Study of Inverted Type Equations of State for Solids at Constant Temperature and High Pressure

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Abstract - In the present paper, have two parameter EOS, three parameter EOS and generalized new three parameter isothermal EOSs. Two parameters EOSs such as Bridgman EOS, Tait EOS, Hayward EOS and three parameter EOSs, such as Shanker-Kushwah EOS, Bose Roy and Bose Roy EOS, Freund Ingalls EOS, Kumari-Dass EOS. A detailed comparison study represented with the Kumari-Dass EOS and Freund-Ingalls EOS. These inverted type equation of state give a large information about the P-V- data and behavior of the solids such as NaCl and MgO and others. Which equation of state express volume ratio as a function of pressure for solid materials at a certain temperature, and pressure range 0-30 (GPa) for NaCl and 0-300 (GPa) for MgO solids and compression range 1-0.647, isothermal bulk modulus range 24-120, first pressure derivative range 5.5-1.63 for NaCl and compression range 1-0.493, isothermal bulk modulus range 157-604,first pressure derivative range 4.37-0.281 for Mgo with Kumari and Dass EOS and with freund-Ingalls EOS V/V0 range 1-0.665, BT range 24-152, B'T range 5.5-3.66 for NaCl and V/V0 range 1-0.539, BT=157-895, B'T range 4.37-1.59 for MgO Solids.

Keywords-Two, Three parameter EOSs, isothermal bulk modulus, First pressure derivatives , high pressure.

I. INTRODUCTION

We find new equations of state for solid, when applied different values data and constant values, if these values are valuable with experimental pressure – volume (P-V) [19-26] data. However, the applying of pressure volume data related to a limited range of pressure does not provide any support for the validity of the new related EOS beyond the range of applying. Stacey Davis and Shanker [18,11] have discussed that new or old, almost every type of EOS, Can be applying to given range of P-V data by arranging the parameters B_0, B_0' and B_0'' these parameters representing the isothermal bulk modulus and its pressure derivatives at zero pressure. The satisfied values of these parameter may not be physically meaningful.

Shanker and Stacey [15, 14] have given statement in favour of curve fitting procedure for the explanation of results on isothermal bulk modulus and isothermal compression describing the P-V relationship. Bose roy also discussed about the isothermal compression, but these arguments are not valid in the view of the observations made by Davis and Stacey [18]. The arguments given by Bose Roy S and Boss Roy P [19], that the bulk modulus and its pressure derivative are not known clearly even for the simple solid like Nacl, but Mgo and such other solids have quite nearly values for B_0 and B_0' Shanker and Kushwah [16] given very close value of B_0, B_0' for solids Nacl, Kcl, Mgo and Cao.

P-V data related equations of state are given by short coming on the inverted type equations of state these equations discussed very carefully on the P-V data relation. In the present study that some of these EOS does not follow basic rules for the validity of an EOS [18]. Roy – Roy [19-25] given some recently drive some inverted type equations of state, which express the volume ratio as a function of pressure. They have tells new nomenclature "realistic equations of state". But in non inverted type equation of state, which expressing pressure as a function of V/V_0. Such as Rydbery – Vinet [15, 16] EOS and Birch – Murnaghun [17] EOS, these equations of state also introduced by new nomenclature unrealistic equation of state. Such a nomenclature for equations of state is not reasonable.

II. INVERTED TYPE EOS:

In the non-inverted type EOS pressure express as a function of volume $\left(V/V_0\right)$ where V_0 is the volume at P = 0 and V/V_0 ratio of volume related to the compression. Non-inverted type equations of state shows as mathematical notation-

$$P = f\left(V/V_0, B_0, B_0', B_0'' \dots\right) \qquad \dots\dots\dots\dots\dots\dots\dots\dots\dots(1)$$

Such types equations of state given by Shanker EOS, Birch-Murnaghan EOS etc. And inverted types EOS shows that the volume express as the function of pressure. The inverted type equation shows as mathematical notation-

$$V/V_0 = f\left(P, B_0, B_0', B_0'' \dots\right) \qquad \dots\dots\dots\dots(2)$$

Where V is the volume and V_0 volume at pressure at P = 0, and B_0 is the bulk modulus, B at P = 0, B_0' and B_0'' are the pressure derivative of bulk modulus $B_0 = \frac{dB}{dP}$ is the first pressure derivative and $B_0'' = \frac{d^2B}{dP^2}$ is the second pressure derivative at P = 0. These have been various EOS to propose inverted type EOS as reviewed earlier given two parameter equation of state by Bridgman EOS [37] , Tait EOS [39] , Hayward EOS[38] and three parameter equation of state by Shanker- Kushwah [11], Kumari- Dass [24], Freund- Ingalls EOS [25], Boss – Roy and Boss – Roy [19].These several types equations of state and applied to many material. In the present study we take following seven equations of state and generalized equations of state ,but detail study on two equations of state such as freund-Ingalls and Kumari-Dass equations of state-

2.1 Bridgman EOS [37]-

$$\frac{V}{V_0} = 1 + aP + bP^2 \qquad \dots\dots\dots\dots\dots\dots\dots\dots(3)$$

2.2 Tait EOS [39] -

$$\frac{V}{V_0} = 1 - a l_n(1 + bP) \qquad \dots\dots\dots\dots\dots\dots(4)$$

2.3 Hayward [38] –

$$\frac{V}{V_0} = 1 - \frac{aP}{b+P} \qquad \dots\dots\dots\dots\dots\dots\dots(5)$$

2.4 Shanker – Kushwah EOS [27]-

$$\left(1 - \frac{V}{V_0}\right) = \frac{(2P+a_1)}{2(P-a_2)}\left[1 - \left\{1 - \frac{4(P-a_2)}{(2P+a_1)}\right\}^{1/2}\right] \qquad \dots\dots\dots\dots(6)$$

2.5 Bose Roy and Bose Roy EOS [19-29]-

$$\frac{V}{V_0} = \left[1 + aP(1 + bP)^C\right]^{-1} \qquad \dots\dots\dots\dots\dots\dots\dots..(7)$$

2.6 Freund – Ingalls EOS [25]-

$$\frac{V}{V_0} = \left[1 - a l'_n(1 + bP)\right]^C \qquad \dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots(8)$$

2.7 Kumari – Dass EOS [24]-

$$l_n\left[{}^{V(P,T)}\!/_{V(0,T)}\right] = -\left({}^{1}\!/_{n}\right)l_n\left[\left\{1+{}^{B_T(0,T)}\!/_{B_T'(0,T)Z}\right\}\{1-\exp\left(-ZP\right)\}\right]-\frac{ZP}{n} \quad ....(9)$$

Above equations (3-5) contains two parameter a and b , equations (6-9) contains three parameters a, b and c. These parameter's have different value for different equations . The expressions for a, b and c in terms of Bo , $B_0' and B_0''$ can be found in references[19-29,37-45]. The expression for isothermal bulk modulus BT = - vdp/dv $B_T' = \frac{dB_T'}{dp} = -\frac{vd^2p}{dpdv}$, $B_T'' = \frac{d^2B_T}{dp^2} = -\frac{vd^3p}{d^2pdv}$, BT B_T', B_T'' be obtained from equation (3-9) by method of successive differentiation with respect to pressure p.

III. General Information about EOSs:

In present valuable comparatively analysis of thermodynamics of solids in the limit of extreme compression, Stacey [13, 14] has given some general information which must be discussed by an EOS for its applicability and valuable validity. The range to which these information are satisfied by some EOSs . We note these information , and discuss them with reference to the inverted type equations (3 - 9).

I. The pressure derivative of isothermal bulk modulus $B_T' = \frac{dB_T}{dP}$ must decrease progressively with the increase in pressure such that B_T' remains greater than 5/3 in the limit of infinitely large pressure, i.e. $P \rightarrow \infty$ and ${}^{V}\!/_{V_0} \rightarrow 0$

II. In the limit ${}^{V}\!/_{V_0} \rightarrow 0$, the pressure should not remain finite but it must approach infinity.

III. The isothermal bulk modulus must increase continuously with the increase in pressure such that $B_T' \rightarrow \infty$ in the limit of infinitely large pressure.

IV. In the limit $P \rightarrow \infty$, the ratio B_T/P remains finite such that $\left(\frac{dB_T}{dP}\right)_\infty = \left(\frac{B_T}{P}\right)_\infty$ for all the equations of the state balancing the condition $B_\infty' > 0.$

V. The volume decreases continuously with the increase in pressure.

VI. These equations in an inverted EOS and therefore pressure can also computed as a function of ${}^{V(P,T)}\!/_{V(0,T)}$

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IV. Results and Discussion

In the present study equation (3-9) the estimating values of v/v0 , BT and BT in case of MgO and NaCl .Calculating the value of v/v0 the input data for MgO B0=157 Gpa, B0 =4.37 Gpa and B0 '=0.040(Gpa) 1 and expected value of pressure starts on 100 Gpa up to 300 Gpa, based on the first principals reported by Hama and Suito [8] ,for NaCl input data have taken B0=24 Gpa ,B0 =5.5 and B0 '=0.223(Gpa)-1 from Anderson [7] B0 ' based on experimental data [6].

Kumara and Dass EOS [24] bassed on the high pressure has been widely used in the recent literature [24]. According to this EOS from equatio(5).

=B0Z+B0 =BT(0,T)Z+BT (0,T)

$$B_T = B_0\left[1+\frac{B_0'}{B_0Z}\{1-\exp\left(-zp\right)\}\right] \quad ....(10)$$

Where $$\left[\frac{\partial^2 B_T(P,T)}{\partial P^2}\right]_T \Big/ \left[\frac{\partial B_T(P,T)}{\partial P}\right] = -Z$$

$$B'_T = B'_0 \exp(-zp) \qquad \text{.................(11)}$$

$$B''_T = -zB'_0 \exp(-zp)$$

Compare with the freund and Ingalls EOS [25] from equation (9)

Where $$a = \left[\left(B_0'^2 - 4B_0B_0''\right)^{1/2} - B_0'\right] \Big/ \left[\left(B_0'^2 - 4B_0B_0''\right)^{1/2} + B_0'\right]$$

$$b = \left[\left(B_0'^2 - 4B_0B_0''\right)^{1/2} + B_0'\right] \Big/ 2B_0 \quad , \quad c = 2 \Big/ \left[\left(B_0'^2 - 4B_0B_0''\right)^{1/2} - B_0'\right]$$

$$B_T = \frac{(1+bP)[1-a\,l_n(1+bP)]}{abc} \qquad \text{..................(12)}$$

$$B'_T = \frac{[-ab+b(1-al_n(1+bP))]}{abc} \qquad \text{....................(13)}$$

$$B''_T = -\frac{b}{c}(1/1+bp)$$

The results from equation (8,9), with equation (10-13) for NaCl and MgO determined in table -1and 2 with comparing study for solids, and graphs (1.a-2.d) also contains with results and comparable study Kumari-Dass EOS with Freund-Ingalls EOS for volume compressions(v/v0), isothermal bulk modulus and first pressure derivative , both solids NaCl and MgO. Kumari-Dass EOS and Freund-Ingalls EOS gives approximate similar results for volume compression, when pressure increases, isothermal bulk modulus have few difference for NaCl and for MgO have more difference ,first pressure derivative have very large difference for NaCl and for MgO some points have less difference but after pressure 50(GPa) B'_T decreases instantaneous with Kumari-Dass EOS and increases with Freund-Ingalls EOS at increasing pressure.

V. CONCLUSIONS

We have thus presented a critical and important test of some inverted type equations of state on the basis of criteria based on the thermodynamics of the solids in the limit of infinite pressure at the constant temperature such as in isothermal conditions . The results for pressure –volume relationship from equation (8,9) and bulk modulus from equation (10,12) and first pressure derivative from equation (11,13) . If pressure is increases for NaCl and Mgo solids then V/V0 and first pressure derivative decreases continuously but isothermal bulk modulus is increases continuously with kumari - dass and freund-Ingalls EOSs shows by table(1,2) and also represented with the help of graphs (1.a-2.c).

REFERENCES

[1] Joshi D.C., Gupta AP and Singh S, Indian J Pure and Appl Physics, 42 (2004) 347.
[2] Kumar M, Indian J Pure and Appl Phys. 40 (2002) 202.
[3] Kean A, Aust J Phys; 7 (1954) 322.
[4] Kumar M, Physica B, 217 (1996) 143.
[5] Kumar M, Physica B, 212 (1995) 391.
[6] Hart S and Green Wool PH, Solid State Commun. 46 (1983) 161.
[7] Anderson OL, Equation of State of Solids for geophysics and Ceramic Science Oxford University Press, New York 1995.
[8] Hamu J and Suito K, J Phys Condens Matter, 8 (1996) 67.
[9] Sushil K, Arunesh K, Singh P.K. Sharma B.S. Physica B, 352 (2004) 134.
[10] Gaurav S. Sharma B.S. Sharma, S.B. and Upadhyay S.C. Physica B. 322 (2002) 328.
[11] Shanker, J. Kushwah SS and Sharma MP, Physica, 271 (1999) 158.
[12] Shanker J, Kushwah SS and Kumar M, Physica B 239 (1997) 337.
[13] Stacey F.D. Phys Earth Planet Inter, 128 (2001) 179.
[14] Stacey F.D., Geo. Phys. J. Int. 143 (2000) 621.
[15] Vinet P, Rose JH Ferrante J and Smith J.R. J. Physics Condens Matter, 1 (1998) 1941.
[16] Rydberg R, Z Phys, 73 (1932) 376.
[17] Birch F, J Geophys Res, 547 (1952) 227.
[18] Stacey F.D. and Davis PM, Phys Earth Planet Inter, 142 (2004) 137.
[19] Bose Roy S and Bose Roy P, Physica B, 350 (2004) 375.
[20] Bose Roy S and Bose Roy P, P Phys Chem Solid 64 (2003) 1305.
[21] Bose Roy S and Bose Roy P, J Phys Condens Matter, 15 (2003) 1643.
[22] Bose Roy S and Bose Roy P, Phys Stat Sol (b) 226 (2001) 125.
[23] Bose Roy S and Bose Roy P, J Phys Condens Matter, 11 (1999) 10375.
[24] Kumari M and Dass NJ Phys Condens Matter 2 (1990) 3219 and 7891.
[25] Freund J. Ingalls R, J Phys Chem Solid 51 (1989) 263.
[26] Grover R, Getting I.G. and Kennedy G.C. Phys Rev B7, (1973) 567.
[27] Shanker J and Kushwah SS High Temp High Pressure 33, (2001) 207.
[28] Parsafar G. and Mason E.A. Phy. Rev B. 49, (1994) 3049.
[29] Anderson OL. Masuda K. and Guo D.J. Physics Earth Pla Inter 85 (1995), 35.
[30] Suzuki I.O. Kajima and Seyak J. Phys Earth 27, (1979) 63.
[31] Murnaghan F.D. Proc Symp Appl. Math. 1 (1949) 158.
[32] Ruoff AL and Chhabildas L.C., High Pressure Science and Technology, Plenum New York. 19 (1979).
[33] Zharkov V.N. and Kalin in V.A., Earths Crust and Upper Mantle (1969) 652.
[34] American Institute of Physics Hand Book McGraw Hill (1972) 4.
[35] Cannon J.F., J. Phys Chem Ref Data 3 (1979) 781.
[36] Merrill L. J. Phys Chemi. Ref. Data 6 (1977) 1205.
[37] Bridgman P.w., The Physics of High Press G. Bell and Sons Ltd. London (1952) 169.
[38] Hayward A.J, J. Appl. Phys 18 (1967) 965.
[39] Borelius G., Solid State Phys New York 6 (1958) 65.
[40] Hung, Y.K. and Chaw C.Y.T. Phys. D App. Phys 7 (1974) 7.
[41] Holzapfel W.B, Rep. Prog. Phys 59 (1906) 29.
[42] Jeanloz R., J. Geophys Rev. B 38 (1988) 805.
[43] Kuchhal P., Kumar R, and Dass N. J. Phys Condens Matter 9 (1997) 2989.
[44] Barsch G.R., Chang Z.P. Natl, Bur. Std. (US) Spec. Publ. 326 (1971) 173.
[45] Kuchhal P and Dass. M.J. Phys. Vol 61. No. 4 (2003) 753-757.
[46] Gibson,R.E., J.Am Chem. Soc,57,(1935)284.
[47] Gibson,R.E.and O.HLffer, J.Am Chem. Soc,63,(1941)898.
[48] Vinet P,Smith J.R.,Ferrante J and Rose J H. J.Phy C19(1986)L467

Table-1 –Values of P ,B_T and B'_T calculated from (a) kumari –Dass EOS (b) Freund Ingalls EOS for NaCl solid.

	(a)			(b)		
P(Gpa)	V/V_0	B_T Gpa	B'_T	V/V_0	B_T Gpa	B'_T
0	1	24	5.5	1	24	5.5
1	0.963	29.4	5.28	0.963	29.4	5.31
2	0.934	34.6	5.07	0.934	34.7	5.15
3	0.909	39.5	4.87	0.909	39.3	5.01
4	0.887	44.3	4.68	0.887	44.7	4.89
5	0.868	48.9	4.49	0.869	49.5	4.79
10	0.798	69.2	3.67	0.799	72.5	4.41
15	0.748	85.8	3	0.753	93.9	4.15
20	0.709	94.4	2.45	0.717	114	3.95
25	0.676	111	2	0.698	133	3.79
30	0.647	120	1.63	0.665	152	3.66

Table-2 –Values of P ,B_T and B'_T calculated from (a) kumari –Dass EOS (b) Freund Ingalls EOS for MgO solid.

	(a)			(B)		
P(Gpa)	V/V_0	B_T Gpa	B'_T	V/V_0	B_TGpa	B'_T
0	1	157	4.37	1	157	4.37
5	0.971	178	4.17	0.971	179	4.19
10	0.945	199	3.99	0.945	199	4.03
20	0.903	237	3.64	0.903	238	3.76
30	0.868	272	3.32	0.865	274	3.55
40	0.838	303	3.03	0.839	309	3.37
50	0.812	332	2.77	0.814	342	3.22
100	0.714	443	1.75	0.721	488	3.65
150	0.643	514	1.11	0.658	610	2.28
200	0.586	558	0.701	0.611	717	1.99
300	0.493	604	0.281	0.539	895	1.59

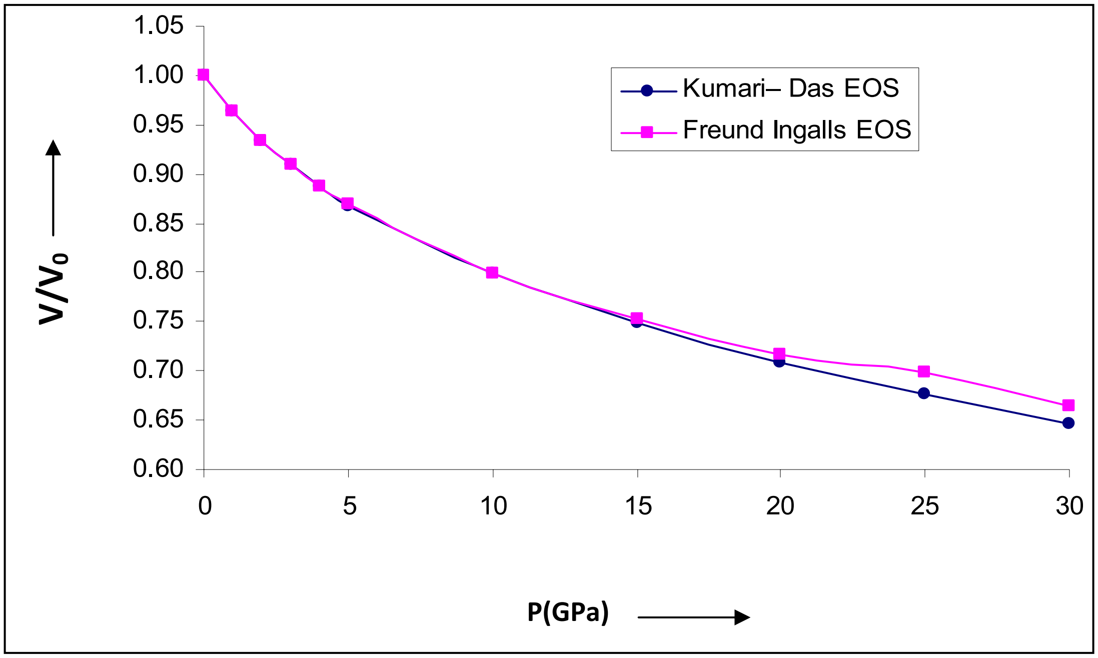

Fig. 1a : Plot between pressure P(GPa) and volume compression (V/V_0) for NaCl solid

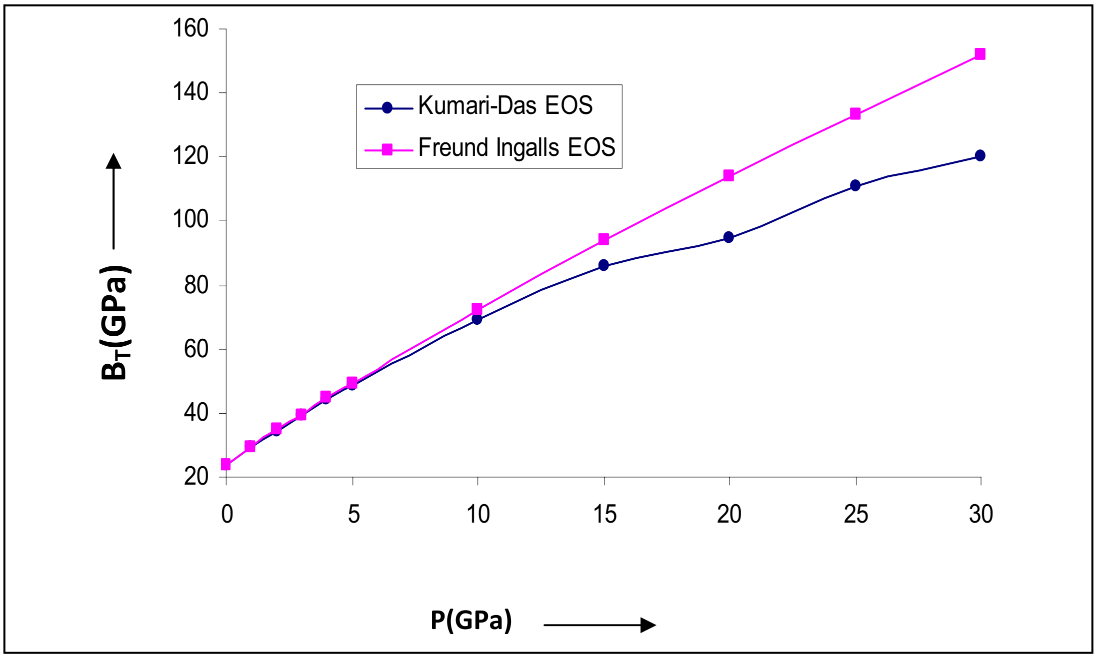

Fig. 1b : Plot between pressure P(GPa) and isothermal bulk modulus B_T (GPa) for NaCl solid.

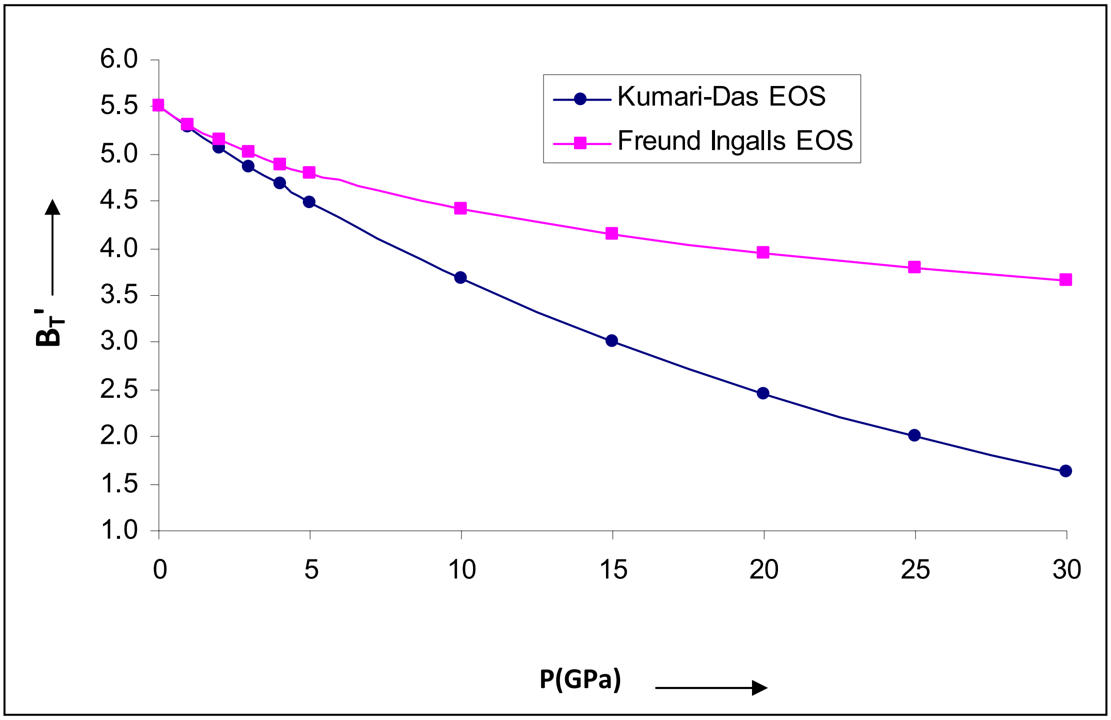

Fig. 1c : Plot between pressure P(GPa) and first pressure derivative B_T' for NaCl solid.

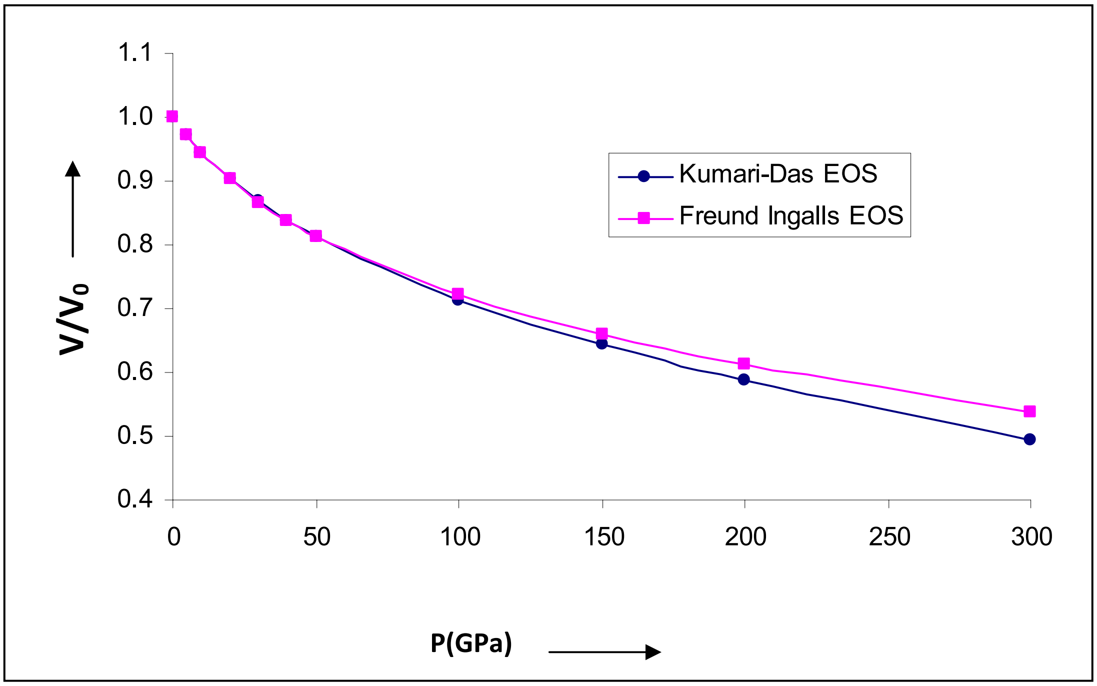

Fig. 2a : Plot between pressure P(GPa) and volume compression (V/V_0) for MgO solid .

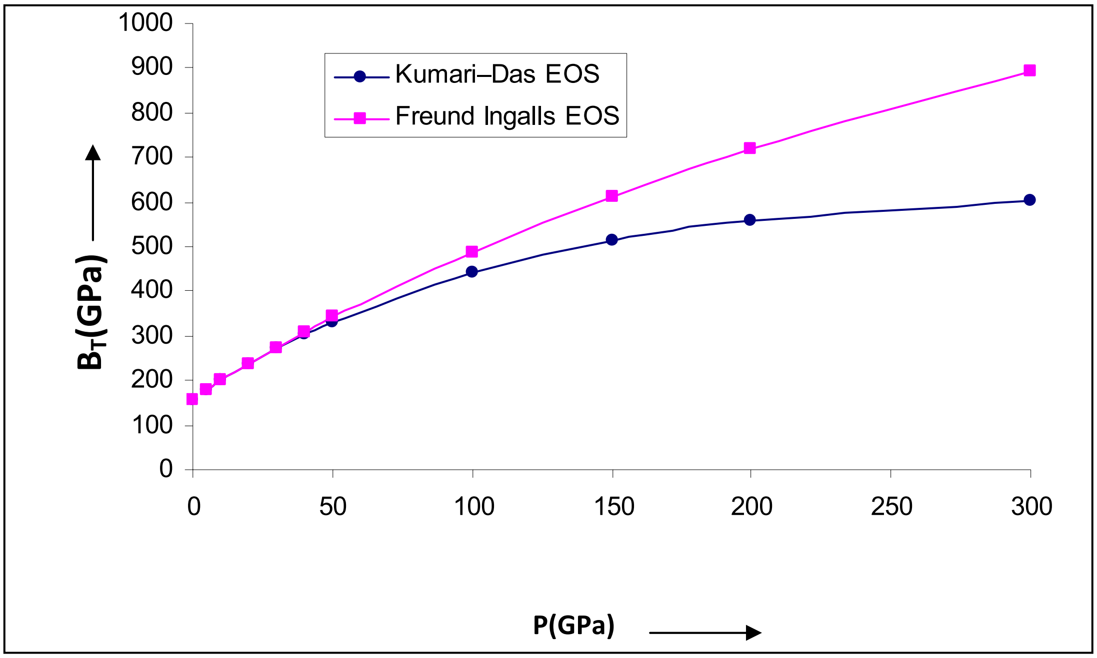

Fig. 2b : Plot between pressure P(GPa) and isothermal bulk modulus B_T (GPa) for MgO solid.

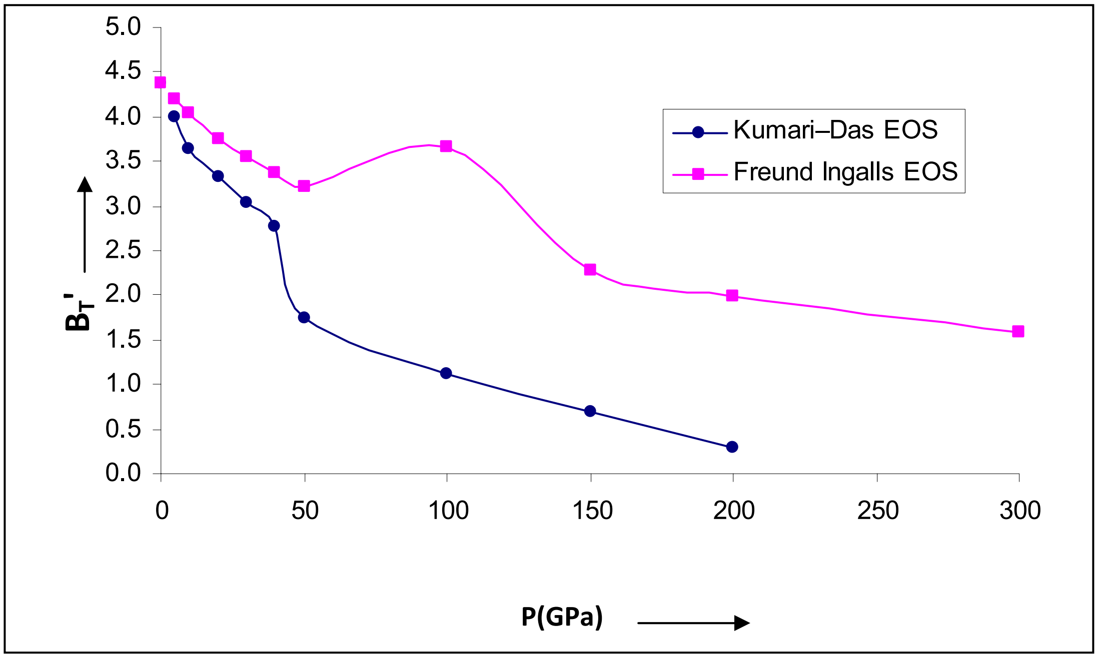

Fig. 2c : Plot between pressure P(GPa) and first pressure derivative B_T' for MgO solid.