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Study on Pressure Volume Temperature Relationship for Diatomic Solids Based On Inverted and Non Inverted Equations of State

Dr. Priti Tiwari*

Assistant Professor, Department of Applied Science and Humanity, Abul Kalam Technical University, Kanpur

***Abstract** – The pressure-volume-temperature (P-V-T) relationship utilizing inverted and non-inverted conditions of state (EOS) for diatomic solids, for example, NaCl, MgO and LiH has been contemplated. It is tracked down that the inverted kind EOS because of yields close concurrence with the outcomes got from the non-inverted conditions due to for isothermal compressions just as isothermal mass modulus. The Roy - Roy inverted EOS has been found to have an extra benefit of foreseeing volumes for a strong at the same time raised pressure and temperature. We have utilized this EOS to get P-V-T results for NaCl and Mgo. The determined qualities present close concurrence with the exploratory data.*

***Keywords** – Pressure, Volume, Temperature, Relationship, Inverted, Non Inverted, Diatomic Solids*

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1. INTRODUCTION

In probes high pressure material science of solids we measure the unit cell volume of packed solids with the assistance of X-beam diffraction relating to various pressures. Subsequently an EOS as volume communicated as a component of pressure is more proper to exploratory data. We hence concentrate on conditions of state VV fP 0 by including warm impacts inside the system of the Debye estimate. These are known as inverted kind condition of state. In the current article we have audited some significant inverted sort conditions of state like the Murnaghan EOS, Bridgman EOS, Borelius EOS, Grover et al EOS, Huang and Chow EOS, Schmidt EOS, Anderson et al EOS (Luban), Tait EOS, Freund and Ingalls EOS , Kumari and Dass EOS , Stacey corresponding B-prepared EOS, Roy-Roy EOS, Roy-Roy logarithmic EOS and Saxena EOS which are relevant to various solids with various synthetic holding. An inverted condition of state can be acquired from the knowledge of pressure reliance of mass modulus which is characterized as

$$B(P) = -V\left[\frac{dP}{dV}\right] \quad \text{.................................(1)}$$

On integrating eq. (1) we get

$$\frac{V}{V_0} = \exp\left[-\int_0^P \frac{dP}{B(P)}\right]. \quad \text{...............................(2)}$$

On the other hand, non-inverted type equations of state are obtained using the following basic relations

$$P = -\left(\frac{dE}{dV}\right) \quad \text{.......................................(3)}$$

And

$$P = -\int_{V_0}^{V} \frac{B(V)}{V} dV \quad \text{.......................................(4)}$$

where E is the total energy of solids. Equation (3) is valid only at T = 0 K

In the accompanying Sections we present a basic assessment of some particular conditions of state with specific accentuation on the limit conditions at outrageous pressure $(V \to 0)$ or $(P \to \infty)$.

2. MURNAGHAN'S EQUATION OF STATE

The condition of state (EOS) is in a general sense significant in concentrating on the high pressure properties of solids. The Murnaghan EOS is notable in the writing which has been inferred based on the direct hypothesis of limited strain. It tends to be communicated in inverted just as non-inverted structures

$$\frac{V}{V_0} = [1 + bP]^{-c} \quad \text{.......................................(5)}$$

where $b = B_0'/B_0$, $c = 1/B_0$ and V_0 is the volume V at pressure P = 0, B0 and B0 are the values of isothermal bulk modulus B, and its first pressure derivative (dB_T/dP) both at zero pressure. The Murnaghan EOS doesn't work sufficiently at higher compressions. This is predominantly in light of the fact that the Murnaghan EOS depends with the understanding that the isothermal mass modulus relies linearily upon pressure

$$B_T = B_0 + B_0'P \quad \text{.......................................(6)}$$

This suggests that the main pressure subordinate of mass modulus is a consistent amount and higher request subsidiaries are zero. Notwithstanding, trial just as hypothetical investigations uncover that second pressure subsidiary of isothermal mass modulus (B_0'') cannot be taken equal to zero. In fact, B_0'' is straightforwardly identified with the fourth request flexible constants which have much higher sizes than that the third request versatile constants. The disappointment of Murnaghan's EOS at higher pressures is because of the insufficiency of the supposition that dB_T/dP s constant. The phenomenological conditions of state can be inferred utilizing the two fundamental structures given by Eqs. (2) and (4)

3. OBJECTIVES OF THE STUDY

1. To study on Murnaghan's equation of state
2. To study on Empirical inverted equations of state

4. EMPIRICAL INVERTED EQUATIONS OF STATE

The connection between pressure (P) and relative volume VV0 at a given temperature is alluded to as an isothermal condition of state (EOS) or an isotherm. EOSs for solids are acquired either exactly by fitting appropriate capacities to the test data or hypothetically by utilization of the Mie-Grüneisen law

$$P = -\left(\frac{\partial P}{\partial V}\right)_{T=0} + \frac{\gamma E_T}{V} \quad \text{..................(7)}$$

where the first term is the pressure due to the potential energy of the compressed solid at T = 0 and the second term is due to lattice vibrations with, γ and E_T being the Grüneisen parameter and the lattice vibrational energy respectively. Different expressions for the potential energy give rise to numerous EOS. They have in common that V/V_0 is the autonomous and P the reliant variable and that they can't be inverted on account of muddled useful structure picked for the possible energy. We call them non-inverted EOS. We need to have an EOS in form $V/V_0 = f(P)$ and its pressure derivatives. We call them inverted EOS.

The simplest two-parameter inverted EOS is the power series given by Bridgman

$$\frac{V}{V_0} = 1 - aP + bP^2 \quad \text{......................(8)}$$

with the definition of the bulk modulus $B = -V(dP/dV)$ we find the pressure derivatives of volume as

$$\frac{dV}{dP} = -\frac{V}{B} \quad \text{........................(9)}$$

And

$$\frac{d^2V}{dP^2} = \frac{V}{B^2}\left(\frac{dB}{dP} + 1\right) \quad \text{..................(10)}$$

Several attempts have been made to formulate inverted type equations. However, they fail to satisfy the criterion given by Stacey according to which $B' \to B/P$ in the limit of infinitely large pressure in the limit of infinitely large pressure $P \to \infty$ The Roy-Roy11 EOS is an inverted kind EOS which fulfils the Stacey basis. An extra benefit of utilizing the Roy-Roy EOS is that we can foresee volumes of solids at the same time raised pressures and temperatures. In the current review, we utilize the Roy-Roy EOS for assessing V (T, P) for NaCl in the reach P = 0 – 30 Gpa and T = 298 – 773 K, and for MgO in the reach P = 0 – 53 GPa and T = 300 – 2474 K.

5. FORMULATION AND METHOD OF ANALYSIS

We consider the following three non-inverted type equations:

Rydberg's EOS

$$P = 3B_0 x^{-2/3}(1 - x^{1/3}) \exp[\eta(1 - x^{1/3})] \quad \text{...............(11)}$$

where $x = \frac{V}{V_0}$, and $\eta = \frac{3}{2}(B_0' - 1)$

Shanker's EOS

$$P = B_0 \frac{x^{-4/3}}{t} \times \left[\left(1 - \frac{1}{t} + \frac{2}{t^2}\right)\{\exp(ty) - 1\} + y\left(1 + y - \frac{2}{t}\right)\exp(ty)\right] \quad \text{.....................(12)}$$

where $x = \frac{V}{V_0}$, $t = B_0' - \frac{8}{3}$ and $y = 1 - \frac{V}{V_0}$

Hama and Suito's EOS

$$P = 3B_0 x^{-5/3}(1 - x^{1/3}) \exp \times \left[\frac{3}{2}(B_0 - 3)(1 - x^{1/3}) + \left(Z - \frac{3}{2}\right)(1 - x^{1/3})^2\right] \quad \text{.........(13)}$$

where $x = \frac{V}{V_0}$, and $Z = \frac{3}{8}(B_0' - 1)(B_0' + 3) + \frac{3}{2} B_0 B_0'' + \frac{1}{3}$

The expression for bulk modulus can be obtained using the relationship:

$$B = -V\left(\frac{dP}{dV}\right)_T \quad \text{.............(14)}$$

The inverted type EOS obtained by Roy and Roy in the form of Eq. (2) is given as follows:

$$\frac{V}{V_0} = \left[1 + aP(1 + bP)^c\right]^{-1} \quad \text{................(15)}$$

$$a = \frac{1}{B_0}$$

$$b = \frac{(4B_0 B_0'' - 5B_0'^2 + 6B_0' - 1)}{6B_0(1 - B_0')}$$

$$c = \frac{3(1 - B_0')^2}{(4B_0 B_0'' - 5B_0'^2 + 6B_0' - 1)} = \frac{1}{B_\infty'} - 1$$

We have calculated the values of pressure P and bulk modulus B for the three solids down to a compression $V/V_0 = 0.65$ using the input parameters are presented in Table 1.

6. RESULTS AND DISCUSSION

The outcomes for pressure-volume (P-V) relationship and mass modulus determined from various EOS are introduced in Tables 2 and 3, separately. To make the correlation of the outcomes dependent on various conditions significant we have utilized similar upsides of information parameters on and ' B_0, B_0', and B_0'' as given in Table 1. It ought to be referenced that ' B0 is an amount of focal significance and its worth remaining parts somewhere in the range of three and six for the vast majority of the solids. We have chosen three solids NaCl, MgO and LiH for which the upsides of ' B0 are 5.50, 4.37 and 3.51, individually. The outcomes for pressure P just as mass modulus B determined from various EOS concur intimately with one another for every one of the three solids under concentrate down to a pressure of V/V0 = 0.65 (Tables 1 and 2). The main finding is that the inverted sort EOS because of Roy and Roy yields great concurrence with other non-inverted sort conditions. Likewise this EOS fulfills the relationship $B/P = B'$ at $P \to \infty$, since $B'_\infty > 0$ is given in the last column of Table 1.

In exploratory investigations, the volumes are estimated with the assistance of X-beam diffraction strategies for a strong at determined states of pressure and temperature. Consequently, an immediate correlation with exploratory data is conceivable provided that an EOS can be utilized to foresee volumes accepting pressure and temperature as info. Non-inverted sort EOS are hard to be settled for getting V(T, P). Then again, an inverted kind EOS, for example, that because of Roy and Roy which yields great concurrence with the grounded non-inverted conditions and is too consistent with the Stacey criterion $B/P = B'_\infty$ in the limit $P \to \infty$ can be utilized to anticipate V(P, T). In the current review, we have, accordingly, utilized the Roy and Roy Eq. to get the outcomes for volumes of NaCl and MgO at all the while raised pressures and temperatures. At high temperatures, Eq.16 can be revamped as:

Table 1 Values of input parameters taken

Table 1—Values of input parameters taken from Refs [2, 11, 21].

	B_0 (GPa)	B'_0	B''_0 (GPa)$^{-1}$	a (GPa)$^{-1}$	b	c	Z	B'_∞
NaCl	24.0	5.50	-0.223	0.0417	0.2170	-0.432	6.649	1.76
MgO	157	4.37	-0.040	0.0064	0.0300	-0.357	0.227	1.56
LiH	39.1	3.51	-0.106	0.0256	0.0987	-0.325	0.244	1.48

Table 2 Values of P (GPa) calculated from (a) Rydberg equation (13), (b) Shanker's Eq.14, (c) Hama-Suito's Eq.15 and (d) Roy-Roy's Eq..16

V/V_0	(a)	(b)	(c)	(d)
		NaCl		
1.00	0	0	0	0
0.95	1.42	1.42	1.42	1.42
0.90	3.36	3.37	3.37	3.37
0.85	6.04	6.06	6.06	6.06
0.80	9.72	9.78	9.77	9.77
0.75	14.8	14.9	14.9	14.9
0.70	21.8	22.0	22.0	22.0
0.65	31.7	32.0	32.4	31.7
		MgO		
1.00	0	0	0	0
0.95	9.03	9.03	9.03	9.03
0.90	20.8	20.8	20.8	20.8
0.85	36.4	36.2	36.4	36.2
0.80	56.3	56.4	56.6	56.3
0.75	82.8	83.1	83.1	82.5
0.70	118	118	120	118
0.65	165	165	166	160
		LiH		
1.00	0	0	0	0
0.95	2.19	2.19	2.20	2.19
0.90	4.94	4.94	4.95	4.94
0.85	8.45	8.34	8.46	8.45
0.80	12.8	12.8	12.9	12.8
0.75	18.3	18.4	18.4	18.4
0.70	25.4	25.5	25.9	25.4
0.65	34.6	34.6	34.9	34.0

$$\frac{V}{V_0}=\left[1+aP^*(1+bP^*)^c\right]^{-1} \quad \text{............(17)}$$

Where

$$P^*=P-\Delta P_{th}$$

and the ΔP_{th} **represents the change in thermal pressure:**

$$\Delta P_{th}=P_{th}(T)-P_{th}(T_0)$$
$$=\alpha B_T(T-T_0) \quad \text{..............................(18)}$$

where α is volume thermal expansion coefficient, BT the isothermal bulk modulus and T_0 is the room temperature. The values of the change in thermal pressure $\alpha B_T =$ 6.3×10^{-3} GPa K^{-1} for MgO and 2.84×10^{-3} GPa K^{-1} for NaCl. These values of αB_T relate to the temperature near the Debye temperature for the solids. The outcomes are introduced in Tables 1 and 2 and contrasted and the accessible test data18−20,22 . The outcomes determined from Roy and Roy EOS are in acceptable concurrence with the test esteems for NaCl and MgO. The outcomes detailed here are predictable with the new discoveries for NaCl.

CONCLUSION

In the current review, we have consequently tracked down that the inverted kind condition of state as of late detailed by Roy and Roy is steady with the other non-inverted sort Eqs for NaCl, MgO and LiH. It is additionally exhibited that the Roy-Roy EOS enjoys a benefit of foreseeing the volumes for a strong at the same time raised pressure and temperature when the impact of warm pressure is considered. We have acquired the aftereffects of V(T, P) for NaCl and MgO at high pressures and high temperatures in close concurrence with the accessible test data up to a pressure of 50 GPa and temperature of 2500 K.

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Corresponding Author

Dr. Priti Tiwari*

Assistant Professor, Department of Applied Science and Humanity, Abul Kalam Technical University, Kanpur