ONE MODEL FOR STABILITY LOSS IN A PLANE IDEAL CRYSTAL UNDER TENSION

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As experiment shows, one form of failure of an ideal crystal in tension is the shear failure, which is characterized by the formation of a slippage system [1, 2] in the case when the Schmidt factor differs from zero, that is, when the direction of tension makes an angle of 5-85° with the slippage plane.

However, it can be expected that under some conditions, plastic deformation can develop, when the Schmidt factor equals zero. We will call this case, when the direction of tension is perpendicular to the slippage plane, the limiting case. This case was investigated theoretically [3, 4] by studying the loss of stability under shear of a plane ideal crystal whose atoms were located in the (111) plane of a metal with a face-centered cubic structure or in the (0001) plane of a metal with a hexagonal close-packed structure. The Lennard-Johnson potential, which is basically characteristic of inert gases, was chosen as the potential for interatomic interactions.

Here we construct a model, which characterizes the loss of stability of a plane ideal crystal under tension in the limiting case. The atomic lattice of the crystal corresponds to the (110) plane of a metal with a face-centered cubic structure. In the investigation, the interatomic potential was chosen in the most general form [4, 5].

We examine a plane ideal crystal with a lattice translation a along the Ox axis and $a/\sqrt{2}$ along the Oy axis. The crystal is stretched by a uniformly distributed load of intensity q along the Ox axis (Fig. 1).

We will assume that the interaction forces between the atoms are potential forces and act only with neighboring atoms. When the crystal is loaded, atoms lying on the vertical (Fig. 1a) relative to each other do not slip and always remain in one line (Fig. 1b). Then the plane crystal can be replaced by a mechanical model, which consists of vertical weightless rods with point masses, which are interconnected by nonlinear spings (dotted lines), whose anchor points coincide with the position of the atoms in the atomic lattice. The force, which acts on the spring side of the atom, is equal to the interatomic potential force σ, and the potential energy of the spring equals the interatomic potential v [4, 5]. The form of σ and v as functions of the interatomic distance ρ in a crystal with a lattice translation b is shown in Fig. 2 (σ_m is either the maximum interaction force of two atoms or the ultimate resistance). Consequently, we represent the crystal deformation under tension in the form of a horizontal displacement and a rotation by an angle θ of the rods in the plane of the drawing, as shown in Fig. 1b.

With the limitations above, it is not difficult to see that the behavior of the whole crystal is characterized by the behavior of an elementary cell, which consists of four atoms and three nonlinear springs (Fig. 3a). When the cell is loaded with an applied force P, its position is determined with the use of the generalized coordinates r and θ (Fig. 3b).

We now examine the behavior of a cell loaded with a force P. It should be expected that for small values of P, the rod B_1B_3 has a single stable equilibrium position $\theta = 0$. When P reaches some critical value P_c, three equilibrium positions of B_1B_3 are possible: an unstable one, corresponding to $\theta = 0$, and two stable ones for which B_1B_3 makes an angle $\theta = \pm\theta_c \neq 0$ with the vertical. This point is a branching point or a bifurcation point. With further loading, the cell has two stable equilibrium positions ($\theta = \pm\theta_1 \neq 0$) and one unstable position ($\theta = 0$).

A slowly loaded crystal behaves similarly: as q grows from zero to q_c, the vertical chains of atoms translate along the Ox axis parallel to the Oy axis, and when q reaches a critical value q_c, the chains of atoms rotate through an angle θ_c or $-\theta_c$ and thereafter develop shear deformations.

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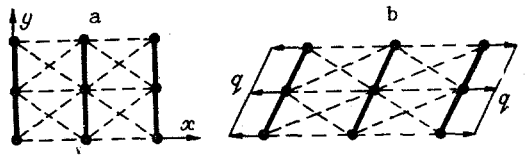

Fig. 1

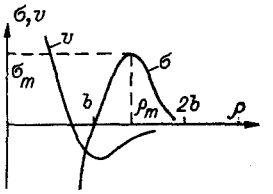

Fig. 2

By using the Lagrange–Dirichlet, Lyapunov, and Chetaev theorems [6] and the methods in [4, 7], we derive the conditions for loss of stability of the atomic axis. We write the potential energy Π of the elementary cell as

$$\Pi = \sum_{s=1}^{3} v_s(\rho_s) - Pr,$$

where $v_s(\rho_s)$ is the potential energy for the interaction of atom B_4 with the atoms B_s (s = 1, 2, 3); $\rho_1 = B_1B_4 = \sqrt{a^2/2 + r^2 - ar\sqrt{2}\sin\theta}$; $\rho_2 = B_2B_4 = r$; and $\rho_3 = B_3B_4 = \sqrt{a^2/2 + r^2 + ar\sqrt{2}\sin\theta}$. The equilibrium conditions have the form

$$\Pi_r = \sum_{s=1}^{3} \frac{\partial v_s}{\partial \rho_s}\frac{\partial \rho_s}{\partial r} - P = 0, \quad \Pi_\theta = \sum_{s=1}^{3} \frac{\partial v_s}{\partial \rho_s}\frac{\partial \rho_s}{\partial \theta} = 0. \tag{1}$$

Here the indices of the function Π indicate partial derivatives with respect to the corresponding variables.

The value of the potential energy Π in the equilibrium position determines its stability or instability [6]: if the potential energy takes a minimum value in the equilibrium position, then the equilibrium position is stable; but if the potential energy does not have a minimum in the equilibrium position, then, according to the theorems of Lyapunov and Chetaev, the equilibrium position is unstable. The presence of a minimum Π is established through the second partial derivatives in the generalized coordinates. We write a matrix A, whose elements are the stability coefficients (second partial derivatives of Π with respect to the generalized coordinates):

$$A = \begin{bmatrix} \Pi_{rr} & \Pi_{r\theta} \\ \Pi_{\theta r} & \Pi_{\theta\theta} \end{bmatrix}.$$

If the matrix A is positive definite, the equilibrium position in question is stable. The point at which this condition is not fulfilled is a bifurcation point.

We now calculate the stability coefficients:

$$\Pi_{rr} = \sum_{s=1}^{3}\left[\frac{\partial^2 v_s}{\partial \rho_s^2}\left(\frac{\partial \rho_s}{\partial r}\right)^2 + \frac{\partial v_s}{\partial \rho_s}\frac{\partial^2 \rho_s}{\partial r^2}\right], \tag{2}$$

$$\Pi_{r\theta} = \sum_{s=1}^{3}\left[\frac{\partial^2 v_s}{\partial \rho_s^2}\frac{\partial \rho_s}{\partial r}\frac{\partial \rho_s}{\partial \theta} + \frac{\partial v_s}{\partial \rho_s}\frac{\partial^2 \rho_s}{\partial r\,\partial \theta}\right], \quad \Pi_{\theta\theta} = \sum_{s=1}^{3}\left[\frac{\partial^2 v_s}{\partial \rho_s^2}\left(\frac{\partial \rho_s}{\partial \theta}\right)^2 + \frac{\partial v_s}{\partial \rho_s}\frac{\partial^2 \rho_s}{\partial \theta^2}\right].$$

Because we are interested in the stability of the vertical position of the rod B_1B_3, we will investigate the stability of the equilibrium position θ = 0. We find the derivatives in Eqs. (2) for θ = 0. Because of symmetry of the cell at θ = 0, we have $\Pi_{r\theta} = \Pi_{\theta r} = 0$; therefore, the stability is determined by the signs of Π_{rr} and $\Pi_{\theta\theta}$: if $\Pi_{rr} > 0$ and $\Pi_{\theta\theta} > 0$, then the equilibrium position is stable; if one of the inequalities is not fulfilled, then the equilibrium position transforms from a stable to an unstable one. The point at which $\Pi_{\theta\theta} = 0$ is the point where the rod B_1B_3 starts to rotate; that is, shear deformation begins to develop in the plane crystal.

Having substituted the values of ρ_s and their derivatives onto [2], we obtain

$$\Pi_{rr} = \dot{\sigma}_* + \frac{2}{\rho^2}\left(r^2\dot{\sigma} + \frac{a^2}{2\rho}\sigma\right), \quad \Pi_{\theta\theta} = \frac{a^2r^2}{\rho^2}\left(\dot{\sigma} - \frac{\sigma}{\rho}\right). \tag{3}$$

Here $\rho_1 = \rho_3 = \rho = \sqrt{a^2/2 + r^2}$; $\rho_2 = r$; $\partial v_1/\partial\rho_1 = \partial v_3/\partial\rho_3 = \sigma$; $\partial v_2/\partial\rho_2 = \sigma_*$; $\partial^2 v_1/\partial\rho_1^2 = \partial^2 v_3/\partial\rho_3^2 = \dot{\sigma}$; and $\partial^2 v_2/\partial\rho_2^2 = \sigma_*$.

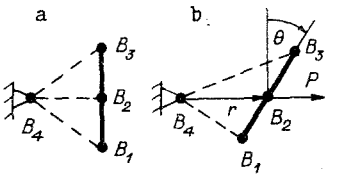

Fig. 3

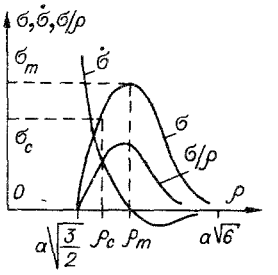

Fig. 4

From Eqs. (3) it follows that, under tension, Π_{rr} does not become zero for any value of r. This condition is theoretically possible: practically the condition $\Pi_{rr} = 0$ means failure of the crystal, because $r > r_m = \sqrt{\rho_m^2 - a^2/2}$; that is, the crystal fails before $\Pi_{rr} = 0$.

The value of $\Pi_{\theta\theta}$ becomes zero for $\rho = \rho_c$, where ρ_c is the solution to the equation

$$\dot{\sigma} - \sigma/\rho = 0. \tag{4}$$

Consequently, the rotation of the rod B_1B_3 occurs when the generalized coordinate r attains a value $r_c = \sqrt{\rho_c^2 - a^2/2}$. Because the explicit form of the interatomic interaction is not always known and an analytical solution of (4) is difficult to find, a geometric solution is shown in Fig. 4 for clarity. From the form of the function $\sigma(\rho)$, it follows that $\rho_c < \rho_m$, and therefore shear deformations occur before the interaction force reaches the ultimate resistance ρ_m.

Having determined ρ_c from Eq. (4) and substituted the results into (1), we find the critical applied force $P_c = \sigma_* + (2r/\rho)\cdot\sigma$, where $r = r_c$, $\rho = \rho_c$, $\sigma_* = \sigma_*(r_c)$, and $\sigma = \sigma(\rho_c)$.

The theoretical calculations presented here show that under some conditions shear deformations can develop even in the limiting case, that is, when the direction of tension is perpendicular to the slippage plane. In the first stage of failure ($q < q_c$), the deformation primarily develops due to a change in the mutual position of the vertical chains of atoms; but in the second ($q = q_c$), rotation of the densely packed chains occurs with destruction of the crystal symmetry, and thereafter deformation develops due to shear displacements.

Note. The discussion presented can properly be applied to the case where $\sigma_*(r_c) < \sigma_{*m}$ (σ_{*m} is the ultimate resistance of the atoms B_2 and B_4).

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