CONTRIBUTIONS OF DEBYE FUNCTIONS TO BOSONS AND ITS APPLICATIONS ON SOME ND METALS, PART II

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Abstract: Internal thermal energy in solids contributes to vibrations (phonons) energy; spin waves (magnons) energy if solid has magnetism and fermions energy across very complicated mechanisms. Debye functions, mathematically, was estimated because they are considered a main term which controls in all equations of those contributions.

Semi-empirical equation has been obtained to nd ($n=3,4,5$) transition metals specific heat to calculate some important physical constants.

Numerical analyses gives an agreement with experimental results on nd transition metals. Comparison between theoretical and experimental was investigated.

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1. Introduction

In solid-state physics and statistical mechanics, bosons mean phonons, magnons, and photons, which subject to Bose–Einstein statistics [1]. There are two kinds of Debye functions family, the first belong to bosons energy, and the second is bosons specific heat. In mathematics, the family of Debye functions defined as [2]:

$$\begin{aligned} E(n, x) &= \frac{n}{x^{n+1}} \int_0^x \frac{t^n}{e^t - 1} dt, \\ C(n, x) &= \frac{n}{x^n} \int_0^x \frac{t^{n+1} e^t}{(e^t - 1)^2} dt, \end{aligned} \quad (1)$$

Here Peter Debye in 1912, analytically computed the heat capacity, with $n = 3$ (of what is now called the Debye model in solid state).

Most components of relationship (1) come from, Bose–Einstein distribution at low temperatures, or Maxwell-Boltzmann distribution at high temperatures [3, 4, 5, 6, 7], and according to the type of particles or quasi-particles, whether they were phonons or magnons.

The temperature-dependent thermal energy or specific heat in most kinds of metals and their alloys must have in its relationship part of equation (1).

The aim of this paper is to mathematically estimate equations (1), and compare this with experimental results. In addition, to get a semi-empirical equation to find transition metals specific heat to calculate some of the physical constants.

2. Quantum Statistical Mechanics Background

Quantum Debye model of phonons thermal energy in solids for all possible frequencies up to the maximum frequency given by [8, 9]:

$$U_{\text{phonons}} = \int_0^{\omega_{\max}} \frac{V \omega^2}{2\pi^2 v_s^3} \frac{\hbar \omega}{e^{\hbar \omega / K_B T} - 1} d\omega. \quad (2)$$

If v_s is identical for all three polarizations, and suppose that:

$$x \equiv \frac{\hbar \omega}{K_B T} \Rightarrow x_{\max} = \frac{\hbar \omega_{\max}}{K_B T} \Rightarrow x_D = \frac{\hbar \omega_D}{K_B T} \equiv \frac{\Theta}{T},$$

where

$$\Theta = \frac{\hbar\omega_D}{K_B} \Rightarrow U_{phonons} = 9NK_B T \left(\frac{T}{\Theta}\right)^3 \int_0^{x_D} \frac{x^3}{e^x - 1} dx = 3NKE(3, x_D). \quad (3)$$

Derivative phonons energy in equation (2) will give phonons specific heat as follows [10]:

$$C_{phonons} = 9Nk_B \left(\frac{T}{\Theta}\right)^3 \int_0^{x_D} \frac{x^4 e^x}{(e^x - 1)^2} dx = 3NkC(3, x_D). \quad (4)$$

For anharmonic phonons energy and specific heat, general expressions may be written as:

$$\begin{aligned} U_{phonons} &= CT^{n+1} \int_0^{x_D} \frac{x^n}{e^x - 1} dx, \\ C_{v(phonons)} &= CT^n \int_0^{x_D} \frac{x^{n+1} e^x}{(e^x - 1)^2} dx \quad n > 3. \end{aligned} \quad (5)$$

In addition, for magnons (spin waves) thermal energy in magnetic solids [11] at temperature T is given by:

$$\begin{aligned} U_{magnons} &= \frac{K_B T}{4\pi^2} \left(\frac{K_B T}{D_{stiff}}\right)^{3/2} \int_0^{x_m} \frac{x^{3/2}}{e^x - 1} dx, \\ \text{where } x &= [\Delta + D_{stiff} k^2] / K_B T. \end{aligned} \quad (6)$$

Here the dispersion relation for magnon in a spin system is [12, 13, 14]:

$$\omega(k) = \Delta + D_{stiff} k^2, \quad (7)$$

D_{stiff} (Alternatively, D) is the spin-stiffness constant, which is a linear combination of the exchange integrals, Δ is being the anisotropy spin wave gap.

The magnons specific heat is usually obtained by thermal energy derivative for long-wavelength of spin waves, which are the dominant excitations at low temperatures, as:

$$C_{magnons} = \frac{dU_{magnons}}{dT} = \frac{K_B}{4\pi^2} \left(\frac{K_B T}{D_{stiff}}\right)^{3/2} \int_0^{x_m} \frac{x^{5/2} e^x}{(e^x - 1)^2} dx. \quad (8)$$

For anharmonic magnons (spin waves) thermal energy and specific heat, general expressions may be written as:

$$\begin{aligned} U_{\text{magnons}} &= CT^{n+1} \int_0^{x_D} \frac{x^n}{e^x - 1} dx, \\ C_{v(\text{magnons})} &= CT^n \int_0^{x_D} \frac{x^{n+1} e^x}{(e^x - 1)^2} dx \quad n > \frac{3}{2}. \end{aligned} \quad (9)$$

Whereas Planck obtained Photons thermal energy law in solids black body radiation's, or may be sometimes named the Stefan-Boltzmann law as follows:

$$U = \frac{8\pi K_B^4 T^4}{(hc)^3} \int_0^\infty \frac{x^3}{e^x - 1} dx \quad (10)$$

where $x = \frac{h\nu}{K_B T} = \beta$.

In addition, the thermal conductivity is given by [15, 16, 17]:

$$K_{\text{phonons}} = \frac{k_B}{2\pi^2 v} \left(\frac{k_B}{\hbar} \right) T^3 \int_0^{x_D} \tau(x) \frac{x^4 e^x}{(e^x - 1)^2} dx, \quad (11)$$

v is the velocity of phonons in solids, $\tau(x)$ is the relaxation time. Thermal conductivity entirely connected with specific heat as follows:

$$K_{\text{phonons}} = \frac{1}{3} C_{\text{phonons}} v \ell, \quad (12)$$

ℓ is the mean free path.

Finally, the electronic (fermions) specific heat, which subject to Fermi-Dirac distribution given be this equation:

Similarly, with bosons specific heat, fermions specific heat may be written as follows:

$$\begin{aligned} C_{\text{fermions}} &= \int_0^\infty d\varepsilon (\varepsilon - \varepsilon_F) D(\varepsilon) \frac{df(\varepsilon)}{dT}, \\ f(\varepsilon) &= \frac{1}{e^{(\varepsilon - \mu)/KT} + 1}, \\ D(\varepsilon) &= \frac{3}{2} \frac{N(\varepsilon)}{\varepsilon_F}. \end{aligned} \quad (13)$$

As was doing in relation (3), electronic (fermions) specific heat given as follows:

$$C_{fermions} = K^2 T D(\varepsilon_F) \int_{-\varepsilon_F/KT}^{\infty} \frac{x^2 e^x}{(e^x + 1)^2} dx, \quad (14)$$

$$\int_{-\infty}^{\infty} \frac{x^2 e^x}{(e^x + 1)^2} dx = \frac{\pi}{3} \quad \text{for } KT \ll \varepsilon_F,$$

$$C_{fermions} = \frac{\pi}{3} K^2 T D(\varepsilon_F),$$

where general formula of fermions specific heat given by:

$$C_{v(fermions)} = AT^n \int_0^{\infty} \frac{x^{n+1}}{(e^x + 1)^2} dx. \quad (15)$$

3. Mathematical Integrals Results of Debye Functions

In all equations $\log(x)$ is the natural logarithm and $\text{Lin}(x) = \text{polylog}(n, x)$ is the polylogarithm function given by:

$$Li_s(x) = \sum_{n=1}^{\infty} \frac{x^n}{n^s} = x + \frac{x^2}{2^s} + \frac{x^3}{3^s} + \dots \frac{n!}{r!(n-r)!}, \quad (16)$$

where

$$Li_0(x) = \frac{x}{1-x}, \quad Li_1(x) = -\log(1-x).$$

In addition, Riemann zeta function describes by [18]:

$$\zeta(s) = \lim_{n \rightarrow \infty} \sum_{n=1}^{\infty} n^{-s} \quad \text{or} \quad \zeta(s) = \frac{1}{\Gamma(s)} \int_0^{\infty} \frac{x^{s-1}}{e^x - 1} dx, \quad (17)$$

where $Li_s(1) = \zeta(s)$, $\Gamma(s)$ is Gamma function.

Many attempt was made to, mathematically, simplify Debye functions [2], the integral formula for Debye energy (1) was given as follows:

$$E(3, x) = -\frac{\pi^4}{5x^5} - \frac{3}{4} + \frac{3}{x} (\ln(1 - e^x) + \frac{9}{x^2} Li_2(e^x) - \frac{18}{x^3} Li_3(e^x) + \frac{18}{x^4} Li_4(e^x)). \quad (18)$$

Moreover, for Debye specific heat [2] was written as follows:

$$C(3, x) = \frac{4\pi^4}{5x^5} + \frac{3xe^{-x}}{(e^{-x} - 1)} + 12(\ln(1 - e^{-x})) - \frac{36}{x}Li_2(e^{-x}) - \frac{72}{x^2}Li_3(e^{-x}) - \frac{72}{x^3}Li_4(e^{-x}). \quad (19)$$

However, for more simplicity, Mathematical programs may help to give solutions for all complicated functions. For $n = 1, 2, 3, 4, 5$, phonon first kind integrals of Debye functions may be given from (1) by the following expressions:

$$E(n, x) = \frac{n}{x^n} \int_0^x \frac{t^n}{e^t - 1} dt, \quad n = 1, 2, 3, 4, 5, \dots,$$

$$\zeta(2)E(1, x) = \frac{1}{x} \left[-\frac{x^2}{2} + x \text{Log}[1 - e^x] + \text{PolyLog}[2, e^x] \right],$$

$$Li_2(1) = \zeta(2) = \frac{\pi^2}{6} \simeq 1.645, \quad (20)$$

$$\zeta(3)E(2, x) = \frac{2}{x^2} \left[-\frac{x^3}{3} + x^2 \text{Log}[1 - e^x] + 2x \text{PolyLog}[2, e^x] - 2 \text{PolyLog}[3, e^x] - 2 \right],$$

$$Li_3(1) = \zeta(3) = 1.202, \quad (21)$$

$$\zeta(4)E(3, x) = \frac{3}{x^3} \left[-\frac{x^4}{4} + x^3 \text{Log}[1 - e^x] + 3x^2 \text{PolyLog}[2, e^x] - 6x \text{PolyLog}[3, e^x] + 6 \text{PolyLog}[4, e^x] - 6 \right],$$

$$Li_4(1) = \zeta(4) = \frac{\pi^4}{90} \simeq 1.082, \quad (22)$$

$$\zeta(5)E(4, x) = \frac{4}{x^4} \left[-\frac{x^5}{5} + x^4 \text{Log}[1 - e^x] + 4x^3 \text{PolyLog}[2, e^x] - 12x^2 \text{PolyLog}[3, e^x] + 24x \text{PolyLog}[4, e^x] - 24 \text{PolyLog}[5, e^x] - 24 \right],$$

$$Li_5(1) = \zeta(5) = 1.037, \quad (23)$$

$$\zeta(6)E(5, x) = \frac{5}{x^5} \left[-\frac{x^6}{6} + x^5 \text{Log}[1 - e^x] + 5x^4 \text{PolyLog}[2, e^x] - 20x^3 \text{PolyLog}[3, e^x] + 60x^2 \text{PolyLog}[4, e^x] - 120x \text{PolyLog}[5, e^x] + 120 \text{PolyLog}[6, e^x] - 120 \right],$$

$$Li_6(1) = \zeta(6) = \frac{\pi^6}{945} = 1.017. \quad (24)$$

For $n = 1, 2, 3, 4, 5$, phonon second kind integrals of Debye functions may be given from (1) by the following expressions where $C'(n, x)$ represents integral part of $C(n, x)$:

$$C(n, x) = \frac{n}{x^n} \int_0^x \frac{t^{n+1} e^t}{(e^t - 1)^2} dt = \frac{n}{x^n} C'(n, x),$$

$$C'(1, x) = -x - \frac{x}{-1 + e^x} + \text{Log}[1 - e^x] + \text{Constant},$$

$$Li_1(1) = \zeta(1) = \infty, \quad (25)$$

$$C'(2, x) = x \left(\frac{e^x x}{1 - e^x} + 2\text{Log}[1 - e^x] \right) + 2\text{PolyLog}[2, e^x] - \frac{\pi^2}{3},$$

$$Li_2(1) = \zeta(2) = \frac{\pi^2}{6} \simeq 1.645, \quad (26)$$

$$C'(3, x) = x^2 \left(\frac{e^x x}{1 - e^x} + 3\text{Log}[1 - e^x] \right) + 6x\text{PolyLog}[2, e^x]$$

$$- 6\text{PolyLog}[3, e^x] - 7.212,$$

$$Li_3(1) = \zeta(3) = 1.202, \quad (27)$$

$$C'(4, x) = -x^4 - \frac{x^4}{-1 + e^x} + 4x^3\text{Log}[1 - e^x] + 12x^2\text{PolyLog}[2, e^x]$$

$$- 24x\text{PolyLog}[3, e^x] + 24\text{PolyLog}[4, e^x] - \frac{24}{90}\pi^4,$$

$$Li_4(1) = \zeta(4) = \frac{\pi^4}{90} \simeq 1.082, \quad (28)$$

$$C'(5, x) = -x^5 - \frac{x^5}{-1 + e^x} + 5x^4\text{Log}[1 - e^x] + 20x^3\text{PolyLog}[2, e^x]$$

$$- 60x^2\text{PolyLog}[3, e^x] + 120x\text{PolyLog}[4, e^x]$$

$$- 120\text{PolyLog}[5, e^x] - 124.44,$$

$$Li_5(1) = \zeta(5) = 1.037. \quad (29)$$

For $n = 1/2, 3/2, 5/2$, magnon integrals of Debye functions may be given from (9) by the following expressions:

$$U_{\text{magnons}} = CT^{n+1} \int_0^{x_D} \frac{x^n}{e^x - 1} dx,$$

$$C_{v(\text{magnons})} = CT^n \int_0^{x_D} \frac{x^{n+1} e^x}{(e^x - 1)^2} dx, \quad n = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}. \quad (30)$$

For $n = 3/2, 5/2$, magnon integrals of Debye functions from (6, 8, 30) was treated as follows:

$$\begin{aligned} \int \frac{x^{3/2} e^x}{(e^x - 1)^2} dx &= -\frac{x^{3/2}}{\ln(e)(e^{x \ln(e)} - 1)} + \int \frac{3}{2} \frac{x^{1/2}}{\ln(e)(e^{x \ln(e)} - 1)} dx \\ &= -\frac{x^{3/2}}{\ln(e)(e^{x \ln(e)} - 1)} + \frac{3}{2} \frac{\int \frac{x^{1/2}}{e^x - 1}}{\ln(e)}, \end{aligned} \quad (31)$$

$$\begin{aligned} \int \frac{x^{5/2} e^x}{(e^x - 1)^2} dx &= -\frac{x^{5/2}}{\ln(e)(e^{x \ln(e)} - 1)} + \int \frac{5}{2} \frac{x^{3/2}}{\ln(e)(e^{x \ln(e)} - 1)} dx \\ &= -\frac{x^{5/2}}{\ln(e)(e^{x \ln(e)} - 1)} + \frac{5}{2} \frac{\int \frac{x^{3/2}}{e^x - 1}}{\ln(e)}. \end{aligned} \quad (32)$$

For Half-Order Integrals in (31, 32), like Fermi-Dirac integrals and Bose-Einstein integrals:

$$f(n, x) = \int \frac{x^{\frac{2n+1}{2}}}{e^x \pm 1} dx. \quad (33)$$

These functions could only be estimated by graphical or numerically evaluation [19, 20, 21, 22, 23, 24].

4. Results and Discussion

Total theoretical specific heat in normal and magnetic metals may be written as follows:

$$C = \gamma T + \beta T^3 + \varepsilon T^{3/2} + \delta T^{-2} + \dots, \quad (34)$$

where the first term is electronic specific heat, the second is phonons or antiferromagnetic magnons specific heat, the third is ferromagnetic magnons specific heat, and the forth is nuclear specific heat.

Calculation of Parameters needs to analysis experimental data and compare with theoretical expressions to get a semi-empirical formula for each parameter.

For this reason, Crude Experimental database for temperature dependence behavior of specific heat to some 3d,4d,5d pure metals(Copper, Silver, Manganese, Iron, Molybdenum, Ruthenium, Rhodium, Palladium, Iridium, Platinum) has been collected [25,26,27,28,29,30,31], and analyzed from many sources.

Figure 1: Specific heat as a function of low and high temperatures for some metals (after [25-31])

Figures 1 show a general diagram shapes between experimental specific heat as a function of low and high temperatures for some metals.

All above Figures 1 appear with the same general graph of specific heat, but interactive content will be different and depending on the type of metal as it was an ordinary or magnetically metal.

Precise mathematical analysis of data show four kinds of metals, normal, ferromagnetic, antiferromagnetic and mix of ferro and antiferromagnetic.

It was found, for normal metals, a power series formula for temperature dependent of specific heat as:

$$C_p = \sum_{n=0}^{\infty} a_n T^n. \quad (35)$$

Here the first term is residual specific heat, the second is fermions contributions (the electronic specific heat,) and remain terms, belong to harmonic and an-harmonic bosons contributions (lattice specific heat), for Cu and Ag relations (36, 37) was found as follows:

$$\begin{aligned} C_p^{Cu} = & a_0 + a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4 + a_5 T^5 \\ & + a_6 T^6 + a_7 T^7 + a_8 T^8 + \dots = \sum_{n=0}^{\infty} a_n T^n \quad (J/mol.K), \quad (36) \end{aligned}$$

$$r^2 = 0.99999983, \quad 0 < T < 60 \text{ K},$$

$$a_0 = 0.003180774, \quad a_1 = -0.0028737059, \quad a_2 = 0.0011088818$$

$$a_3 = -8.3841194e - 05, \quad a_4 = 5.5776841e - 06, \quad a_5 = 2.179094e - 08,$$

$$a_6 = -4.9216696e - 09, \quad a_7 = 8.6450629e - 11, \quad a_8 = -4.6874092e - 13,$$

$$\begin{aligned} C_p^{Ag} = & a_0 + a_1 T + a_2 T^2 + a_3 T^3 + a_4 T^4 + a_5 T^5 \\ & + a_6 T^6 + a_7 T^7 + a_8 T^8 + \dots = \sum_{n=0}^{\infty} a_n T^n \quad (J/kg.K), \quad (37) \end{aligned}$$

$$r^2 = 0.99999974, \quad 0 < T < 30 \text{ K},$$

$$a_0 = 0.0018995098, \quad a_1 = 0.011940065, \quad a_2 = -0.0097313301,$$

$$a_3 = 0.0058459452,$$

$$a_4 = -0.00083125759, \quad a_5 = 7.888871e - 05, \quad a_6 = -3.589049e - 06,$$

$$a_7 = 7.7363885e - 08, \quad a_8 = -6.4691298e - 10.$$

One has to know that the problem of ferro or antiferromagnetic in transition metals are belongs to a crystal structure of metal [32, 33, 34, 35, 36].

Where generally, Fe, Co, Ni are ferromagnetic; Cr and γ -Mn are (FCC), but crystal structure of α -Mn (BCC) possess ferromagnetic behavior at low temperatures and antiferromagnetic at high temperatures, and Fe (BCC) is ferromagnetic, but Fe (FCC) is antiferromagnetic. In addition, according of crystal structure, platinum group metals (ruthenium, rhodium, palladium, osmium, iridium, and platinum) may be ferro or antiferromagnetic, e.g. BCC ruthenium, possibility to be ferromagnetic.

For antiferromagnetic metals, they have total specific heat formula look like relation (35). It is difficult to discriminate between formula of phonons and magnons (spin waves) antiferromagnetic, because, for example, A T^3 term in the expressions for both harmonic lattice and spin waves complicates the separation of their contributions, but phonons contributions may be evaluated above Neel temperature (T_N), and then calculate magnons below Neel temperature. γ -Mn has antiferromagnetic behavior and a similar trend was found for AFM Cr, analyses specific heat data for γ -Mn give this expression:

$$C_p^{\gamma-Mn} = a_0 + a_1T + a_2T^2 + a_3T^3 + a_4T^4 + a_5T^5 + a_6T^6 + a_7T^7 + a_8T^8 + \dots = \sum_{n=0}^{\infty} a_n T^n \quad (J/mol.K), \quad (38)$$

$$\begin{aligned} r^2 &= 0.99999959 & 0 < T < 60 \text{ K} \\ a_0 &= -0.0033683733 & a_1 &= 0.015595686, \\ a_2 &= -0.0028299466 & a_3 &= 0.00052908612 \\ a_4 &= -3.6004464e-05 & a_5 &= 1.3775614e-06 \\ a_6 &= -2.8142022e-08 & a_7 &= 2.878235e-10 \\ a_8 &= -1.1616613e-12. \end{aligned}$$

As for ferromagnetic, may be found a double power series of specific heat like this:

$$C_p = \sum_{n=0}^{\infty} a_n T^n + \sum_{n=0}^{\infty} a_n T^{\frac{2n+1}{2}}. \quad (39)$$

The first series belongs to fermion and phonons contributions, and the second belong to magnons contributions, analyses data of α -Fe and α -Mn specific heat as a function of temperature gave an expression like (39) relation, where coefficients values as in (40):

$$C_p^{\alpha-Fe} = a_0 + a_1T^{0.5} + a_2T + a_3T^{1.5} + a_4T^2 + a_5T^{2.5}$$

$$+ a_6 T^3 + a_7 T^{3.5} + a_8 T^4 + a_9 T^{4.5} + a_{10} T^5 + \dots \quad (J/gm.K), \quad (40)$$

$$\begin{aligned} r^2 &= 0.99999959, \quad 0 < T < 80 \text{ K} \\ a_0 &= 4.9978926e^{-5}, \quad a_1 = 0.0013777828, \\ a_2 &= -0.0046838768 \quad a_3 = 0.0064275355 \\ a_4 &= -0.0045659346, \quad a_5 = 0.0018966612 \quad a_6 = -0.00047873697, \\ a_7 &= 7.376948e^{-5} \\ a_8 &= -6.70225767e^{-6} \quad a_9 = 3.2836596e^{-7} \quad a_{10} = 6.6913669e^{-9}. \end{aligned}$$

Moreover, for manganese:

$$C_p^{\alpha-Mn} = a_0 + a_1 T + a_2 T^{1.5} + a_3 T^{2.5} + a_4 T^3 + \dots \quad (J/mol.K), \quad (41)$$

$$\begin{aligned} r^2 &= 0.99992258, \quad 0 < T < 30 \text{ K}, \\ a_0 &= 0.0050833471, \quad a_1 = 0.044095211 \\ a_2 &= 0.0040370956, \quad a_3 = -0.00028232669, \\ a_4 &= 7.395301e^{-05}. \end{aligned}$$

In addition, Ruthenium has a same behavior like α -Mn as in relation (42):

$$C_p^{Ruthenium} = a_0 + a_1 T + a_2 T^{1.5} + a_3 T^{2.5} + a_4 T^3 + \dots \quad (J/mol.K),$$

$$\begin{aligned} r^2 &= 0.99974742 \quad 0 < T < 20 \text{ K} \\ a_0 &= 0.0009141367 \quad a_1 = 0.00026509099 \quad a_2 = 0.0018888998 \\ a_3 &= -0.00022421412 \quad a_4 = 5.0439565e^{-05}. \end{aligned}$$

In this way, from theoretical values of Debye functions, all constants in theoretical equations (3,4,6,12) could be found, for example, $a_3 T^3$ represent an experimental harmonic phonons term in Cu and Ag specific heat(36,37), and one can calculate Debye temperature (ω_D), phonon(sound) speed(v), number density of vibrations modes (N/V) and force constant(β), from expression (4,28,36) as follows:

$$a_3 T^3 = 9Nk_B \left(\frac{T}{\Theta} \right)^3 C'(4, x),$$

$$C'(4, x) = -x^4 - \frac{x^4}{-1 + e^x} + 4x^3 \text{Log}[1 - e^x] + 12x^2 \text{PolyLog}[2, e^x]$$

$$-24x \text{PolyLog}[3, e^x] + 24 \text{PolyLog}[4, e^x] - \frac{24}{90} \pi^4,$$

$$\Theta = \left(\frac{9Nk_B}{a_3} C'(4, x) \right)^{\frac{1}{3}}$$

where

$$\Theta = \frac{\hbar\omega_D}{K_B} = \frac{v}{K_B} \left(\frac{6\pi^2 N}{V} \right)^{\frac{1}{3}} = \frac{h\nu}{K_B} \left(\frac{3n}{4\pi} \right)^{\frac{1}{3}},$$

and

$$\omega_D = 2 \left(\frac{\beta}{M} \right)^{\frac{1}{2}} \equiv \text{lattice cut - off frequency},$$

β = force constant, M = Molecular weight,

n = number of atoms in unit volume.

Thermal conductivity from (11) become:

$$K_{\text{phonons}} = \frac{1}{3} C_{\text{phonons}} v \ell = \frac{1}{3} a_3 T^3 v \ell \quad (44)$$

In addition, for magnons, stiffness constant (D_{stiff}) may be found as follows:

$$a_3 T^{1.5} = \frac{K_B}{4\pi^2} \left(\frac{K_B T}{D_{\text{stiff}}} \right)^{3/2} \int_0^{x_m} \frac{x^{5/2} e^x}{(e^x - 1)^2} dx$$

$$D_{\text{stiff}}^{3/2} = \frac{K_B^{5/2}}{a_3 4\pi^2} \int_0^{x_m} \frac{x^{5/2} e^x}{(e^x - 1)^2} dx \Rightarrow$$

$$D_{\text{stiff}}^{3/2} = \frac{K_B^{5/2}}{a_3 4\pi^2} \left(-\frac{x^{5/2}}{\ln(e)(e^{x \ln(e)} - 1)} + \frac{5}{2} \frac{\int \frac{x^{3/2}}{e^x - 1}}{\ln(e)} \right). \quad (45)$$

The last term in (45) may be estimated by graphical or numerically evaluation.

5. Conclusions

Semi-empirical equations has been found to some (3,4,5)d transition metals specific heat to calculate some of the physical constants, there are an excellent agreement between bosons Debye functions, quantum theoretical expressions and experimental results.

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