MECHANICAL PROPERTIES, PHYSICS OF STRENGTH, AND PLASTICITY

Description of the Thermoelastic Effect in Solids in a Wide Temperature Range

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Abstract—The change in temperature under adiabatic elastic deformation of solids (thermoelastic effect) at low and high temperatures has been calculated taking into account the quantum properties of thermal dynamics. In the high-temperature range, a quantum-mechanical correction to the classical Kelvin formula has been found. In the low-temperature range, a new formula for the description of the thermoelastic effect has been derived.

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Thermoelastic effect, a change in temperature under adiabatic elastic deformation of solids, has been known for a long time: it was discovered by Joule and described by Kelvin in 1853 [1].

The temperature change ΔT under elastic deformation of solids in the realistic range of applied stress up to ~1–2 GPa is small: $\Delta T/T \sim 10^{-3}$–10^{-2}. Therefore, the thermoelastic effect is primarily of theoretical interest. However, it can be noted that progress made in the infrared phonon detection technology has led to the development and fabrication of commercial sensors for detection and analysis of elastic stresses in technical objects via a change in temperature [2]; i.e., the thermoelastic effect has found practical applications.

We now turn to the description of the thermoelastic effect.

Kelvin proposed the classical (which is natural for those times) formula for the dependence of the temperature of a solid on the applied uniaxial external stress σ

$$\frac{\Delta T}{T} = -\frac{\alpha}{C}\sigma,$$

where T and ΔT are the temperature and its change, respectively; α is the linear coefficient of thermal expansion (CTE); and C is the specific heat.

The presence of the CTE in the Kelvin formula indicated that the nature of the thermoelastic effect is associated with a nonlinearity of the atom–atom interaction and, accordingly, with an anharmonicity of the thermal oscillations of atoms.

In addition to such an important physical indication, the Kelvin formula raised questions on the conditions and limits of its applicability to the description

of thermoelasticity of objects with different structures and in different temperature ranges.

The development of the thermodynamic description of the thermoelastic effect in the classical temperature range can be found in [3–5]. A separate question is the influence of the quantum character of the thermal dynamics (which was unknown at the Kelvin time) on the behavior of thermoelasticity, which is typical of solids.

The simplest manifestations of the quantum character of the thermal dynamics are changes in the specific heat and CTE with variations in the temperature (vanishing of both quantities at $T \longrightarrow 0$). An attempt of taking this factor into account by introducing the dependences $C(T)$ and $\alpha(T)$ into the Kelvin formula leads to an obviously incorrect result. As is known, the ratio $\alpha(T)/C(T)$ is nearly constant (the Grüneisen relation, see, e.g., [6]) and thus the ratio $\Delta T/T$ in the Kelvin formula remains finite at an arbitrary $\sigma \neq 0$, which is unrealistic at $T \longrightarrow 0$. Therefore, thermoelasticity requires special consideration with the inclusion of quantum properties of solids from the very beginning. This work is aimed at carrying out such an analysis in a wide temperature range.

Since in many cases nonlinear effects can be described by the model of a solid as a system of oscillators, it seems reasonable to use this model to clarify the effect of quantum properties on the process of adiabatic deformation of materials. In this work, the energy of the ensemble of nonlinear oscillators is calculated with the use of the virial theorem [7]. According to this theorem, the average kinetic energy of the system can be expressed as [7]

$$\langle E_{\text{kin}} \rangle = -\frac{1}{2}\sum_i \langle \mathbf{F}_i \mathbf{r}_i \rangle, \tag{1}$$

where $\mathbf{F}_i$ is the force acting on the ith particle and $\mathbf{r}_i$ is the coordinate of this particle. In the ensemble of non-linear oscillators considered below, this expression takes the form (per oscillator)

$$2\langle E_{\mathrm{kin}}\rangle = \langle zU'(z)\rangle. \qquad (2)$$

Here, $U(z)$ is the potential energy of the oscillator and the prime sign denotes the derivative with respect to the coordinate z. The angle brackets in Eqs. (1) and (2) denote both the thermodynamic averaging (over the ensemble) and quantum-mechanical averaging. Since we consider below the effects associated with small changes in temperature at a low mechanical load, the interatomic potential can be approximated by the cubic parabola

$$U(z) = \frac{f}{2}z^2 - \frac{g}{3}z^3 - Fz, \qquad (3)$$

where f is the coefficient of linear elasticity, g is the anharmonicity constant, and F is the external force applied to the solid and transmitted to each bond in the model of a one-dimensional crystal. The displacement z from the equilibrium position can be expressed as a sum ($z = x + a$) of two terms: the instantaneous displacement x and the average displacement a, the magnitude of which is found from the condition of the thermodynamic equilibrium of the system. This condition is knowingly zero average force acting on the oscillator: $\langle U'(z)\rangle = 0$. In this case, the kinetic energy (1) described in terms of the virial theorem takes the form

$$2\langle E_{\mathrm{kin}}\rangle = \langle xU'(x+a)\rangle.$$

To calculate the thermodynamic characteristics of the ensemble of anharmonic oscillators, we use the self-consistent Einstein approximation, the essence of which is to approximate the free energy of a nonlinear system by the known probe system of harmonic oscillators (see, e.g., [8]). This probe system of quantum harmonic oscillators is described by the distribution function over the coordinates x of the form

$$\rho(x) = \sqrt{\frac{n\omega\tanh q}{\pi\hbar}}\exp\left(-\frac{m\omega}{\hbar}x^2\tanh q\right), \qquad (4)$$

where

$$q = \frac{\hbar\omega}{2kT},$$

m is the particle mass, T is the absolute temperature, $\hbar$ and k are the Planck's and Boltzmann constants. The free energy has a minimum at the thermodynamic equilibrium, which leads to the set of equilibrium equations [9]

$$\begin{aligned}\langle U'(x)\rangle_0 &= fa - g\langle x^2\rangle - ga^2 - F = 0,\\ m\omega^2 &= f - 2ga = m\omega_0^2 - 2ga.\end{aligned} \qquad (5)$$

The first equation here describes zero average force acting on the oscillator and the second one specifies the best approximation of the free energy of the ensemble of nonlinear oscillators under consideration by the harmonic system; $\omega_0 = \sqrt{f/m}$. The model of a one-dimensional crystal generally requires taking into account that m in Eq. (5) must be set equal to a half of the atomic mass, since each atom belongs to two interatomic bonds (in the nearest-neighbor approximation).

The expressions for the components of the internal energy E of the oscillator (without the field term proportional to the external force in Eq. (3)) calculated with the use of Eq. (4) have the form

$$\langle E_{\mathrm{kin}}\rangle = \frac{\langle x^2\rangle}{2}(f - 2ga) = \frac{1}{4}\hbar\omega\coth\left(\frac{\hbar}{2kT}\right)(f - 2ga),$$

$$U_{\mathrm{int}} = \langle U\rangle = \frac{\langle x^2\rangle}{2}(f - 2ga) + \frac{f}{2}a^2 - \frac{g}{3}a^3 \qquad (6)$$

$$= \frac{1}{4}\hbar\omega\coth\left(\frac{\hbar\omega}{2kT}\right) + \frac{f}{2}a^2 - \frac{g}{3}a^3.$$

Let us consider adiabatic mechanical loading of the system. In this case, as was shown in [9], the internal energy $E_2 \approx E_1 + F^2/2f$ (to the second order in force) is conserved in the low- and high-temperature limits.

In the high-temperature region ($\hbar\omega/kT \ll 1$), from Eq. (6) we obtain

$$k\Delta T + \frac{gkT}{f^2}F - \frac{g(\hbar\omega_0)^2}{12f^2 kT} = 0,$$

which yields the expression for the temperature change (thermoelastic effect)

$$\frac{\Delta T}{T} \approx -\frac{g}{f^2}F\left(1 - \frac{1}{12}\left(\frac{\hbar\omega_0}{kT}\right)^2\right). \qquad (7)$$

The first term in Eq. (7) corresponds to the classical Kelvin formula for the thermoelastic effect and the second one is the correction caused by the quantum effects; i.e., there is a quantum-mechanical correction to the classical Kelvin formula.

Let us present the expression for the equilibrium temperature–force strain, which follows from Eq. (5) and also includes the quantum-mechanical correction to the classical value:

$$a \approx \frac{F}{f} + \frac{gkT}{f^2}\left(1 + \frac{1}{12}\left(\frac{\hbar\omega_0}{kT}\right)^2\right). \qquad (8)$$

Now, we construct using Eqs. (5) and (6) the solutions in the opposite limiting case of low temperatures $\hbar\omega/kT \gg 1$

$$\frac{\Delta T}{T} \approx -\frac{kT}{\hbar\omega_0}\ln\left(1 + \frac{\hbar\omega_0 g}{kT f^2}F\right), \qquad (9)$$

$$a \approx \frac{F}{f} + \frac{g\hbar\omega_0}{2f^2}\left(1 + 2e^{-\frac{\hbar\omega_0}{kT}}\right). \tag{10}$$

As is seen, Eq. (9) for the thermoelastic effect in this limiting case cannot be generally reduced to the classical Kelvin formula with some quantum-mechanical correction but rather has a specific, essentially different functional form.

Remarkably, Eq. (9) leads to zero thermoelastic effect at $T \longrightarrow 0$, which is physically reasonable.

At the same time, quantum-mechanical formula (9) asymptotically transforms to the classical Kelvin formula at high temperatures ($\hbar\omega/kT \ll 1$). This allows using Eq. (9) as an approximation in the entire temperature range.

Equations (7)−(10) hold at low applied loads $gF/f^2 \ll 1$ and a small ratio of the ground-state energy to the dissociation energy: $\hbar\omega_0/2D \ll 1$, where $D = f^3/6g^2$.

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