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Fig. 1

Figure 1: Fig. 1

Abstract

Full Text

PHYSICS

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ON THE TEMPERATURE DEPENDENCE OF THE HEAT CAPACITY OF SOLIDS

The quantum theory of the heat capacity of monatomic solids was first developed by A. Einstein (^1), who assumed that all atoms in a solid have the same frequency of oscillation. Using Planck' s distribution, which makes it possible to express the mean energy of an oscillator as a function of temperature, Einstein obtained the following expression for the internal energy of a solid:

$$\Delta U = 3N \frac{h\nu}{e^{h\nu/kT} - 1}.$$

The great fundamental significance of Einstein' s work lay in the fact that the temperature dependence of heat capacity was theoretically derived, being in character close to that observed experimentally, and also in the fact that it clarified the fundamental role of the characteristic temperature $\theta = h\nu/k$, which is an important constant associated with many properties of solids.

In Debye' s theory (^2), which at present is in fact the generally accepted theory of the vibrational heat capacity of the lattice of solids, a distribution of frequencies over the spectrum is adopted, described by the parabolic law $dz/d\nu = B\nu^2$ (Fig. 1). Very important in this respect are the works of M. Born and T. Karman (^3) and M. Blackman (^4).

As follows from a number of considerations, as well as from data of direct experiments and calculations (^4), the actual distribution of frequencies in a solid is closer to a Gaussian law, different from Debye' s distribution, to which A. F. Ioffe (^5) drew special attention.

Fig. 1

In the present work we shall show the possibility of calculating the temperature dependence of the heat capacity of solids with allowance for a frequency distribution described by a law close to the Gaussian one. In a previous note (^6) attention was drawn to the necessity of allowing for dimensionality in the

Fig. 2

Figure 2: Fig. 2

distribution of frequencies, which subsequently was also considered by a number of authors (([7,]8) and others). With the approach adopted here to the problem of calculating the temperature dependence of heat capacity, it is also possible to allow for dimensionality, as follows from the expressions obtained; however, we shall restrict ourselves to the case of an isotropic solid.

The frequency distribution adopted by us, to a known approximation, can be described by an expression of the form

$$\frac{dz}{d\nu} = A\nu^p e^{-\alpha\nu^n}. \tag{1}$$

However, for simplification, apparently without making a large error, we shall confine ourselves to approximating the curve of the frequency distribution over the vibration spectrum by an equation of the form (Fig. 1)

$$\frac{dz}{d\nu} = A\nu^p e^{-\alpha\nu}. \tag{1a}$$

Since the total number of vibrations z in a gram-atom of a solid is equal to $3N$, we have

$$z = 3N = \int_0^\infty A\nu^p e^{-\alpha\nu}\, d\nu = A\frac{\Gamma(p+1)}{\alpha^{p+1}}, \tag{2}$$

whence $A = 3N\alpha^{p+1}/\Gamma(p+1)$, and the frequency ν_0 corresponding to the maximum on the distribution curve, which we shall take as the characteristic frequency, will then be equal to $\nu_0 = p/\alpha$. Then the characteristic temperature θ will be equal to

Fig. 2

$$\theta = \frac{h\nu_0}{k} = \frac{hp}{k\alpha}. \tag{3}$$

In this case the total vibrational energy, or the internal energy of the solid, will be equal to

$$\Delta U = A\int_0^\infty \frac{h\nu \cdot \nu^p e^{-\alpha\nu}\, d\nu}{e^{h\nu/kT} - 1}, \tag{4}$$

whence, with sufficient approximation, we obtain

$$\Delta U = 3RT \left(\frac{T}{\theta}\right)^{p+1} \frac{p^{p+1}}{(pT/\theta + 1)^{p+1}}. \tag{5}$$

Since for an isotropic solid one may put $p \geq 2$, in this case, for $p = 2$,

$$\Delta U = 24RT \frac{(T/\theta)^3}{(2T/\theta + 1)^3}. \tag{6}$$

On the basis of formula (6), for the temperature dependence of the heat capacity of an isotropic solid we obtain

$$C = 3Rp^{p+1} \frac{(T/\theta)^{p+1} \left[pT/\theta + p + 2\right]}{(pT/\theta + 1)^{p+2}}; \tag{7}$$

for $p = 2$

$$C = 3R \frac{(T/\theta)^3 (2T/\theta + 4)}{(T/\theta + 1/2)^4}.$$

Figure 2 shows the curve of the change in the vibrational heat capacity of the lattice of a solid as a function of T/θ. The adopted characteristic temperature is approximately three times smaller than the Debye temperature.

Experimental data on the temperature dependence of the heat capacity of various solids are well described by the expression obtained. The simplicity of the resulting law for the variation of the heat capacity of solids as a function of temperature opens broad possibilities for its application in the most diverse thermodynamic and other physical calculations.

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