Research Article

Temperature Dependence of Thermoelastic Properties for NaCl Crystal

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Recently developed isothermal Kholiya's EOS is modified to study the temperature dependent volume expansion and applied for NaCl crystal. The results obtained with the present model are in quite close agreement to the experimental values. The model is therefore extended to study the variation of bulk modulus and the coefficient of volume thermal expansion with temperature. Comparison of the obtained results with the experimental data demonstrates that an isothermal EOS may also be modified to study the temperature dependent elastic properties. The present study also reveals that the quasi harmonic approximation, that is, the product of bulk modulus and the coefficient of volume thermal expansion as constant, is valid in case of NaCl crystal.

1. Introduction

The behavior of solids under the effect of high pressure and high temperature has truly developed into an interdisciplinary area which has important implications for an application in the area of physics, biology, engineering, and technology apart from the discovery of various novel and unexpected phenomena, high pressure high temperature research has provided new insight into the behavior of matter [1]. Strength and elastic properties of a solid depend on the strength of its interatomic forces. Therefore, the application of temperature which changes the interatomic distance of the substances changes its physical properties. The EOS gives us valuable information about the relationship between the changes in thermodynamic variable, namely, pressure, volume, and temperature. Every thermodynamic system has its own EOS, independent of others. An EOS expresses the peculiar behavior of one individual system which distinguishes it from the others. In order to determine the EOS of a system, the thermodynamic variables of the system are accurately measured and a relation is expressed between them. Attempts have been made to derive a compressibility equation from molecular theory, but none of them has resulted in convenient equation expressing the results of

experiments with adequate accuracy. To meet this need some empirical equations have been proposed, the sole justification of which is that it works.

In spite of impressive advances on the theoretical front over the past decades, the need for the search of an EOS continues to exist. Although, modern electronic band structure calculation allows the predictions of EOS for solids yet the calculation is time consuming as well as expensive. In the literature, there are number of equations of states, and these arise from an unchecked and improvable assumption concerning an assumed interatomic potential, an assumed strain function, or an assumed boundary condition that is not testable [2]. Recently, Kholiya have developed an isothermal EOS to study the high pressure behavior of nanomaterials [3]. The main advantage of this EOS is that it follows the basic requirements revealed from the fundamental thermodynamics for solids in the limit of extreme compressions, as given by Kholiya et al. [4]. In the present paper our aim is to modify isothermal Kholiya's EOS to study the temperature dependent elastic properties of the solid. For understanding the thermodynamic behavior of solids at high temperature it is useful to have reliable values of volume thermal expansion coefficient (α), isothermal bulk modulus (B_T) [5–8]. For this

purpose NaCl is taken as an example because NaCl is the most widely used internal pressure standard in high pressure diffraction experiments due to the availability of the large body of experimental data. NaCl has a stable structure (B1) up to a pressure of about 30 GPa and its melting temperature is nearly 1074 K. Thus we have a wide range of pressures and temperatures for studying the equation of state and thermoelastic properties of NaCl. Besides this, numerous attempts have been made to understand the high pressure and high temperature [9–16] behavior of NaCl using equation of state and thus the experimental/theoretical data is available which can be useful to check the validity of our proposed temperature dependent EOS.

2. Method of Analysis

Recently, to study the high pressure elastic properties of nanomaterials Kholiya [3] has expended pressure in powers of density up to the quadratic term and achieved the EOS as

$$P(V, T_0) = \frac{B_0}{2} \left[(B'_0 - 3) - 2(B'_0 - 2) \left(\frac{V}{V_0} \right)^{-1} + (B'_0 - 1) \left(\frac{V}{V_0} \right)^{-2} \right] \quad (1)$$

Here B_0 and B'_0 are the bulk modulus and first order pressure derivative of bulk modulus at $P = 0$ and $T = T_0$, respectively.

Equation (1) can also be written in the inverted form as

$$\left(\frac{V}{V_0} \right)^{-1} = \frac{(B'_0 - 2)}{(B'_0 - 1)} [1 + X], \quad (2)$$

where $X = [1 - ((B'_0 - 1)/(B'_0 - 2)^2) \{B'_0 - (2P(V, T_0)/B_0) - 3\}]^{1/2}$.

This EOS may be used to determine the pressure for different compression or vice-versa at the reference temperature (which is generally room temperature) (T_0) and it is shown by Kholiya [3] that (2) gives the better results for the compression behavior of nanomaterials than some well-known EOS, namely, usual Tait, Murnaghan, and Shanker EOS. To make (2) temperature dependent we have used the basic equation of state which is in terms of thermal pressure as [2]

$$P(V, T) = P(V, T_0) + P_{TH}, \quad (3)$$

where thermal pressure P_{TH} may be given as

$$P_{TH} = \int_{T_0}^T (\alpha B_T) dT. \quad (4)$$

In the quasi harmonic approximation considering $\alpha B_T = \text{Constant} = \alpha_0 B_0$, (5) gives

$$P_{TH} = \alpha_0 B_0 (T - T_0). \quad (5)$$

Using (4) and (6), (3) may be written as

$$\left(\frac{V}{V_0} \right)^{-1} = \frac{(B'_0 - 2)}{(B'_0 - 1)} [1 + Y], \quad (6)$$

where $Y = [1 - ((B'_0 - 1)/(B'_0 - 2)^2) \{B'_0 - (2P(V, T)/B_0) + 2\alpha_0(T - T_0) - 3\}]^{1/2}$.

The bulk modulus is defined as

$$B = -V \left(\frac{\partial P}{\partial V} \right)_T. \quad (7)$$

Thus, (6) gives

$$B = B_0 Y (1 + Y) \times \frac{(B'_0 - 2)^2}{(B'_0 - 1)}. \quad (8)$$

The coefficient of volume thermal expansion is defined as

$$\alpha = \left(\frac{1}{V} \right) \left(\frac{\partial V}{\partial T} \right)_P. \quad (9)$$

Therefore, (6) gives

$$\alpha = \frac{\alpha_0}{Y (1 + Y)} \times \frac{(B'_0 - 1)}{(B'_0 - 2)^2}. \quad (10)$$

If the pressure $P(V, T) = 0$ the expression for, (V/V_0) , bulk modulus B , and coefficient of volume thermal expansion α comes out to be

$$\left(\frac{V}{V_0} \right)^{-1} = \frac{(B'_0 - 2)}{(B'_0 - 1)} [1 + Z], \quad (11)$$

$$B = B_0 Z (1 + Z) \times \frac{(B'_0 - 2)^2}{(B'_0 - 1)}, \quad (12)$$

$$\alpha = \frac{\alpha_0}{Z (1 + Z)} \times \frac{(B'_0 - 1)}{(B'_0 - 2)^2}, \quad (13)$$

where $Z = [1 - ((B'_0 - 1)/(B'_0 - 2)^2) \{B'_0 + 2\alpha_0(T - T_0) - 3\}]^{1/2}$.

3. Results and Discussion

To study the volume change, bulk modulus, and coefficient of volume thermal expansion at high temperature, the present model requires three input parameters, namely, B_0 , B'_0 , and α_0 . For NaCl, the experimental values of B_0 , B'_0 , and α_0 are 24 GPa, 5.5, and 11.8×10^{-5} , respectively [2]. Equation (11) is used to calculate the variation of volume (V/V_0) with temperature for NaCl crystal. The obtained results are given in Table 1 along with other theoretical and experimental data. From the table it is clear that our calculated values are quite close to the experimental findings in comparison to the other theoretical results. This close agreement between our theoretical results and the experimental findings motivated us to apply the model for the study of temperature dependence of bulk modulus and coefficient of volume thermal expansion. Tables 2 and 3 represent our calculated, experimental, and other theoretical values of bulk modulus and coefficient of volume thermal expansion at different temperatures. From these tables it may be revealed that the present model gives

TABLE 1: Variation of volume (V/V_0) with temperature for NaCl crystal.

T (K)	V/V_0		
	Present (11)	Reference [13]	Reference [11]
300	1	1	1
350	1.0060	1.0060	1.0060
400	1.0123	1.0122	1.0127
450	1.0188	1.0186	1.0194
500	1.0256	1.0253	1.0259
550	1.0328	1.0322	1.0332
600	1.0403	1.394	1.0409
650	1.0483	1.0469	1.0491
700	1.0567	1.0547	1.0580
750	1.0657	1.0629	1.0679

TABLE 2: Variation of bulk modulus with temperature for NaCl crystal.

T (K)	Bulk modulus (In GPa)		
	Present (12)	Reference [15]	Exp. [2]
300	24	24	24
350	23.2	—	23.2
400	22.4	21.97	22.4
450	21.6	—	21.6
500	20.8	19.99	20.8
550	19.9	—	19.9
600	19.0	18.09	19.0
650	18.1	—	18.1
700	17.2	15.12	17.3
750	16.3	—	16.5

TABLE 3: Variation of coefficient of volume thermal expansion with temperature for NaCl crystal.

T (K)	Volume thermal expansion coefficient (α) (In 10^{-5} K^{-1})		
	Cal. (11)	Reference [16]	Exp. [2]
300	11.8	11.8	11.8
350	12.2	12.1	12.2
400	12.6	12.5	12.7
450	13.1	12.8	13.2
500	13.6	13.2	13.7
550	14.2	13.7	14.3
600	14.9	14.1	14.8
650	15.6	14.6	15.4
700	16.4	15.2	16.0
750	17.4	15.7	16.6

the results better than other theoretical models. The present study also shows that the quasi harmonic approximation, that is, the product of bulk modulus and the coefficient of volume thermal expansion as constant, is valid in case of

NaCl crystal. From the overall discussion it may be concluded that an isothermal EOS may also be modified to study the temperature dependent elastic properties.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

References

- [1] R. Chidambaram and S. M. Sharma, "Frontiers in high-pressure physics research," *Current Science*, vol. 60, pp. 397–408, 1991.
- [2] O. L. Anderson, *Equations of State of Solids for Geophysics and Ceramic Science*, Oxford University Press, Oxford, UK, 1994.
- [3] K. Kholiya, "High pressure isothermal equation of state for nanomaterials," *Indian Journal of Physics*, vol. 87, no. 4, pp. 339–343, 2013.
- [4] K. Kholiya, J. Chandra, and S. Verma, "Analysis of equation of states for the suitability at high pressure: MgO as an example," *The Scientific World Journal*, vol. 2014, Article ID 289353, 5 pages, 2014.
- [5] J. L. Tallon, "The thermodynamics of elastic deformation-I. Equation of state for solids," *Journal of Physics and Chemistry of Solids*, vol. 41, no. 8, pp. 837–850, 1980.
- [6] S. Yamamoto, I. Ohno, and O. L. Anderson, "High temperature elasticity of sodium chloride," *Journal of Physics and Chemistry of Solids*, vol. 48, no. 2, pp. 143–151, 1987.
- [7] O. L. Anderson and K. Zou, "Formulation of the thermodynamic functions for mantle minerals: MgO as an example," *Physics and Chemistry of Minerals*, vol. 16, no. 7, pp. 642–648, 1989.
- [8] X. Xia and J. Xiao, "Thermal expansivity of periclase at high temperature and high pressure," *Journal of Physics and Chemistry of Solids*, vol. 54, no. 5, pp. 629–633, 1993.
- [9] S. S. Kushwah and J. Shanker, "Thermal expansivity and bulk modulus of NaCl crystal at high temperatures," *High Temperatures—High Pressures*, vol. 27–28, no. 2, pp. 177–182, 1995.
- [10] L. M. Thomas and J. Shanker, "Analysis of the pressure dependence of the thermal expansivity of NaCl crystal," *Physica Status Solidi (b)*, vol. 195, no. 1, pp. 67–71, 1996.
- [11] S. S. Kushwah and J. Shanker, "Analysis of thermal expansivity of NaCl and KCl crystals," *Journal of Physics and Chemistry of Solids*, vol. 59, no. 2, pp. 197–199, 1998.
- [12] J. Shanker and S. S. Kushwah, "Temperature dependence of thermal expansivity along isobars for NaCl and MgSiO_3 -perovskite," *Physica B: Condensed Matter*, vol. 254, no. 1–2, pp. 45–51, 1998.
- [13] Z. H. Fang, "Pressure dependence of thermal expansivity in solids," *High Temperatures—High Pressures*, vol. 31, no. 5, pp. 507–510, 1999.
- [14] S. S. Kushwah and J. Shanker, "On the temperature dependence of thermal expansivity of NaCl crystal," *Indian Journal of Pure and Applied Physics*, vol. 36, no. 1, pp. 46–48, 1998.
- [15] M. Kumar, "Temperature dependence of interatomic separation and bulk modulus for ionic solids," *Physica B: Physics of Condensed Matter*, vol. 205, no. 2, pp. 175–179, 1995.
- [16] Z. H. Fang, "Thermal expansion of ionic materials at high temperatures," *Journal of Applied Physics*, vol. 102, no. 1, Article ID 013523, 2007.