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Short Communication

Elastic Behaviour of Diborides Under High Pressure

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Abstract

The present study deals with the elastic behaviour of diborides (BeB_2, MgB_2 and NbB_2) under high pressure with the help of equation of state (EOS) using the elastic data reported by Islam *et al.* It is concluded that EOS, which are based either on quantum statistical model or pseudopotential model, only are capable of explaining high pressure behaviour of the solids under study. Moreover the value of first order pressure derivative of bulk modulus at infinite pressure (K'_∞) is greater than 5/3 and thus the diborides under study do not behave as Thomas-Fermi electron gas under high compression.

Keywords: Equation of state; High Pressure; Diborides.

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The equation of state (EOS) is fundamentally important in studying the high pressure physics of solids. The knowledge of EOS, based on either calculation or experiment, is of primary importance in both basic and applied sciences. It provides insight into the nature of solid state theories. Up to now a number of workers have endeavoured to search for a simple form of the EOS, which has small number of parameters. The parameters are determined by using available low-pressure data such as the equilibrium volume V_o , the isothermal bulk modulus K_o and its pressure derivatives K'_o and K''_o at zero pressure. Some widely used EOS are due to Murnaghan (M) [1], Birch-Murnaghan III (B-MIII) [2], Brennan-Stacey (BS) [3], Born-Mayer (B-Ma) [2], Birch-Murnaghan IV (B-MIV) [2], Sikka (Si) [4], Misra and Goyal (M-S) [5], Usual-Tait (UT) [2] and Hama-Suito (H-S) [6]. In order to compute the values of pressure (*P*) at different compression (η) using the above mentioned EOS we require the values of K_o , K'_o and K''_o. The values of input data are taken from Islam *et al.* [7, 8]. The results are shown in Fig. 1.

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It is interesting to note from Fig. 1 that the values of pressure (*P*) obtained with the help of different equations of state up to compression *V/Vo*=0.80 are almost the same in nature except the value of pressure obtained by Murnaghan equation of state at high compression. However, the magnitude of pressure at same compression is different in all the three cases. The calculated pressure at the same compression for the compounds are in the order MgB_2< BeB_2 < NbB_2. The higher value of pressure in case of NbB_2 may be due to the contribution of *d* core electrons under high pressure.

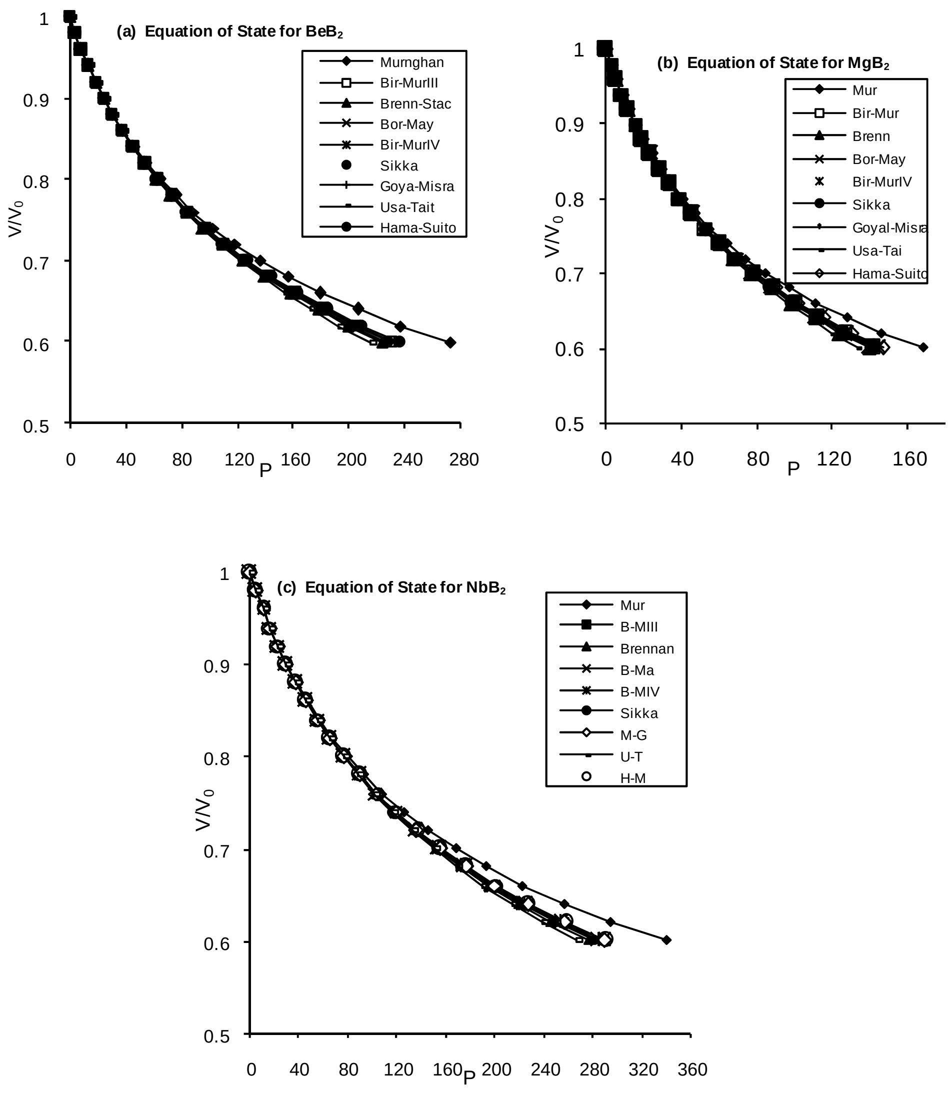


Fig. 1. Isothermal compression curves from various EOS for (a) BeB_2, (b) MgB_2, and (c) NbB_2.

With the increase of ionic radii of the cation, elastic softening becomes evident. But this is not the case with transition metal cation. It is apparent from the above figures that different EOS show distinct behaviour under high compression, i.e., for *V/Vo*=0.80-0.55. The most important reason to know about K'_∞ is that it provides a close control on the curvature of the plot of K'_o versus *P/K* and therefore the thermodynamic parameters can be inferred from such a plot. According to Brennan and Stacey [3] the essential significance of K'_∞ is that it is the reciprocal of $(P/K)_{P\to\infty}$, so that a plot of K' versus *P/K* has a fixed 'End Point' corresponding to the infinite pressure extrapolation. Therefore a computation of K'_∞ may help in analysing the applicability of various EOS in diborides.

K_o and K'_o data are taken from Islam *et al.* [7, 8] and K''_o are computed following the procedure described by Misra and Goyal [5]. With the help of these parameters we have computed and plotted the dimensionless isothermal curves K' as a function of *P/K* (Fig. 2) for MgB_2, BeB_2 and NbB_2 using EOS as shown below:

Misra-Goyal

$$K(\eta) = V\frac{dP}{dV}$$

$$= \frac{K_0}{20}\left[\alpha\left\{12\eta^{-2} - 25\eta^{-5/3} + \frac{40}{3}\eta^{-4/3} - \frac{1}{3}\eta^{-1/3}\right\} + \beta\left\{6\eta^{-2} - \frac{20}{3}\eta^{-4/3} + \frac{2}{3}\eta^{-1/3}\right\} + \gamma\left\{2\eta^{-2} - \frac{1}{3}\eta^{-1/3}\right\}\right] \quad (1)$$

$$K'(\eta) = \frac{dK}{dP} = \left[\alpha\left\{24\eta^{-3} - \frac{125}{3}\eta^{-8/3} + \frac{160}{9}\eta^{-7/3} - \frac{1}{9}\eta^{-4/3}\right\} + \beta\left\{12\eta^{-3} - \frac{80}{9}\eta^{-7/3} + \frac{2}{9}\eta^{-4/3}\right\}\right.$$
$$\left. + \gamma\left\{4\eta^{-3} - \frac{1}{9}\eta^{-4/3}\right\}\right] \times \left[\alpha\left\{12\eta^{-3} - 25\eta^{-8/3} + \frac{40}{3}\eta^{-7/3} - \frac{1}{3}\eta^{-4/3}\right\}\right.$$
$$\left. + \beta\left\{6\eta^{-3} - \frac{20}{3}\eta^{-7/3} + \frac{2}{3}\eta^{-4/3}\right\} + \gamma\left\{2\eta^{-3} - \frac{1}{3}\eta^{-4/3}\right\}\right]^{-1} \quad (2)$$

Hama-Suito

$$K(\eta) = \frac{P}{3} * \frac{2\eta\left(\xi - \frac{3}{2}\right)(1-\eta)^2 + \eta(1-\eta)\left\{\left(\frac{3}{2}(K'_0 - 1)\right) - 3\right\} - 4\eta + 5}{(1-\eta)} \quad (3)$$

$$K'(\eta) = \frac{K_T}{P} + \frac{P}{9K_T}\left[\mu^2\left\{(2\xi - 3) - \frac{1}{(1-\eta)^2}\right\} + 5\right] - \frac{1}{3} \quad (4)$$

Brennan-Stacey

$$K(\eta) = K_0(\eta)^{-1/3}\left[\exp\left(\left(K_0 - \frac{5}{3}\right)\left(1 - \frac{V}{V_0}\right)\right)\right] + \frac{4}{3}P \quad (5)$$

$$K`(\eta) = \left(1 - \frac{4}{3}\frac{P}{K_T}\right)\left[\left(K_0 - \frac{5}{3}\right)\frac{V}{V_0} + \frac{5}{3}\right] + \frac{16}{9}\frac{P}{K_T} \quad (6)$$

Brich-Murnaghan III

$$K(\eta) = K_0\eta^{-5/3}\left[1 + \left(\frac{3}{2}K_0^{`} - \frac{5}{2}\right)\left(\eta^{-2/3} - 1\right)\right] + \frac{9}{8}\left(K_0K_0^{``} + K_0^{`}[K_0^{`} - 4] + \frac{35}{9}\right)\left(\eta^{-2/3} - 1\right) \quad (7)$$

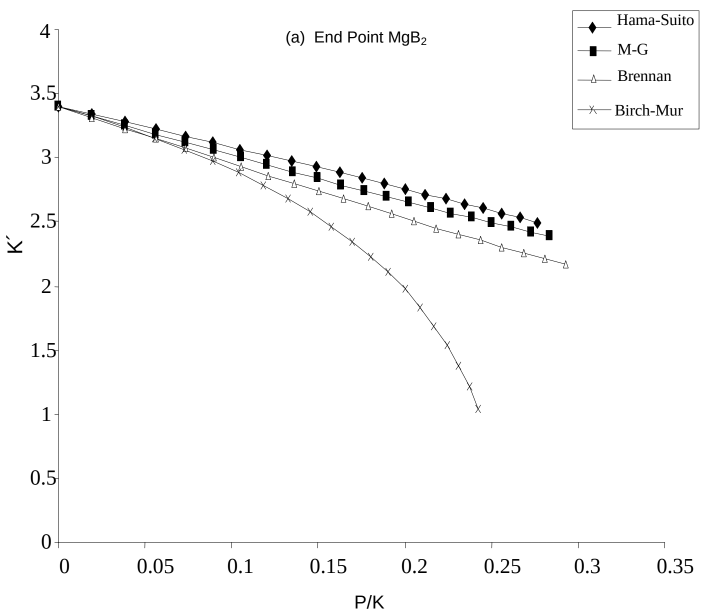
$$K`(\eta) = \left(K_0^{`} + \frac{3}{2}K_0K_0^{``}\right)\left(\eta^{-2/3} - 1\right) \quad (8)$$

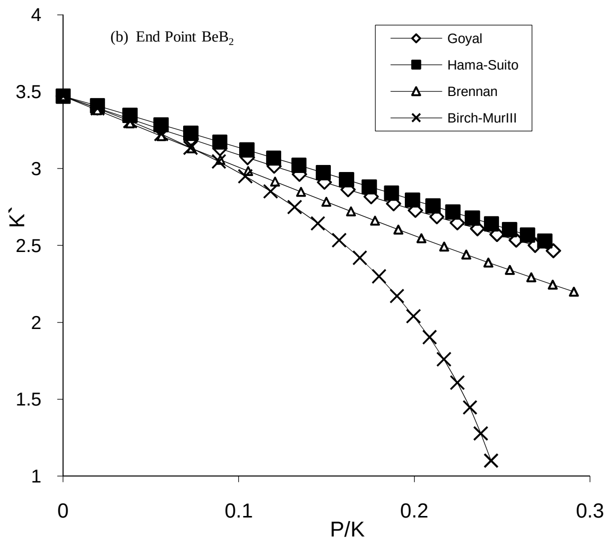
where $\eta = \left(\frac{V}{V_0}\right)^{1/3}$, V is volume of unit cell, $t = B_0^{`} - \frac{8}{3}$, $y = \left(1 - \frac{V}{V_0}\right)$,

$a_1 = \frac{3}{2}\left(K_0 - 4\right)$, $a_2 = \frac{3}{2}\left(K_0K_0^{`} + (K_0 - 7) + \frac{143}{9}\right]$, $f = \frac{1}{2}\left(\left(\frac{V}{V_0}\right)^{2/3} - 1\right)$,

$\sigma = \frac{3}{2}\left(K_0^{`} - 1\right) + \left[\frac{9}{4}\left(K_0^{`}\right)^2 - 6K_0^{`} + 12\right]^{1/2}$ and $\xi = \frac{\left(\eta^2 + 6\eta + 2 + 9K_0K_0^{``}\right)}{6}$,

$\alpha = 6 + 9K_oK_o'' + \left(3K_o' - 4\right)\left(3K_o' - 7\right)$, $\beta = 2\left(3K_o' - 7\right)$ and $\gamma = 12$.





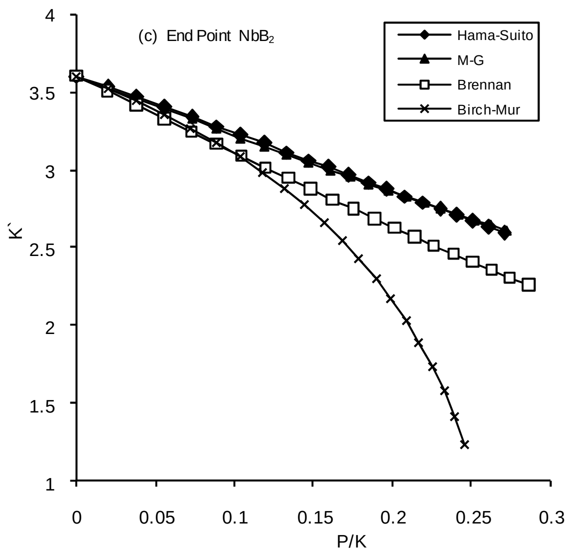


Fig. 2. Dimensionless isothermal curves *K`* versus P/K for (a) MgB_2, (b) BeB_2, (c) NbB_2 using different EOS.

It is encouraging to note from Fig. 2 that the curves for end point plotted with the help of EOS by Hama-Suito [6] and Misra-Goyal [5] are almost the same for all the three diborides under study. The calculation yields the value of K'_o as 3.0, which is greater than 5/3. It is thus concluded that these diborides do not behave as Thomas-Fermi electron gas [9] under high compression. The present study reveals that EOS, which are based either on quantum statistical model [6] or on pseduopotential model [5], are only seen to explain successfully high pressure behavior of the solids under study.

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