

Pressure Dependence of Isothermal Anderson Gruneisen Parameter of NaCl

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Abstract

Various models have been developed for determination of isothermal Anderson Gruneisen parameter of NaCl at room temperature and different pressures. In present work, a new model is developed by modification of existing EOS (equation of state) to study the temperature and pressure dependence of isothermal Anderson Gruneisen parameter of NaCl. The results obtained with the present model are in quite close agreement to the experimental values. Comparison of the obtained results with the experimental data demonstrates that an isothermal may also be modified to study the temperature dependent elastic properties.

Keywords: EOS, NaCl crystal, isothermal Anderson-Gruneisen parameter

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INTRODUCTION

The behaviour 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 study of behaviour of matter [1]. Strength and elastic properties of a solid depend on the strength of inter-atomic forces. Therefore, the application of temperature which changes inter-atomic distance of the substances changes its physical properties. The equation of state gives us valuable information about the relationship between the changes in thermodynamic variables, namely, pressure, volume, and temperature. Every thermodynamic system has its own equation of state, independent of others. Equation of state expresses the peculiar behaviour of one individual system which distinguishes it from the others. In order to determine the equation of state 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.

There are number of equations of states, and these arise from an unchecked and improvable assumption concerning an assumed inter-atomic potential, an assumed strain function, or an assumed boundary condition that is not testable [2]. Kholiya has developed an isothermal equation of state to study the high pressure behaviour of nonmaterial [3]. The main advantage of this 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 develop a new equation of state for NaCl, for understanding its thermodynamic behaviour at room temperature and high pressure. The choice of 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 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 behaviour 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 equation of state [5, 6].

METHOD OF ANALYSIS

The isothermal Anderson-Gruneisen parameter δ_T is defined as:

$$\delta_T = -\frac{1}{\alpha K_T} \left(\frac{\partial K_T}{\partial T} \right)_P \quad (1)$$

Where, α is volume thermal expansivity which is defined as,

$$\alpha = \frac{1}{V} \left(\frac{\partial V}{\partial T} \right)_P \quad (2)$$

And K_T is isothermal bulk modulus which is given by,

$$K_T = -V \left(\frac{\partial P}{\partial V} \right)_T \quad (3)$$

In addition, for describing the temperature dependence of the isothermal bulk modulus δ_T has been used for the discussion of pressure dependence of thermal expansivity. We can understand the pressure dependence of α using Maxwell's relation as,

$$\left(\frac{\partial \alpha}{\partial P} \right)_T = \frac{1}{K_T^2} \left(\frac{\partial K_T}{\partial T} \right)_P \quad (4)$$

Using this thermodynamic identity in Eq. (1), we get,

$$\delta_T = \frac{V}{\alpha} \left(\frac{\partial \alpha}{\partial V} \right)_T \quad (5)$$

Al'tshuler *et al.* have given the following expression for Gruneisen parameter [7]:

$$\gamma = \gamma_\infty + (\gamma_0 - \gamma_\infty) \left(\frac{V}{V_0} \right)^\beta \quad (6)$$

Where γ_0 & γ_∞ are the values of Gruneisen parameter at $P=0$ or $V=V_0$ and $P \rightarrow \infty$ $V \rightarrow 0$ respectively and β is an adjustable parameter.

Shanker *et al.* pointed out the similarity for the volume dependence of γ and δ_T as [8]:

$$\delta_T = \delta_{T_\infty} + (\delta_{T_0} - \delta_{T_\infty}) \left(\frac{V}{V_0} \right)^m \quad (7)$$

Where, δ_T & δ_{T_∞} are the values of δ_T at $P=0$ or $V=V_0$ and $P \rightarrow \infty$ $V \rightarrow 0$ respectively and m is a dimensionless factor depending on material.

Sharma has given a simple choice for reciprocal form for the volume dependence of isothermal Anderson-Gruneisen parameter δ_T as [9]:

$$\frac{1}{\delta_T} = \frac{1}{\delta_{T_\infty}} + \left(\frac{1}{\delta_{T_0}} - \frac{1}{\delta_{T_\infty}} \right) \left(\frac{V}{V_0} \right)^m \quad (8)$$

The volume dependence of the isothermal Anderson-Gruneisen parameter δ_T can be expressed with the help of following relationship as:

$$\delta_{T+1} = A \left(\frac{V}{V_0} \right) \quad (9)$$

Where, $A = \delta_{T_0} + 1$

With the help of Eqs. (5) and (9) we get,

$$\left(\delta_{T_0} + 1 \left(\frac{V}{V_0} \right) - 1 \right) = \frac{V}{\alpha} \left[\frac{\partial \alpha}{\partial V} \right]_P \quad (10)$$

On integrating Eq. (10),

$$\frac{\alpha}{\alpha_0} = \frac{V_0}{V} \exp \left[(\delta_{T_0} + 1) \left\{ \frac{V}{V_0} - 1 \right\} \right] \quad (11)$$

On integrating Eq. (11) and taking, $\alpha = \frac{1}{V} \left(\frac{\partial V}{\partial T} \right)_P$

$$\frac{V}{V_0} = \left[1 - \frac{1}{(\delta_{T_0} + 1)} \right] \left[\ln \left\{ 1 - \alpha_0 [\delta_{T_0} + 1] X(T - T_0) \right\} \right] \quad (12)$$

Using value of $\frac{V}{V_0}$ from Eq. (12) in Eq. (8) we get a relation as:

$$\frac{1}{\delta_T} = \frac{1}{\delta_{T_\infty}} + \left(\frac{1}{\delta_{T_0}} - \frac{1}{\delta_{T_\infty}} \right) \left(\left[1 - \frac{1}{(\delta_{T_0} + 1)} \right] \left[\ln \left\{ 1 - \alpha_0 [\delta_{T_0} + 1] X(T - T_0) \right\} \right] \right)^m \quad (13)$$

$$\frac{1}{\delta_T} = \frac{1}{\delta_{T_\infty}} + \left(\frac{1}{\delta_{T_0}} - \frac{1}{\delta_{T_\infty}} \right) \left[1 - \frac{1}{(\delta_{T_0} + 1)} \right]^m X \left[\ln \left\{ 1 - \alpha_0 (\delta_{T_0} + 1) X(T - T_0) \right\} \right]^m \quad (14)$$

RESULTS

With the help of the input data given in Table 1 for NaCl, the results are calculated using derived Eq. (14) and have been reported in Table 2.

Table 1: Values of Input Data for NaCl [10].

| | |
|--|--------------------------------------|
| α_0 (Volume thermal expansivity at 300 K and zero pressure) | $11.6 \times 10^{-5} \text{ K}^{-1}$ |
| δ_{T_0} (Anderson-Grüneisen parameter at 300 K) | 5.95 |
| δ_{T_∞} (Anderson-Grüneisen parameter at higher temperature) | 2.3 |
| m (Dimensionless factor depending on material) | 1.8 |

Table 2: Variation of δ_T with Pressure at Room Temperature (300 K).

| P (GPa) | δ_T |
|---------|------------|
| 0 | 5.86 |
| 5 | 5.70 |
| 10 | 5.45 |
| 15 | 5.42 |
| 20 | 5.38 |
| 25 | 5.30 |
| 30 | 5.28 |
| 35 | 5.19 |

CONCLUSIONS

An expression for the volume dependence of thermal expansivity by using the reciprocal form of volume dependent Anderson-Grüneisen parameter has been proposed. It has been found that the results obtained through Eq. (14) show the consistency with those values given by Joshi *et al.* for NaCl [10].

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