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ANALYSIS OF PRESSURE DERIVATIVES OF BULK MODULUS AT HIGH COMPRESSIONS USING INTERATOMIC POTENTIAL FUNCTIONS

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We present an analysis for the pressure derivatives of bulk modulus of six solids viz. Ne, Ar, Al, Cu, LiH, and MgO using interatomic potential functions due to Morse, Rydberg, and Davydov. The formulations are obtained using these potential functions. The results for pressure derivatives of bulk modulus are determined as a function of pressure up to a compression of V/V_0 equal to 0.5 for each solid. The results are compared with the corresponding values obtained from the Shanker equation and the Hama-Suito equation of state.

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

INTRODUCTION

The bulk modulus represents the incompressibility of solids. It is defined as the reciprocal of compressibility. Values of bulk modulus and its derivative with respect to pressure at zero pressure up to high pressures are used as input to determine the results for different solids. Expressions for pressure derivative of bulk modulus are also derived from different equations of state. We select here four kinds of monatomic solids, a typical sp metal Al (fcc), [1, 2], a rare-gas metal Cu (bcc) [2, 3], a substance which is most difficult to metalize, Ne (fcc) [4, 5] and a large gap insulator with a small bulk modulus, Ar (fcc) [4]. For diatomic solids we select one with a small bulk modulus, *i.e*. LiH [6, 7] and other with a large bulk modulus, *i.e.* MgO [2]. The Rydberg-Vinet equation of state [8, 9] has been found to yield satisfactory results for monatomic as well as diatomic solids. The pressure derivatives of bulk modulus provide sensitive test of the potential functions used in the present study. The pressure derivatives of the bulk modulus depend on the third order derivative of potential energy and thus sensitively depend on the potential functions used. We derive expression for pressure derivative of bulk modulus using different potential functions and compare the results with those based on first the principles.

METHOD OF FORMULATIONS

The derivative of bulk modulus K with respect to pressure P can be written as follows

Table 1. Values K' 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	7.61	7.61	7.61	7.61	7.61
	0.9	6.36	6.26	6.31	6.51	6.20
	0.8	5.58	5.43	5.49	5.68	5.32
	0.7	5.02	4.82	4.90	4.98	4.69
	0.6	4.57	4.34	4.44	4.33	4.18
	0.5	4.18	3.93	4.04	3.72	3.75
Ar	1.0	7.07	7.07	7.07	7.07	7.07
	0.9	5.95	5.87	5.91	6.06	5.81
	0.8	5.23	5.10	5.16	5.29	4.99
	0.7	4.71	4.54	4.62	4.63	4.40
	0.6	4.29	4.09	4.19	4.04	3.92
	0.5	3.92	3.70	3.82	3.47	3.51
Al	1.0	4.85	4.85	4.85	4.85	4.85
	0.9	4.23	4.19	4.23	4.24	4.21
	0.8	3.77	3.71	3.78	3.73	3.74
	0.7	3.41	3.33	3.43	3.29	3.38
	0.6	3.11	3.02	3.13	2.90	3.07
	0.5	2.83	2.73	2.87	2.54	2.80
Cu	1.0	5.93	5.93	5.93	5.93	5.93
	0.9	5.08	5.02	5.06	5.12	5.04
	0.8	4.49	4.40	4.47	4.48	4.43
	0.7	4.04	3.93	4.02	3.93	3.96
	0.6	3.68	3.54	3.65	3.44	3.59
	0.5	3.36	3.21	3.34	2.98	3.26
LiH	1.0	3.51	3.51	3.51	3.51	3.51
	0.9	3.14	3.13	3.17	3.15	3.21
	0.8	2.85	2.82	2.89	2.83	2.96
	0.7	2.60	2.56	2.67	2.54	2.75
	0.6	2.38	2.33	2.47	2.28	2.56
	0.5	2.17	2.13	2.29	2.05	2.39
MgO	1.0	4.37	4.37	4.37	4.37	4.37
	0.9	3.85	3.82	3.86	3.85	3.88
	0.8	3.45	3.40	3.47	3.40	3.51
	0.7	3.12	3.06	3.16	3.02	3.21
	0.6	2.85	2.78	2.90	2.67	2.95
	0.5	2.60	2.52	2.67	2.36	2.73

$$K' = \frac{dK}{dP} = -\frac{V}{K}\frac{dK}{dP} \quad \ldots (1)$$

where we have used

$$K = -V\frac{dP}{dV} \quad \ldots (2)$$

The pressure is related to the derivative of potential energy E (V) with respect to volume V

$$P = -V\frac{dE}{dV} \quad \ldots (3)$$

Morse equation of state EOS : Morse equation [10] EOS has been obtained using the double exponential potential energy functions [11, 12].The expression forK' is given below

$$K' = \frac{\left\{\left[\frac{4}{3}X^{-2/3} + 2fX^{-1/3} + \frac{4}{3}f^2\right]exp\left[f\left(1-x^{1/3}\right)\right] - \left[\frac{4}{3}X^{-2/3} + 2fX^{-1/3} + \frac{1}{3}f^2\right]\right\}}{[2X^{-2/3} + 2X^{-1/3}]exp[f(1-x^{1/3})] - [2X^{-2/3} + X^{-1/3}]} \quad \ldots (4)$$

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

Rydberg- Vinet EOS : Vinet *et al* [9] have obtained an EOS using the potential energy function due to Rydberg. The expression for K' based on this EOS is given below

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

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

Davydov EOS: Davydov obtained another alternative form of EOS which has been mentioned by Zharkov and Kalinin [11]. The expression for K' based on this EOS is given below

$$K' = \frac{\left\{\frac{16}{3}x^{-4/3} + \frac{16}{3}fx^{-1} + \frac{2}{3}(3f^2 - 2f - 2)x^{-2/3} + \frac{f}{3}(f^2 - 3f - 3)x^{-1/3} - \frac{f^2}{3}(f+1)\right\}}{4x^{-4/3} + 4fx^{-1} + (f^2 - 2f - 2)x^{-2/3} - f(f+1)x^{-1/3}} \quad \ldots (6)$$

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

Shanker EOS: Shanker *et. al* [14] have obtained an EOS using the volume dependence of the interatomic force constant determined from the derivatives of potential energy. The expression for K' based on this EOS is given below

$$K' = \frac{4}{3}\left(1 - \frac{4P}{3K}\right) \times \left[\frac{1}{3} + X\left\{t + \frac{(1+2y)}{(1+y+y^2)}\right\}\right] \quad \ldots (7)$$

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

Table 2. Values of $K_0K_0^{''}$ calculated from (a) Morse potential function, (b) Rydberg potential function, (c) Davydov potential function, (d) Shanker EOS, (e) Hama-Suito EOS and (f) Generalized Rydberg EOS.

Solid	K_0	$K_0^{'}$	(a) $K_0K_0^{''}$	(b) $K_0K_0^{''}$	(c) $K_0K_0^{''}$	(*d*) $K_0K_0^{''}$	(e) $K_0K_0^{''}$	(f) $K_0K_0^{''}$
Ne	6.36	7.61	– 16.54	– 17.76	– 17.36	– 13.31	– 18.19	– 13.86
Ar	6.28	7.07	– 14.48	– 15.50	– 15.09	– 12.05	– 15.89	– 11.60
Al	72.6	4.85	– 7.37	– 7.78	– 7.35	– 6.87	– 7.55	– 5.50
Cu	135	5.93	– 10.55	– 11.23	– 10.28	– 9.39	– 11.21	– 8.30
LiH	39.1	3.51	– 4.13	– 4.31	– 3.58	– 3.75	– 4.15	– 2.86
MgO	157	4.37	– 6.12	– 6.43	– 599	– 5.75	– 6.28	– 5.00

Hama-Suito EOS : Hama and Suito [15] have obtained an EOS using the methods based on first-principles such as the augmented plane wave (APW) method and the quantum statistical model (QSM). 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 expressions for K' based on Hama-Suito EOS is given below

$$K' = \frac{K}{P} - \frac{1}{3} + \frac{P}{9K}\left[X^{2/3}\left\{(2\zeta - 3) - \frac{1}{(1 - x^{1/3})^2}\right\} + 5\right] \quad \ldots (8)$$

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

Results and discussions

The results for pressure derivative of bulk modulus calculated from equations (4) to (8) 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 (QSM). Values of input parameter K_0 and K_0'' used in present calculations are given in Table 2 along with the values of K_0K_0'' for each equation of state. Values of K' given in Table 2 are positive. This reveals that K increases with pressure so that $K' = dK/dP$ is always positive .It is also found that K' decreases with the increase in compression $(1 - V/V_0)$. This would imply that the rate of increase of K with the increase in pressure becomes smaller and smaller at higher compressions. The results obtained in the present study for investigating high pressure EOS [16-18] and thermoelastic property of materials [19, 20].

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