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ORIGINAL ARTICLE

Equations of State based on Exponential Potential Energy Function for Some Solids

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ABSTRACT

The pressure–volume relationships have been calculated for monoatomic and diatomic solids with different nature of chemical bonds. We have selected four kinds of monoatomic solids a typical sp metal (Al), a substance which is most difficult to metallize (Ne), a rare–gas metal (Cu) and a large–gap insulator with a small bulk modulus (Ar). For diatomic solids, we selected one with a small bulk modulus, i.e. LiH and the other with large bulk modulus, i.e. MgO. We have studied equations of state based on potential energy functions, viz. Birch– Murnaghan Fourth Order EOS, Morse EOS, Rydberg EOS and Davydov EOS. The results are compared with the corresponding values obtained from the Shanker EOS and Hama-Suito EOS. The Rydberg–Vinet equation departed from the theoretical pressures at a larger value of V/V_0 for diatomic solids than for monoatomic solids, but it is still in good agreement with theoretical values among the others.

Key words: *Equation of state, bulk modulus, potential energy functions, solids*

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INTRODUCTION

The equation of state of solids is fundamentally important in many fields such as condensed matter physics and geophysics. An EOS provides useful information about the relationship between pressure, volume and temperature which helps us to understand the behaviour of materials under the effect of high pressures and high temperatures (Anderson and Isaak, 1993; Shanker and Thomas, 1997). The bulk modulus is fundamentally related to the second order derivatives of free energy with respect to volume. The pressure derivatives of bulk modulus are therefore related to the higher order derivatives of potential energy and their evaluation is very sensitive to the forms of potential energy functions or of equation of state used (Stacey, 1991 and Shanker *et al*. 1997). Thus a study of bulk modulus not only provides an adequate description for pressure–volume relationship under different thermodynamic conditions, but is also useful for the development of models determining higher derivative thermoelastic properties of solids (Stacey and Isaak 2001; Stacey, 2005). We studied equations of state based on potential energy functions, viz. Birch–Murnaghan Fourth Order EOS, Morse EOS, Rydberg EOS and Davydov EOS. The parameters appearing in the potential energy functions are determined using the zero–pressure or atmospheric pressure values of bulk modulus and its pressure derivative at reference temperature. Equations of state representing isothermal pressure–volume relationships are then used to predict the

compressions of materials at high pressures and also to determine the values of bulk modulus as a function of pressure and temperature. The results obtained from the equations based on potential energy functions have been compared with the corresponding values determined from the Shanker EOS and Hama-Suito EOS for different solids.

METHOD OF ANALYSIS

The pressure–volume relationships for different EOS used are given below.

Birch-Murnaghan Fourth–Order EOS:

Using the strain and the method of Stacey, we obtain the following expression.

$$P = \frac{9}{16} K_0 \left[-B_1 x^{-5/3} + B_2 x^{-7/3} - B_3 x^{-3} + B_4 x^{-11/3} \right] \quad \text{....(1)}$$

where $x = \frac{V}{V_0}$, and

$$B_1 = K_0 K_0'' + (K_0' - 4)(K_0' - 5) + \frac{59}{9}$$

$$B_2 = 3K_0 K_0'' + (K_0' - 4)(3K_0' - 13) + \frac{129}{9}$$

$$B_3 = 3K_0 K_0'' + (K_0' - 4)(3K_0' - 11) + \frac{105}{9}$$

$$B_4 = K_0 K_0'' + (K_0' - 4)(K_0' - 3) + \frac{35}{9}$$

Morse EOS:

Morse EOS (Morse, 1929) has been obtained using the double exponential potential energy function and it can be expressed as

$$P = \frac{3K_0}{f} x^{-2/3} \left[e^{2f\left(1 - x^{1/3}\right)} - e^{f\left(1 - x^{1/3}\right)} \right] \quad \text{....(2)}$$

where $x = \frac{V}{V_0}$ and $f = K_0' - 1$

Rydberg – Vinet EOS:

Vinet *et al*. 1989 have obtained the following EOS which is based on the potential energy function due to Rydberg, 1932.

$$P = 3K_0 x^{-2/3} \left(1 - x^{1/3}\right) \exp\left[f\left(1 - x^{1/3}\right)\right] \quad \text{....(3)}$$

where $x = \frac{V}{V_0}$ and $f = \frac{3}{2}(K_0' - 1)$

Davydov EOS:

Davydov obtained another alternative form which has been mentioned by Zharkov and Kalinin, 1971 based on a different potential energy function which yields

$$P = \frac{3K_0}{(f + 2)} \left[x^{-4/3} + f x^{-1} - (f + 1) x^{-2/3} \right] \exp\left[f\left(1 - x^{1/3}\right)\right] \quad \text{....(4)}$$

where $x = \frac{V}{V_0}$, $f = \frac{3}{4}\left[(K_0' - 3) + \left\{(K_0' + 1)\left(K_0' - \frac{5}{3}\right)\right\}^{1/2}\right]$

Shanker EOS:

Shanker *et al*. 1997 have obtained an EOS using the volume dependence of the interatomic force constant determined from the derivatives of potential energy

$$P = \frac{K_0 x^{-4/3}}{t}\left[\left(1 - \frac{1}{t} + \frac{2}{t^2}\right)\{\exp(ty) - 1\} + y\left(1 + y - \frac{2}{t}\right)\exp(ty)\right] \quad \text{....(5)}$$

where $x = \frac{V}{V_0}$, $t = K_0' - \frac{8}{3}$ and $y = 1 - \frac{V}{V_0}$

Hama-Suito EOS:

Hama and Suito 1996 have obtained an EOS using methods based on first–principles such as the APW method and the quantum statistical method. The Hama–Suito EOS has been found to be consistent with the ab initio results for different types of solids, for the entire range of compressions corresponding to low pressure, intermediate pressures and extremely high pressures. The expressions based on the Hama–Suito EOS are given below

$$P = 3K_0 x^{-5/3}(1 - x^{1/3})\exp\left[\frac{3}{2}(K_0' - 3)(1 - x^{1/3}) + \left(z - \frac{3}{2}\right)(1 - x^{1/3})^2\right] \quad \text{....(6)}$$

where $x = \frac{V}{V_0}$ and $Z = \frac{3}{8}(K_0' - 1)(K_0' + 3) + \frac{3}{2}K_0 K_0'' + \frac{1}{3}$ ....(7)

The values of the bulk modulus at zero pressure, K_0 and of its pressure derivative at zero–pressure, K_0', are used as input data to determine bulk modulus of different solids as a function of pressure. Now, the expressions for K derived from different equations of state are given below.

Birch – Murnaghan Fourth order EOS:

$$K = \frac{9}{16}K_0\left[-B_1\left(\frac{5}{3}\right)x^{-5/3} + B_2\left(\frac{7}{3}\right)x^{-7/3} - B_3(3)x^{-3} + B_4\left(\frac{11}{3}\right)x^{-11/3}\right] \quad \text{....(8)}$$

where $x = \frac{V}{V_0}$, and

$$B_1 = K_0 K_0'' + (K_0' - 4)(K_0' - 5) + \frac{59}{9}$$

$$B_2 = 3K_0 K_0'' + (K_0' - 4)(3K_0' - 13) + \frac{129}{9}$$

$$B_3 = 3K_0 K_0'' + (K_0' - 4)(3K_0' - 11) + \frac{105}{9}$$

$$B_4 = K_0 K_0'' + (K_0' - 4)(K_0' - 3) + \frac{35}{9}$$

Morse EOS:

$$K = \frac{K_0}{f}\left[\{2x^{-2/3} + 2fx^{-1/3}\}\exp\{2f(1 - x^{1/3})\} - \{2x^{-2/3} + fx^{-1/3}\}\exp\{f(1 - x^{1/3})\}\right] \quad \text{....(9)}$$

where f= K_0'-1

Rydberg EOS:

$$K = K_0 x^{-1/3}\left[2x^{-1/3} - 1 + \frac{3}{2}(K_0' - 1)(1 - x^{-1/3})\right]\exp\left[\frac{3}{2}(K_0' - 1)(1 - x^{-1/3})\right] \quad \text{....(10)}$$

Davydov EOS:

$$K = \frac{K_0}{(f+2)}\left\{4x^{-4/3} + 4fx^{-1} + (f^2 - 2f - 2)x^{-2/3} - f(f+1)x^{-1/3}\right\}\exp\left\{f(1 - x^{1/3})\right\} \quad \text{....(11)}$$

where $f = \frac{3}{2}\left[(K_0' - 3) + \left\{(K_0' + 1)\left(K_0' - \frac{5}{3}\right)\right\}^{1/2}\right]$

Shanker EOS:

$$K = K_0 x^{-1/3}(1 + y + y^2)\exp(ty) + \frac{4}{3}P \quad \text{....(12)}$$

where $x = \frac{V}{V_0}$, $t = K_0' - \frac{8}{3}$ and $y = 1 - \frac{V}{V_0}$

Hama – Suito EOS:

$$K = \frac{P}{3}\left[\left\{5 + \frac{x^{1/3}}{(1 - x^{1/3})}\right\} + x^{1/3}\left\{\frac{3}{2}(K_0' - 1) + 2Z(1 - x^{1/3}) + 3x^{1/3} - 6\right\}\right] \quad \text{....(13)}$$

where $Z = \frac{3}{8}(K_0' - 1)(K_0' + 3) + \frac{3}{2}K_0K_0'' + \frac{1}{3}$

Now we study the variation of $K' = dK/dP$ with the change in compression (V/V_0). The value of K' depends on the third derivative of potential energy function. The expression for K' derived from different equations of state are given below.

Birch–Murnagham Fourth order EOS:

$$K' = \frac{-B_1\left(\frac{5}{3}\right)^2 x^{-5/3} + B_2\left(\frac{7}{3}\right)^2 x^{-7/3} - B_3(3)^2 x^{-3} + B_4\left(\frac{11}{3}\right)^2 x^{-11/3}}{-B_1\left(\frac{5}{3}\right)x^{-5/3} + B_2\left(\frac{7}{3}\right)x^{-7/3} - B_3(3)x^{-3} + B_4\left(\frac{11}{3}\right)x^{-11/3}} \quad \text{....(14)}$$

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

Morse EOS:

$$K' = \frac{\left[\left\{\frac{4}{3}x^{-2/3} + 2fx^{-1/3} + \frac{4}{3}f^2\right\}\exp\left\{f(1 - x^{1/3})\right\} - \left\{\frac{4}{3}x^{-2/3} + fx^{-1/3} + \frac{1}{3}f^2\right\}\right]}{\left\{2x^{-2/3} + 2fx^{-1/3}\right\}\exp\left\{f(1 - x^{1/3})\right\} - \left\{2x^{-2/3} + fx^{-1/3}\right\}} \quad \text{....(15)}$$

where $f = K_0' - 1$ and $x = \frac{V}{V_0}$

Rydberg EOS:

$$K' = \frac{\left\{f^2(1 - x^{1/3}) + f(3x^{-1/3} - 1) + x^{-1/3}(4x^{-1/3} - 1)\right\}}{3\left\{2x^{-2/3} - x^{-1/3} + f(x^{-1/3} - 1)\right\}} \quad \text{....(16)}$$

where $f = \frac{3}{2}(K_0' - 1)$

Davydov EOS:

$$K' = \frac{\left\{\frac{16}{3}x^{-4/3} + \frac{16}{3}fx^{-1} + \frac{2}{3}\left(3f^2 - 2f - 2\right)x^{-2/3} + \frac{f}{3}\left(f^2 - 3f - 3\right)x^{-1/3} - \frac{f^2}{3}\left(f + 1\right)\right\}}{4x^{-4/3} + 4fx^{-1} + \left(f^2 - 2f - 2\right)x^{-2/3} - f\left(f + 1\right)x^{-1/3}} \quad \text{.(17)}$$

where $f = \frac{3}{4}\left[\left(K_0' - 3\right) + \left\{\left(K_0' + 1\right)\left(K_0' - 5/3\right)\right\}^{1/2}\right]$

Shanker EOS:

$$K' = \frac{4}{3} + \left(1 - \frac{4P}{3K}\right)\left\{\frac{1}{3} + x\left(t + \frac{(1+2y)}{(1+y+y^2)}\right)\right\} \quad \text{....(18)}$$

where $t = K_0' - \frac{8}{3}$ and $y = 1 - \frac{V}{V_0}$

Hama – Suito EOS:

$$K' = \frac{K}{P} - \frac{1}{3} + \frac{P}{9K}\left[x^{2/3}\left\{(2Z-3) - \frac{1}{\left(1 - x^{1/3}\right)^2}\right\} + 5\right] \quad \text{....(19)}$$

where $Z = \frac{3}{8}\left(K_0' - 1\right)\left(K_0' + 3\right) + \frac{3}{2}K_0K_0'' + \frac{1}{3}$

RESULTS, DISCUSSIONS AND CONCLUSIONS

We have calculated the values of P for the six solids viz. Ne, Ar, Al, Cu, LiH and MgO. The input data used in our calculations for K_0, K_0' and K_0'' are taken from ab initio results reported by Hama and Suito 1996 and given in Table 1. We have used the same input data in all the EOS without any adjustments in the values of K_0, K_0' and K_0''so as to make the comparison of the results meaningful.

The results for P are reported in Table 2 for the compression range down to V/V_0 = 0.5. This range of compressions corresponds to very high pressures, which are several times larger than the values of K_0 for the solids under study. It is found from the results given in Table 2 that the EOS based on the potential functions yield good agreement with each other and also with the Hama – Suito EOS derived from the first principles based on the augmented plane wave APW method and the quantum statistical model. The pressure required for different solids to produce the maximum compression V/V_0 = 0.5 are quite different from each other. Thus Ne and Ar are more compressible (less amount of pressure is required at V/V_0 = 0.5) as compared to other solids e.g. Cu and MgO. The bulk modulus represents incompressibility of a material. For Cu and MgO, the bulk moduli have largest values (Table 1) and therefore these solids are highly incompressible, requiring large amounts of pressures for producing high compressions. The relationship between P and V through different equations of state depends on the value of K_0 as well as K_0'. A material would be more incompressible if K_0 and K_0' both are high. For example in case of Cu, K_0 is some what less than that for MgO, but K_0' is larger for Cu than that for MgO. This makes Cu to be more incompressible than MgO. This is evident from the results which reveal P = 620 GPa for Cu, and P = 430 GPa for MgO both at V/V_0 = 0.5, the maximum compression.

Table 1: Values of input-data K_0(GPa), K_0' and K_0'' $(GPa)^{-1}$ all at P=0 and Z, obtained from the Augmented plane wave (APW) method [13]

Material	K_0 (GPa)	K_0'	K_0' $(GPa)^{-1}$	Z
Ne	6.36	7.61	−2.86	−1.385
Ar	6.28	7.07	−2.53	−1.141
Al	72.6	4.85	−0.104	0.253
Cu	135	5.93	−0.083	0.191
LiH	39.1	3.51	−0.106	1.417
MgO	157	4.37	−0.04	1.101

$$Z = \frac{3}{8}(K_0' - 1)(K_0' + 3) + \frac{3}{2}K_0K_0'' + \frac{1}{3}$$

Table 2: Values of P(GPa) calculated from (a) Birch-Murnaghan fourth order EOS (b) Morse EOS (c) Rydberg EOS (d) Davydov EOS (e) Shanker EOS and (f) Hama-Suito EOS

Material	V/V_0	(a)	(b)	(c)	(d)	(e)	(f)
Ne	1.0	0	0	0	0	0	0
	0.9	0.994	1.00	0.995	1.00	1.00	0.993
	0.8	3.23	3.25	3.23	3.24	3.31	3.21
	0.7	8.31	8.41	8.24	8.32	8.65	8.11
	0.6	20.3	20.7	19.8	20.2	21.2	19.3
	0.5	51.4	52.0	48.3	49.8	51.9	46.0
Ar	1.0	0	0	0	0	0	0
	0.9	0.954	0.96	0.995	0.96	0.96	0.953
	0.8	3.01	3.03	3.01	3.02	3.07	2.99
	0.7	7.46	7.56	7.43	7.50	7.70	7.31
	0.6	17.6	17.9	17.3	17.5	18.1	16.7
	0.5	42.5	42.9	40.4	41.6	42.3	38.4
Al	1.0	0	0	0	0	0	0
	0.9	9.83	9.84	9.84	9.86	9.85	9.84
	0.8	27.4	27.5	27.4	27.5	27.5	27.4
	0.7	59.1	59.5	59.2	59.7	59.4	59.4
	0.6	117	120	118	121	119	120
	0.5	224	240	235	243	232	240
Cu	1.0	0	0	0	0	0	0
	0.9	19.3	19.4	19.3	19.4	19.4	19.3
	0.8	57.3	57.4	57.3	57.5	57.7	57.3
	0.7	132	133	132	133	134	133
	0.6	286	290	284	289	289	286
	0.5	618	635	610	629	614	621
LiH	1.0	0	0	0	0	0	0
	0.9	4.94	4.94	4.94	4.96	4.94	4.95
	0.8	12.8	12.8	12.8	12.8	12.8	12.9
	0.7	25.3	25.5	25.4	25.7	25.5	25.9
	0.6	45.7	46.8	46.6	47.5	46.6	48.4
	0.5	78.7	84.3	83.5	86.6	83.3	89.6
MgO	1.0	0	0	0	0	0	0
	0.9	20.7	20.7	20.8	20.8	20.8	20.8
	0.8	56.2	56.3	56.3	56.6	56.4	56.6
	0.7	117	119	118	119	118	120
	0.6	223	231	229	233	229	236
	0.5	404	445	438	453	433	463

Table 3: Values of K_T(GPa) calculated from (a) Birch-Murnaghan fourth order EOS (b) Morse EOS (c) Rydberg EOS (d) Davydov EOS (e) Shanker EOS and (f) Hama-Suito EOS

Material	V/V_0	(a)	(b)	(c)	(d)	(e)	(f)
Ne	1.0	6.36	6.36	6.36	6.36	6.36	6.36
	0.9	13.1	13.2	13.1	13.1	13.3	13.1
	0.8	26.1	26.5	26.0	26.2	27.2	25.7
	0.7	52.5	53.6	51.5	52.2	55.4	50.0
	0.6	110	112	104	107	113	99.4
	0.5	249	248	221	231	235	205
Ar	1.0	6.28	6.28	6.28	6.28	6.28	6.28
	0.9	12.3	12.4	12.3	12.4	12.4	12.3
	0.8	23.5	23.8	23.5	23.6	24.3	23.2
	0.7	45.6	46.2	44.6	45.3	47.1	43.3
	0.6	90.5	92.1	86.7	89.1	91.7	82.2
	0.5	194	194	176	184	182	163
Al	1.0	72.6	72.6	72.6	72.6	72.6	72.6
	0.9	117	117	117	117	117	117
	0.8	186	187	186	187	187	187
	0.7	294	301	297	302	298	300
	0.6	465	497	484	500	480	495
	0.5	717	852	816	864	787	851
Cu	1.0	135	135	135	135	135	135
	0.9	239	240	239	240	241	240
	0.8	417	421	416	419	423	415
	0.7	730	742	725	737	741	731
	0.6	1306	1344	1289	1328	1306	1312
	0.5	2428	2549	2382	2507	2341	2466
LiH	1.0	39.1	39.1	39.1	39.1	39.1	39.1
	0.9	55.4	55.4	55.4	55.5	55.5	55.7
	0.8	78.4	78.8	78.6	79.3	78.8	80.1
	0.7	111	113	113	115	113	117
	0.6	155	166	164	171	163	178
	0.5	204	251	246	263	242	282
MgO	1.0	157	157	157	157	157	157
	0.9	241	241	241	242	242	242
	0.8	367	370	369	372	370	374
	0.7	555	573	567	578	568	586
	0.6	825	907	888	920	879	945
	0.5	1143	1488	1438	1527	1388	1598

Table 4: Values of K_T' calculated from (a) Birch-Murnaghan fourth order EOS (b) Morse EOS (c) Rydberg EOS (d) Davydov EOS (e) Shanker EOS and (f) Hama-Suito EOS

Material	V/V_0	(a)	(b)	(c)	(d)	(e)	(f)
Ne	1.0	7.61	7.61	7.61	7.61	7.61	7.61
	0.9	6.28	3.36	6.26	6.31	6.51	6.21
	0.8	5.50	5.58	5.43	5.49	5.68	5.33
	0.7	4.99	5.02	4.82	4.90	4.97	4.71
	0.6	4.63	4.57	4.34	4.44	4.32	4.21
	0.5	4.36	4.18	3.92	4.04	3.71	3.80
Ar	1.0	7.07	7.07	7.07	7.07	7.07	7.07
	0.9	5.88	5.95	5.87	5.91	6.60	5.81
	0.8	5.16	5.23	5.10	5.16	5.29	5.00
	0.7	4.68	4.71	4.54	4.62	4.63	4.42
	0.6	4.33	4.29	4.09	4.19	4.03	3.95
	0.5	4.06	3.92	3.69	3.82	3.47	3.56
Al	1.0	4.85	4.85	4.85	4.85	4.85	4.85
	0.9	4.20	4.23	4.19	4.23	4.23	4.22
	0.8	3.69	3.77	3.71	3.78	3.73	3.76
	0.7	3.22	3.41	3.33	3.43	3.29	3.40
	0.6	2.72	3.11	3.01	3.13	2.89	3.11
	0.5	1.98	2.83	2.73	2.87	2.54	2.86
Cu	1.0	5.93	5.93	5.93	5.93	5.93	5.93
	0.9	5.04	5.08	5.02	5.06	5.12	5.04
	0.8	4.43	4.49	4.40	4.47	4.48	4.44
	0.7	3.97	4.05	3.93	4.02	3.93	3.98
	0.6	3.59	3.68	3.54	3.65	3.43	3.62
	0.5	3.22	3.36	3.30	3.34	2.98	3.32
LiH	1.0	3.51	3.51	3.51	3.51	3.51	3.51
	0.9	3.12	3.14	3.12	3.17	3.15	3.21
	0.8	2.77	2.85	2.82	2.89	2.83	2.97
	0.7	2.39	2.60	2.56	2.67	2.54	2.77
	0.6	1.91	2.38	2.33	2.47	2.30	2.61
	0.5	1.07	2.17	2.12	2.29	2.08	2.46
MgO	1.0	4.37	4.37	4.37	4.37	4.37	4.37
	0.9	3.81	3.85	3.82	3.86	3.84	3.88
	0.8	3.33	3.45	3.40	3.47	3.40	3.52
	0.7	2.86	3.12	3.06	3.16	3.01	3.23
	0.6	2.26	2.85	2.77	2.90	2.67	2.99
	0.5	1.21	2.60	2.52	2.67	2.35	2.78

Table 5: Values of P/K calculated from (a) Birch-Murnaghan fourth order EOS (b) Morse EOS (c) Rydberg EOS (d) Davydov EOS (e) Shanker EOS and (f) Hama-Suito EOS

Material	V/V_0	(a)	(b)	(c)	(d)	(e)	(f)
Ne	1.0	0.00	0.00	0.00	0.00	0.00	0.00
	0.9	0.07	0.07	0.07	0.07	0.07	0.07
	0.8	0.12	0.12	0.12	0.12	0.12	0.12
	0.7	0.15	0.15	0.16	0.15	0.15	0.16
	0.6	0.18	0.18	0.19	0.18	0.18	0.19
	0.5	0.20	0.20	0.21	0.21	0.22	0.22
Ar	1.0	0.00	0.00	0.00	0.00	0.00	0.00
	0.9	0.07	0.07	0.08	0.07	0.07	0.07
	0.8	0.12	0.12	0.12	0.12	0.12	0.12
	0.7	0.16	0.16	0.16	0.16	0.16	0.16
	0.6	0.19	0.19	0.19	0.19	0.19	0.20
	0.5	0.21	0.22	0.22	0.22	0.23	0.23
Al	1.0	0.00	0.00	0.00	0.00	0.00	0.00
	0.9	0.08	0.08	0.08	0.08	0.08	0.08
	0.8	0.14	0.14	0.14	0.14	0.14	0.14
	0.7	0.20	0.19	0.19	0.19	0.19	0.19
	0.6	0.25	0.24	0.24	0.24	0.24	0.24
	0.5	0.31	0.28	0.28	0.28	0.29	0.28
Cu	1.0	0.00	0.00	0.00	0.00	0.00	0.00
	0.9	0.08	0.08	0.08	0.08	0.08	0.08
	0.8	0.13	0.13	0.13	0.13	0.13	0.13
	0.7	0.18	0.17	0.18	0.18	0.18	0.18
	0.6	0.21	0.21	0.22	0.21	0.22	0.21
	0.5	0.25	0.24	0.25	0.25	0.26	0.25
LiH	1.0	0.00	0.00	0.00	0.00	0.00	0.00
	0.9	0.08	0.08	0.08	0.08	0.08	0.08
	0.8	0.16	0.16	0.16	0.16	0.16	0.16
	0.7	0.22	0.22	0.22	0.22	0.22	0.22
	0.6	0.29	0.28	0.28	0.27	0.28	0.27
	0.5	0.38	0.33	0.33	0.32	0.34	0.31
MgO	1.0	0.00	0.00	0.00	0.00	0.00	0.00
	0.9	0.08	0.08	0.08	0.08	0.08	0.08
	0.8	0.15	0.15	0.15	015	0.15	0.15
	0.7	0.21	0.20	0.20	0.20	0.25	0.20
	0.6	0.27	0.25	0.25	0.25	0.26	0.24
	0.5	0.35	0.29	0.30	0.29	0.31	0.28

Table 6: Values of 1/K' calculated from (a) Birch-Murnaghan fourth order EOS (b) Morse EOS (c) Rydberg EOS (d) Davydov EOS (e) Shanker EOS and (f) Hama-Suito EOS

Material	V/V_0	(a)	(b)	(c)	(d)	(e)	(f)
Ne	1.0	0.13	0.13	0.13	0.13	0.13	0.13
	0.9	0.15	0.15	0.15	0.15	0.15	0.16
	0.8	0.18	0.17	0.18	0.18	0.17	0.18
	0.7	0.20	0.19	0.20	0.20	0.20	0.21
	0.6	0.21	0.21	0.23	0.22	0.23	0.23
	0.5	0.22	0.23	0.25	0.24	0.26	0.26
Ar	1.0	0.14	0.14	0.14	0.14	0.14	0.14
	0.9	0.17	0.16	0.17	0.16	0.15	0.17
	0.8	0.19	0.19	0.19	0.19	0.18	0.20
	0.7	0.21	0.21	0.22	0.21	0.21	0.22
	0.6	0.23	0.23	0.24	0.23	0.24	0.25
	0.5	0.24	0.25	0.27	0.26	0.28	0.28
Al	1.0	0.20	0.20	0.20	0.20	0.21	0.20
	0.9	0.23	0.23	0.23	0.23	0.23	0.23
	0.8	0.27	0.26	0.26	0.26	0.26	0.26
	0.7	0.31	0.29	0.30	0.29	0.30	0.29
	0.6	0.36	0.32	0.33	0.31	0.34	0.32
	0.5	0.51	0.35	0.36	0.34	0.39	0.34
Cu	1.0	0.16	0.16	0.16	0.16	0.16	0.16
	0.9	0.19	0.19	0.19	0.19	0.19	0.19
	0.8	0.22	0.22	0.22	0.22	0.23	0.22
	0.7	0.25	0.24	0.25	0.24	0.25	0.25
	0.6	0.27	0.27	0.18	0.27	0.29	0.27
	0.5	0.31	0.29	0.30	0.29	0.34	0.30
LiH	1.0	0.28	0.28	0.28	0.28	0.28	0.28
	0.9	0.32	0.31	0.32	0.31	0.31	0.31
	0.8	0.36	0.35	0.35	0.34	0.35	0.33
	0.7	0.41	0.38	0.39	0.37	0.39	0.36
	0.6	0.52	0.42	0.42	0.40	0.43	0.38
	0.5	0.93	0.46	0.47	0.43	0.48	0.40
MgO	1.0	0.22	0.22	0.22	0.22	0.22	0.22
	0.9	0.26	0.25	0.26	0.25	0.26	0.25
	0.8	0.30	0.28	0.29	0.28	0.29	0.28
	0.7	0.34	0.32	0.32	0.31	0.33	0.30
	0.6	0.44	0.35	0.36	0.34	0.37	0.33
	0.5	0.82	0.38	0.39	0.38	0.42	0.35

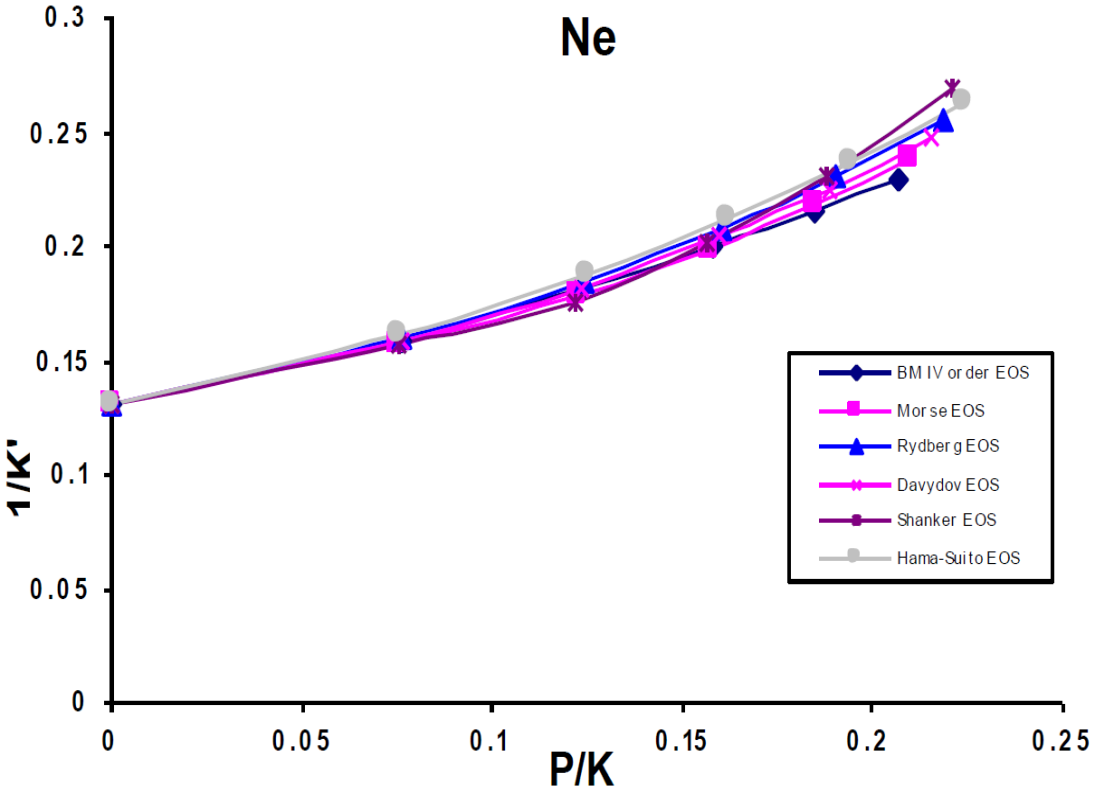

Fig. 1: Plots between P/K and 1/K' for Ne

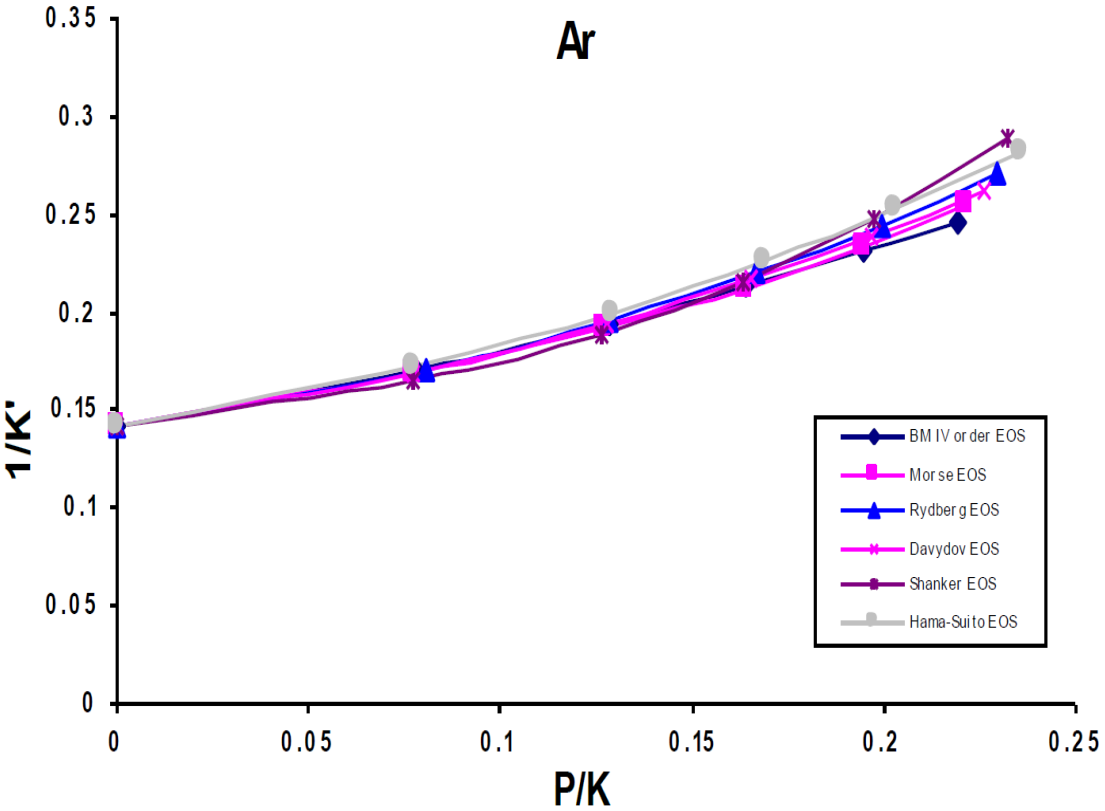

Fig. 2: Plots between P/K and 1/K' for Ar

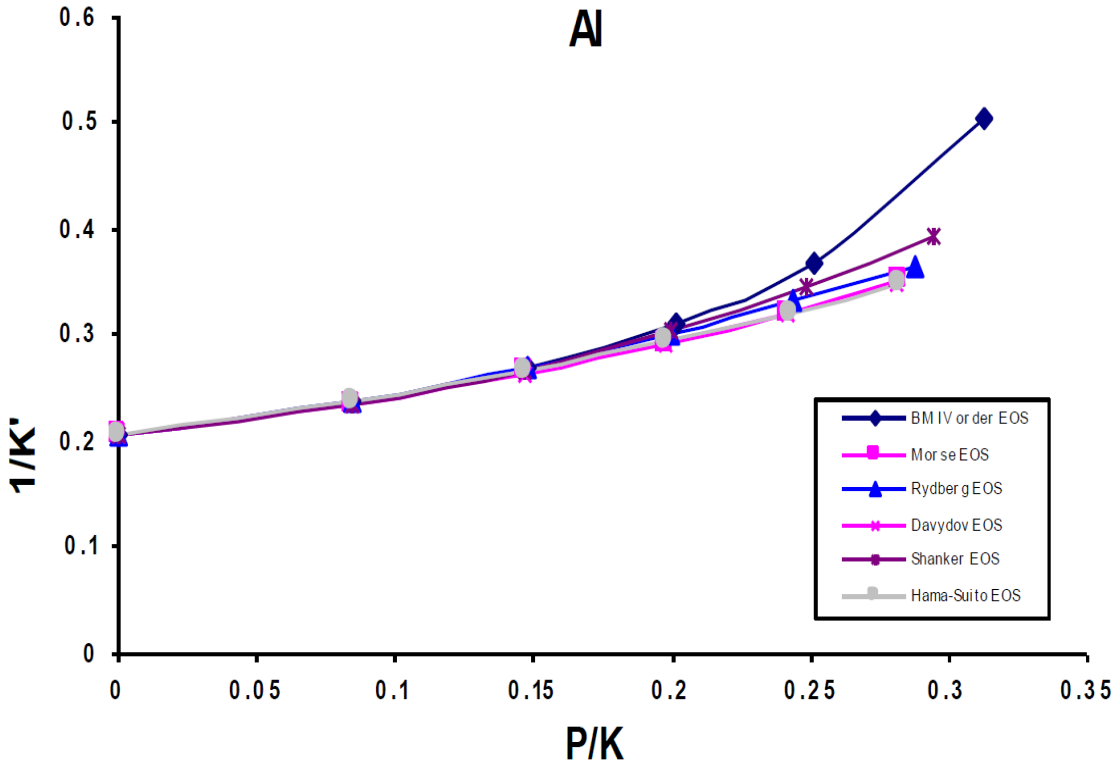

Fig. 3: Plots between P/K and 1/K' for Al

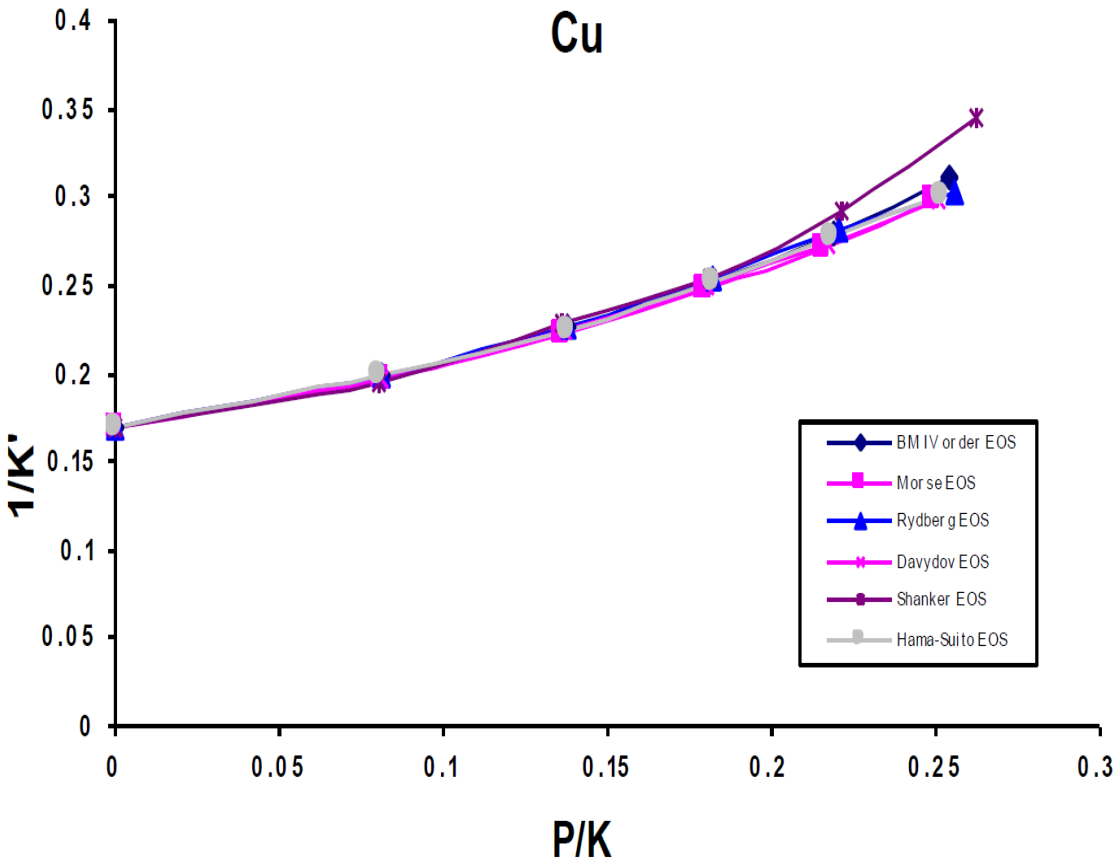

Fig. 4: Plots between P/K and 1/K' for Cu

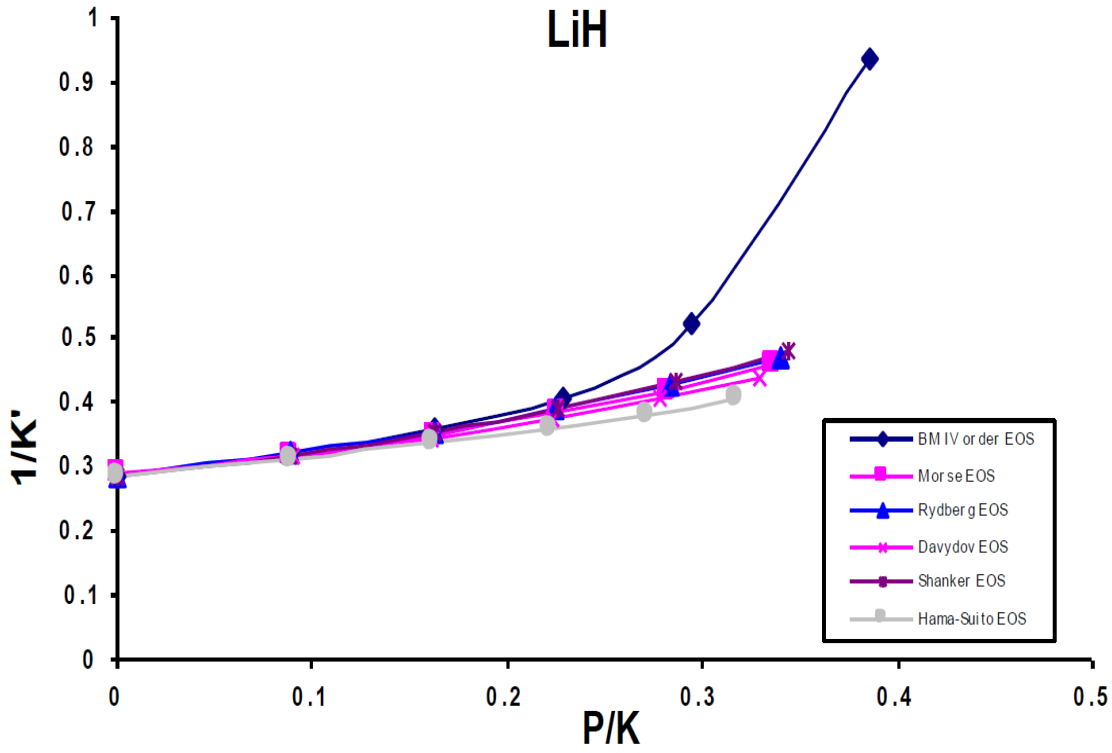

Fig. 5: Plots between P/K and 1/K' for Lih

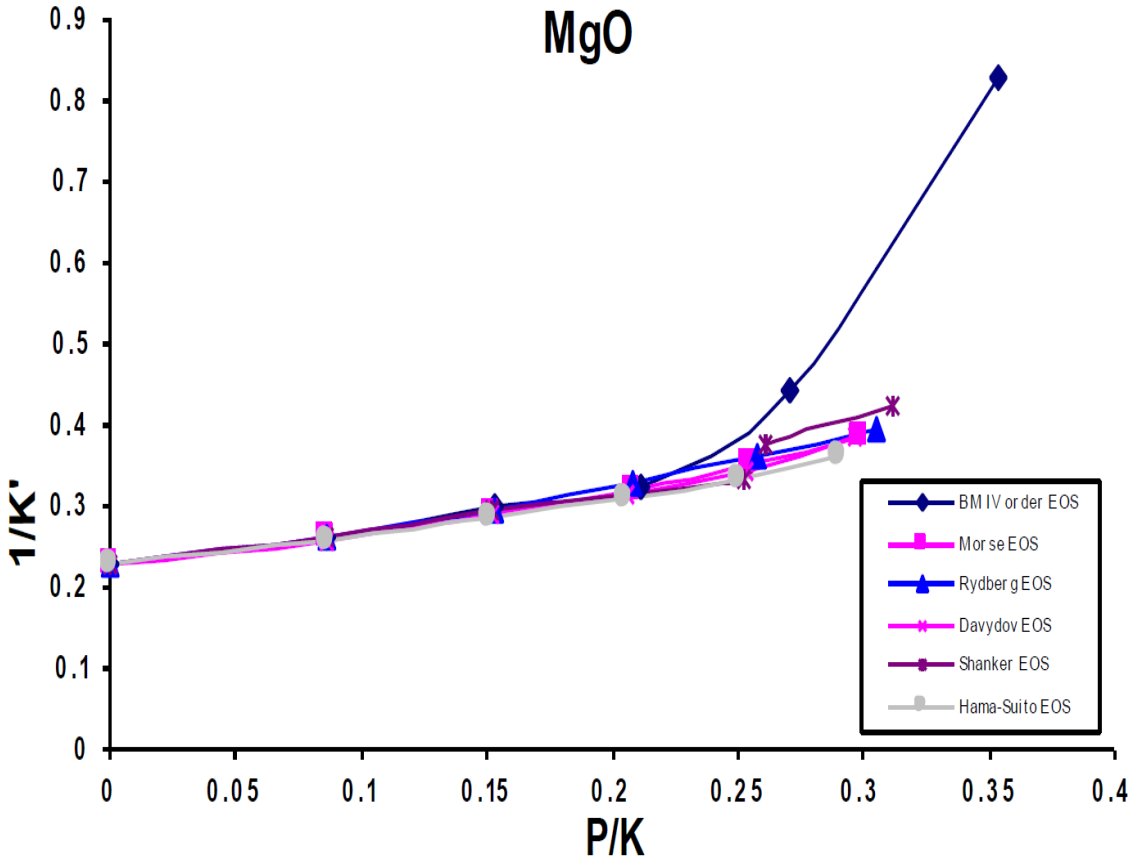

Fig. 6: Plots between P/K and 1/K' for MgO

The results for isothermal bulk modulus K calculated from equations (8 to 13) are given in Table 3. From this table, we note that the equations based on different potential energy functions yield good agreement with each other and also with the Hama–Suito EOS. The bulk modulus increases with the increase in pressure or compression. The rate of increase of K_T depends on the value of K_0' and to some extent also on the value of K_0. For Ne and Ar, the values of K_0' are more than 7 and values of K_0 are small as compared to those for other solids, it is found that K_T increases faster and becomes 30 to 40 times at $V/V_0 = 0.5$ to its value at zero pressure.

The results for pressure derivatives of isothermal bulk modulus K' calculated from equations (14 to 19) are given in Table 4. A critical discussion regarding the validity of various EOS for solids has been presented by Stacey, 1999. The importance of the work of Stacey has been demonstrated by Gaurav *et al*., 2002 studying the relationship between P, K and K'. Of particular importance is the variation of K' with the increase in compression or pressure. It is found that P/K and $1/K'$ both show similar trends of variations with the increase in compression (Tables 5, 6). In the limit of extreme compression (volume $V \to 0$, pressure $P \to \infty$), the following condition is satisfied.

$$\frac{1}{K'_\infty} = \left(\frac{P}{K}\right)_\infty \qquad \text{....(20)}$$

We have plotted 1/K' versus P/K for Ne, Ar, Al, Cu, LiH and MgO solids (Singh, 2012; Kushwah *et al*., 2012; Vidyarti and Singh, 2013; Vijay, 2014; Kushwah *et al*., 2014; Shanker *et al*., 2014; Dharmendra, 2015 and 2016) in Figures 1–6. It is found that there is a linear relationship between $1/K'$ and P/K based on the results predicted from different equations of state. Only the fourth–order Birch Murnaghan EOS gives the results which deviate significantly from the linear relationship. The deviations are more in case of LiH and MgO for the Birch–Murnaghan EOS.

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