THE TWO-PARAMETER DEBYE MODEL

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When analyzing thermodynamic and kinetic properties of crystals whose anisotropy is not large and the considered effects do not relate to the existence of singled-out directions in crystals, one may use a more simple model of an isotropic medium with a good accuracy, after having chosen its parameters in an optimal way. Based on the quantum mechanical description it is shown that the method of approximation of the moduli of elasticity of a crystal by the model of an isotropic medium, proposed earlier in [2], follows from the requirement of the minimal difference between the free energies of a crystal and an approximating isotropic medium. The two-parameter Debye model is formulated, which, in contrast to the standard model where the average velocity of phonons is introduced, takes into account the existence in an isotropic medium of both longitudinal and transverse phonons. The proposed model contains, except the Debye energy, an additional dimensionless parameter and, consequently, the law of corresponding states for the heat capacity being characteristic of the standard model does not hold. With taking account of the two phonon branches the structure of the density of phonon states proves to be more complex as compared to the standard model and has a singularity that resembles Van Hove singularities in real crystals. As an example, an application of the two-parameter Debye theory to such crystals of the cubic system as tungsten, copper, lead is considered. It is shown that the calculation of the low-temperature heat capacity of these crystals by means of the approximated moduli of elasticity within the framework of the two-parameter model leads to a considerably better agreement with experiment than in the case of the standard Debye model.

Key words: moduli of elasticity, phonon, free energy, heat capacity, Debye energy

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I. INTRODUCTION

The elastic properties of an isotropic medium are characterized by two elastic moduli, for example, the Lame coefficients \( \lambda \) and \( \mu \) [1]. A crystal is an anisotropic medium, and therefore its elastic properties differ from those of an isotropic body and are characterized by a large number of parameters. If the degree of the anisotropy is sufficiently small, then, obviously, the properties of a crystal will slightly differ from the properties of an isotropic medium and the analysis of the properties of a crystal can be replaced by a more simple analysis of the properties of a model isotropic medium, which parameters are selected in an optimal way. In [2] it is proposed to find the elastic moduli of an approximating isotropic body from the condition of minimum of the quantity

\[
G = (\lambda_{iklm} - \lambda_{iklm}^{(0)})^2,
\]

where \( \lambda_{iklm} \) is the elastic moduli tensor of a crystal, and

\[
\lambda_{iklm}^{(0)} = \lambda \delta_{ik} \delta_{lm} + \mu (\delta_{il} \delta_{km} + \delta_{im} \delta_{kl}),
\]

is the elastic moduli tensor of an isotropic medium. The extremum conditions \( \partial G / \partial \lambda = \partial G / \partial \mu = 0 \) give a relation between the approximating Lame coefficients and the invariants of the elastic moduli tensor of a crystal:

\[
\lambda = \frac{1}{15} (2 \lambda_{ikkk} - \lambda_{ikik}), \quad \mu = \frac{1}{30} (3 \lambda_{ikik} - \lambda_{ikkk}).
\]

This approximation is quite reasonable for a qualitative, and in many cases quantitative, analysis of the integral properties of a crystal and those effects that are not related to the existence of distinguished directions in crystals and can be described in the approximation of an isotropic medium. In [2] such an approach was developed for the theory

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of elastic waves in crystals. A similar approach can be used when nonlinear effects are taken into account in crystals, for example, to simplify the calculations of the matrix elements of the interaction between phonons in crystals of any system. In this paper we restrict ourselves to the framework of the linear theory of elasticity.

Condition (11) is convenient in that it leads to a system of linear algebraic equations. However, in principle, other criteria for the closeness of the elastic moduli tensors of a real and a model media are possible, which contain, for example, the difference modulus of a higher degree. It is natural to require that the approximating elastic moduli are chosen so that the free energies of real and model media would be as close as possible.

The purpose of this work is to show on the basis of quantum consideration that the elastic moduli of an isotropic model medium, obtained from the condition of the extremum of the quantity $G$ (11), do indeed lead to the free energy being as close as possible to the free energy of a crystal.

The well-known Debye model (5) is widely used to describe the thermodynamic properties of solids in the approximation of an isotropic medium. In the standard Debye model, which is formulated for an isotropic medium, a further simplification is made consisting in the fact that an isotropic medium, instead of two parameters, is characterized by a single parameter – the average phonon velocity and its corresponding energy. However, such a simplification is not necessary and it seems natural to formulate a theory for an isotropic medium with two elastic moduli and, accordingly, with two types of phonons – longitudinal and transverse. Obviously, such a theory cannot be less accurate than the Debye model in the standard formulation (5) and, possibly, will allow us to describe some more subtle effects. In addition, using the approximation of the elastic moduli (3), it becomes possible to apply the model to the calculation of crystals of various systems. Thus, another goal of this work is to formulate the Debye model which takes into account the existence of longitudinal and transverse phonons in an isotropic medium. As an example, we consider the application of the proposed two-parameter Debye theory to crystals of the cubic system. The approximating elastic moduli are found for tungsten, copper, and lead. The calculation of their low-temperature heat capacities using the calculated moduli shows that the two-parameter model describes the thermodynamic properties with a much better approximation than the standard Debye model.

II. OPTIMAL APPROXIMATION OF ELASTIC PROPERTIES OF A CRYSTAL BY THE MODEL OF AN ISOTROPIC MEDIA

The density of the Hamiltonian of a crystal, as an elastic medium, is given by the expression

$$H(r) = \pi_a(r)^2 \rho + \frac{1}{2} \lambda_{abj} u_{ai}(r) u_{bj}(r),$$

(4)

where the deformation tensor in the linear approximation has the form

$$u_{ij} = \frac{1}{2} (\nabla_i u_j + \nabla_j u_i),$$

(5)

$u_i(r)$ is the displacement vector, $\pi_a(r) = \rho \dot{u}_a(r)$ is the canonical momentum, $\rho$ is the density, $\lambda_{abj}$ is the elastic moduli tensor of a crystal. In (4) and in the following, the rule of summation over repeated indices is used.

Let us try to approximate the Hamiltonian (4), which contains the elastic moduli of a real crystal, by a model isotropic medium, choosing its Hamiltonian in the form

$$H_S(r) = \pi_a(r)^2 \rho + \frac{1}{2} \tilde{\lambda}_{abj} u_{ai}(r) u_{bj}(r) + \varepsilon_0,$$

(6)

where

$$\tilde{\lambda}_{abj} = \tilde{\lambda} \delta_{ai} \delta_{bj} + \tilde{\mu} (\delta_{ai} \delta_{ij} + \delta_{aj} \delta_{ib}),$$

(7)

and the Lame coefficients $\tilde{\lambda}$, $\tilde{\mu}$ will be considered as parameters determined from the condition of the best approximation of the crystal Hamiltonian (4) by the Hamiltonian of an isotropic medium (6), which will be introduced below. Here and in what follows the elastic moduli of an approximating isotropic medium will be denoted by the tilde sign at the top. The Hamiltonian (6) contains the energy density $\varepsilon_0$, which is caused by the fact that replacing the exact elasticity tensor $\lambda_{abj}$ with the approximate isotropic one $\tilde{\lambda}_{abj}$ can lead, generally speaking, to a change in the ground undeformed state of a crystal as well. The total initial Hamiltonian $H = \int H(r) dr$ can be represented in the form $H = H_S + H_C$, where the total approximating Hamiltonian is singled out:

$$H_S = \int \left[ \frac{\pi_a(r)^2}{2\rho} + \frac{1}{2} \tilde{\lambda}_{abj} u_{ai}(r) u_{bj}(r) \right] dr + V\varepsilon_0,$$

(8)
and the correlation Hamiltonian

\[ H_C = \frac{1}{2} \int \left( \lambda_{abj} - \tilde{\lambda}_{abj} \right) \nabla_i u_a \nabla_j u_b \, d\mathbf{r} - V \varepsilon_0 \]  

characterizes the difference between the exact and approximating Hamiltonians.

In the quantum description, which will be used, the deformation vector \( u_a(\mathbf{r}) \) and the canonical momentum \( \pi_a(\mathbf{r}) \) should be considered as operators for which the known commutation relations hold

\[ \pi_a(\mathbf{r}) u_b(\mathbf{r}') - u_b(\mathbf{r}') \pi_a(\mathbf{r}) = -i \hbar \delta_{ab} \delta(\mathbf{r} - \mathbf{r}'), \]

\[ u_a(\mathbf{r}) u_b(\mathbf{r}') - u_b(\mathbf{r}') u_a(\mathbf{r}) = 0, \quad \pi_a(\mathbf{r}) \pi_b(\mathbf{r}') - \pi_b(\mathbf{r}') \pi_a(\mathbf{r}) = 0. \]  

(10)

Let us use the expansion of the field operators

\[ u_a(\mathbf{r}) = \frac{1}{\sqrt{V}} \sum_{k, \alpha} \sqrt{\frac{\hbar}{2 \rho \omega(k, \alpha)}} e_a(k, \alpha) (b_{k\alpha} + b_{k\alpha}^+ e^{i k \cdot \mathbf{r}}), \]

\[ \pi_a(\mathbf{r}) = -i \frac{1}{\sqrt{V}} \sum_{k, \alpha} \sqrt{\frac{\rho \hbar \omega(k, \alpha)}{2}} e_a(k, \alpha) (b_{k\alpha} - b_{k\alpha}^+ e^{i k \cdot \mathbf{r}}), \]  

(11)

where \( e(k, \alpha) \) are the complex polarization vectors \((\alpha = 1, 2, 3)\), such that \( e(-k, \alpha) = e^*(k, \alpha) \), for which the conditions of orthogonality and completeness hold

\[ e(k, \alpha)e^*(k', \alpha') = \delta_{\alpha \alpha'}, \quad \sum_{\alpha} e_i^*(k, \alpha)e_j(k, \alpha) = \delta_{ij}. \]  

(12)

The creation \( b_{k\alpha}^+ \) and annihilation \( b_{k\alpha} \) operators of phonons obey the usual commutation relations: \([b_{k\alpha}, b_{k'\alpha'}^+] = \delta_{kk'} \delta_{\alpha \alpha'}, [b_{k\alpha}, b_{k'\alpha'}] = [b_{k\alpha}^+, b_{k'\alpha'}^+] = 0\). When describing an isotropic medium, it is convenient to choose one of the polarization vectors directed along the wave vector: \( e(k, 3) = \hat{i}(k/k) = \mathbf{m} \). The other two polarization vectors with \( \alpha = 1, 2 \) lie in a plane perpendicular to the wave vector. With this in mind, the approximating Hamiltonian \([\mathbf{R}]\) can be written in the diagonal form

\[ H_S = \sum_k \left( 2 \hbar \omega_{kt} b_{k\alpha}^+ b_{kt} + \hbar \omega_{kt} b_{k\alpha}^+ b_{kt} \right) + \sum_k \left( \hbar \omega_{kt} + \frac{1}{2} \hbar \omega_{kt} \right) + V \varepsilon_0. \]  

(13)

Here phonons with the transverse polarization \((\alpha = 1, 2)\) are denoted by the single index \( t \), and phonons with the longitudinal polarization \((\alpha = 3)\) are denoted by the index \( l \). It is also taken into account that the transverse phonons have two degrees of freedom. As a result of reducing the Hamiltonian to the diagonal form \([\mathbf{L}]\), we find the phonon dispersion laws \( \omega_{kt} = c_t k, \omega_{kl} = c_l k \), where the velocities of the transverse and longitudinal phonons are given by the well-known expressions \([\mathbf{J}]\):

\[ c_t = \sqrt{\frac{\mu}{\rho}}, \quad c_l = \sqrt{\frac{\lambda + 2 \mu}{\rho}}. \]  

(14)

In the following we will calculate the average quantities by means of the statistical operator

\[ \hat{\rho} = \exp(\beta (F - H_S)), \]  

(15)

where \( \beta = 1/T \) is the inverse temperature. The normalization condition \( \text{Sp} \hat{\rho} = 1 \) leads to the formula for the free energy in the self-consistent field model

\[ F = V \varepsilon_0 + \sum_k \left( \hbar \omega_{kt} + \frac{1}{2} \hbar \omega_{kl} \right) + 2T \sum_k \ln(1 - e^{-\beta \hbar \omega_{kt}}) + T \sum_k \ln(1 - e^{-\beta \hbar \omega_{lt}}). \]  

(16)

The energy of the undeformed state \( \varepsilon_0 \) in such a model is found from the condition of equality of the averages for the exact and approximating Hamiltonians \( \langle H \rangle = \langle H_S \rangle \), or, equivalently, from the condition \( \langle H_C \rangle = 0 \). This gives

\[ \varepsilon_0 = \frac{1}{2V} \int \left[ (\lambda_{abj} - \tilde{\lambda}_{abj}) \left( \nabla_i u_a \nabla_j u_b \right) \right] d\mathbf{r}. \]  

(17)
Calculating the average in (17) by means of the statistical operator (15), we arrive at the following formula

$$\varepsilon_0 = \frac{\hbar}{4\rho V} \left( \lambda_{aibj} - \tilde{\lambda}_{aibj} \right) \sum_k k_i k_j \left[ A_{kl} \delta_{ab} + (A_{kl} - A_{kt}) n_a n_b \right],$$

where the quantities

$$A_{kt} = \frac{1 + 2f_{kt}}{\omega_{kt}}, \quad A_{kl} = \frac{1 + 2f_{kl}}{\omega_{kl}}$$

are expressed through the distribution functions of the longitudinal $f_{kt} = \left[ \exp \beta \hbar \omega_{kt} - 1 \right]^{-1}$ and transverse $f_{kl} = \left[ \exp \beta \hbar \omega_{kl} - 1 \right]^{-1}$ phonons. The sums over wave vectors entering into (18), after passing from summation to integration and integrating over angles, can be represented in the form

$$\sum_k k_i k_j A_{kt} = \frac{V}{6\pi^2} \delta_{ij} I_t, \quad \sum_k k_i k_j n_a n_b (A_{kl} - A_{kt}) = \frac{V}{30\pi^2} (\delta_{ij} \delta_{ab} + \delta_{ia} \delta_{jb} + \delta_{ib} \delta_{ja}) (I_t - I_i),$$

where

$$I_t = \int_0^{k_D} dk k^4 \frac{(1 + 2f_{kt})}{\omega_{kt}} = \frac{k_D^4 D}{4 c_t} \Phi \left( \frac{\Theta_t}{T} \right), \quad I_i = \int_0^{k_D} dk k^4 \frac{(1 + 2f_{kl})}{\omega_{kl}} = \frac{k_D^4 D}{4 c_t} \Phi \left( \frac{\Theta_i}{T} \right).$$

Here $\Theta_t = \hbar c_t k_D$, $\Theta_i = \hbar c_i k_D$ are the Debye energies defined through the velocities of the transverse and longitudinal phonons, $k_D = (6\pi^2 N/V)^{1/3}$ is the Debye wave number, $N$ is the particle number. In (21) there is defined the function

$$\Phi(x) = 1 + (8/3x) D(x), \quad D(x) = \frac{3}{x^3} \int_0^x \frac{z^3 dz}{e^z - 1}.$$ (22)

As a result, we find

$$\varepsilon_0 = \frac{3NT}{16V} \left[ \left( \frac{\lambda_t}{x_t} - x_t \right) \Phi(x_t) + 2 \left( \frac{\lambda_i}{x_t} - x_t \right) \Phi(x_t) \right],$$

where for brevity we introduce the following notation:

$$x_t \equiv \frac{\Theta_t}{T} = \frac{\hbar c_t k_D}{T}, \quad x_i \equiv \frac{\Theta_i}{T} = \frac{\hbar c_t k_D}{T}, \quad \lambda_t \equiv \frac{\hbar^2 k_D^2}{15\rho T^2} (2\lambda_B + \lambda_A), \quad \lambda_i \equiv \frac{\hbar^2 k_D^2}{30\rho T^2} (3\lambda_B - \lambda_A).$$

Here $\lambda_A \equiv \lambda_{aiii}$, $\lambda_B \equiv \lambda_{iiai}$ are the invariants of the crystal elastic moduli tensor. As a result, taking into account (10), we obtain the free energy as a function of temperature, volume, number of particles and two parameters $x_t, x_i$:

$$F = \frac{3NT}{16} \left[ \Phi(x_t) \left( \frac{\lambda_t}{x_t} - x_t \right) + 2 \Phi(x_t) \left( \frac{\lambda_i}{x_t} - x_t \right) \right] + \frac{3NT}{8} (x_t + 2x_i) + \frac{NT}{3} \left[ 3 \ln(1 - e^{-x_t}) - D(x_t) \right] + \frac{2NT}{3} \left[ 3 \ln(1 - e^{-x_i}) - D(x_i) \right].$$

(25)

For arbitrary values of the parameters $x_t, x_i$, the free energy (25) describes a system in a state of incomplete thermodynamic equilibrium. The equilibrium values of these parameters and, consequently, the optimal values of the elastic coefficients of a model isotropic medium $\lambda$ and $\tilde{\mu}$ should be found from the conditions of the extremum of the free energy (25):

$$\frac{\partial F}{\partial x_t} = 0, \quad \frac{\partial F}{\partial x_i} = 0.$$ (26)

As a result, we obtain the equations:

$$\left( \frac{\lambda_A}{x_A^2} - 1 \right) [x_A \Phi'(x_A) - \Phi(x_A)] = 0,$$

(27)
where $\alpha = l, t$. The function in the second brackets does not vanish in the field of its definition, so that the relation $x^2_\alpha = \lambda_\alpha$ should hold, or in more detail:

$$c_l^2 = \frac{1}{15\rho}(2\lambda + \lambda_0), \quad c_t^2 = \frac{1}{30\rho}(3\lambda_0 - \lambda_0).$$

(28)

Hence, according to (14), formulas for the Lame coefficients of an isotropic medium that model a crystal have the form

$$\lambda = \frac{1}{15}(2\lambda_0 - \lambda_0), \quad \mu = \frac{1}{30}(3\lambda_0 - \lambda_0).$$

(29)

These formulas coincide with the formulas (33) obtained on the basis of another criterion introduced in [2]. As was also shown here, such approximation proves to be valid at an arbitrary temperature. Here are the approximating formulas for the bulk modulus $\tilde{K}$, the Young modulus $\tilde{E}$ and the Poisson ratio $\tilde{\sigma}$:

$$\tilde{K} = \frac{1}{9}\lambda_0, \quad \tilde{E} = \frac{\lambda_0 (3\lambda_0 - \lambda_0)}{3(3\lambda_0 + \lambda_0)}, \quad \tilde{\sigma} = \frac{2\lambda_0 - \lambda_0}{3\lambda_0 + \lambda_0}.$$

(30)

Note that the bulk modulus of the approximating continuous medium is determined by the single invariant of a crystal $\lambda_0 \equiv \lambda_{1111}$.

III. THE TWO-PARAMETER DEBYE MODEL

The Debye model [2] describes the thermodynamic properties of an isotropic elastic medium. The elastic properties of such a medium are characterized by two elastic moduli, which can be chosen, for example, as the Lame coefficients $\lambda$ and $\mu$ or any two other moduli [50]. Accordingly, there are two sound modes corresponding to the longitudinal and transverse vibrations and the two velocities $c_l$ and $c_t$ of propagation of such waves [14]. In the standard Debye theory [2] an additional simplification is used: instead of two velocities, the average velocity of sound vibrations $c_D$ is introduced, which is defined by the relation:

$$\frac{1}{c_D^2} + \frac{1}{\rho} = 2 + \frac{1}{c_l^2} + \frac{1}{c_t^2} = \frac{\rho^{3/2}}{2} + \frac{1}{(\lambda + 2\mu)^{3/2}}.$$

(31)

A consequence of this approximation is that an isotropic elastic medium is characterized by a single parameter $\Theta_D = \hbar c_D k_D$ – the Debye energy, and the heat capacity proves to be a function of only the ratio $\Theta_D/T$. The definition (31) means that the inverse cubes of velocities are actually averaged. However, one can define the average velocity in another way, for example, by the relation

$$c_0^2 = \frac{1}{3}(2c_l^2 + c_t^2) = \frac{\lambda + 4\mu}{3\rho},$$

(32)

which arises in an approach based on the description of interacting phonons in the self-consistent field model [6, 7]. The definition (32) seems more natural, since for $\mu \to 0$ and $c_l \to 0$ from (31) it follows that $c_D \to 0$ as well, while the definition (32) gives in this case a finite value of the average velocity $c_0$. The ratio of the average velocities defined by the formulas (31) and (32) depends on the ratio of the Lame coefficients

$$\frac{c_0^2}{c_D^2} = \frac{1}{3^{2/3}}(4 + \lambda/\mu)^{2/3} \left[2 + \frac{1}{(2 + \lambda/\mu)^{3/2}}\right]^{2/3},$$

(33)

where $\lambda/\mu > -2/3$ [1]. The dependence of the velocities ratio $c_0/c_D$ on the ratio $\lambda/\mu$ is shown in Fig. 1. As the ratio $\lambda/\mu$ increases, the difference in the average velocities determined by the formulas (31) and (32) increases. The question may arise which averaging should be considered correct. If we consider the average velocity and the Debye energy as phenomenological parameters, then this question, apparently, is not fundamental. At the same time, it is obvious that the transition from the use of two parameters characterizing an elastic medium to a single parameter is not necessary, and it is more natural to construct a theory with taking into account both phonon velocities. In doing so the complication of the theory proves to be insignificant, and the question as to the way of introducing the average velocity does not arise at all. It can be expected that a theory with two Debye energies will sometimes describe more
Figure 1: Dependence of the ratio of the phonon average velocities \( c_0/c_D \), defined by the formulas (31) and (32), on the ratio of the Lame coefficients \( \lambda/\mu \).

subtle effects. In addition, it becomes possible to apply such a model for calculating crystals of various symmetries with the help of the elastic moduli, if we make use of the method of the approximating isotropic medium that was considered above.

In this section, we formulate the Debye model without using the averaging of the phonon velocity. It is natural to call such a model a two-parameter one. The usual Debye model will also be called one-parameter model. With an optimal choice of the phonon velocities (28), the free energy takes the form

\[
F = \frac{3N}{8}(\Theta_l + 2\Theta_t) + \frac{NT}{3}\left[3\ln(1 - e^{-\beta\Theta_l}) + D(\beta\Theta_l)\right] + \frac{2NT}{3}\left[3\ln(1 - e^{-\beta\Theta_t}) - D(3\beta\Theta_t)\right].
\] (34)

The entropy \( S = \partial F/\partial T \) and the energy \( E = F + TS \) are given by the formulas:

\[
S = -\frac{N}{3}\left[3\ln(1 - e^{-\beta\Theta_l}) - 4D(3\beta\Theta_l)\right] - \frac{2N}{3}\left[3\ln(1 - e^{-\beta\Theta_t}) - 4D(3\beta\Theta_t)\right],
\] (35)

\[
E = \frac{3N}{8}(\Theta_l + 2\Theta_t) + NTD(3\beta\Theta_l) + 2NTD(3\beta\Theta_t).
\] (36)

The heat capacity \( C_V = T(\partial S/\partial T) \), with taking into account (35), is determined by the formula

\[
C_V = N\left[4D(3\beta\Theta_l) - \frac{3\beta\Theta_l}{e^{3\beta\Theta_l} - 1}\right] + 2N\left[4D(3\beta\Theta_t) - \frac{3\beta\Theta_t}{e^{3\beta\Theta_t} - 1}\right].
\] (37)

Here, the Debye energies are defined in the same way as above \( \Theta_l = \hbar c_l k_D, \Theta_t = \hbar c_t k_D \), but now the velocities are expressed through the invariants of the elastic moduli tensor of a crystal by the optimal relations (28). If in the formulas (34) – (37) the Debye energies are formally set equal, then we obtain the corresponding formulas of the standard Debye theory. However, since the inequality \( c_l/c_t > \sqrt{4/3} \) holds in an isotropic medium, the same inequality \( \Theta_l/\Theta_t > \sqrt{4/3} \) holds as well for the Debye energies, and therefore these energies cannot be equal.

Since it is more common to use one energy instead of two Debye energies, let us introduce instead of the two parameters of the energy dimension \( \Theta_l, \Theta_t \), the single average Debye energy \( \Theta \) and one dimensionless parameter, for which it is convenient to choose the angle \( \chi \):

\[
\Theta^2 = \frac{1}{3}(2\Theta_l^2 + \Theta_t^2), \quad \sin\chi = \sqrt{\frac{2}{3}}(\Theta_l/\Theta_t), \quad \cos\chi = \frac{1}{\sqrt{3}}(\Theta_l/\Theta_t), \quad \tan\chi = \frac{\Theta_l}{\Theta_t}.
\] (38)

The average Debye energy \( \Theta \) determined in such a way corresponds to the averaging of velocities (32). Owing to the given above inequality \( \Theta_l/\Theta_t > \sqrt{4/3} \) for the ratio of the Debye energies, the tangent of the angle \( \chi \) introduced in (38) takes the maximum value at the angle \( \chi_m \), which is determined by the condition \( \tan\chi_m = \sqrt{3/2} \), whence \( \chi_m = 0.886 \)
and, accordingly, $\cos \chi_m = \sqrt{2/5}$, $\sin \chi_m = \sqrt{3/5}$. Thus, the angle can vary within the range $0 \leq \chi < \chi_m$. Here are also given the expressions for the parameters defined in (38) in terms of the invariants of the crystal elasticity tensor:

$$\Theta^2 = \frac{\hbar^2 k_D^2}{9 \rho} \lambda_B, \quad \sin^2 \chi = \frac{(3 \lambda_B - \lambda_A)}{5 \lambda_B}, \quad \cos^2 \chi = \frac{(2 \lambda_B + \lambda_A)}{5 \lambda_B}. \quad (39)$$

Let us consider in more detail the behavior of the heat capacity (37) with temperature. As is known, in the standard Debye theory the heat capacity is a universal function of the ratio $T/\Theta_D$ [5]. According to this model the heat capacities of all bodies being in corresponding states, i.e. having the same $T/\Theta_D$, should be the same. For real bodies this law, obviously, is not satisfied. In the proposed two-parameter model, as we see, the law of the corresponding states does not hold, since the heat capacity also depends on the parameter $\chi$ which is different for different bodies [39]. At high temperatures $T \gg \Theta$, the formula for the heat capacity has visually the same form as in the usual theory

$$C_V = 3N \left[1 - \frac{1}{20} \left(\frac{\Theta}{T}\right)^2\right]. \quad (40)$$

Here, the average Debye energy is determined by the relations (38), (39) and the dependence on the parameter $\chi$ falls out in this approximation. At low temperatures $T \ll \Theta$, the same as in the usual theory, the cubic dependence on temperature is preserved

$$C_V = \frac{12}{5} \pi^4 N f(\chi) \left(\frac{T}{\Theta}\right)^3, \quad (41)$$

but in this case the coefficient also depends on the parameter $\chi$ through the function

$$f(\chi) = \frac{1}{3^{5/2}} \left(\frac{1}{\cos^3 \chi} + \frac{2^{5/2}}{\sin^3 \chi}\right) \quad (42)$$

and turns out to be different for different substances. The influence of the second parameter $\chi$ is manifested most significantly at low temperatures. At high temperatures, the main difference of the two-parameter theory consists in that the average Debye energy (38), (39) is defined differently here and, moreover, it is related to the invariants of the elasticity tensor of a crystal of a certain symmetry [39].

Figure 2: The densities of phonon states $g(\omega) (2\pi^2 c_0/k_D^2)$ as functions of the frequency $\omega = \omega/c_0 k_D$; 1 – the one-parameter model, 2 – the two-parameter model. The calculation is made for $\lambda/\mu = 2$. 
Let us also give an expression for the density of phonon states, which in this case is determined by the formula

\[ g(\omega) = \int \frac{d\mathbf{k}}{(2\pi)^3} \left[ \delta(\omega - c_l k) + 2\delta(\omega - c_t k) \right]. \]  

(43)

As a result, we have

\[ g(\omega) \frac{2\pi}{2} = \begin{cases} \omega^2 \left( \frac{1}{c_l^3} + \frac{2}{c_t^3} \right), & \omega < k_D c_t, \\ \omega^2 / c_l^3, & k_D c_t < \omega < k_D c_l, \\ 0, & \omega > k_D c_l. \end{cases} \]  

(44)

The form of the density of phonon states is shown in Fig. 2. Due to the presence of the two phonon branches in the function \( g(\omega) \), a jump appears at the frequency \( \omega = k_D c_t \) and, therefore, the structure of the density of states proves to be more complicated than in the standard model. As is known [8, 9], there are van Hove features in the density of phonon states of real crystals, so that the two-parameter model is closer in this respect to real crystals.

IV. CRYSTALS OF THE CUBIC SYSTEM

As an example, we consider the application of the two-parameter Debye theory to crystals of the cubic system, which are most close to an isotropic medium and are characterized by three elastic moduli. In this case the two invariants are given by the expressions \( \lambda_A = 3c_{11} + 6c_{12}, \lambda_B = 3c_{11} + 6c_{44} \) in terms of three elastic moduli of the cubic crystal in the standard notation [2], and the approximating Lame coefficients are:

\[ \tilde{\lambda} = \frac{1}{5}(c_{11} + 4c_{12} - 2c_{44}), \quad \tilde{\mu} = \frac{1}{5}(c_{11} - c_{12} + 3c_{44}). \]  

(45)

The values of these quantities for some cubic crystals at low temperatures are shown in Table 1.

Table 1: The values of the adiabatic elastic moduli of tungsten, copper and lead at low temperatures [8], the invariants \( \lambda_A, \lambda_B \) and the approximating Lame coefficients (45) (in units of \( 10^{12} \) dyn/cm).

| Crystal | \( c_{11} \) | \( c_{12} \) | \( c_{44} \) | \( \lambda_A \) | \( \lambda_B \) | \( \lambda \) | \( \tilde{\mu} \) |
|---------|--------|--------|--------|--------|--------|--------|--------|
| W       | 5.326  | 2.049  | 1.631  | 28.272 | 25.764 | 2.052  | 1.634  |
| Cu      | 1.762  | 1.249  | 0.818  | 12.78  | 10.194 | 1.024  | 0.593  |
| Pb      | 0.555  | 0.454  | 0.194  | 4.389  | 2.829  | 0.397  | 0.137  |

Table 2 shows the density, the transverse and longitudinal phonon velocities calculated using the data of Table 1 and the average velocities determined by the formulas (31) and (32).

Table 2: The values of the density \( \rho \) (g/cm\(^3\)), transverse \( c_t \) and longitudinal \( c_l \) velocities (28) and also average velocities \( c_D \) (31) and \( c_0 \) (32) (in units of \( 10^6 \) cm/s).

| Crystal | \( \rho \) | \( c_t \) | \( c_l \) | \( c_D \) | \( c_0 \) |
|---------|--------|--------|--------|--------|--------|
| W       | 1.551  | 0.292  | 0.524  | 0.225  | 0.385  |
| Cu      | 9.018  | 0.257  | 0.495  | 0.199  | 0.355  |
| Pb      | 11.60  | 0.109  | 0.240  | 0.085  | 0.165  |

Table 3 gives the Debye wave number \( k_D \), parameter \( \chi \) [33], value of the function \( f(\chi) \) (42) and Debye temperatures calculated by the formulas \( \Theta_t = \hbar c_t k_D, \Theta_l = \hbar c_t k_D, \Theta_D = \hbar c_D k_D, \Theta = \Theta_0 = \hbar c_0 k_D \), where the velocity values are taken from Table 2, as well as the experimental low-temperature value of the Debye temperature \( \Theta_{D\text{exp}} \) [8].

Table 3: The wave number \( k_D \) (in \( 10^8 \) cm\(^{-1}\)), Debye temperatures in Kelvin degrees (K).

| Crystal | \( k_D \) | \( \Theta_t \) | \( \Theta_l \) | \( \Theta = \Theta_0 \) | \( \Theta_D \) | \( \Theta_{D\text{exp}} \) | \( \chi \) | \( f(\chi) \) |
|---------|--------|--------|--------|----------------|--------|----------------|--------|--------|
| W       | 1.551  | 346    | 621    | 456            | 266    | 400            | 0.665  | 1.676  |
| Cu      | 1.717  | 337    | 650    | 466            | 261    | 343            | 0.632  | 1.882  |
| Pb      | 1.263  | 105    | 232    | 159            | 82     | 105            | 0.569  | 2.427  |
As we can see, the Debye temperatures $\Theta_D$ calculated in the standard one-parameter model from the values of elastic constants prove to be much lower than the measured Debye temperatures $\Theta_{Dexp}$. The calculation of the Debye temperatures in the proposed two-parameter model from the values of elastic constants gives values greater than $\Theta_{Dexp}$. Introducing to the theory the second parameter most appreciably affects the calculation of thermodynamic quantities at low temperatures. Figure 3 shows the calculated temperature dependencies of the heat capacity of copper at low temperatures. The calculations are performed using the approximated values of the elastic moduli for the one-parameter (curve 1) and two-parameter (curve 2) models. Curve 3 is plotted using the experimental value of the Debye temperature. The relative error $\delta = (C_V - C_{Vexp})/C_{Vexp}$ in the one-parameter model for copper is $\delta_1 = 1.27$. In the two-parameter model the discrepancy with the experimental value proves to be much smaller: $\delta_2 = 0.25$. The values of these deviations for tungsten are $\delta_1 = 2.7$, $\delta_2 = 0.57$, and for lead $\delta_1 = 1.1$, $\delta_2 = 0.3$. As seen, the calculation in the one-parameter model gives a greater discrepancy with experimental data. At the same time, the two-parameter model leads to much better agreement with experiment and can be used for theoretical estimates of the Debye temperature from the values of the crystal elastic moduli.

![Graph](image)

Figure 3: The temperature dependence of the heat capacity of copper at low temperatures: 1 – the calculation through the approximated elastic moduli in the one-parameter model, 2 – the similar calculation in the two-parameter model, 3 – the dependence in the standard model, where the Debye temperature is considered as a phenomenological parameter. The Debye temperature for Cu $\Theta_{Dexp} = 343$ K.

V. CONCLUSIONS

It is shown that the proposed earlier method [2] of describing the elastic properties of crystals on the basis of a comparison with an isotropic medium follows from the requirement of the maximal closeness of the free energies of a crystal and an isotropic medium. In this work it is proposed a model of an isotropic elastic medium which is similar to the standard Debye model and in which the existence of both transverse and longitudinal phonons is taken into account. In this model, besides the Debye energy, an additional parameter is introduced, so that the law of corresponding states characteristic of the usual Debye theory ceases to be fulfilled. The calculation of the heat capacity at low temperatures using the approximated elastic moduli leads to much better agreement with experimental data than for the usual theory using the average phonon velocity.

There are two extreme points of view on the Debye model. Often it is given an unduly general meaning to the Debye model and, when processing experimental data, observable quantities are adjusted to the relations of this theory assuming that the Debye energy depends on temperature. The opposite point of view consists in that the relations of the Debye theory are considered as crude interpolation formulas [1, 9]. The Debye model, of course, is a quite approximate and simple (in what its value consists) model of the solid body, but, in our opinion, its value is not limited only to the possibility of constructing a single interpolation formula that would correctly describe the behavior of a body in the limit of low and high temperatures. This model, as shown above, allows further development and, in particular, generalization with taking into account the interaction of phonons [6, 7], and also can be extended to describe surface phenomena in solids.
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