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Theoretical prediction of equation of state for lithium halides

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ABSTRACT

Equation of state for solids developed by Born-Mayer, Birch and Poirier- Tarantola have been used here to determine the pressure-volume relationships for LiF, LiCl, and LiBr solids. The results obtained through the Born-Mayer and Birch equation of states are in good agreement with each other but the calculated values obtained from Poirier- Tarantola EOS are different at higher compression ranges. The computed results suggest the validity of Born-Mayer and Birch equation of states for the prediction of pressure-volume relationships for Lithium Halides is good at higher compression ranges but Poirier- Tarantola EOS shows its validity only at low compression range specially upto the compression range (from $V/V_0=1.0$ to 0.77). The validity of these equation of states are due to the consideration of different approximation regarding change in strain due to the compression.

Keywords: Pressure volume relation, lithium halides, Equation of state.

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INTRODUCTION

The compressibility of the alkali metals is very large, and the large volume reduction with application of pressure affects significantly the otherwise free-electron like electronic structure. As a consequence, these metals undergo several pressure-induced structural transformations. These have been studied experimentally as well as by theoretical methods [1-10] and references therein.

Although the experimental data on the compression behaviour of lithium halides is not abundant but the available data for LiF rock salt (B1) upto the compression ratio (from $V/V_0=1.0$ to 0.75) gives the clear idea about its variation [11].

The equation of state (EOS) of a solid (pressure-volume relation) plays an important role in condensed matter physics, because the knowledge of the EOS is of central importance for the general understanding of the behaviour and the application of condensed matters. The EOS of crystalline solids has been a long-standing topic and extensively investigated. A lot of interesting and important phenomena have been observed [12].

In the present work, pressure of three lithium halides viz. LiF, LiCl, LiBr, have been calculated at different compression ranges using various equation of state (EOS) viz. Born-Mayer EOS, Birch EOS and Poirier- Tarantola EOS. Comparative study has also been made among the calculated values of pressure to test the validity of various equation of states. It is found that the Poirier- Tarantola EOS is suitable only upto low compression range while the rest of two equation of states are suitable upto higher compression range.

THEORY**(1) Born-Mayer Equation of State**

When we use an exponential function for Φ [such as $b \exp \{-K(V/V_0)\}^{1/3}$ and eliminating b and K in terms of K_0 and K'_0 using the relationship for potential parameter [13] we get Born-Mayer EOS which is

$$P = \frac{3K_0}{(\eta - 2)} \left[\left(\frac{V}{V_0} \right)^{-2/3} \exp \left\{ \eta \left[1 - \left(\frac{V}{V_0} \right)^{1/3} \right] \right\} - \left(\frac{V}{V_0} \right)^{-4/3} \right] \quad (1)$$

$$\text{where } \eta = \frac{3(K'_0 - 1)}{2} + \left[\frac{9(K'_0 - 1)^2}{4} - 6K'_0 + 12 \right]^{1/2}$$

(2). Birch Equation of State

On the basis of finite strain theory [14] in which the expansion of Helmholtz free energy is considered as a polynomial series in terms of Eulerian Strain and taking third order approximation Birch obtained an EOS [15] which is as follows

$$P = \frac{3K_0}{2} \left[\left(\frac{V}{V_0} \right)^{-7/3} - \left(\frac{V}{V_0} \right)^{-5/3} \right] \left[1 - \frac{3(4 - K'_0)}{4} \left\{ \left(\frac{V}{V_0} \right)^{-2/3} - 1 \right\} \right] \quad (2)$$

(3) Poirier-Tarantola Equation of State

Poirier and Tarantola [16] derived an equation similar to Birch EOS but define strain as

$\epsilon = \log(V_0/V)$ rather than Eulerian Strain $f = 1/2[(V/V_0)^{-2/3} - 1]$ used by Birch and give an EOS as

$$P = K_0 \left(\frac{V_0}{V} \right) \left[\ln \left(\frac{V_0}{V} \right) + \left\{ \left(\frac{K'_0 - 2}{2} \right) \right\} \left\{ \ln \left(\frac{V_0}{V} \right)^2 \right\} \right] \quad (3)$$

RESULTS AND DISCUSSION

The pressure have been calculated at different compression ranges (from $V/V_0=1.0$ to 0.1) for different Lithium halides viz. LiF, LiCl and LiBr, using three different isothermal equation of state viz. Born-Mayer EOS, Birch EOS and Poirier Tarantola EOS from equation (1-3). The calculated values are displayed in table (2-4). The input values of isothermal bulk modulus (K_0) and its first pressure derivative (K'_0) at zero pressure are taken from the literature [17] displayed in table (1). The logarithmic values of calculated pressure obtained by using different isothermal EOS have been plotted against the logarithmic values of unit cell volume ratio (V/V_0) and shown graphically, displayed in figure (1-3). The result thus obtained shows very interesting pattern i.e. the graph plotted between logarithmic values of pressure vs logarithmic value of unit cell volume ratio (V/V_0) appears linear characteristic fig. (1-3).

Another remarkable characteristic is observed that the variation in value of pressure from compression range $V/V_0 = 1.0$ to 0.5 are minimum but as the compression increases the variation in the values of pressure also increases. Pressure (P) vs. unit cell volume ratio (V/V_0) relation for all the three Lithium Halides are almost same with slight variation upto $V/V_0 = 0.5$ but as the compression increases variation in pressure gradually increases and after $V/V_0 = 0.3$ it increases abruptly which is crystal clear from figure (1-3).

When we consider about the success of equation of state derived from certain scientists, we have observed that two EOS viz Born-Mayer EOS and Birch EOS show very good agreement with each other except the validity of Poirier Tarantola EOS only upto the short compression range[11]. The Poirier-Tarantola proposed an equation of state

derived using Hencky logarithmic strain [18] equivalent to the Eulerian strain for small strain and better behaved for large strain. The reference strain is neither the initial nor the final configuration, but the instantaneous configuration of the body being deformed. In uniaxial deformation as the instantaneous volume (V) of the body is increased by an infinitesimally small increment dV , the ratio (dV/V) is considered as an increment of the current state of strain $dE=(dV/V)$

When the solid goes from volume V_0 to V the total finite strain or normal strain also called the Hencky measure of strain.

$$E_H=(1/3) \log (V/V_0)$$

As it is obvious from the above expression that the Hencky strain varies as a function of the ratio (V_0/V) thus we conclude that, as the compression increases this potential deviates from other potential and successively it shows a pseudo linear characteristic. Because of this basic difference in the assumptions made for the deduction of Poirier Tarantola EOS, it is valid upto the short compression range only[11]

Table-1 The input values of isothermal bulk modulus (K_0) & its first pressure derivative (K_0') at zero pressure [18]

S.No.	Sample	K_0 (GPa)	K_0'
1	LiF	66.51	5.31
2	LiCl	29.68	5.63
3	LiBr	23.52	5.68

Table -2 Calculated values of pressure (P) in GPa as a function of V/V_0 at different compressions using different equation of state from equations (1-3) for "LiF"

V/V_0	P (GPa) Born-Mayer EOS (1)	P (GPa) Birch EOS (2)	P (GPa) Poirer -Tarantola EOS (3)
1.00	0.00	0.00	0.00
0.90	9.27	9.27	8.23
0.80	26.89	26.85	20.32
0.70	61.38	61.28	37.71
0.60	132.35	132.49	62.67
0.50	289.76	293.01	98.93
0.40	679.75	705.64	153.26
0.30	1824.82	2015.21	239.46
0.20	6314.19	8090.99	391.86
0.10	39068.92	76966.36	736.10

Table -3 Calculated values of pressure (P) in GPa as a function of V/V_0 at different compressions using different equation of state from equations (1-3) for "LiCl"

V/V_0	P (GPa) Born-Mayer EOS (1)	P (GPa) Birch EOS (2)	P (GPa) Poirer -Tarantola EOS (3)
1.00	0.00	0.00	0.00
0.90	4.21	4.20	3.73
0.80	12.47	12.38	9.30
0.70	29.17	28.74	17.43
0.60	64.81	63.24	29.21
0.50	147.09	142.46	46.43
0.40	360.62	349.78	72.38
0.30	1023.34	1019.80	113.75
0.20	3809.99	4188.87	187.17
0.10	26278.57	40922.94	353.67

Fig. -1: The logarithmic graph between calculated values of pressure (P) against V/V₀ of LiF using different equation of state from equations (1-3)

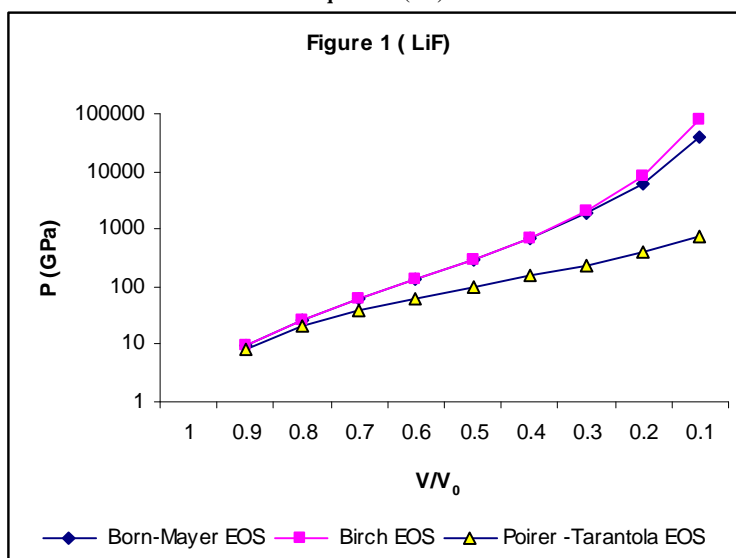


Fig. -2: The logarithmic graph between calculated values of pressure (P) against V/V₀ of LiCl using different equation of state from equations (1-3)

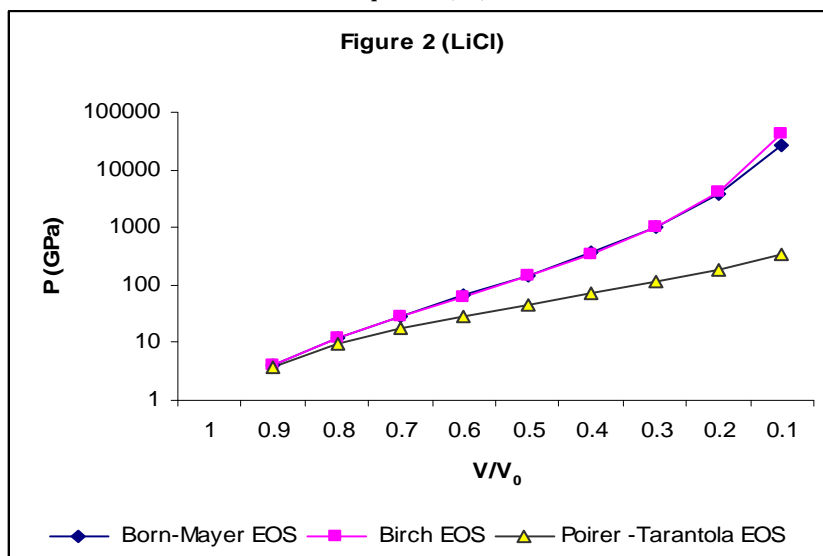
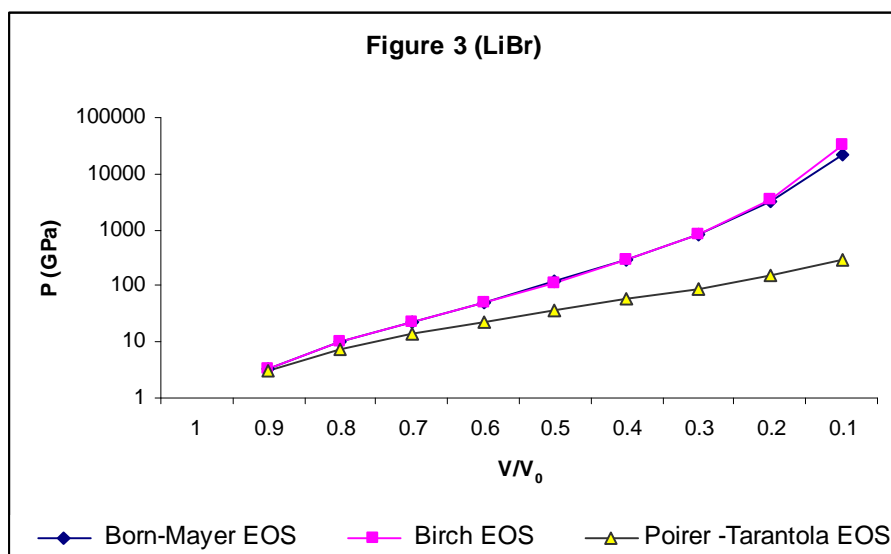


Table -4 Calculated values of pressure (P) in GPa as a function of V/V₀ at different compressions using different equation of state from equations (1-3) for "LiBr"

V/V ₀	P (GPa) Born-Mayer EOS (1)	P (GPa) Birch EOS (2)	P (GPa) Poirer -Tarantola EOS (3)
1.00	0.00	0.00	0.00
0.90	3.35	3.34	2.96
0.80	9.94	9.86	7.40
0.70	23.36	22.95	13.89
0.60	52.15	50.65	23.30
0.50	119.06	114.40	37.09
0.40	294.03	281.67	57.87
0.30	842.05	823.67	91.03
0.20	3173.02	3393.95	149.91
0.10	22278.54	33276.42	283.51

Fig. -3: The logarithmic graph between calculated values of pressure (P) against V/V_0 of LiBr using different equation of state from equations (1-3)



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