Pressure –Volume Behavior of some Ionic solids and Geophysical Minerals (CsCl)

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Abstract— Various forms of the equation of state for studying high-pressure behavior of solids have been developed by numerous investigators using phenomenological approaches. A common feature of the phenomenological equation is that they present the relationship between pressure and volume which can be expressed analytically involving two quantities only, viz Bo, B0' respectively, the isothermal bulk modulus and its first pressure derivative, both at zero pressure. The present proposal which intend to compare the efficiency of the four equations under close examination reports the V/V_o versus P derived from the new modified forms of Murnaghan equation –NMME1 and NMME2, Birch equation (BE) and Freund- Ingalls (FIE) equation obtained for the best agreement with the experimental data of Drickamer et.al.

Key words: Equation of State, NMME1, NMME2, Birch Equation (BE), Freund-Ingalls (FIE)

I. Introduction

The material include in this study is CsCl, as it is commonly used as a standard for pressure measurements. Experimental studies on the P-V data include the direct measurement by Bridgeman [1], Vaidya and Kennedy [2], Boehler and Kennedy [3], and Chhabildas and Ruoff [4] based on measurement of length under hydrostatic pressure. The highest pressure reaches in this studies is 4.5GPa by Vaidya and Kennedy. As against this ultrasonic interferometry technique used by Frankel et al. [5] goes to a pressure of 27GPa. The Physical properties included in the Table are (i) the structure with lattice constant a and c (ii) the zero pressure density ρ_o and (iii) the max. Pressure P_{max} reached in the particular study together with the technique used the original reference.

A. Physical Properties of CsCl

Solid	Lattice Structure a, c in (Å)	ρ_o(g/cm3)	P_{max}(GPa)
CsCl	a = 4.1	3.99	4.5 Hydrostatic [1-4] 27 Ultrasonic [5] 25x-ray diffraction [6]

Table 1: Physical Properties

The values of B_o, B_o', and B_o'' as determined from the polynomial fit with the P-V data are listed below.

1) Polynomial fit values of B_o, B_o', B_o'':

CsCl	B_o(GPa)	B_o'	$B_o''(GPa^{-1})$
	18.9	5.52	0.22

The values have been numerically determined from equation as,

$$B = -V\left(\frac{dP}{dV}\right)_T \quad (1)$$

$$B = \frac{1+\sum_1 ai([P])^{-1}}{\sum_1 ia_1([P])^{1-1}} \quad (2)$$

In the limit P = 0, we get

$$B_0 = -\frac{1}{a_1} \quad (3)$$

Successive differentiation of eqn. (1) with respect to P and then on taking the limit as P=0 yield

$$\frac{dB}{dP} = B_o' = -1 + \frac{2a_2}{a_1^2} \quad (4)$$

$$\frac{d^2B}{dP^2} = B_0'' = \frac{2a_2}{a_1} + \frac{6a_3}{a_1^2} - \frac{8a_2}{a_1^3} \quad (5)$$

and so on. The suffix o indicates the value at zero pressure. It is observed that contrary to expectation B_o'' is positive in this case. However numerical values of B_o'' evaluated at high pressures show that this derivative takes negative values for the entire pressure range starting from P=20 or 30 GPa that is nearly the zero pressure. The positive values may therefore be due to small undulation caused by the numerical program. The four equation under examination are the NMME1 [7], NMME2 [7], FIE [8] and BE[9]. The two equations which have been designed as NMME1 and NMME2 indicate that they are new modified forms of Murnaghan equation. The Freund–Ingalls three parameter equation FIE [8] and the Birch equation BE [9] have also been used for comparing the derived equations with these two equations which are known to be giving very good results in similar studies. The equations used for fitting the P-V data are explicitly given here for ready reference.

$$P = (3\frac{B_0}{2})\{(\frac{V_0}{V})^{\frac{7}{3}} - ([\frac{V_0}{V}])^{\frac{5}{3}}\}\{1 + (\frac{3}{4})(B_0' - 4)[([\frac{V_0}{V}])^{\frac{2}{3}} - 1]\} \quad (6)$$

(Birch equation)

$$\frac{V}{V_0} = \{1 - a\ln(1 + bP)\}^c \quad (7)$$

(Freund and Ingalls equation)

$$\frac{V}{V_0} = (1+P)^{-\frac{1}{n}}[1 + (\frac{m}{6n})\{b(P+1)^2 + 3(1-2b)(P+1) + 3b - 6(1-b)\ln(P+1) - \frac{(3-2b)}{(P+1)}\}] \quad (8)$$

(New modified form of Murnaghan equation NMME2)

This equation easily goes into NMME1 for b=1

II. Results and Discussion

The present study which intends to compare the efficiency of the four equations under close examination reports the V/V_o versus P derived from the new modified forms of Murnaghan equation –NMME1 and NMME2, Birch equation (BE) and Freund- Ingalls (FIE) equation obtained for the best agreement with the experimental data of Drickamer et.al. The shock wave data published by Drickamer et.al covers a pressure range for the normal metal phase of these materials. The graph obtained by plotting these values against P together is shown in figure 1.

B_o	B_o'	B_o''	source
16.2	5.40	-	BE
16.5	5.57	-	NMME1
17.0	5.80	- 4.98	NMME2
17.2	5.04	-	FIE
17.1	5.09	-	Ref[10]
16.9	5.54	-0.24	Ref[10]
16.8	5.98	-0.42	Ref[12]
17.4	5.50	-	Ref[13]

Table 1: The best fit value for B_o, B_o', B_o'' .

P	A	B	C
0	1.0679	1.0684	1.0647
10	0.9995	0.9997	0.9972
20	0.9499	0.9499	0.9487
30	0.912	0.912	0.9109
40	0.8803	0.8803	0.8801
50	0.8544	0.8544	0.8541
60	0.8318	0.8318	0.8317

Table 2: Values of volume compressions at different pressures P(GPa) for CsCl (T=673K)

P	A	B	C
0	1.1256	1.1288	1.109
10	1.0339	1.0349	1.0248
20	0.9726	0.9729	0.9678
30	0.9284	0.9285	0.9248
40	0.8919	0.8919	0.8903
50	0.8632	0.8633	0.8617
60	0.8383	0.8384	0.8372

Table 3: Values of volume compressions at different pressures P (GPa) for CsCl (T=873K)

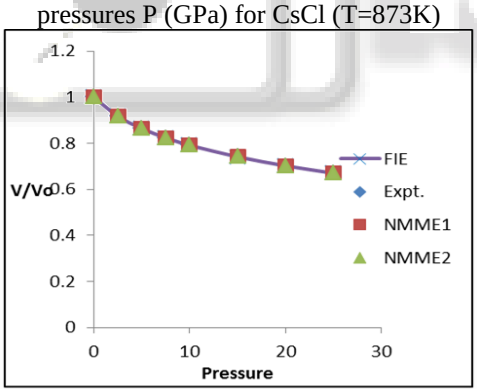

Fig. 1: Graph

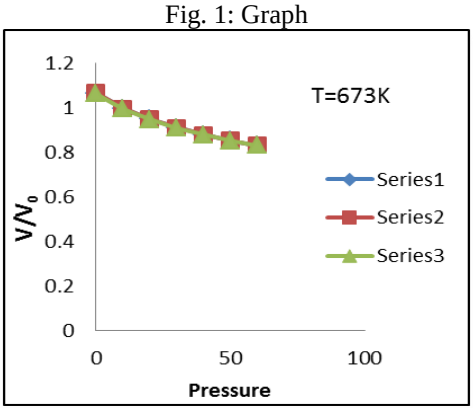

Fig. 2: Values of volume compressions at different pressures P(GPa) for CsCl (T=673K)

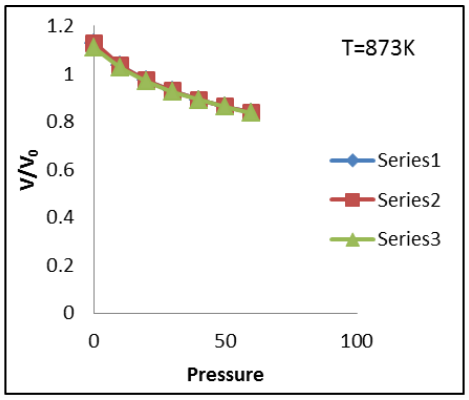

Fig. 3: Values of volume compressions at different pressures P(GPa) for CsCl (T=873K)

ACKNOWLEDGEMENT

The financial support from Madhya Pradesh Council of Science & Technology Madhya Pradesh Bhopal (India) under the research project is gratefully acknowledged. The authors are very much thankful to the Department of Physics.

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