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ANALYSIS OF PRESSURE DERIVATIVES OF BULK MODULUS FOR NaCl AND MgO

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*Abstract:*We have used the Holzapfel adapted polynomial of second order (AP2) equation of state (EOS) for determining pressure derivatives of bulk modulus up to third order for NaCl and MgO corresponding to different values of volume compression. It has been found that there exists a quadratic relationship for $1/K'$ in terms of P/K where K' is the first pressure derivative of bulk modulus K at pressure P. Values of pressure derivatives of bulk modulus up to third order have also been calculated using the quadratic equation. The results are found to present good agreement with the corresponding values based on the Holzapfel AP2 EOS establishing the validity of quadratic relationship between $1/K'$ versus P/K.

Keywords: Holzapfel AP2 EOS, Pressure derivative of bulk modulus, Quadratic relationship for pressure derivative of bulk modulus, NaCl, MgO

I. INTRODUCTION

An EOS which has successfully been applied for the entire range of compressions was formulated by Holzapfel [1, 2] on the basis of the Thomas-Fermi gas model in the limit of extreme compression. It has been found by Belonoshko et al. [3, 4] that the Holzapfel adapted polynomial of second order (AP2) EOS is consistent with the ab initio molecular dynamics results [5, 6] and gives a correct Thomas–Fermi limit for materials at extreme compression [7]. The Holzapfel AP2 EOS has been used recently [8, 9] to determine thermoelastic properties of bridgmanite ($MgSiO_3$) and forsterite (Mg_2SiO_4). It has thus become evident that the Holzapfel EOS has a fundamental physical origin, and gives accurate results up to very high pressures.

In the present study we apply the Holzapfel AP2 EOS for determining pressure-volume relationship, bulk modulus and its pressure derivatives for NaCl and MgO corresponding to different volume compressions V/V0. The results thus obtained have been used to establish a quadratic relationship between reciprocal of pressure derivative of bulk modulus K' and ratio P/K pressure P, and bulk modulus K.

II. Method of Analysis and Results

The Holzapfel AP2 EOS can be written as [10, 11]

$$P = 3K_0 x^{-5}(1-x)[1 + c_2 x(1-x)]\exp[c_0(1-x)] \tag{1}$$

where $x = (V/V_0)^{1/3}$, K_0 is the zero-pressure value of bulk modulus K, and

$$c_0 = -\ln\left(\frac{3K_0}{P_{FG0}}\right) \tag{2}$$

$$P_{FG0} = a_{FG}\left(\frac{Z}{V_0}\right)^{5/3} \tag{3}$$

and

$$c_2 = \frac{3}{2}\left(K_0' - 3\right) - c_0 \quad (4)$$

Here K_0' is the value of pressure derivative of bulk modulus $K' = dK/dP$ at zero-pressure. P_{FG0} is the pressure of Fermi gas with a_{FG}. For NaCl and MgO, we have Z, the number of electrons multiplied by the Avogadro number, and V_0.

On differentiating Eq.(1), we get

$$K = -V\frac{dP}{dV} = -\frac{x}{3}\frac{dP}{dx} \quad (5)$$

and

$$K' = \frac{dK}{dP} = -\frac{x}{3K}\frac{dK}{dx} \quad (6)$$

where

$$\frac{dK}{dx} = -\frac{x}{3}\frac{d^2P}{dx^2} - \frac{1}{3}\frac{dP}{dx} \quad (7)$$

The second order pressure derivatives of bulk modulus are obtained by differentiation of Eq.(6)

$$KK'' = \frac{x^2}{9K}\frac{d^2K}{dx^2} - K'\left(K' + \frac{1}{3}\right) \quad (8)$$

where

$$\frac{d^2K}{dx^2} = -\frac{x}{3}\frac{d^3P}{dx^3} - \frac{2}{3}\frac{d^2P}{dx^2} \quad (9)$$

where $K'' = d^2K/dP^2$, K'' has been multiplied by K, in order to make them dimensionless quantities.

An expression for the third order pressure derivative of bulk modulus K^2K''' written as dimensionless parameter, where K''' is d^3K/dP^3 , has been derived as follows

$$K^2K''' + \left(3K' + \frac{1}{3}\right)KK'' = -\frac{x^2}{9K}\left[\left(K' + \frac{2}{3}\right)\frac{d^2K}{dx^2} + \frac{x}{3}\frac{d^3K}{dx^3}\right] \quad (10)$$

Where

$$\frac{d^3K}{dx^3} = -\frac{x}{3}\frac{d^4P}{dx^4} - \frac{d^3P}{dx^3} \quad (11)$$

The input parameters used in calculations are given in Table 1. Results for P, K, K', KK'' and K^2K''' are given in Tables 2 and 3 for NaCl and MgO corresponding to different values of V/V_0. It was pointed out by Stacey[12,13] that there exists a linear relationship between $1/K'$ and P/K. In order to investigate a relationship we have plotted $1/K'$ versus P/K using the results based on the Holzapfel AP2 EOS for NaCl in Figures 1 and for MgO in Figure 2. It is found from these figures that the relationship between $1/K'$ and P/K is not linear, but represented more appropriately by the following expression [14-16]

$$\frac{1}{K'} = A + B\left(\frac{P}{K}\right) + C\left(\frac{P}{K}\right)^2 \quad (12)$$

At P=0, $K' = K_0'$ and there for Eq.(12) gives

$$A = \frac{1}{K_0'} \quad (13)$$

On differentiating Eq.(12) with respect to pressure P, we get the following expression for second pressure derivatives of bulk modulus

$$KK'' = -K'^2\left(B + 2C\frac{P}{K}\right)\left(1 - \frac{P}{K}K'\right) \tag{14}$$

At P=0, Eq.(14) gives

$$B = -\frac{K_0 K_0''}{(K_0')^2} \tag{15}$$

In the limit of infinite pressure, we can write according to Knopoff [17]

$$\frac{1}{K'_\infty} = \left(\frac{P}{K}\right)_\infty \tag{16}$$

Using Eq.(16) in Eq.(12) we find

$$\frac{1}{K'_\infty} = \frac{1}{K'_0} + \frac{-K_0 K_0''}{(K_0')^2}\left(\frac{P}{K}\right)_\infty + C\left(\frac{P}{K}\right)_\infty^2 \tag{17}$$

On solving Eq.(17) we get

$$C = \left(\frac{K'_\infty}{K_0'^2}\right)\left[K_0 K_0'' + K_0'(K_0' - K'_\infty)\right] \tag{18}$$

We drive an expression for third order pressure derivative K^2K''' by differentiating Eq.(14) with respect to P. Thus we get

$$K^2K''' = KK''\left[\frac{2C\left(1 - K'\left(\frac{P}{K}\right)\right)}{B + 2C\left(\frac{P}{K}\right)} + \frac{2KK''}{K'} - 2K' - \frac{KK''\left(\frac{P}{K}\right)}{1 - K'\left(\frac{P}{K}\right)}\right] \tag{19}$$

Values of the dimensionless parameters A, B and C determined from Eqs. (13), (15) and (18) are given in Table 1. The results are given in Figures 3-8.

III. Discussion and conclusions

We have found that the results for pressure derivatives of bulk modulus up to third order obtained from the Holzapfel AP2 EOS in case of NaCl and MgO satisfy well the quadratic relationships between $1/K'$ and P/K. The Holzapfel AP2 EOS used in present study is based on K'_∞, the pressure derivative of bulk modulus in the limit of infinite pressure, is equal to 5/3 corresponding to the Thomas-Fermi model. It should be emphasized that the quadratic equation use for K' Eq.(12) in the present work is more general than the linear relationship proposed by Stacey [12,13]. Eq.(12) is used to the Stacey reciprocal K-prime EOS when C=0. In this case we get from Eq.(18) the following expression (C=0).

$$K_0 K_0'' = -K_0'(K_0' - K'_\infty) \tag{20}$$

The results obtained from the Holzapfel AP2 EOS do not satisfy Eq.(20). This reveals that C is Eqs. (12) and (18) deviate significantly from zero. Appropriate values of A, B and C are given in Table 1 which reproduce the adequate results for the pressure derivatives of bulk modulus up to third order.

TABLE 1- Input parameters appearing in the Holzapfel AP2 equation of state for NaCl and MgO at room temperature and atmospheric pressure.

Material	NaCl	MgO
K(GPa)	24.0	162
K'	5.35	4.15
KK''	10.16	4.88
c_0	2.70	1.69
c_2	0.83	0.038
Z	28	20
P_{FG0} (GPa)	1065.62	2626
V_0 (cm^3/mol.)	27.015	11.248
a_{FG} (GPa nm^5)	0.02337	0.02337
A	0.187	0.241
B	0.317	0.283
C	0.619	0.525

TABLE 2- Results obtained from the Holzapfel AP2 EOS for pressure derivatives of bulk modulus for NaCl.

V/V0	P (GPa)	K (GPa)	K'	KK"	K^2K'''
1.00	0.00	24.00	5.35	-9.10	99.74
0.95	1.411	31.24	4.95	-6.97	68.05
0.90	3.341	40.44	4.61	-5.47	48.08
0.85	5.977	52.20	4.33	-4.37	34.94
0.80	9.587	67.37	4.09	-3.55	25.97
0.75	14.55	87.14	3.89	-2.92	19.66
0.70	21.43	113.2	3.70	-2.42	15.11
0.65	31.06	148.0	3.54	-2.03	11.76

TABLE 3- Results obtained from the Holzapfel AP2 EOS for pressure derivatives of bulk modulus for MgO.

V/V0	P (GPa)	K (GPa)	K'	KK"	K^2K'''
1.00	0.00	162.0	4.15	-4.88	40.85
0.95	9.24	199.3	3.93	-3.98	30.63
0.90	21.22	245.0	3.73	-3.28	23.36
0.85	36.80	301.7	3.56	-2.73	18.06
0.80	57.18	372.6	3.41	-2.29	14.13
0.75	84.04	462.2	3.27	-1.93	11.17
0.70	119.8	576.7	3.15	-1.64	8.89
0.65	167.8	725.2	3.04	-1.40	7.13
0.60	233.4	920.9	2.93	-1.19	5.74
0.55	324.6	1184	2.84	-1.02	4.64
0.50	453.9	1544	2.75	-0.88	3.76

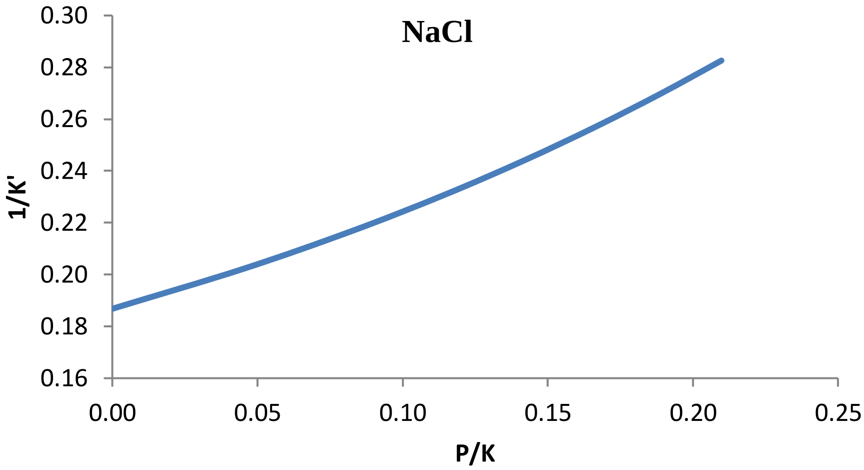

Figure 1- Variation of $1/K'$ vs P/K for NaCl based on the Holzapfel AP2 EOS.

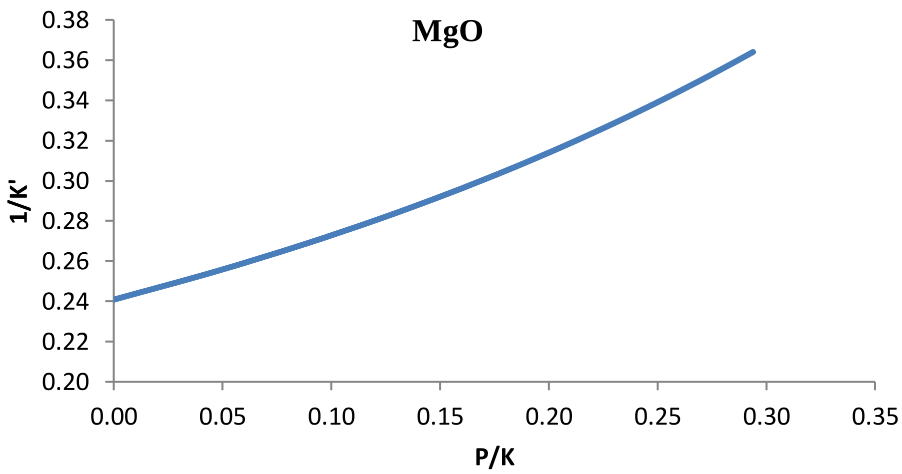

Figure 2- Variation of $1/K'$ vs P/K for MgO based on the Holzapfel AP2 EOS.

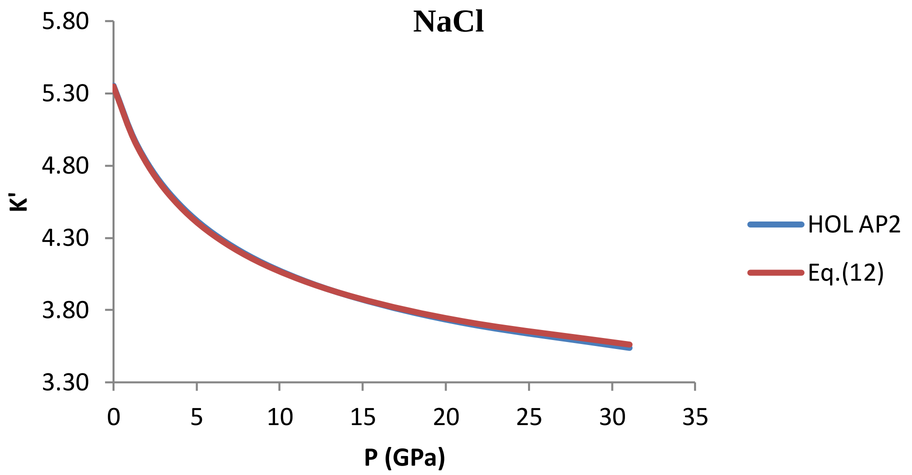

Figure 3- Plots of K' versus P calculated from the Holzapfel AP2 EOS and compared with those based on Eq.(12).

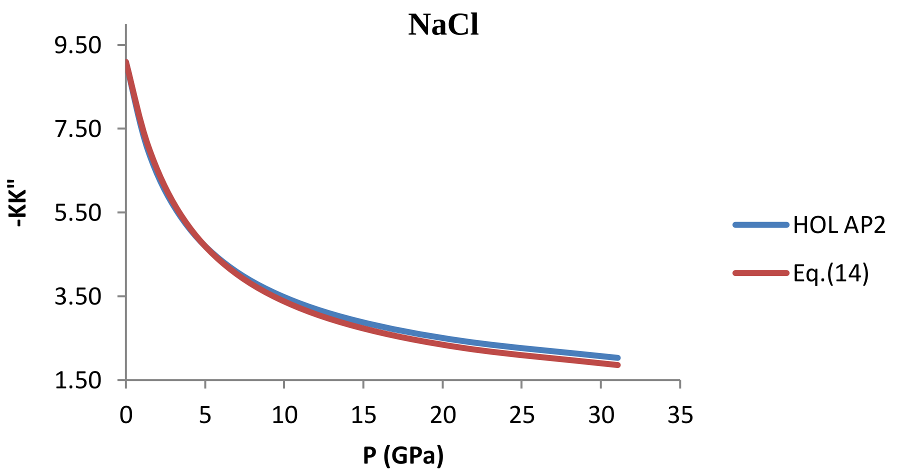

Figure 4- Plots of KK'' versus P calculated from Holzapfel AP2 EOS and compared with those based on Eq.(14).

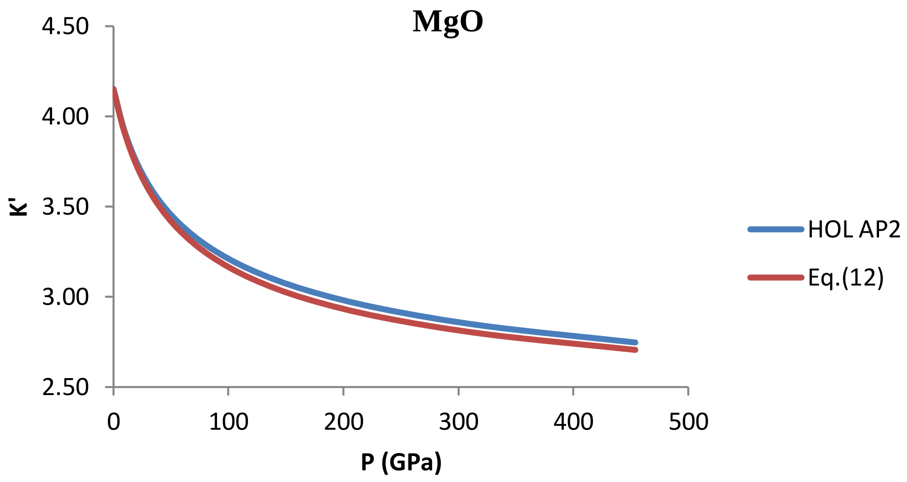

Figure 5- Plots of K' versus P calculated from Holzapfel AP2 EOS and compared with those based on Eq.(12).

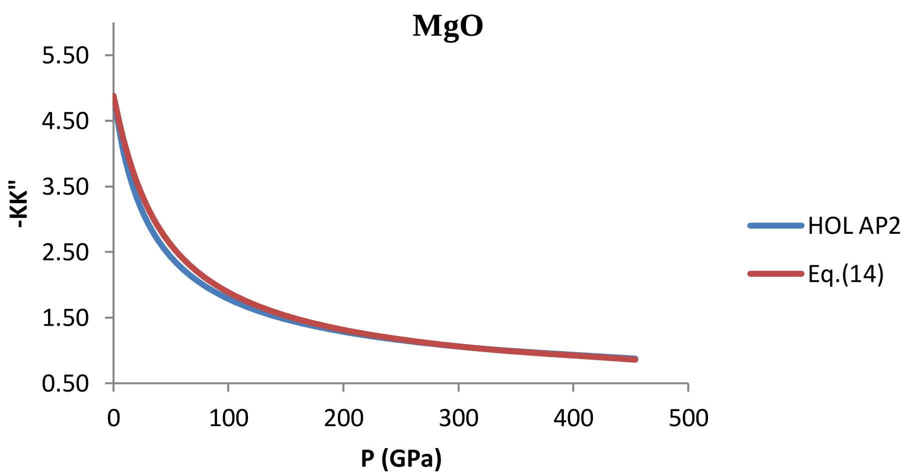

Figure 6- Plots of KK'' verses P calculated from Holzapfel AP2 EOS and compared with those based on Eq.(14).

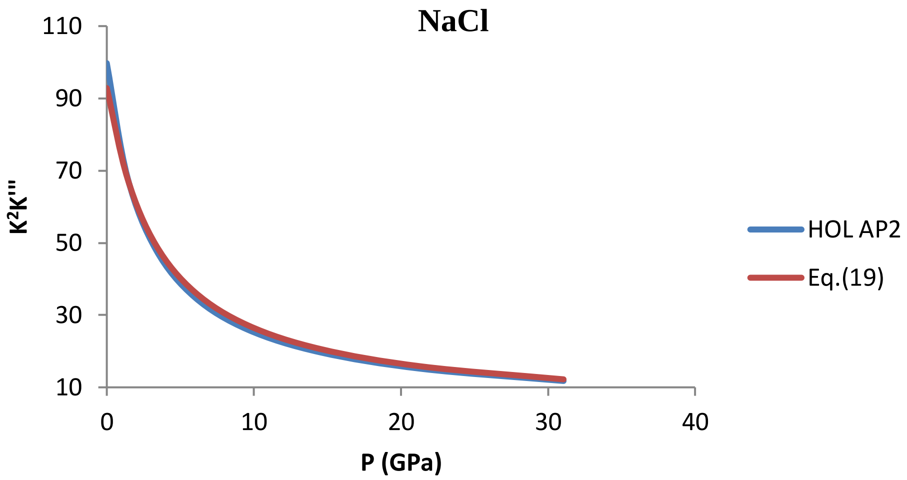

Figure 7- Plots of K^2K''' versus P calculated from Holzapfel AP2 EOS and compared with those based on Eq.(19).

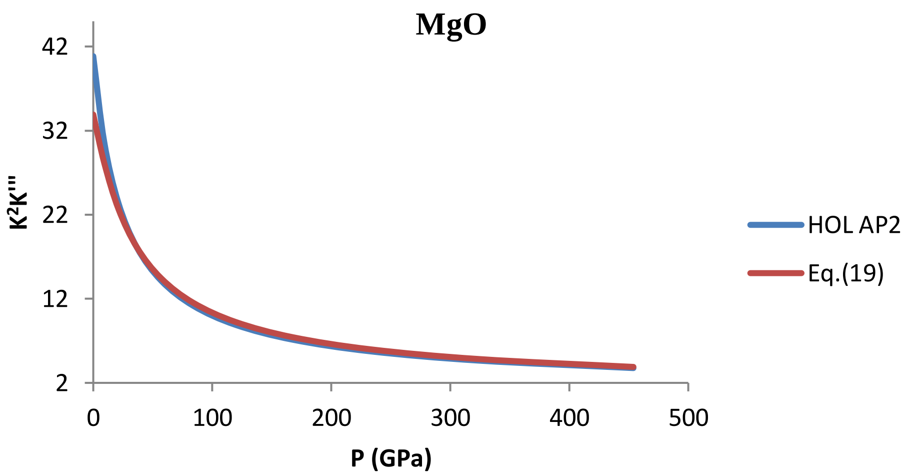

Figure 8- Plots of K^2K''' versus P calculated from Holzapfel AP2 EOS and compared with those based on Eq.(19).

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