International Journal of Education, Modern Management, Applied Science & Social Science (IJEMMASSS)
ISSN : 2581-9925, Impact Factor: 5.143, Volume 02, No. 04, October - December, 2020, pp.202-206

HIGHER PRESSURE DERIVATIVE OF BULK MODULUS AT DIFFERENT COMPRESSIONS

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ABSTRACT

Equation of state (EOS) Plays an important role in understanding the properties of matter under extreme conditions of pressure and temperature. In the present paper we shall consider four EOSs such as Vinet Rydberg EOS, Shanker EOS, Shanker – Kushwah EOS and Kean's EOS to study the behavior of five solids viz Ne, Cu, Al, LiH and MgO upto very high Compressions.

Keywords: *Equations of State, Bulk Modulus, Monoatomic and Diatomic Solids*.

Introduction

Equation of state (EOS) normally means a relationship between pressure P, Volume V and temperature T for a material [1]. An EOS can be classified into two categories, viz (i) Inverted type EOS, and (ii) non-inverted type EOS [2]. Shanker and Kushwah [3] have formulated an equation of state which can be expressed inverted as well as non-inverted forms with the help of this EOS, we can determine V/Vo as a function of pressure and vice-versa. This EOS has been found most suitable for the materials for which the pressure derivative of isothermal bulk modulus at P=0 ie B'_0 is less than four. 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'o which are respectively the isothermal bulk modulus and its first pressure derivative both at zero pressure. Shanker et al. have developed a method within the framework of the theory of lattice Potential for ionic crystals to obtain analytical forms of EOS containing B_0 and B'_0 [4, 5]. Morse [6] presented an early quantum mechanical theory with two exponential terms to explain molecular vibration speetra. The morse potential was first used in a finite strain theory by slater [7]. Rydberg [8] tried the Morse potential in a study of the vibrational spectrum of molecular hydrogen. This is the potential favoured more recently and advocated as 'universal' by Vinet et al. [9]. The first true B-primed equation was developed by Keane [10]. Keane recognized the significance of the extrapolation of B' to infinite pressure that is B'_∞.

Formulation and Method of Analysis

We consider the following four equations:

- Vinet- Rydberg EOS
- Shanker EOS
- Shanker – Kushwah EOS
- Kean's EOS

Vinet-Rydherg EOS

$$B_T = B_0(x)^{\frac{-2}{3}}\left[1+\left\{\eta(x)^{\frac{1}{3}}+1\right\}\left\{1-(x)^{\frac{2}{3}}\right\}\right]exp\left[\eta\left\{1-(x)^{\frac{1}{3}}\right\}\right]$$

$$B'_T = \frac{1}{3}\left[\frac{(x)^{\frac{1}{3}}(1-\eta)+2\eta(x)^{\frac{2}{3}}}{1+\left[\eta(x)^{\frac{1}{3}}+1\right]\left[1-(x)^{\frac{1}{3}}\right]}+\eta(x)^{\frac{1}{3}}+2\right]$$

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

$$B_T B_T'' - \frac{1}{9}(x)^{\frac{1}{3}} \left[\frac{\left\{(1-\eta)x^{\frac{1}{3}} + 2\eta x^{\frac{2}{3}}\right\}\left\{(\eta - 1) - 2\eta(x)^{\frac{1}{3}}\right\}}{\left\{1 + \left[\eta(x)^{\frac{1}{3}} + 1\right]\left[1 - (x)^{\frac{1}{3}}\right]\right\}^2} + \frac{\left\{(\eta - 1) - 4\eta(x)^{\frac{1}{3}}\right\}}{\left\{1 + \left[\eta(x)^{\frac{1}{3}} + 1\right]\left[1 - (x)^{\frac{1}{3}}\right]\right\}} \eta \right] \quad \dots\dots\dots(1)$$

At $\frac{V}{V_0} = 0$, $B_T B_T'' = 0$

Shanker EOS

$$B_T = B_0 x^{\frac{-1}{3}}(1 + y + y^2)\exp(ty) + \frac{4}{3}P$$

$$B_T' = \frac{4}{3} + \left(1 - \frac{4}{3}\frac{P}{K_T}\right)\left[\frac{1}{3} + x\left\{t + \frac{(1+2y)}{(1+y+y^2)}\right\}\right]$$

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

$$B_T'' = \left(1 - \frac{4}{3}\frac{P}{B_T}\right)\left[\left(\frac{-x}{B}\right)\left\{t + \frac{1+2y}{1+y+y^2}\right\} + x\left\{\frac{2\left(\frac{x}{B}\right)}{1+y+y^2} - \frac{(1+2y)\left\{\frac{x}{B} + 2y\left(\frac{x}{B}\right)\right\}}{(1+y+y^2)^2}\right\}\right] - \frac{4}{3}\left(\frac{1}{B_T} - \frac{PB_T'}{B_T^2}\right)\left\{\frac{1}{3} + x\left(t + \frac{1+2y}{1+y+y^2}\right)\right\}$$

$$B_T B_T'' = \left(\frac{4}{3}\frac{P}{B_T} - 1\right)x\left[\left(t + \frac{1+2y}{1+y+y^2}\right) - x\left\{\frac{1-2y-2y^2}{(1+y+y^2)^2}\right\}\right] - \frac{4}{3}\left(1 - \frac{PB_T'}{B_T}\right)\left\{\frac{1}{3} + x\left(t + \frac{1+2y}{1+y+y^2}\right)\right\} \quad \dots\dots\dots(2)$$

At $x = 0$, $B_T' = \frac{B_T}{P} = \frac{4}{3}$ and therefore $B_T B_T'' = 0$

Shanker-Kushwah EOS

$$B_T' = \frac{4(a_1 + a_2) - (a_1 + 2a_2)\left(\frac{V}{V_0}\right)}{a_1\left[2 - \left(\frac{V}{V_0}\right)\right] + 2a_2\left[1 - \left(\frac{V}{V_0}\right)\right]}$$

Where $a_1 = B_0$ and $a_2 = B_0(B_0' - 3)/2$

$$B_0 \; and \; B_0' \; are \; the \; values \; of \; B_T \; and \; \frac{dB_T}{dP} \; at \; V = V_0$$

$$B_T'' = \frac{B_T\left(\frac{V}{V_0}\right)^2\left[-(a_1+2a_2)\frac{1}{V_0}\frac{dV}{dP}\right]-\left[B_T'\left(\frac{V}{V_0}\right)^2+2B_T\frac{V}{V_0^2}\frac{dV}{dP}\right]\left[4(a_1+a_2)-(a_1+2a_2)\frac{V}{V_0}\right]}{B_T^2\left(\frac{V}{V_0}\right)^4}$$

$$B_TB_T'' = \frac{\left[(a_1+2a_2)\frac{V}{V_0}\right]-(B_T'-2)\left[4(a_1+a_2)-(a_1+2a_2)\frac{V}{V_0}\right]}{a_1\left(2-\frac{V}{V_0}\right)+2a_2\left(1-\frac{V}{V_0}\right)} \qquad \dots\dots\dots(3)$$

At $\frac{V}{V_0} = 0,\quad B_T' = B_\infty' = 2$ and therefore $B_TB_T'' = 0$

Keane's EOS

$$B_T = B_0\left[1+\frac{B_0'}{B_\infty'}\left(x^{-B_\infty'}-1\right)\right]$$

Where $x = \frac{V}{V_0}$

$$B_T' = B_\infty' + (B_0' - B_\infty')\frac{B_0}{B_T^2}$$

$$B_T'' = -B_T'(B_0' - B_\infty')\frac{B_0}{B_T^2}$$

$$B_TB_T'' = -B_T'(B_0' - B_\infty')\frac{B_0}{B_T} \qquad \dots\dots\dots(4)$$

Results and Discussion

We have calculated the values of B_TB_T'' using the Vinet- Rydberg EOS, the Shanker EOS, the Shanker-Kushwah EOS and the Kean's EOS as function of $\frac{V}{V_0}$ down to 0.1 for the solids under study taking input parameters are presented in Table 1 based on first principal reported by Hama and Suito [11] and by Anderson [12] based on experimental data. It should be mentioned that B'_0 is a quantity of central importance and its value remains between three and eight for most of the solids. We have selected five solids Ne, Cu, Al LiH and MgO. For which the value of B'_0 are 7.61, 5.93, 4.85, 3.51 and 4.37 respectively. The results for B_TB_T'' calculated from different EOS (eqn 1 to 4) are presented in Table 2,3,4,5, and 6. The values of B_TB_T'' obtained from Kean's EOS are decreasing most rapidly as compared to other EOS. Value of B_TB_T'' are negative because B'_T decreases with the increase in pressure and attains a constant value $B'_T=B'_\infty$ in the limit of infinite pressure. Therefore B_TB_T'' become zero in the limit $P \to \infty$ or $V \to 0$. At infinity large compressions $V \to 0$, $P \to \infty$ $B_T' \to B_\infty'$ and $\left(\frac{B_T}{P}\right) \to B_\infty'$. Using these limits and value of B_∞' for different EOS it can be verified that B_TB_T'' vanish at $\frac{V}{V_0} \to 0$ for all the EOS under study.

Value of input parameters for the solids based on first principles reported by Hama and Suito [11] and for NaCl reported by Anderson [12] based on experimental ultrasonic data value of B'_∞ are based on the Stacey formulation.

Table 1

Material	**B_0 (GPa)**	B_0'	B_0'' **(GPa^{-1})**	B'_∞
Ne	6.36	7.61	2.86	5.22
Al	72.6	4.85	0.104	3.29
Cu	135	5.93	0.083	4.04
LiH	39.1	3.51	0.106	2.33
MgO	157	4.37	0.040	2.93

Table 2

Values of $-B_T\ B_T''$ with the variation of V/V_0 for Ne calculated from (a) Vinet-Rydberg EOS (b) Shanker EOS (c) Shanker-Kushwah EOS (d) Keane's EOS

V/V_0	(a)	(b)	(c)	(d)
1.0	17.8	13.3	37.1	18.2
0.9	9.19	8.34	13.7	7.36
0.8	5.56	6.01	6.58	3.28
0.7	3.72	4.71	3.60	1.47
0.6	2.65	3.77	2.11	0.621
0.5	2.02	2.99	1.28	0.233
0.4	1.53	2.30	0.776	0.072
0.3	1.19	1.16	0.455	0.016
0.2	0.906	0.975	0.236	0.002
0.1	0.634	0.391	0.096	0.00005

Table 3

Values of $-B_T\ B_T''$ with the variation of V/V_0 for Al calculated from (a) Vinet-Rydberg EOS (b) Shanker EOS (c) Shanker-Kushwah EOS (d) Keane's EOS

V/V_0	(a)	(b)	(c)	(d)
1.0	7.78	6.87	10.9	7.57
0.9	4.95	4.96	5.98	4.13
0.8	3.37	3.75	3.55	2.34
0.7	2.42	2.90	2.23	1.33
0.6	1.79	2.24	1.44	0.736
0.5	1.36	1.75	0.931	0.382
0.4	1.03	1.23	0.596	0.177
0.3	0.798	0.828	0.366	0.067
0.2	0.595	0.469	0.202	0.018
0.1	0.402	0.181	0.084	0.002

Table 4

Values of $-B_T\ B_T''$ with the variation of V/V_0 for Cu calculated from (a) Vinet-Rydberg EOS (b) Shanker EOS (c) Shanker-Kushwah EOS (d) Keane's EOS

V/V_0	**(a)**	**(b)**	**(c)**	**(d)**
1.0	10.4	9.39	19.4	11.2
0.9	6.58	6.36	8.99	5.42
0.8	4.26	4.69	4.86	2.78
0.7	2.95	3.62	2.85	1.44
0.6	2.15	2.84	1.75	0.716
0.5	1.62	2.20	1.10	0.328
0.4	1.24	1.64	0.687	0.130
0.3	0.956	1.23	0.412	0.040
0.2	0.720	0.569	0.224	0.008
0.1	0.494	0.255	0.093	0.0005

Table 5

Values of $-B_T\ B_T''$ with the variation of V/V_0 for LiH calculated from (a) Vinet-Rydberg EOS (b) Shanker EOS (c) Shanker-Kushwah EOS (d) Keane's EOS

V/V_0	(a)	(b)	(c)	(d)
1.0	4.31	3.75	3.79	4.14
0.9	3.06	3.06	2.57	2.63
0.8	2.24	2.24	1.79	1.69
0.7	1.69	1.92	1.26	1.09
0.6	1.29	1.45	0.884	0.687
0.5	0.998	1.06	0.615	0.416
0.4	0.768	0.730	0.417	0.234
0.3	0.579	0.452	0.269	0.115
0.2	0.432	0.235	0.155	0.044
0.1	0.285	0.079	0.068	0.009

Table 6

Values of $-B_T\ B_T'$ with the variation of V/V_0 for MgO calculated from (a) Vinet-Rydberg EOS (b) Shanker EOS (c) Shanker-Kushwah EOS (d) Keane's EOS

V/V_0	(a)	(b)	(c)	(d)
1.0	6.43	5.75	7.99	6.29
0.9	4.25	4.13	4.70	3.62
0.8	2.97	3.30	2.94	2.14
0.7	2.16	2.57	1.91	1.27
0.6	1.66	1.96	1.26	0.739
0.5	1.23	1.68	0.836	0.406
0.4	0.948	1.06	0.544	0.202
0.3	0.725	0.697	0.338	0.085
0.2	0.538	0.394	0.189	0.026
0.1	0.360	0.247	0.080	0.003

Conclusions

In the present study we have thus found that all values of $B_T\ B_T''$ are negative and tend to zero as $\frac{V}{V_0} = 0$.

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