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About Debye Temperature In Crystals At $T = 0$ K

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ABSTRACT

Based on the analysis of the Debye function, which relates the Debye temperature θ_D and the measured temperature of the object T , it is shown that the Debye temperature of crystals decreases with temperature decreasing from room temperature to absolute zero.

It is shown that the Debye temperature at temperature $T = 0$ K does not depend on the Debye function, but depends only on the mass of the atom and the amplitude of the zero-point oscillations. Based on the analysis of the thermal crystal lattice oscillations Debye theory basic assumptions and experimental data accumulated for recent years, a formula is proposed that relates the Debye temperature at moderate temperatures θ_b and at absolute zero temperature ($T = 0$ K) θ_0 . It is shown that the calculated Debye temperature θ_0 at the absolute zero temperature according to the proposed formula in the range from ~ 2 to ~ 13 % coincides with the experimental data taken from literature for a number of substances of different classes.

KEYWORDS

Thermal crystal lattice oscillations, Debye temperature, Debye theory, moderate temperatures, absolute zero temperature.

INTRODUCTION

The Debye temperature θ_b is one of the important characteristics of a crystal characterizing its thermo-physical and

strength properties. To successfully use these characteristics in practice and manage them based on the scientifically justified methods, it

is important to know the nature and thermal vibrations mechanisms of atoms. In the theory of thermal vibrations of atoms in crystals, the Debye temperature θ_D is assumed to be almost constant (in the limit $\sim 10\%$ for a given substance) at temperatures $300-0\text{ K}$ ($T < \theta_D$) [1,2,3]. Apparently, at that period of time this was probably due to lacking relevant experimental data on low-temperature dependence of the Debye temperature. Recent experimental data show that the Debye temperature decreases from 22% to 40% for various compounds, such as TiC [4] $Zr_2Nb_{1-z}C_xN_y$ [5] and gallium monochalcogenides [6] in the temperature range $300-0\text{ K}$. In some recent publications, θ_0 is given a value greater than θ_D [7]. Thus, the question if Debye temperature either decreases or increases or remains constant with decrease in the temperature of the matter to absolute zero is still open. Is it possible to find an unambiguous answer to this question? Is it possible to find an expression connecting the Debye temperatures at high θ_D and at cryogenic temperature θ_0 ? The purpose of this paper is to analyze the nature of the change in the Debye temperature in the temperature range $300-0\text{ K}$ and find an expression relating the Debye temperature at room temperature

θ_D ($T=300\text{ K}$) and at absolute zero temperature ($T=0\text{ K}$) θ_0 .

THEORETICAL ANALYSIS

According to Debye's theory of atoms thermal oscillations in a crystal lattice, the thermal oscillations of atoms in crystals are considered to be similar to the thermal excitation of quasiparticles – phonons, like to thermal excitation of photons. In this model, vibration energy of the crystal lattice, that is, the phonon energy should be considered a quantized quantity. In experiment, energy quantization of elastic waves in lattice is indeed manifested when these waves interact with X-rays and neutrons. At these interaction, the energy and impulse of X-rays and neutrons change so that these changes correspond exactly to the occurrence or absorption of one or more phonons [8, 9].

According to the X-ray and neutron scattering theory, the relationship between the amplitude of thermal oscillations of atoms in a crystal and the Debye temperature is determined by the following transcendental equation [8, 9]:

$$\theta_D = \frac{9h^2}{4\pi^2 \cdot k \cdot m \cdot u^2} \cdot \left[\frac{\Phi(x)}{x} + \frac{1}{4} \right], \quad (1)$$

where θ_D is the Debye temperature, u is the mean square amplitude of the thermal oscillations of atoms in the element (or atomic complex in alloys) conditioned by thermal oscillations of atoms, h is the Planck constant, k is the Boltzmann constant, m is the average atomic mass in the element (or atomic

complex in the alloys), $x = \theta_D/T$ is the ratio of the Debye temperature to the measured temperature T (in K), and $\Phi(x)$ is the tabulated Debye function, which is known from the specific heat theory and is defined as follows:

$$\Phi(x) = \frac{1}{x} \int_0^x \frac{\xi d\xi}{\lambda^\xi - 1}, \quad (2)$$

where $\xi = \frac{h\omega}{kT}$, ω -cyclic frequency of thermal oscillations. Let us analyze formula (1) in the absence of phase transformations at cryogenic temperatures. (In the case of phase transformations, the thermo physical characteristics of the matter may undergo an abnormal transformation). Equation (1) includes two variables that depend on the temperature: the Debye function and the mean square amplitude of the thermal vibrations of atoms $\overline{u^2}$. According to the properties of the Debye function $\Phi(x)$ [9], the ratio $\Phi(x)/x$ in the expression (1) decreases with decreasing temperature T (with

increasing $x = \theta_D/T$), and as T approaches absolute zero ($T \rightarrow 0$ K), the ratio $\Phi(x)/x$ highly rapidly (exponentially) approaches zero (Fig.1). This should lead to a decrease in the Debye temperature θ_D at $T \rightarrow 0$ K. Although, as the temperature decreases $\overline{u^2}$ also decreases, which, according to (1), should lead to an increase in θ_D . However, $\overline{u^2}$ decreases much slower than the Debye function. If the amplitude of thermal oscillations of atoms is usually 5-7% of the mean atomic distance at room temperature, then at $T = 0$ K, the amplitude of zero-point oscillations is 2-3% of the average atomic distance.

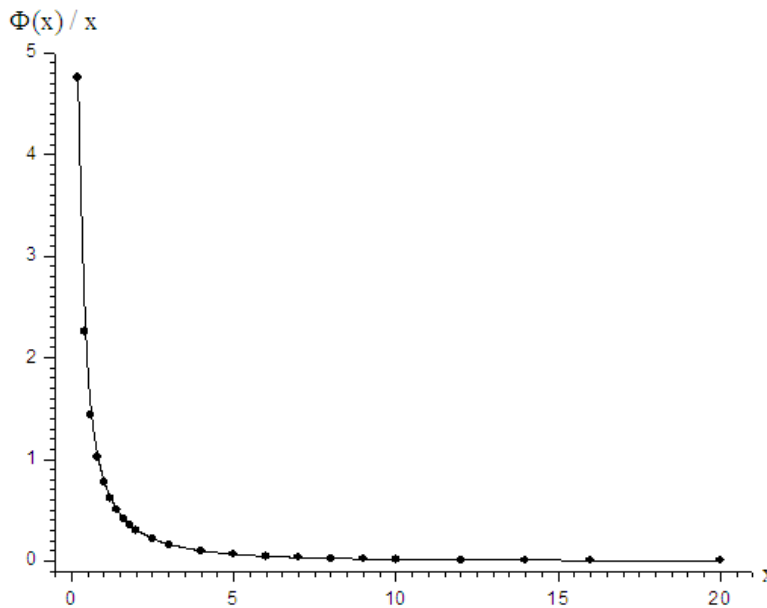


Fig. 1. Dependence of $\Phi(x)/x$ function on x (according to the data from [9]).

Therefore, one can see that decrease of $\overline{u^2}$ in the temperature interval 300 - 0 K is not as big as the decrease in the expression for $\Phi(x)/x$, which decreases several times sharply with decreasing temperature in the interval 300 - 0

K. Thus, analysis of formula (1), which relates the Debye temperatures and the mean square amplitude of the thermal oscillations of atoms through the Debye function, makes it possible to state that at cryogenic temperature with

the Debye temperature changing from θ_0 to θ , a strong decrease in the Debye function plays determining role leading to decrease in the temperature.

On the other hand, this conclusion can be also drawn by analyzing formulas (1) and (2). Let's

calculate $\Phi(x)$ function at the temperature $T = 0$ K. At $T = 0$ K, the integral in expression (2) has the following form:

$$\Phi(x) = \frac{1}{x} \int_0^\infty \frac{\xi d\xi}{\lambda^\xi - 1}, \quad (3)$$

By taking into account that the integral (3) is [10]

$$\int_0^\infty \frac{\xi d\xi}{\lambda^\xi - 1} = \frac{\pi^2}{6}.$$

Then from (3) and from the condition $T = 0$ K one can obtain the following expression:

$$\Phi(x) = \frac{1}{x} \int_0^\infty \frac{\xi d\xi}{\lambda^\xi - 1} = \frac{T}{\theta} \times \frac{\pi^2}{6} = 0 \quad (4)$$

According to the condition (4) and expression (1), at $T = 0$ K for the Debye temperature one can obtain the following expression:

$$\theta_0 = \frac{9h^2}{4\pi^2 \cdot k \cdot m \cdot \overline{u_0^2}} \cdot \left(\frac{\Phi(x)}{x} + \frac{1}{4} \right)_{T=0} = \frac{9h^2}{4\pi^2 \cdot k \cdot m \cdot \overline{u_0^2}} \cdot \frac{1}{4} = \frac{9h^2}{16\pi^2 \cdot k \cdot m \cdot \overline{u_0^2}}. \quad (5)$$

It is seen from expression (5) that at the temperature $T = 0$ K, the Debye temperature will be determined by the mean square displacement of the atom and the mass of the atom. This means that at the temperature $T = 0$ K, the Debye temperature θ_0 does not depend on the Debye function, that is, on the

phonon spectrum, but depends only on the mass of the atom and the mean square amplitude of zero-point oscillations of atoms (on the energy of zero-point oscillations).

Thus, theoretical analysis shows that the Debye temperature decreases with decreasing temperature below room temperature, and at temperature $T = 0$ K does not depend on the Debye function (thermal vibration spectrum), but depends only on the mass of the atom and the amplitude of zero-point oscillations (zero-point energy). Of course, this assertion is correct if there are no phase transitions in the crystal with decreasing temperature. Let's now proceed to find the connection between the Debye temperatures at room temperature and at absolute zero.

RESULTS AND DISCUSSION

According to the theory of crystal lattice oscillations, the energy of a normal lattice oscillation is equal to the energy of a quantum oscillator with a mass equal to the mass of vibrating atoms, and its frequency is equal to the frequency of the normal oscillations [1]. If the crystal consists of N atoms making bound oscillations, the total energy of the crystal will be equal to the sum of the energy of $3N$ independent normal linear harmonic oscillators. The lattice thermal oscillations energy quantum or a quantum oscillator is called phonon.

It is known that the energy of one quantum oscillator or a phonon is quantized and described by the following formula [1]:

$$\varepsilon_n = (n+1/2)h\nu_0, \quad (6)$$

where ν_0 is zero oscillations frequency of oscillator, n – is quantum number that takes integer values ($n = 0, 1, 2, \dots$) and characterizes degree of thermal excitation of oscillator. The energy corresponding to the value $n = 0$ is

called the zero-point energy $\varepsilon_0 = (1/2)h\nu_0$, which is not thermal energy. It is appropriate to note here that according to some educational literature (for example, in [11]), the zero-vibration energy of one phonon is determined by the expression

$$\varepsilon_0 = \frac{9\eta}{8} \omega_{\max} = \frac{9h}{8} \nu_{\max},$$

where ω_{\max} is the maximum frequency (Debye frequency) of thermal oscillations excited at a temperature called the Debye temperature $T = \theta$. However, this expression is incorrect. The incorrectness of this expression is that the energy of zero-point oscillations cannot be determined by the maximum frequency $\omega_D = \omega_{\max}$. It should be determined by the frequency of zero-point oscillations ω_0 , which lies between the frequencies 0 and ω_{\max} . Zero oscillation does not carry and does not transmit energy. It is not an elastic vibration, and is determined by the quantum nature of the atoms. The energy of zero-point oscillations of a crystal is constant and must be additively added to the thermal energy of the lattice. The fallacy of expression (2) follows from the fact that, first, when determining the total crystal energy as an integral sum of the thermal oscillations of individual oscillators, the expression of zero-point oscillations $\hbar\omega_0/2$ also contribute to the integral [1-3, 11] as a variable. This cannot be done, since it does not depend on temperature on temperature and is a constant value for a given crystal. Secondly, for the lower boundary of integration, which determines the total energy of thermal oscillations of oscillators, they take not the frequency of zero oscillations ω_0 , but the frequency 0 , which is also not correct.

Zero-point energy corresponds to zero-point oscillations, which do not depend on the temperature of the crystal and do not decay even at $T = 0$ K. These oscillations do not carry and do not transmit thermal energy.

The existence of zero-point vibrations is related to the uncertainty relation of quantum mechanics, according to which, $\Delta x \times \Delta p_x \geq \hbar/2$. From this relation it follows that an exact definition of coordinate of an oscillating atom in the space ($x \rightarrow 0$) causes a large uncertainty in its momentum, and, accordingly, in its kinetic energy. On the other hand, an increase in the particle

coordinate $\frac{k\Delta x^2}{2}$ determination region

would lead to an increase in the potential energy, which is also not energetically favorable. Consequently, the zero-point oscillations energy is the minimum value of energy that an atom can have. Thus, atoms in a crystal at a temperature $T = 0$ K oscillate with zero frequency corresponding to zero energy.

According to the existing thermal lattice vibrations theory, at certain temperature $T = \theta_D$, called the Debye

temperature, all possible oscillations in a crystal with frequencies from ν_0 to ν_{max} are excited [1, 2]. This temperature is called the Debye temperature. The energy quantum of one quantum oscillator corresponding to a given temperature and frequency ν_{max} can be defined as $\varepsilon_{max} = h\nu_{max}$. ν_{max} is the frequency that corresponds to the imaginary wavelength $\lambda_{min} = 2a$ (a – is lattice period) and creates standing waves in the lattice. At frequencies $\nu < \nu_{max}$, it is difficult for standing waves to appear. They are weakly excited and rapidly damped. Waves with wavelength $\lambda > \lambda_{min} = 2a$ become stable after excitation at the frequency ν_{max} [2]. Consequently, at the temperature $T = \theta_D$, at the first energy level ($n = 1$), the energy of one phonon with frequency $\nu = \nu_{max}$ will be determined according to the expression (6), as follows [12]:

$$\varepsilon_{max} = h\nu_{max} = (1 + 1/2)h\nu_0 = \frac{3}{2} h\nu_0. \tag{7}$$

The frequency ν_{max} can be determined through the Debye temperature from the following condition [1]:

$$k\theta_D = \hbar\omega_{max} = h\nu_{max}. \tag{8}$$

It follows that

$$\nu_{max} = \frac{k}{h}\theta_D. \tag{9}$$

Similarly to expression (9), for zero-point oscillations frequency one can write that

$$\nu_0 = \frac{k}{h} \theta_0. \tag{10}$$

where θ_0 is the Debye temperature corresponding to the zero-point oscillations frequency of the atoms. From the expressions (7), (9) and (10) it follows that

$$\theta_0 = \frac{2}{3} \theta_D. \tag{11}$$

Indeed, such relation can be supported by experimental data described in recent Table 1 presents published data on determination of the Debye temperature at room and cryogenic temperatures T_1 and T_2 ($T_1=0$ K and $T_2= 78$ K), respectively. Because of the proximity of T_1 and T_2 , it is observed that $\theta_0(T_1) \approx \theta_0(T_2)$ for compounds of different classes (for semiconductors, refractory binary and multicomponent interstitial alloys) and tin and data obtained by formula (11).

CONCLUSION

Formula that relates the Debye temperature and the mean-square amplitude of thermal oscillations of atoms through the Debye function is analyzed. It is shown that when the temperature drops below room temperature, despite the decrease in the amplitude of thermal oscillations of atoms in a lattice, which is inversely proportional to the Debye temperature, a strong decrease in the Debye function plays determining role, which in turn leads to a decrease in temperature .

publications.

Based on the analysis the main principles of the Debye theory of thermal lattice oscillations and of the theory of X-ray and thermal neutron scattering by real crystals and the recently accumulated experimental data, the formula is proposed that relates Debye temperatures at moderate temperatures (θ_D) and at temperature $T = 0$ K (θ_0). Note that this reasoning is valid only when there are no phase transitions at cryogenic temperatures. It is shown that the value $\theta_0(\text{calc})$ calculated via the proposed formula (11) in the range from ± 2 to ± 13 % coincide with the experimental data for a number of substances of different classes.

It is shown that the Debye temperature of a crystal at the absolute zero temperature does not depend on the Debye function (the frequency spectrum of thermal oscillations) but depends only on an atomic mass and root-mean-square amplitude of zero oscillations of atoms in a lattice.

Table 1. Debye temperature θ_0 at room and cryogenic temperatures θ_0 ($\theta_0(\text{exp})$) and $\theta_0(\text{calc})$ – experimental and calculated data, respectively, temperature in K).

№	Substance	θ_D , T= 300 K	θ_0 (exp.)		θ_0 (cal c.)	$\Delta\theta$ o	$\Delta\theta_0/\theta_{0ca}$ Ic.r %
			T = 0 K	T = 78 K			
1	GaS	454 [6]*	263 [6]*		302	39	12.9
2	GaTe	267 [6]*	165 [6]*		177	12	6.7
3	TiC _{0.97}	860 [4] **		520 [4] **	573	53	9.2
4	TiC _{0.88}	700 [4] **		480 [4] **	467	13	2.8
5	TiC _{0.70}	590 [4] **		440 [4] **	393	47	11.9
6	Zr _z Nb _{1-z} C _x N _y	710 [5]*	462 [5]*		473	11	2.3
7	α -Sn (gray)	230 [13]***	148 [13]***		153	5	3.3

Note. θ_0 (exp.) is experimentally; θ_0 (calc.) is calculated by expression (6); $\Delta\theta_0 = |\theta_0(\text{exp.}) - \theta_0(\text{calc.})|$. The Debye temperatures are determined by: * - calculations from the heat capacity data, ** - neutron diffraction, *** - calculations of the Mossbauer spectrum thermal factor, given in [13].

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