emphasize that for the nonideal system, this difference can exceed 25–30% (see [3, Fig. 70]). Therefore, in calculating the theoretical strength, it is reasonable to introduce a correction for shear strains, and in Novozhilov's integral criteria of brittle strength, it is expedient to use a refined estimate of the theoretical strength of crystals.

**Remark.** The nonideality of a system [3] can be modeled by the presence of an impurity atom in the cell. In such a system, loss of stability occurs much earlier. For example, for a chain of atoms, the critical loads for the ideal system and the system with impurity atoms can differ by one or two orders of magnitude [9]. We note that references on the real physical potentials and calculation results for ten different pairs of atoms are given in [9].

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