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About a new semi-empirical equations of temperature dependence of heat capacity and thermal expansion coefficient of solids

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The empirically established polynomial form of the Cp equations for solids at T > 298.15 K recommended by Maier and Kelley (1932), Haas and Fisher (1976), Berman and Brown (1985), as a rule, can be used for the data interpolation. In 1986 Fei and Saxena, and, independently, Khodakovsky, are proposed semi-empirical equations, using well known C_V approaches to $3Rn$ constant value (where R is the gas constant, and n is a number of atoms) at $T \to \infty$, and thermodynamic relation $C_P - C_V = \alpha^2 V K_T T$ as well. However, their forms C_P equations approach to ∞ (not to zero) at $T \to 0$.

The equation (1): $Cp = a[1 - 1/(1 + cT^2)] + bT$ was proposed by Kuznetsov and Kozlov (1988). This new type equation, unlike previous ones, corresponds to third law of thermodynamic ($C_P = 0$ at $T = 0$), but dose not obey the «Debye T^3 law» at low temperatures (*i.e.* the temperature dependence is not expressed in terms of AT^3 where A is a constant). The equation (2): $C_P = Rn\{[a_3T^3/(1 + a_3T^3)] + [b_2T^2/(1 + b_2\mathrm{T})] + [c_1T/(1 + c_1T)]\} + \alpha^2 V K_T T$ was proposed by Khodakovsky in 2000. The equation (2) are examined using the C_p experimental data for different types of solids. In this paper, as a result of preliminary investigations, it is found that the last term of an equation (2) should be excluded, but a new adjusting parameter ***k*** should be included:

$$C_v = Rn[\boldsymbol{k}L_D + (3 - \boldsymbol{k})L_E], \text{ where } L_D = [1 - 1/(1 + bT^3)] \text{ and } L_E = [1 - 1/(1 + bT^2)]$$

The empirically established form of the α equations recommended by different authors can be used for the data interpolation only. Because the ratio $C_P/\alpha \approx$ const, the following equations: $\alpha = a\,[1 - 1/(1 + bT^2)]$ may be good for representation, estimation, and high (low) temperature extrapolation of α. In this case the thermodynamic limitations: $\alpha = 0$, and $C_P - C_V = \alpha^2 V K_T T = 0$ at $T = 0$ will be obeyed exactly.

Key words: thermodynamic, thermophisics, heat capacity of minerals

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