

SOME ASPECTS OF THE THERMAL PROPERTIES OF SOLIDS

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ABSTRACT

The article outlines the main principles about the thermal movement of particles in crystals. Thermal expansion is caused by an increase in the energy of vibrating particles. The vibrations become anharmonic (non-harmonic). If, when heated, a solid body does not have the opportunity to expand freely, then very large stresses arise, which must be taken into account in practice.

Keywords: Thermal motion, internal energy, solid body, interatomic distance, quasi-elastic, vibration amplitude, crystallographic axis .

INTRODUCTION

The thermal motion of particles in crystals differs significantly from the thermal motion of molecules in gases and liquids. Particles in crystals vibrate near equilibrium positions—the nodes of the crystal lattice. When a particle deviates from its equilibrium position, a force arises that tends to return it to its equilibrium position. For small deviations, these forces are quasi-elastic and the vibrations of the particles are harmonic. At room temperatures, the vibration amplitude is ~ 0.1 interatomic distance, which means 1 – 2 nm.

Thermal vibrations of particles do not have a specific orientation. These are complex vibrations that are determined by bonds with neighboring particles. The energy of vibrational motion of particles depends on temperature and determines the internal energy of the crystal. As the temperature decreases, the internal energy decreases. However, as $T \rightarrow 0$, the internal energy

does not tend to zero, but, according to quantum theory, to a certain value U_0 , which is called zero energy. Zero-point energy is usually much less than the interaction energy of particles. When heated, solids expand. As the temperature increases, the vibration amplitude and particle energy increase. However, an increase in the amplitude of vibrations cannot explain the thermal expansion of solids, because with increasing amplitude the equilibrium position of the particles should not change.

Thermal expansion is caused by an increase in the energy of vibrating particles. The vibrations become anharmonic (not harmonic).

Let's consider the curve of the potential energy of particles versus the distance between them (Fig. 1):

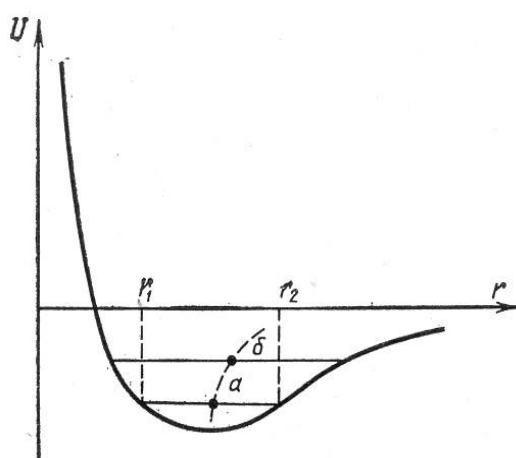


Fig.1. Thermal expansion of crystals

Let the horizontal straight line a show the energy level of an atom in a crystal lattice at room temperature. The points of intersection of the straight line with the energy curve determine the extreme positions of the atom r_1 and r_2 , which it occupies during vibrations. The midpoint of the line determines the equilibrium position of the atom at a given temperature. As the temperature increases, the atom moves to a higher energy level, which is determined by straight line b. Due to the different dependence of attractive and repulsive forces on the distance between atoms, the potential energy curve is asymmetrical in the upper part.

Due to the asymmetry of the dependence curve $U(r)$, the center of straight line b is shifted relative to the center of straight line a to the right, which means a shift in the equilibrium position of the atom, i.e. increase in interatomic distance. Consequently, the reason for the thermal expansion of solids when heated is not an increase in the amplitude of atomic vibrations, but an increase in interatomic distances that characterize the new equilibrium position.

the length of the body be l at temperature T_1 , and l' at temperature T_2 . Experiments have shown:

$$\frac{l' - l}{l} = \alpha (T_2 - T_1) \text{ and } \frac{\Delta l}{l} = \alpha \Delta T \quad (1)$$

where the proportionality coefficient α is the coefficient of linear expansion, $\Delta l / l$ is the relative elongation.

From (1):

$$\alpha = \frac{\Delta l}{l} \frac{1}{\Delta T} \quad (2)$$

The coefficient of linear expansion is numerically equal to the relative elongation with an increase in temperature by 1 K.

For most solids $\alpha \approx 10^{-5} - 10^{-6} \text{ K}^{-1}$. The value of α decreases slightly with decreasing temperature.

Due to the anisotropy of crystals, the linear expansion coefficient is different for different directions. Therefore, if you draw an arbitrary straight line in a crystal, then when the temperature increases, it will not remain straight.

However, in any crystal there are directions along which the straight line will remain straight even during thermal expansion of the crystal. Such directions are called crystallographic axes

The values of the linear expansion coefficient along these axes are called principal. Depending on the type of lattice, crystals can have one (uniaxial), two (biaxial), three (triaxial) crystallographic axes and, accordingly, one, two, or three main linear expansion coefficients. When heated, the volume of the solid increases. It has been established that the relative change in body volume is proportional to the change in temperature:

$$\frac{\Delta V}{V} = \beta \Delta T \quad (3)$$

where $\Delta V / V$ is the relative change in the volume of the body when the temperature changes by ΔT . The proportionality coefficient β is called the coefficient of volumetric expansion:

$$\beta = \frac{\Delta V}{V} \frac{1}{\Delta T} \quad (4)$$

The coefficient of volumetric expansion is numerically equal to the relative change in volume with a temperature change of 1 K.

If $\alpha_1, \alpha_2, \alpha_3$ are the main coefficients of linear expansion of the crystal, then the coefficient of its volumetric expansion is determined by the expression:

$$\beta = \alpha_1 + \alpha_2 + \alpha_3 \quad (5)$$

For crystals with a cubic lattice and for all isotropic bodies:

$$\alpha_1 = \alpha_2 = \alpha_3 = \alpha \quad (6)$$

For these bodies:

$$\beta = 3\alpha \quad (7)$$

If, when heated, a solid body does not have the opportunity to expand freely, then very large stresses arise, which must be taken into account in practice.

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