International Journal of Physics and Applications.
ISSN 0974-3103 Volume 2, Number 1 (2010), pp. 57--60

http://www.irphouse.com

Pressure - Volume Behaviour for NaCl Crystal

Pankaja Singh, Tanveer Ahmad Wani*, Mahendra Mehra and A.S. Khan

Department of Physics, MVM Bhopal M.P., India
**E-mail: wani_mvm@yahoo.com*

Abstract

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

Keywords: Equation of State, NMME1, NMME2, BE, FIE.

PACS: 64.30.-t, 64.10.+h, 62.20.-x.

Introduction

The material included in this study is the ionic compound NaCl, as it is commonly used as a standard for pressure measurements and is perhaps the most investigated solid. 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 measurements of length under hydrostatic pressure. The highest pressure reached in these 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 27 GPa and the shock waves technique used by Fritz et al. [6] reports the measurements upto more than 23GPa.

Some physical properties of NaCl are listed below. The properties included in the

Table are (i) the structure with lattice constants a and c (ii) the zero pressure density ρ_0 and (iii) the max. pressure P_{max} reached in the particular study together with the technique used and the original reference.

Physical Properties

NaCl	Structure a, c in A^0	$\rho_{0\ (g/cm^3)}$	Pmax (GPa)
	a=2.81	2.13	4.5 Hydrostatic [1-4]
			27 Ultrasonic [5]
			23 Shock wave [6]
			25 x-ray diffraction [7]

The values of B_o, $B_o`$ and $B_o``$ as determined from the polynomial fit with the p-v data are listed below

Polynomial fit values of B_O, $B_O`$ and $B_o``$:

NaCl	$B_{O\ (}$GPa)	$B_O`$	$B_O``$ (GPa^{-1})
	22.60	5.74	0.034

The values have been numerically determined from equations as,

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

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

In the limit P=0, we get

$$B_0 = -\frac{1}{a_1} \tag{3}$$

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

$$\frac{dB}{dP} = B_O` = -1 + \frac{2a_2}{a_1{}^2} \tag{4}$$

$$\frac{d^2B}{dP^2} = B_0`` = \frac{2a_2}{a_1} + \frac{6a_3}{a_1{}^2} - \frac{8a_{2^2}}{a_1{}^3} \tag{5}$$

and so on. The suffix o indicates value at zero pressure. It is observed that contrary to expectations $B_o``$ 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 undulations caused by the numerical programme. The four equations under examination are the NMME1 [8], NMME2 [8], FIE [9] and BE [10]. The two equations which have been designated as NMME1 and NMME2 indicate that they are new modified forms of Murnaghan equation. The

Freund-Ingalls three parameter equation FIE [9] and the Birch equation BE [10] 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.

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

(Birch equation)

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

(Freund and Ingalls equation)

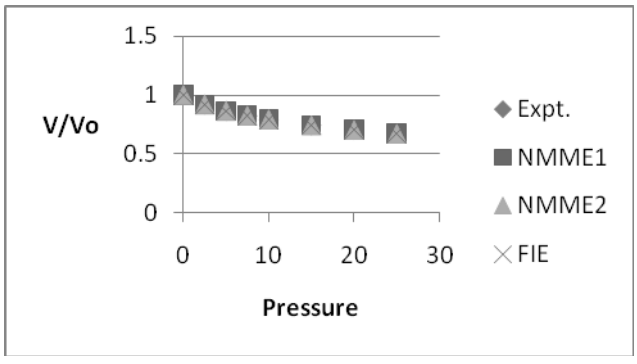
$$V/V_t0 = [(1+p)]^{(-1/n)}[1+(m/6n)\{b(p+1)^2+3(1-2b)(p+1)+3b-6(1- \quad b)\ln[(p+1)-((3-2b))/((p+1))]\}] \quad (8)$$

(New modified form of Murnaghan equation NMME2)

This equation easily goes into NMME1 for b=1

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 values derived from the NMME1, NMME2, BE and FIE 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.



The best fit values for B_O, $B_O`$, $B_O``$ and $B_O```$ are listed in Table 1.

B_O	$B_O`$	$B_O``$	$B_O```$	Source
25.16	4.50	-	-	BE
23.65	4.82	-0.035	-	NMME1
23.64	4.82	-0.035	-0.014	NMME2
22.79	5.73	-0.45	-	FIE
23.88	5.2	-	-	Ref.[11]
23.60	5.2	-0.45	-	Ref.[12]
23.6	5.85	-0.08	-	Ref.[13]

23.84	5.35	-0.068	-	Ref.[14]
23.7	5.59	-0.068	-	Ref.[15]
26.4	3.9	-	-	Ref.[16]

Acknowledgement
The authors acknowledge thanks due to departmental teachers and researchers.

References

[1] Bridgeman P.W., 1940, Proc. Am. Acad. Arts. Sci., 74, 21.
[2] Vaidya S.N., and Kennedy G.C., 1971, J Phys. Chem. Solids, 41, 517.
[3] Boehler R., and Kennedy G.C, 1980, J Phys. Chem. Solids, 41, 517.
[4] Chhabildas L.C., and Ruoff A.L., 1976, J Appl. Phys., 47, 4182.
[5] Frankel J., Rich J.F., and Homan C.G., 1976, J. Geophys. Res., 81, 6357.
[6] Fritz J.N., Marsh S.P., Carter W.J., and McQueen R.G., 1971, The Hugornioe equation of state of sodium chloride in the sodium chlorid structure, in accurate characterization of the high pressure environment. (Edited by Leoyd E.C., NBS special publication 326, Washington D.C).
[7] Borelius G., Solid State Phys., Edited by F. Seitz and D. Turnbull, 1958, Academic press, New York, 6, 65.
[8] Singh P. and Verma M.P., 1994, Proc. Nat. Acad. Sci. India, 64 (A), I.
[9] Freund J. and Ingalls R., 1989, J. Phys. Chem. Solids, 50, 263.
[10] Birch F.J., 1952, J. Geo. Phys. Res., 57, 227.
[11] Hadjicontics V., Ftasias K.E., and Varotsoes C., 1989, J Phys. Chem. Solids
[12] Birch F.J., 1986, J. Geo. Phys. Res., 91, 4949.
[13] Boehler R., and Kennedy G.C., 1979, J Phys. Chem. Solids, 41, 517.
[14] Spetzler H., Sammis C.G., and O`connel R.J., 1972, J Phys. Chem. Solids, 33, 1727.
[15] Swenson C.A., and Anderson M.S., 1983, Shock waves in condensed matter, chapter II, 7.
[16] Drickmer H.G., Lynch R.W., Clender R.L., and Perez-Albueme E.A., 1966, Solid State Physics, 19, 225.