

Dependence of the temperature factor of X-ray scattering intensity on the shape of the lattice frequency spectrum

N. N. Sirota

1962

SovietRxiv

View the original and related papers at <https://sovietsrxiv.org/items/ru-196201.15761>

Source: Math-Net.Ru and CyberLeninka. Machine translation. Verify with the original.

Abstract

Full Text

Reports of the Academy of Sciences of the USSR
1962. Volume 144, No. 1

PHYSICAL CHEMISTRY

Academician of the Academy of Sciences of the Belorussian SSR N. N. SIROTA

DEPENDENCE OF THE TEMPERATURE FACTOR OF THE INTENSITY OF X-RAY SCATTERING ON THE FORM OF THE FREQUENCY SPECTRUM OF THE LATTICE

In the physics of condensed media, in X-ray and neutron studies of solids, knowledge of the temperature factor of the intensities of scattering of X-rays, neutrons, electrons, etc., by lattice vibrations is of great importance.

The Debye-Waller temperature factor $M_{T,D}$ plays a fundamental role in a number of areas of physics and, above all, in solid-state physics. The theory of the Debye-Waller factor has been developed (¹⁻³) for the Debye frequency spectrum

$$dz = \frac{9N}{\nu_m^3} \nu^2 d\nu,$$

where ν_m is the limiting Debye frequency of lattice vibrations; the Debye characteristic temperature is $\theta = h\nu_m/k$.

In this case the expression for the temperature factor has the form

$$B_{T,D} = \frac{6h^2}{mk\theta} \left[\frac{1}{4} + \frac{\Phi(X)}{X} \right], \quad (1)$$

where

$$\Phi(X) = \frac{1}{X} \int_0^X \frac{x dx}{e^x - 1}; \quad x = \frac{h\nu}{kT}; \quad X = \frac{h\nu_m}{kT} = \frac{\theta}{T}; \quad B_{D,T} = M_{T,D} \left(\frac{\lambda}{\sin \vartheta} \right)^2.$$

In the present work we investigate the influence of the form of the frequency spectrum on the magnitude of the temperature factor. Let us consider a comparatively wide range of forms of frequency spectra, which can be combined by the general expression

$$dz = A\nu^p e^{-\alpha\nu^n} d\nu. \quad (2)$$

Since the total sum of all frequencies of a gram-atom of a solid is equal to $3N$, it follows that the constant multiplier of the phonon distribution curve (2), and from the condition $\partial^2 z / \partial \nu^2 = 0$, is determined as

$$A = \frac{3N}{\int_0^\infty \nu^p e^{-\alpha\nu^n} d\nu} = 3N \frac{n\alpha^{(p+1)/n}}{\Gamma((p+1)/n)}, \quad \text{where } \alpha = \frac{p}{n\nu_0^n}.$$

Following the scheme of the Debye-Waller theory ⁽²⁾, we shall find expressions for the mean-square displacements $\overline{u_{R,T}^2}$ and the temperature factor B_T as applied to the case of the type of frequency spectra under consideration, restricting ourselves at this stage to harmonic vibrations.

As is known, the mean value of the square of the displacement of a harmonic oscillator $\overline{x^2}$ is equal to one half of the square of the vibration amplitude, $\overline{x^2} = a^2/2$. On the other hand, the energy of the oscillator is $W = 2\pi^2\nu^2 m a^2$, or $a^2 = W/2\pi^2\nu^2 m$.

The mean-square displacement $\overline{u_{S,T}^2}$ of the coupled oscillators of the lattice of a gram-atom of a solid over the entire vibrational spectrum may be expressed by the relation

$$\overline{u_{S,T}^2} = \frac{1}{3N} \int_0^\infty \frac{a^2}{2} dz = \frac{1}{4\pi^2 m \cdot 3N} \int_0^\infty \frac{W}{\nu^2} dz. \quad (3)$$

Expressing, as is customary, the mean energy of a quantized oscillator according to Planck, with allowance for the zero-point energy,

$$W = h\nu \left(\frac{1}{2} + \frac{1}{e^{h\nu/kT} - 1} \right),$$

substituting it into (3), and expanding the values of dz and A , we obtain:

$$\begin{aligned} \overline{u_{S,T}^2} &= \frac{n(p/n\nu_0^n)^{(p+1)/n}}{4\pi^2 m \Gamma\left(\frac{p+1}{n}\right)} \int_0^\infty W \nu^{p-2} e^{-\alpha\nu^n} d\nu = \\ &= \frac{n}{4\pi^2 m \Gamma((p+1)/n)} \left(\frac{p}{n}\right)^{(p+1)/n} \frac{1}{\nu_0^{p+1}} \int_0^\infty W \nu^{p-2} e^{-\alpha\nu^n} d\nu. \end{aligned} \quad (4)$$

Hence, expanding the value of W , we shall have:

$$\overline{u_{S,T}^2} = \frac{n}{4\pi^2 m} \frac{(p/n)^{(p+1)/n}}{\Gamma((p+1)/n) \nu_0^{p+1}} \left\{ \frac{1}{2} \int_0^\infty h\nu^{p-1} e^{-\alpha\nu^n} d\nu + \int_0^\infty \frac{h\nu^{p-1} e^{-\alpha\nu^n}}{e^{h\nu/kT} - 1} d\nu \right\}. \quad (5)$$

Taking the first integral and carrying out simple transformations, we obtain

$$\overline{u_{S,T}^2} = \frac{\hbar^2 n (p/n)^{(p+1)/n}}{mk\theta \Gamma((p+1)/n)} \left\{ \frac{1}{2} \frac{\Gamma(p/n)}{n (p/n)^{p/n}} + \frac{1}{X^p} I(X, p, n) \right\}, \quad (6)$$

where

$$\begin{aligned} \frac{1}{X} &= \frac{kT}{h\nu_0}; & x &= \frac{h\nu}{kT}; & \theta &= \frac{h\nu_0}{k}; & \beta &= \frac{p}{n} \left(\frac{T}{\theta} \right)^n; & I(X, p, n) &= \\ & & & & & & & & = \int_0^\infty \frac{x^{p-1} e^{-\beta x^n}}{e^x - 1} dx. \end{aligned}$$

Since the temperature factor is related to the mean-square displacement by the relation $B_T = 8\pi^2 \cdot \overline{u_{S,T}^2}$, then

$$B_T = \frac{2\hbar^2}{mk\theta} \left\{ \frac{n \left(\frac{p}{n} \right)^{(p+1)/n}}{\Gamma((p+1)/n)} \right\} \left\{ \frac{1}{2} \frac{\Gamma(p/n)}{n (p/n)^{p/n}} + \frac{1}{X^p} I(X, p, n) \right\}. \quad (7)$$

In particular, for $p = 2$, $n = 1$

$$B_T = \frac{4\hbar^2}{mk\theta} \left\{ \frac{1}{4} + \frac{2}{X^2} I_{2,1}(X) \right\}^*. \quad (7a)$$

When comparing the values of the temperature factor calculated for the type of frequency spectrum under consideration with the Debye one, it is necessary to take into account that the Debye characteristic temperatures differ from the characteristic temperatures of other types of frequency spectra determined from the ordinates of the maxima of the distribution curves. For correct comparison it is necessary to introduce conversion corrections. In the simplest case one may use approximate conversion factors.

* The values of the integrals $I(X, p, n)$ as functions of (T/θ) were calculated on an electronic computer by T. D. Sokolovskii and I. M. Kuntsevich.

The expressions obtained may be used to calculate the temperature factor of anisotropic bodies having chain and layered structures, with allowance for the dimensionality of atomic vibrations.

Analogous calculations for the properly Gaussian frequency spectrum $dz = Ae^{-\alpha\Delta\nu^2} d\nu$ lead to the expressions:

$$\overline{u^2}_{S,T} \text{ (Gaussian)} = \frac{4h}{4\pi^2 m} \sqrt{\frac{\alpha}{\pi}} [\varphi + 2\psi(X)], \quad (8)$$

$$B_T \text{ (Gaussian)} = \frac{4h}{m} \sqrt{\frac{\alpha}{\pi}} \left[\frac{\varphi}{2} + \psi(x) \right], \quad (9)$$

where

$$\psi(X) = \int_0^\infty \frac{e^{-\beta\Delta x^2}}{x(e^x - 1)} dx, \quad \varphi = \int_0^\infty \nu^{-1} e^{-\alpha\Delta\nu^2} d\nu,$$

with α characterizing the reciprocal magnitude of the variance of the curve of the normal law of frequency distribution; here $\beta = \alpha(kT/h)^2$.

Analysis of the results of the present investigation shows that the form of the frequency spectrum affects the magnitude of the temperature factor. It follows from this that, in particular, the determination of characteristic temperatures by X-ray and similar methods should be carried out with allowance for the form of the frequency spectrum of the vibrations of ions in the lattice.

Department of Solid-State Physics and Semiconductors
Academy of Sciences of the BSSR

Received
30 I 1962

REFERENCES

1. P. Debye, *Ann. d. Phys.*, **39**, 789 (1912); **43**, 49 (1914).
2. I. Waller, *Zs. f. Phys.*, **17**, 398 (1923); **51**, 213 (1928).
3. P. James, *The Optical Principles of the Diffraction of X-Rays*, Moscow, 1950.

Note: Figure translations are in progress. See original paper for figures.

Source: Math-Net.Ru and CyberLeninka. Machine translation. Verify with the original.