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Theory of thermal expansivity and bulk modulus

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Abstract

The expression for thermal expansivity and bulk modulus, claimed by Shanker et al. to be new [Physica B 233 (1977) 78; 245 (1998) 190; J. Phys. Chem. Solids 59 (1998) 197] are compared with the theory of high pressure–high temperature reported by Kumar and coworkers. It is concluded that the Shanker formulation and the relations based on this are equal to the approach of Kumar et al. up to second order.

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Keywords: Thermal expansivity; Bulk modulus; Equation of state

1. Introduction

Shanker et al. [1–3] have claimed to have derived a new relation to study the properties of solids under varying conditions of pressures and temperatures. Using the Gruneisen theory of thermal expansivity, Shanker et al. [1] obtained the following relations:

$$\frac{V}{V_0} - 1 = \frac{1 - [1 - 2\{(K_0' + 1)/K_0\}P_{\mathrm{Th}}]^{1/2}}{(K_0' + 1)}, \qquad (1)$$

where V/V_0 is the relative change in volume, K is the isothermal bulk modulus, K' is the first-order pressure derivative of K, P_{Th} the thermal pressure, subscript 0 refers to their value at room temperature and atmospheric pressure. Eq. (1) is valid at $P = 0$. Shanker and Kushwah [2,3] discussed that Eq. (1) may be rewritten as follows, when pressure, $P \neq 0$,

$$\frac{V}{V_0} - 1 = \frac{1 - [1 - 2\{(K_0' + 1)/K_0\}(P_{\mathrm{Th}} - P)]^{1/2}}{(K_0' + 1)}, \qquad (2)$$

where

$$P_{\mathrm{Th}} = \alpha_0 K_0 (T - T_0). \qquad (3)$$

These authors [1–3] claimed that Eqs. (1,2) emerge from their analysis, and therefore, referred to it as the Shanker et al. formulation [2,3]. The purpose of present paper is to demonstrate that the formulae reported by Shanker et al. [1–3] are not new.

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2. Mathematical analysis

In Eq. (1), the term within bracket may be regarded as $(1-x)^n$, the expansion of which reads as follows (neglecting higher-order terms)

$$(1-x)^n = 1 - nx + \frac{n(n-1)}{2}x^2. \tag{4}$$

Thus, we can write

$$\left\{1 - 2\left(\frac{K_0'+1}{K_0}\right)P_{\mathrm{Th}}\right\}^{1/2} = 1 - \left(\frac{K_0'+1}{K_0}\right)P_{\mathrm{Th}} - \frac{1}{2}\left\{\left(\frac{K_0'+1}{K_0}\right)P_{\mathrm{Th}}\right\}^2$$

or

$$1 - \left\{1 - 2\left(\frac{K_0'+1}{K_0}\right)P_{\mathrm{Th}}\right\}^{1/2} = \left(\frac{K_0'+1}{K_0}\right)P_{\mathrm{Th}} + \frac{1}{2}\left\{\left(\frac{K_0'+1}{K_0}\right)P_{\mathrm{Th}}\right\}^2 \tag{5}$$

dividing both sides of Eq. (5) by $(K_0'+1)$, we get

$$\frac{1 - \left[1 - 2\{(K_0'+1)/K_0\}P_{\mathrm{Th}}\right]^{1/2}}{(K_0'+1)} = \frac{1}{K_0'+1}\left[\left(\frac{K_0'+1}{K_0}\right)P_{\mathrm{Th}} + \frac{1}{2}\left\{\left(\frac{K_0'+1}{K_0}\right)P_{\mathrm{Th}}\right\}^2\right]. \tag{6}$$

From Eq. (1) and (6) we get

$$\frac{V}{V_0} - 1 = \frac{1}{K_0'+1}\left[\left(\frac{K_0'+1}{K_0}\right)P_{\mathrm{Th}} + \frac{1}{2}\left\{\left(\frac{K_0'+1}{K_0}\right)P_{\mathrm{Th}}\right\}^2\right]. \tag{7}$$

Similarly, Eq. (2) may be rewritten as follows:

$$\frac{V}{V_0} - 1 = \frac{1}{(K_0'+1)}\left[\left(\frac{K_0'+1}{K_0}\right)(P_{\mathrm{Th}} - P) + \frac{1}{2}\left\{\left(\frac{K_0'+1}{K_0}\right)(P_{\mathrm{Th}} - P)\right\}^2\right]. \tag{8}$$

3. Theory of Kumar

A theoretical analysis of high pressure–high temperature equation of state has already been reported by Kumar and Bedi [4]. The detailed analysis is available elsewhere [4] and the mathematical relation reads as follows:

$$\frac{V}{V_0} - 1 = -\frac{1}{(K_0'+1)}\ln\left[1 - \left(\frac{K_0'+1}{K_0}\right)(P_{\mathrm{Th}} - P)\right]. \tag{9}$$

The term within bracket in Eq. (9) may be regarded as ln $(1-x)$. The expansion of which reads as follows (neglecting higher-order terms):

$$\ln(1-x) = -x - \frac{x^2}{2}. \tag{10}$$

Thus, Eq. (9) may be rewritten as follows:

$$\frac{V}{V_0} - 1 = \frac{1}{(K_0'+1)}\left[\left(\frac{K_0'+1}{K_0}\right)(P_{\mathrm{Th}} - P) + \frac{1}{2}\left\{\left(\frac{K_0'+1}{K_0}\right)(P_{\mathrm{Th}} - P)\right\}^2\right]. \tag{11}$$

At $P = 0$, Eq. (11) reads as follows:

$$\frac{V}{V_0} - 1 = \frac{1}{(K_0'+1)}\left[\left(\frac{K_0'+1}{K_0}\right)P_{\mathrm{Th}} + \frac{1}{2}\left\{\left(\frac{K_0'+1}{K_0}\right)(P_{\mathrm{Th}})\right\}^2\right]. \tag{12}$$

4. Results and analysis

If, I compare Eq. (7) with Eq. (12), and Eq. (8) with Eq. (11) these are same relations. Thus, the Shanker formulation is in agreement with the earlier formulation of Kumar and coworker [4,11]. The expression of thermal pressure (P_{Th} at $P = 0$), in terms of the change in volume ($\Delta = V - V_0$) as presented by Shanker and coworkers [1–3] reads as follows:

$$P_{\mathrm{Th}} = K_0\left(\frac{\Delta}{V_0}\right) - \frac{1}{2}\left(\frac{\Delta}{V_0}\right)^2 K_0(K_0'+1). \tag{13}$$