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Temperature dependence of Debye frequency and Grüneisen parameter in the low temperature range

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The Debye temperature (Θ) is an important characteristic of a crystal and the Θ values for specific substances are presented in many reference books and monographs. However, for many substances, the experimentally determined Θ value changes with temperature (T). It is shown that in the presence of a functional dependence $\Theta(T)$, the expressions for entropy and isochoric heat capacity should include terms with the first and second derivatives of the $\Theta(T)$ function with respect to temperature. Therefore, for the fulfillment of the third law of thermodynamics for an n-dimensional crystal, the function $\Theta(T)$ and the temperature dependence of the Grüneisen parameter $\gamma(T)$ at low temperatures must change according to the dependence $(T/\Theta_0)^{n+1}$. At this, the Θ_0 value differs from the Θ_{0s} value, which was determined from the experimental temperature dependence of the heat capacity, without taking into account the dependence $\Theta(T)$. It is shown that if the $\Theta(T)$ function decreases, then the $\gamma(T)$ function increases with increasing temperature from the values $\Theta_0 > \Theta_{0s}$ and $\gamma_0 > \gamma_{0s}$, respectively. At average temperatures, the $\Theta(T)$ function has a minimum, and the $\gamma(T)$ function has a maximum. If the $\Theta(T)$ function increases from $\Theta_0 < \Theta_{0s}$ to a maximum, then the $\gamma(T)$ function decreases from $\gamma_0 < \gamma_{0s}$ to a minimum. A method for determining the temperature dependence of the $\Theta(T)$ function was proposed.

Keywords: entropy, isochoric heat capacity, Debye temperature, Grüneisen parameter, graphene.

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Introduction

The Debye temperature (Θ) is an important parameter that determines various properties of a substance. The Θ value also approximates the temperature limit below which quantum effects begin to affect. Therefore, much attention is paid to the determination of the Θvalue in both experimental and theoretical studies.

In the traditional Debye theory, it is assumed that the Θ value does not dependent on temperature (T) [1,2]. Then the expressions for calculating free energy (F_D), entropy ($S_D = -(\partial F_D/\partial T)_V$) and isochoric heat capacity ($C_D = T(\partial S_D/\partial T)_V = -T(\partial^2 F_D/\partial T^2)_V$) of an n-dimensional molecular crystals are obtained in the following form

$$f_D^* = \frac{F_D}{nN_A n_i k_B} = \frac{n\Theta}{2(n+1)} + T\ln\left[1-\exp\left(-\frac{\Theta}{T}\right)\right] - \frac{T}{n}\mathrm{Deb}_n\left(\frac{\Theta}{T}\right), \tag{1}$$

$$s_D^* = \frac{S_D}{nN_A n_i k_B} = -\left(\frac{\partial f_D^*}{\partial T}\right)_V = -\ln\left[1-\exp\left(-\frac{\Theta}{T}\right)\right] + \frac{(n+1)}{n}\mathrm{Deb}_n\left(\frac{\Theta}{T}\right), \tag{2}$$

$$c_D^* = \frac{C_D}{nN_A n_i k_B} = -T\left(\frac{\partial^2 f_D^*}{\partial T^2}\right)_V = (n+1)\,\mathrm{Deb}_n\left(\frac{\Theta}{T}\right) - \frac{n\left(\frac{\Theta}{T}\right)}{\exp\left(\frac{\Theta}{T}\right)-1}. \tag{3}$$

Here N_A is the Avogadro number, n_i is the number of ions (or atoms) in a molecule, k_B is the Boltzmann constant, V is the crystal volume, $n = 1, 2, 3$, $\mathrm{Deb}_n(x)$ is the Debye function for an n-dimensional crystal, which has the form [3]:

$$\mathrm{Deb}_n(x) = \frac{n}{x^n}\int_0^x \frac{t^n}{[\exp(t)-1]}\,dt. \tag{4}$$

At low temperatures, the $\mathrm{Deb}_n(x)$ function can be transformed to the form

$$\mathrm{Deb}_n(x \gg 1) \cong \frac{nA_n}{x^n} - n\exp(-x) \cong \frac{nA_n}{x^n}, \tag{5}$$

where $A_n = n!\,\xi(n+1)$, $\xi(n+1)$ is the Riemann zeta function [3]: $\xi(2) = \pi^2/6$, $\xi(3) = 1.202057$, $\xi(4) = \pi^4/90$, i.e. $A_1 = \pi^2/6$, $A_2 = 2.404114$, $A_3 = \pi^4/15$.

The Θ value for specific substances, experimentally determined based on the temperature dependence of the heat capacity under the assumption of independence of Θ from T, are presented in many reference books and monographs. At the same time, many substances show a dependence of the Θ value on the temperature [1,2,4–11]. If we take into account the presence of such a dependence, then the expressions $(2)-(3)$ will contain derivatives of the $\Theta(T)$ function in temperature and will have a more complex form [12]:

$$s^* = \frac{S}{nN_A n_i k_\mathrm{B}} = s_D^* - \left[\frac{n}{2(n+1)} + \left(\frac{T}{\Theta}\right)\mathrm{Deb}_n\left(\frac{\Theta}{T}\right)\right] \times \left(\frac{\partial\Theta}{\partial T}\right)_V, \tag{6}$$

$$c^* = \frac{C}{nN_A n_i k_\mathrm{B}} = c_D^*\left[1 - \left(\frac{T}{\Theta}\right)\left(\frac{\partial\Theta}{\partial T}\right)_V\right]^2 - \left[\frac{n}{2(n+1)} + \left(\frac{T}{\Theta}\right)\mathrm{Deb}_n\left(\frac{\Theta}{T}\right)\right] T\left(\frac{\partial^2\Theta}{\partial T^2}\right)_V, \tag{7}$$

where S and C is the entropy and isochoric heat capacity of a substance in which the Θ value is found to depend on temperature.

These expressions have the following form for the low temperature region $(T \ll \Theta(T))$

$$s_{low}^* = \left(\frac{S}{nN_A n_i k_\mathrm{B}}\right)_{low} \cong s_{D\,low}^* - \frac{n}{2(n+1)}\left(\frac{\partial\Theta}{\partial T}\right)_V, \tag{8}$$

$$c_{low}^* = \left(\frac{C}{nN_A n_i k_\mathrm{B}}\right)_{low} \approx c_{D\,low}^*\left[1 - \frac{T}{\Theta}\left(\frac{\partial\Theta}{\partial T}\right)_V\right]^2 - \frac{n}{2(n+1)} T\left(\frac{\partial^2\Theta}{\partial T^2}\right)_V. \tag{9}$$

Here the functions $s_{D\,low}^*$ and $c_{D\,low}^*$ have the traditional Debye form [1,2]:

$$s_{D\,low}^* \cong \frac{(n+1)}{n}\mathrm{Deb}_n\left(\frac{\Theta}{T} \gg 1\right) = (n+1)A_n\left(\frac{T}{\Theta(T)}\right)^n, \tag{10}$$

$$c_{D\,low}^* \cong (n+1)\,\mathrm{Deb}_n\left(\frac{\Theta}{T} \gg 1\right) = (n+1)nA_n\left(\frac{T}{\Theta(T)}\right)^n. \tag{11}$$

It can be seen from (9) that if the Θ parameter in the low temperature region has a functional dependence on temperature, then the $\Theta(T)$ value should be determined from the experimental dependence $c^*(T)_{low}$ using a differential equation. However, even today, the $\Theta(T)$ value is determined using the power equation (11) [1,2,4–11].

At low temperatures, the $\Theta(T)$ function should have such a dependence that (8) and (9) satisfy the third law of thermodynamics in Planck's statement

$$\lim_{T\to 0\,\mathrm{K}} \frac{S}{nN_A n_i k_\mathrm{B}} = 0, \quad \lim_{T\to 0\,\mathrm{K}} \frac{C}{nN_A n_i k_\mathrm{B}} = 0. \tag{12}$$

This imposes certain restrictions on the functional dependency $\Theta(T)$. These constraints are studied in this paper and a correct dependence is obtained for the $\Theta(T)$ function in the low temperature region.

1. Calculating method and results

Since in most cases the experimentally determined dependence $\Theta(T)$ decreases with increasing temperature from $\Theta_0 = \Theta(T = 0\,\mathrm{K})$ [1,2,4–11], we assume the formula of the folllowing form for the $\Theta(T)$ function at low temperatures

$$\Theta(T)_{low} = \Theta_0\left[1 - \chi_n\left(\frac{T}{\Theta_0}\right)^k\right], \tag{13}$$

where χ_n is a numerical coefficient.

Then from $(8)-(11)$, limiting to linear terms in $(T/\Theta_0)^n$ with $T \ll \Theta_0$, it is easy to obtain

$$s_{low}^* \cong s_{D\,low}^* - \frac{n}{2(n+1)}\left(\frac{\partial\Theta}{\partial T}\right)_V = (n+1)A_n\left(\frac{T}{\Theta_0}\right)^n + \frac{n}{2(n+1)}k\chi_n\left(\frac{T}{\Theta_0}\right)^{k-1}, \tag{14}$$

$$c_{low}^* \cong c_{D\,low}^* - \frac{n}{2(n+1)} T\left(\frac{\partial^2\Theta}{\partial T^2}\right)_V = (n+1)nA_n\left(\frac{T}{\Theta_0}\right)^n + \frac{n}{2(n+1)}k(k-1)\chi_n\left(\frac{T}{\Theta_0}\right)^{k-1}. \tag{15}$$

It can be seen from (14) and (15) that for any χ_n, the functions s_{low}^* and c_{low}^* are zero at $T = 0\,\mathrm{K}$. However, in order to comply with the dependency $c_{low}^* \propto (T/\Theta_0)^n$, the condition $k \geq n+1$ must be met. In addition, the following condition must be met for $s_{low}^* \geq 0$ and $c_{low}^* \geq 0$ to be satisfied with $\chi_n < 0$

$$\frac{2(n+1)^2}{nk}A_n\left(\frac{T}{\Theta_0}\right)^{n+1-k} \geq -\chi_n = |\chi_n| > 0. \tag{16}$$

It follows from (16) that it is necessary to assume $k = n+1$ for the $\chi_n < 0$ value to be independent of temperature. Also, it follows from (16) with $\chi_n < 0$ and $k > n+1$ that the functions s_{low}^* and c_{low}^* have maxima for $T_\mathrm{max}/\Theta_0 > 0$, after which the functions s_{low}^* and c_{low}^* will decrease with the increase of T/Θ_0. Since the presence of these maxima contradicts the experiments, we must assume $k = n+1$. The values of the maxima are easily found from (14) and (15):

$$\frac{T_{\mathrm{max}(s)}}{\Theta_0} = \left[\frac{2(n+1)^2A_n}{k(k-1)|\chi_n|}\right]^{1/[k-(n+1)]},$$

$$\frac{T_{\mathrm{max}(c)}}{\Theta_0} = \left[\frac{2(n+1)^2nA_n}{k(k-1)^2|\chi_n|}\right]^{1/[k-(n+1)]}. \tag{17}$$

It can be seen from (17) that in order for the temperatures of the maxima to coincide, i.e. to meet the condition: $T_{\mathrm{max}(s)} = T_{\mathrm{max}(c)}$, $k = n+1$ must also be satisfied. At the same time, the values of the maxima go to infinity, i.e. become unattainable. Thus, it can be argued that for an

n-dimensional crystal, the parameters included in (13) must satisfy the conditions

$$k = n + 1, \quad \chi_n > -\frac{2(n+1)A_n}{n}. \tag{18}$$

An expression for the Grüneisen parameter in the following form can be obtained from the dependence (13)

$$\gamma(T)_{low} = -\left(\frac{\partial \ln \Theta(T)_{low}}{\partial \ln V}\right)_T$$

$$= \gamma_0 + \frac{\chi_n\left[(n+1)\gamma_0 + \left(\frac{\partial \ln \chi_n}{\partial \ln V}\right)_T\right]\left(\frac{T}{\Theta_0}\right)^{n+1}}{\left[1 - \chi_n\left(\frac{T}{\Theta_0}\right)^{n+1}\right]}$$

$$\cong \gamma_0 + \chi_n[(n+1)\gamma_0 - \lambda_0]\left(\frac{T}{\Theta_n}\right)^{n+1}. \tag{19}$$

The following designations are introduced here:

$$\gamma_0 = -\left(\frac{\partial \ln \Theta_0}{\partial \ln V}\right)_{T=0\,\mathrm{K}}, \quad \lambda_n = -\left(\frac{\partial \ln \chi_n}{\partial \ln V}\right)_T. \tag{20}$$

The Grüneisen parameter determines the degree of increase in the Debye temperature during isothermal compression of the crystal. The λ_n parameter determines the degree of increase of the χ_n value in case of the isothermal compression of the crystal. It should be noted that there are two Grüneisen parameters in the literature (depending on the method of experimental determination): vibrational and thermodynamic [4,13–15]. The Grüneisen vibration parameter is determined by the change in the frequency of atomic vibrations (ω) in case of crystal compression: $\gamma = (\partial \ln \omega / \partial \ln V)_T$. The Grüneisen thermodynamic parameter is determined by the ratio of the isobaric coefficient of thermal expansion ($\alpha_p = (\partial \ln V / \partial T)_P$), the isothermal elastic modulus ($B_T = -V(\partial P / \partial V)_T$), volume ($V$) and isochoric heat capacity (C): $\gamma_{\mathrm{Th}} = \alpha_p B_T V / C$. It should be noted that this expression for γ_{Th} is incorrect in case of a presence of the temperature dependence $\Theta(T)$ [15]. This is due to the fact that, according to (7), the heat capacity will include terms with the first and second derivatives of the function $\Theta(T)$ in temperature, and the value $\alpha_p B_T = (\partial S / \partial V)_T$ will depend on the first derivative of the function $\Theta(T)$ in temperature. This leads to a difference between the values γ and γ_{Th}. Here we study the Grüneisen vibration parameter γ.

The dependence in (15) will correspond to the experimental one for $k = n + 1$, but the calculation of the Θ_0 value will need to be performed not from (11), but from the expression that follows from (15):

$$c^*_{low} \cong \left[(n+1)nA_n + \frac{n^2}{2}\chi_n\right]\left(\frac{T}{\Theta_0}\right)^n. \tag{21}$$

This leads to a correction in the Debye temperature calculated from (11) at $T = 0\,\mathrm{K}$. By equating the expressions for the heat capacities from (11) and (21), we can obtain

$$\Theta_0 \cong \Theta_{0s}\left[1 + \frac{n}{2(n+1)A_n}\chi_n\right]^{1/n}, \tag{22}$$

where Θ_{0s} is the value determined from the experimental values of the heat capacity without taking into account the dependence $\Theta(T)_{low}$, i.e. Θ_{0s} is calculated from the power equation (11).

The expression for the Grüneisen parameter will have the following form from Eq. (22)

$$\gamma_0 = -\left(\frac{\partial \ln \Theta_0}{\partial \ln V}\right)_{T=0\,\mathrm{K}} = \gamma_{0s} + \frac{\chi_n \lambda_n}{2(n+1)A_n + n\chi_n}. \tag{23}$$

where γ_{0s} is the value of the Grüneisen parameter determined from the function $\Theta_{0s}(V)$, i.e. without taking into account the temperature dependence $\Theta(T)_{low}$:

$$\gamma_{0s} = -\left(\frac{\partial \ln \Theta_{0s}}{\partial \ln V}\right)_{T=0\,\mathrm{K}}.$$

Thus, the function $\Theta(T)_{low}$ decreases at $\chi_n > 0$ with increasing temperature (this follows from (13)), and the function $\gamma(T)_{low}$ increases (this follows from (19)). The function $\Theta(T)_{low}$ decreases from $\Theta_0 > \Theta_{0s}$ (this inequality follows from (22)), and the function $\gamma(T)_{low}$ increases from $\gamma_0 > \gamma_{0s}$ (this follows from (23)). Since at high temperatures ($T \gg \Theta_0$) the function $\Theta(T)$ does not go into the range of negative values (as it should be following (13)), but has a positive value comparable to Θ_0 (as it follows from the experimental data), the function $\Theta(T)$ should have a minimum in the range of average temperatures. The function $\gamma(T)$ at high temperatures does not go to infinity (as it should be, following (19)), and has a finite value, therefore, the function $\gamma(T)$ should have a maximum in the range of average temperatures. It should be noted that our formulas do not imply the presence of these extremes, since these formulas are obtained under the condition $T \ll \Theta_0$. Therefore, it is impossible to estimate the position of these extremes from these formulas. However, the existence of these extremes follows from the physical definition of the functions $\Theta(T)$ and $\gamma(T)$, according to which these functions must have a finite positive value. The presence of extremes has also been pointed out in many papers, for example, in Res. [1,2,4,5,10].

At $\chi_n < 0$, the picture changes to the opposite: the function $\Theta(T)_{low}$ increases with increasing temperature from $\Theta_0 < \Theta_{0s}$, and the function $\gamma(T)_{low}$ decreases from $\gamma_0 < \gamma_{0s}$. In both cases, the change in the functions $\Theta(T)_{low}$ and $\gamma(T)_{low}$ must be proportional to the dependence $(T/\Theta_0)^{n+1}$ for fulfillment of the third principle of thermodynamics in the form of (12). It should be noted that in the case of $\chi_n > 0$ and $k > n + 1$, or for $\chi_n = 0$, the functions $s^*(T)_{low}$ and $c^*(T)_{low}$ will follow Debye dependencies, and the values Θ_0 and γ_0 will match the values of Θ_{0s} and γ_{0s}, due to the disappearance of corrections to Debye dependencies in Eqs. (14) and (15). This is obvious in the case of $\chi_n = 0$. And in the case of $\chi_n > 0$ and $k > n + 1$, the second terms in (14) and (15) at T/Θ_0, close to zero, will be much smaller than the first terms, and therefore they can not take into account both Θ_0 values and γ_0 values in calculations.

Debye temperature values, which are determined from the heat capacity and the elastic properties of the crystal [16], and the χ_3 values calculated from them using Eq. (25)

Crystal	Θ_{0s}, K	Θ_0^{el}, K	χ_3
C-diam	2220	2252	0.7597
Si	645	655	0.8180
Ge	374	379	0.7039
3*C*-SiC	1080	1108	1.3821
c-BN	1850	1900	1.4424
AlN	825	903	5.3907
AlP	588	553	−2.9119
AlAs	417	411	−0.7368
ZnO	399.5	418.8	2.6330
ZnS	340	349	1.4119

The following method can be proposed to estimate the χ_n value. It is known that the Debye temperature can also be determined by the elastic modulus of a crystal $(B_T = -V(\partial P/\partial V)_T)$ [4,16–22]. However, the Θ_0^{el} value determined from the elastic modulus Θ_0^{el} differs from the value of the Debye temperature, which is determined from the temperature dependence of the isochoric heat capacity (Θ_{0s}), i.e. from Eq. (11). Since the calculation of the elastic modulus of a crystal does not use derivatives of free energy with respect to temperature, it can be assumed that the Θ_0^{el} value coincides with the Θ_0 value, or is very close to it. Then the χ_n value can be estimated from the expression that follows from (22):

$$\chi_n = \frac{2(n+1)A_n}{n}\left[\left(\frac{\Theta_0^{\mathrm{el}}}{\Theta_{0s}}\right)^n - 1\right]. \qquad (24)$$

For a three-dimensional crystal, (24) is transformed to the form

$$\chi_3 = \frac{8\pi^4}{45}\left[\left(\frac{\Theta_0^{\mathrm{el}}}{\Theta_{0s}}\right)^3 - 1\right] = 17.317\left[\left(\frac{\Theta_0^{\mathrm{el}}}{\Theta_{0s}}\right)^3 - 1\right]. \qquad (25)$$

The table shows the χ_3 values, which are calculated using (25) for some crystals. The Debye temperatures, which are determined from the heat capacity (Θ_{0s}) and the elastic properties (Θ_0^{el}) of the crystal at $T = 0\,\mathrm{K}$, are taken from Ref. [16, Table 4].

The table shows that in most cases the function $\Theta(T)_{low}$ decreases with increasing temperature from Θ_0^{el}. It should be noted that the values Θ_{0s} and Θ_0^{el}, as indicated in Ref. [16], have a certain range of variance, which is quite different from different authors. Therefore, the estimates of χ_3 from the table are also approximate. However, estimates of the $\Theta(T)_{low}$ function carried out by other, more complex methods in Res. [1,2,4–11] also indicate that the $\Theta(T)_{low}$ function decreases with increasing temperature for most of the studied substances. We also note that in Ref. [15] we proposed another method for estimating the χ_n value of single-component crystals based on the parameters of the paired interatomic potential. However, the method from (25), despite its simplicity, is also applicable to multicomponent crystals.

2. Discussion of the results

Unfortunately, not all dependencies obtained for the function $\Theta(T)_{low}$ satisfy the above conditions: incorrect dependencies have been obtained in many studies. For example, a quadratic dependence was obtained for three-dimensional crystals in Res. [8,16]: $\Theta(T)_{low} \propto T^2$, and a linear increase in the function $\Theta(T)_{low}$ with growth of T was obtained in Ref. [23]. The quadratic dependence for $\Theta(T)_{low}$ leads to a linear dependence of entropy and heat capacity on temperature in (8) and (9), and the linear dependence for $\Theta(T)_{low}$ leads to a violation of the third law of thermodynamics (12) for entropy.

A formula with six fitting constants was proposed for the function $\Theta(T)$ in Ref. [11]: „calorimetric Debye temperature", which has the form [11, Eq. (12)]:

$$\Theta_{cal}(T) = a_1\exp(-b_1T) + a_2[1 - \exp(-b_2T^2)] + c.$$

However, substituting this dependence into Eq. (8) leads to a violation of the third law of thermodynamics (12) due to the following relations:

$$\left(\frac{\partial\Theta_{cal}}{\partial T}\right)_V = -a_1b_1\exp(-b_1T) + a_2b_2zT^{z-1}\exp(-b_1T^2),$$

$$\lim_{T\to 0\,\mathrm{K}}\left(\frac{\partial\Theta_{cal}}{\partial T}\right)_V = -a_1b_1 \neq 0.$$

Recently, the Debye model has also been used to study the heat capacity of two-$(2D)$ [24,25] and one-dimensional $(1D)$ structures [26]. At the same time, a linear decrease in the function $\Theta(T)_{low}$ was obtained in Ref. [24] for the $2D$-layer of Ne with increasing temperature. A linear growth of the function $\Theta(T)_{low}$ with temperature increase was obtained in Ref. [25] for $2D$-graphene. However, for fulfillment of the third principle of thermodynamics in the form of (12), the change in the function $\Theta(T)_{low}$ for $2D$-structures should be proportional to the dependence of $(T/\Theta_0)^3$, and for $1D$-structures it should be proportional to $(T/\Theta_0)^2$. Using an incorrect dependence for the $\Theta(T)_{low}$ function can lead to incorrect temperature dependences of other crystal properties that are associated with this function.

In order to get rid of the problem of correctly accounting for the temperature dependence of the Debye temperature in theoretical models, we can follow a simple path, assuming (as Einstein and Debye did) that the function Θ depends only on density and does not change with an isochoric increase in temperature. This was done in

Res. [20–22,27,28], where the Θ value was calculated either from the elastic properties of the crystal [20–22], or from the parameters of the paired interatomic potential [27,28]. This method allowed both observing the third principle of thermodynamics and obtaining good agreement with experimental data.

Conclusion

If, at low temperatures, the Debye temperature for a n-dimensional crystal changes with temperature, then the $\Theta(T)$ values should be determined from the experimental dependence of $c^*(T)_{low}$ by solving the differential equation (7) or (9), and not from the power equation (11). In this case, the Grüneisen thermodynamic parameter should differ from the Grüneisen vibration parameter: $\gamma_{\text{Th}} \neq \gamma$.

For fulfillment of the third principle of thermodynamics, the function $\Theta(T)$ at low temperatures must change according to the dependence

$$\Theta(T)_{low} = \Theta_0[1 - \chi_n(T/\Theta_0)^{n+1}].$$

In this case, the Grüneisen parameter should vary depending on (19). To find the values of Θ_0 and χ_n, it is also possible to use a power equation that follows from Eqs. (15) and (18):

$$c^*(T)_{low} \cong c_D(T)^*_{low} + \frac{n^2}{2}\chi_n\left(\frac{T}{\Theta_0}\right)^n$$

$$= n\left[(n+1)A_n + \frac{n}{2}\chi_n\right]\left(\frac{T}{\Theta_0}\right)^n.$$

It is shown that at $\chi_n > 0$, the function $\Theta(T)_{low}$ decreases, and the function $\gamma(T)_{low}$ increases with increasing temperature from $\Theta_0 > \Theta_{0s}$ and $\gamma_0 > \gamma_{0s}$, respectively. In the average temperature range, the function $\Theta(T)$ should have a minimum, and the function $\gamma(T)$ should have a maximum. At $\chi_n < 0$, the picture changes to the opposite: the function $\Theta(T)_{low}$ increases with increasing temperature from $\Theta_0 < \Theta_{0s}$ to maximum, and the function $\gamma(T)_{low}$ decreases from $\gamma_0 < \gamma_{0s}$ to minimum.

For any $\chi_n \neq 0$, the Θ_0 value differs from the Θ_{0s} value, which is determined from the experimental values of the heat capacity without taking into account the dependence $\Theta(T)_{low}$. In the case of $\chi_n > 0$ and $k > n + 1$, or for $\chi_n = 0$, the functions $s^*(T)_{low}$ and $c^*(T)_{low}$ will follow Debye dependencies, and the values of Θ_0 and γ_0 will match the values of Θ_{0s} and γ_{0s} due to the disappearance of corrections to Debye dependencies.

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Conflict of interest

The author declares that he has no conflict of interest.

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