STABILITY OF A ONE-DIMENSIONAL CRYSTAL WITH A
SHORT-RANGE INTERACTION BETWEEN ATOMS IN THE
HARMONIC APPROXIMATION

G. M. Bartenev, I. V. Razumovskaya,
and E. S. Savin

UDC 539.424

There has been increasing interest in the strength and destruction mechanisms for ideal (flawless) structures in recent years, for two reasons: first, various ideal solids have been produced in the laboratory, e.g., whiskers of a wide variety of materials [1], high-strength glass [2], and glass fibers [3]. The outlook for the use of the high strength of these materials (if not directly, then as a component part of some composite material) seems good. Second, in studying the destruction mechanism of ordinary (flawed) solids, we are studying the rupture of interatomic bonds near the flaws in the most overstressed microscopic volumes which do not themselves contain flaws. The strength of the material in these microscopic volumes is quite high and corresponds to the strength of the ideal structure.

The simplest strength characteristic of the ideal structure is the theoretical strength [4] — the stress at which a uniformly deformed structure becomes unstable at $0°K$. An analogous characteristic — the maximum strength — can be introduced for discussing the ideal structure at $T > 0°K$ [5]. Here only the average statistical effect of the temperature is taken into account, through the thermal pressure, as an additive correction to the external mechanical effect.

This stability with respect to purely mechanical effects (or to a combination of mechanical and quasimechanical effects) could be arbitrarily called the "mechanical stability." Analysis of the mechanical stability of an ideal structure [5] is actually a first approximation of the strength calculation for an arbitrary temperature and for rapid destruction, in which case fluctuation effects are ruled out.

Account of the real spectrum of thermal vibrations in a solid constitutes the next approximation and yields information about the dynamic stability. The role of the external effect (deformation) reduces to one of changing the spectrum by changing the interatomic distances and interaction forces.

A crystal is known to be microscopically stable if its potential energy increases with an arbitrary small virtual displacement of any atoms from their equilibrium positions. In an analysis of the set of all small deformations in terms of normal coordinates, this condition requires that the vibration frequency be real, $\omega^2(\kappa, s) > 0$, for all wave vectors κ and polarizations s. If the frequency is not real, the vibration amplitude increases as time elapses, and this circumstance is equivalent to destruction of the lattice. Here we cannot make the a priori assertion that for critical conditions (high temperature, deformation, etc.) the crystal becomes unstable with respect to its entire frequency spectrum at once. It is extremely probable that the "destructive" frequencies occupy only finite part of the spectrum which depends on the external conditions. Using a model of a linear chain of identical particles, Born showed that stability at all wavelengths follows from the mechanical stability with respect to uniform extension of the chain if the second derivative of the potential for the interatomic interaction is positive for any pair of nearest neighbors and is negative for any pair of more remote neighbors. This condition probably always holds in a real material, but the converse assertion — that macroscopic (mechanical) instability of the crystal automatically leads to instability with respect to all waves — turns out to be incorrect, as we will show below.

The problem of crystal stability is usually formulated in terms of an increase in temperature (melting) instead of in terms of a mechanical effect [7]. Below we analyze the stability of a uniformly deformed one-dimensional lattice in which there is a short-range interaction between atoms.
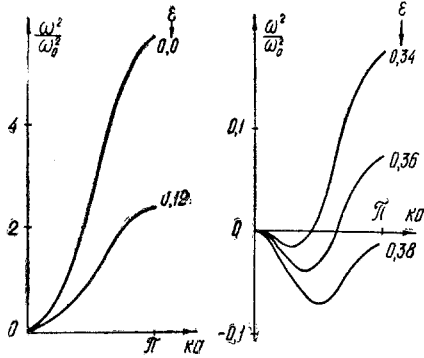
Fig. 1. Dispersion curves of a one dimensional crystal as functions of the deformation of ε.

1. We consider a linear chain of identical atoms of mass M whose Hamiltonian can be written as

$$H = \sum_l \frac{P_l^2}{2M} + \frac{1}{2} \sum_{l \neq m} U(R_l - R_m), \tag{1}$$

where P_l and R_l are the momentum and coordinate operators for an atom at site l. In the harmonic approximation the normal-mode frequencies $\omega(\kappa)$ corresponding to Hamiltonian (1) are found from the solution of the equation

$$M\omega^2(\kappa) = 2 \sum_h^\infty \Phi^h (1 - \cos \kappa a h), \tag{2}$$

where Φ^h is the force constant; a is the distance between nearest neighbors; and κ is the wave vector. To find the dependence of the frequency on the chain length or on the elongation, we expand the potential energy of the crystal in terms of the quantity $a = (1 + \varepsilon)a_0$, where a_0 is the equilibrium distance between atoms at a deformation of $\varepsilon = 0$.

Normal-mode frequencies (2) can be evaluated if we know the explicit binary interaction potential in Hamiltonian (1). We use the Morse potential

$$U(R) = D[(e^{-\alpha(R-r_0)} - 1)^2 - 1], \tag{3}$$

where r_0 is the equilibrium distance between atoms; D is the depth of the potential well; and $1/\alpha$ represents the well width.

Using (3), we convert Eq. (2) to

$$M\omega^2(\kappa) = 4\alpha^2 D \sum_h [2e^{-2\alpha(ha-r_0)} - e^{-\alpha(ha-r_0)}](1 - \cos \kappa a h). \tag{4}$$

Carrying out the summation, we find the following expression for the normal-mode frequencies taking into account the interactions of all neighbors and for a given distance a between nearest atoms:

$$\omega^2(\kappa) = \frac{f}{M(\kappa)} \sin^2 \frac{\kappa a}{2}, \tag{5}$$

where $f = 8\alpha^2 D$ and

$$M(\kappa) = M \frac{2(\operatorname{ch} 2\alpha a - \cos \kappa a)(\operatorname{ch} \alpha a - \cos \kappa a)}{2e^{2\alpha r_0} \operatorname{cth} \alpha a (\operatorname{ch} \alpha a - \cos \kappa a) - e^{\alpha r_0} \operatorname{cth} \frac{\alpha a}{2}(\operatorname{ch} 2\alpha a - \cos \kappa a)}.$$

Equation (5) is of the same form as the familiar equation for a lattice in which there is an interaction between nearest neighbors only. In Eq. (5), however, the mass depends on the wave vector.

The equilibrium distance between atoms in the chain for a deformation $\varepsilon = 0$ is found from

$$\sum_h U'(ha) h = 0. \tag{6}$$

Using (3), we can convert Eq. (6) to

$$2 \operatorname{ch} \frac{\alpha a}{2} = e^{\frac{\alpha r_0}{2}}.$$

The critical interatomic distance $a_c(\varepsilon)$, at which we have $\omega = 0$, is found from a solution of the equation

$$x^3 + (1 - e^{\alpha r_0})x^2 + \left(e^{\alpha r_0} \cos \kappa a - \cos^2 \frac{\kappa a}{2}\right)x - \cos^2 \frac{\kappa a}{2} = 0, \tag{7}$$

where $x = \cosh \alpha a$.

We see from Eq. (7) that the critical atomic distance and the critical deformation depend on κ (i.e., on the wavelength).

Figure 1 shows the dispersion curves for the linear crystal ($\alpha r_0 = 2.5$) which we calculated for various deformations on an MIR-1 computer. This figure shows that waves with small κ "vanish" first (at $\varepsilon' \approx 30\%$); i.e., the crystal first becomes unstable with respect to long-wave vibrations. As the deformation increases, the spectral range corresponding to the instability expands until the entire spectrum becomes imaginary at some deformation ε''. The crystal thus becomes completely "unstable" over some deformation interval $\varepsilon' - \varepsilon''$.

Solving the stability problem for a linear crystal in the usual approximation, in which only the interaction between nearest neighbors is taken into account, we find the critical value $a_c(\varepsilon)$ to be equal for all wavelengths:

$$a_c = r_0 + \frac{\ln 2}{\alpha}.$$

2. We can show that the critical value $a_c(\varepsilon)$ at which we have $\omega = 0$ for long-wave vibrations (as $\kappa \to 0$) corresponds to the a_{max} value which governs the theoretical strength σ_m of a linear crystal. In other words, the theoretical strength is the value of the external stress at which the crystal becomes unstable with respect to long-wave vibrations (it is macroscopically unstable since long-wave vibrations are directly related to macroscopic elastic properties, e.g., the elastic moduli).

By definition we have

$$\sigma_m = \left(\frac{\partial U}{\partial a}\right)_{a_{max}},$$

where a_{max} is found from

$$\sum_h \Phi^h h^2 = 0. \tag{8}$$

For long-wave vibrations, Eq. (2) becomes

$$M\omega^2(\kappa) = 4 \sum_h \Phi^h \sin^2 \frac{\kappa a h}{2} \approx (\kappa a)^2 \sum_h \Phi^h h^2,$$

and the critical value of $a_c(\varepsilon)$ at which we have $\omega = 0$, is found from the solution of $\sum_h \Phi^h h^2 = 0$, which is the same as condition (8).

CONCLUSIONS

1. The model of a uniformly deformed one-dimensional lattice in which there is a short-range interaction between atoms is unstable with respect to long-wave vibrations in the harmonic approximation.

2. The critical deformation, at which the crystal becomes unstable with respect to long-wave vibrations, corresponds to the theoretical strength.

LITERATURE CITED

1. É. M. Nadgornyi, Usp. Fiz. Nauk, 77, 229 (1962).
2. F. F. Vitman, G. S. Pugachev, and V. R. Pukh, Steklo i Keramika, 9, 12 (1965).
3. G. M. Bartenev, Silikattechnik, 18, 315 (1967).
4. G. M. Bartenev and I. V. Razumovskaya, Dokl. Akad. Nauk SSSR, 133, 341 (1960).
5. G. M. Bartenev, I. V. Razumovskaya, and E. S. Savin, Dokl. Akad. Nauk SSSR, 192, 775 (1970).
6. M. Born, Proc. Camb. Phil. Soc., 36, 160 (1940).
7. J. S. Dugdale and D. K. C. McDonald, Phys. Rev., 96, 57, 1905 (1954).