

ANALYSIS OF BULK MODULUS FOR MATERIALS AT HIGH PRESSURES USING INTERATOMIC POTENTIAL FUNCTIONS

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We present an analysis of bulk modulus for solids such as Ne, Ar, Al, Cu, LiH, and MgO using interatomic potential functions due to Morse, Rydberg, and Davydov. The formulations for bulk modulus have been obtained using these potential functions. The results for bulk modulus as a function of pressure are determined up to a compression of $V/V_0 = 0.5$. The results are compared with the corresponding values obtained from the Shanker equation of state and the Hama-Suito equation of state. There is a good agreement between the results determined from different equations of state.

KEYWORDS : Equation of state, interatomic potential functions, bulk modulus, Metals and Non-metals.

INTRODUCTION

The bulk modulus represents the incompressibility of material. It is defined as the reciprocal of compressibility. Values of bulk modulus at ambient pressure K_0 and of its derivative with respect to pressure K'_0 are used as input to determine bulk modulus of different solids under high pressure. The expressions for bulk modulus are derived from different equations of state. Bulk modulus for monatomic and diatomic solids with different nature of chemical bonds. We select here four kinds of monatomic solids (a) a typical sp metal Al (fcc), [1], (b) a rare-gas metal Cu (bcc) [2], (c) a substance which is the most difficult to metalize, Ne (fcc) and (d) a large gap insulator with a small bulk modulus, Ar (fcc) [3]. For diatomic solids we select one with a small bulk modulus, *i.e.*, and other with large bulk modulus, *i.e.* MgO [2]. It should be mentioned that the calculation of bulk modulus is sensitive to the potential functions used. The bulk modulus depends on the second derivative of potential energy whereas the pressure-volume relationship depends on the first derivative of potential energy. We have therefore calculated bulk modulus for monatomic solids as well as diatomic solids using different equations of state (EOS). It is found that the Vinet-Rydberg EOS [6, 7] work satisfactorily for the solids under the high pressures.

METHOD OF FORMULATIONS

Morse equation of state (EOS) : Morse [8] EOS has been obtained using the double exponential potential energy functions and can be expressed as follows :

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

where $x = V/V_0$, $f = K'_0 - 1$ and V_0 is the volume V at $P = 0$.

The expression for $K = -V(dP/V_0)$ is derived by differentiating equation (1) with respect to V as follows

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

Rydberg-Vinet EOS : Vinet *et. al.* [7] have obtained the following EOS which is based on the potential energy function due to Rydberg [9]

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

The expression for K derived from equation (3) is given below :

$$K = K_0 x^{-1/3} \left[2x^{-1/3} - 1 + \frac{3}{2} (K'_0 - 1) (1 - x^{-1/3}) \right] \exp \left[\frac{3}{2} (K'_0 - 1) (1 - x^{-1/3}) \right]$$

where $\eta = \frac{3}{2} (K'_0 - 1)$.

Davydov EOS : Davydov obtained another alternative form of EOS which has been mentioned by Zharkov and Kalinin [9]. This EOS is based on a different potential energy function which yields

$$P = \frac{3K_0}{(f+2)} \left[x^{-4/3} + f x^{-1} - (f+1)x^{-2/3} \right] \exp f (1 - x^{1/3}) \quad \dots (5)$$

The expression for K derived from equation (3) is given as follows

$$K = \frac{K_0}{(f+2)} \left\{ 4x^{-4/3} + 4f x^{-1} + (f^2 - 2f - 2)x^{-2/3} - f(f+1)x^{-1/3} \right\} \exp[f(1-x^{1/3})] \quad \dots (6)$$

where $f = \frac{3}{4} \left\{ (K'_0 - 3) + \left[(K'_0 + 1) \left(K'_0 - \frac{5}{3} \right) \right]^{1/2} \right\}$.

Shanker EOS : Shanker *et al* [10] have obtained an EOS using the volume dependence of the interatomic force constant determined from the derivatives of potential energy. This EOS is written as follows

$$P = \frac{K_0}{t} x^{-4/3} \left[\left(1 - \frac{1}{t} + \frac{2}{t^2} \right) \left\{ \exp(ty) - 1 \right\} + y \left(1 + y - \frac{2}{t} \right) \exp(ty) \right] \quad \dots (7)$$

The expression for K has been derived from equation (7) as follows

$$K = K_0 x^{-1/3} (1 + y + y^2) \exp(ty) + \frac{4}{3} P \quad \dots (8)$$

where $t = K'_0 - \frac{8}{3}$ and $y = 1 - \frac{V}{V_0}$.

Hama-Suito EOS : Hama and Suito [11] have obtained an EOS using methods based on first-principles such as the augmented plane wave (APW) methods and the quantum statistical model. 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 pressures, intermediate pressures and extremely high pressures. The Hama-Suito EOS is given below

$$P = 3K_0 x^{-5/3} (1 - x^{1/3}) \exp \left[\frac{3}{2} (K'_0 - 3)(1 - x^{1/3}) + \left(\zeta - \frac{3}{2} \right) (1 - x^{1/3})^2 \right] \dots (9)$$

The expression for K derived from equation (9) is given below

$$K = \frac{P}{3} \left[\left\{ 5 + \frac{x^{1/3}}{(1 - x^{1/3})} \right\} + x^{1/3} \left\{ \frac{3}{2} (K'_0 - 1) + 2\zeta(1 - x^{1/3}) + 3x^{1/3} - 6 \right\} \right] \dots (10)$$

where $\zeta = \frac{3}{8} (K'_0 - 1)(K'_0 + 3) + \frac{3}{2} K_0 K''_0 + \frac{1}{3}$.

RESULTS AND DISCUSSIONS

The results for isothermal bulk modulus K calculated from equations (2), (4), (6), (8), and (10) are given in Table 1. We note that the equations based on different potential energy functions yield good agreement with each other and also with the Hama-Suito EOS derived from the first-principles based on the APW method and the quantum statistical model. The bulk modulus increases with the increases in pressure or compression. The rate of increases of K 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 value of K_0 are small as compared to those for other solids, it is found that K increases faster, and becomes 30 to 40 times at $V/V_0 = 0.5$ to its value at zero pressure. For other solids, bulk modulus K_0 is larger and K'_0 is smaller, the ratio K/K_0 at $V/V_0 = 0.5$ remains smaller as compared to that for Ne and Ar (Table 2). The results obtained in the present study are useful for investigating high-pressure equations of state [12-15] and thermoelastic properties of materials [16-19].

Table 1. Values K (GPa) calculated from (a) Morse EOS, (b) Rydberg EOS, (c) Davydov EOS, (d) Shanker EOS and (e) Hama- Suito EOS

Material	V/V_0	(a)	(b)	(c)	(d)	(e)
Ne	1.0	6.36	6.36	6.36	06.36	6.36
	0.9	13.2	13.1	13.1	13.3	13.1
	0.8	26.5	26.0	26.2	27.2	25.6
	0.7	53.6	51.4	52.2	55.4	49.9
	0.6	112	104	107	113	99.0
	0.5	248	220	231	235	205
Ar	1.0	6.28	6.28	6.28	6.28	6.28
	0.9	12.4	12.3	12.4	12.5	12.3
	0.8	23.8	23.5	23.6	24.3	23.1
	0.7	46.2	44.5	45.3	47.1	43.2

	0.6	92.1	86.5	89.1	91.7	82.2
	0.5	194	175	184	182	163
Al	1.0	72.6	72.6	72.6	72.6	72.6
	0.9	117	117	117	117	117
	0.8	187	185	187	187	186
	0.7	301	296	302	298	300
	0.6	497	483	500	480	494
	0.5	852	815	864	787	850
	Cu	1.0	135	135	135	135
0.9		240	239	240	241	240
0.8		421	416	419	423	417
0.7		742	724	737	741	730
0.6		1344	1286	1328	1306	1310
0.5		2549	2376	2507	2341	2462
LiH	1.0	39.1	39.1	39.1	93.1	39.1
	0.9	55.4	55.4	55.5	55.5	55.7
	0.8	78.8	78.5	79.3	78.9	80.0
	0.7	113	112	115	113	117
	0.6	166	164	171	164	178
	0.5	251	246	263	243	281
MgO	1.0	157	157	157	157	157
	0.9	241	241	242	242	242
	0.8	370	368	372	370	374
	0.7	573	566	578	568	585
	0.6	907	887	920	879	944
	0.5	1488	1436	1527	1388	1596

Table 2. The ratio K for different solids calculated at $V/V_0 = 0.5$ using (a) Morse EOS, (b) Rydberg EOS, (c) Davydov EOS, (d) Shanker EOS and (e) Hama- Suito EOS

Material	(a)	(b)	(c)	(d)	(e)
Ne	39	35	36	37	32
Ar	31	28	29	29	26
AL	12	11	12	11	12
Cu	19	17	18	17	18
LiH	6	6	7	6	7
MgO	9	9	10	9	10

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