

Analysis of the first Pressure Derivative of the Isothermal Bulk Modulus using the Brennan-Stacey, Ullmann-Pankov, and Vinet-Redberg Equations of State for MgO and CaO Solids

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Abstract: In order to extend a prior study and derive accurate values for the and its initial pressure derivative, isothermal bulk modulus, the main objective of the current study is to analyse the link between the three EOSs. The three EOSs that are taken into account are the Vinet-Redberg, Walzer-Ullmann-Pankov, and Brennan-Stacey equations of state. We utilized all three EOS experiments in comparison for two solids. The compression and pressure range variation have been used to assess the applicability.

Keywords: Brennan-Stacey equation of state, Ullmann –Pan’kov Equation of state and Vinet - Redberg.

I. INTRODUCTION

The equation of state, also referred to as the relationship between pressure and volume, can help you grasp some of the material's physical characteristics [1-3].

K and signify the bulk modulus, respectively (the value of K). It is defined by the equation

$$K = -V \frac{dP}{dV} \text{----- (1)}$$

The derivative of pressure with regard to volume is $\frac{dP}{dV}$. Here, P stands for pressure, and V for the solid's initial volume.

However, we follow that based on the relationship between density and volume.

$$K = \rho \frac{dP}{d\rho} \text{----- (2)}$$

In this instance, the initial density is and $\frac{dP}{d\rho}$ is the derivative of pressure with respect to density. At constant temperature, the isothermal bulk modulus is defined as the fractional relationship between the fractional change in volume and the change in pressure. [4-6]. The volume of a solid does not vary much when solids, liquids, and gases are all subjected to the same pressure, as is widely known. Since solids are denser than other states, they have a greater bulk modulus [7].

II. METHOD OF ANALYSIS

[A] Brennan-Stacey Equation of State

The pressure-volume relation, which is a key component of the equation of state (EOS) of a solid, can be used to express the volume dependence of A [6].

$$A = A_0 f\left(\frac{V}{V_0}\right) \text{----- (3)}$$

Where $f(V/V_0)$ is a function of (V/V_0) . Brennan-Stacey [10,11] used an exponential form for the function f appearing in equation (3) which as follows.

$$f\left(\frac{V}{V_0}\right) = \exp\left\{-K\left(\frac{V}{V_0}\right)\right\} \text{----- (4)}$$

Where A_0 and K are constants independent of volume and pressure. Whereas the exponential form equation (3) and equation (4) yields

$$\frac{V dA}{A dV} = -K \frac{V}{V_0} \text{----- (5)}$$

And

$$\frac{V^2 d^2A}{A dV^2} = K^2 \left(\frac{V}{V_0}\right)^2 \text{----- (6)}$$

The constant K are determined by substituting equation (5) in equation and applying consider that $\frac{dK}{dP} = K_0'$ at $P=0$ and $V=V_0$, values of K is found to be equal to $(K_0' - 5/3)$. Similarly using the relation (5) and (6) based as the exponential form in the respective

$$K = K_0 \left(\frac{V}{V_0}\right)^{-1/3} \exp\left\{\left(K_0' - \frac{5}{3}\right)\left(1 - \frac{V}{V_0}\right)\right\} + \frac{4}{3}P \text{----- (7)}$$

$$\frac{dK}{dP} = \left(1 - \frac{4P}{3K}\right)\left(K \frac{V}{V_0} + \frac{5}{3}\right) + \frac{16P}{9K} \text{----- (8)}$$

$$\frac{d^2K}{dP^2} = -\frac{1}{K} \frac{dK}{dP} - \frac{1}{K} \left(\frac{dK}{dP}\right)^2 + \left(\frac{1}{K} - \frac{4P}{3K^2}\right)\left(K^2 \left(\frac{V}{V_0}\right)^2 + 2K \left(\frac{V}{V_0}\right) + 4\right) + \frac{112P}{27K^2} \text{----- (9)}$$

Equations (7)-(9) can be used to predict the values of K , $\frac{dK}{dP}$ and $\frac{d^2K}{dP^2}$ as the function pressure with help of input data on K_0 and K_0' only[12].

[B] Ulmann –Pan’kov Equation of State

This equation of state could be used to calculate the relationship between atomic potentials and strain[11,12]. Consider a solid with $N \gg 1$, where N is the total number of atoms occupying a volume V with r separation between neighbours, as defined by Stacey [13].

$$V = Nf_2 r^3 \text{----- (10)}$$

Where f_2 is the structure factor of order unity

We can explain the total atomic interaction energy ε in terms of averaged interaction between a neighbouring pair of atoms $E(r)$.

$$\varepsilon = 3 Nf_1 E(r) \text{----- (11)}$$

Differentiating of equation (10) this with respect to r then we get

$$\frac{dV}{dr} = 3Nf_2 r^2 \text{----- (12)}$$

The thermodynamic definition of pressure is used to determine the equation of state, the relationship between pressure and volumetric strain.

$$P = -\left(\frac{d\varepsilon}{dV}\right) \text{----- (13)}$$

$$= -\frac{dr d\varepsilon}{dV dr}$$

So therefore equation (13) can be written as

$$P = -\frac{dr d}{dV dr} [3 Nf_1 E(r)]$$



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$$P = -\frac{3Nf_1 dE/dr}{dV/dr} = -\frac{3Nf_1 dE/dr}{3Nf_2 r^2}$$

$$P = -\frac{1}{r^2} \frac{f_1 dE}{f_2 dr} \dots\dots\dots (14)$$

Differentiating of equation (14) this with respect to r then we get

$$\frac{dP}{dr} = -\frac{1}{r} \frac{f_1}{f_2} \left(\frac{1}{r} \frac{d^2 E}{dr^2} - \frac{2}{r^2} \frac{dE}{dr} \right) \dots\dots\dots (15)$$

The isothermal bulk modulus K which is the inverse of the isothermal compressibility is defined as

$$K = -V \left(\frac{dP}{dV} \right)_T \dots\dots\dots (16)$$

$$K = -V \left(\frac{dP/dr}{dV/dr} \right) = -\frac{V \left[-\frac{1}{r} \frac{f_1}{f_2} \left(\frac{1}{r} \frac{d^2 E}{dr^2} - \frac{2}{r^2} \frac{dE}{dr} \right) \right]}{3Nf_2 r^2}$$

$$K = \frac{f_1}{3f_2} \left(\frac{1}{r} \frac{d^2 E}{dr^2} - \frac{2}{r^2} \frac{dE}{dr} \right) \dots\dots\dots (17)$$

Differentiating of equation (17) this with respect to r then we get

$$\frac{dK}{dr} = -\frac{1}{r} \frac{f_1}{3f_2} \left(\frac{3}{r} \frac{d^2 E}{dr^2} - \frac{d^3 E}{dr^3} - \frac{4}{r^2} \frac{dE}{dr} \right) \dots\dots\dots (18)$$

On using first pressure derivative of isothermal bulk modulus K'

$$K' = \left(\frac{dK}{dP} \right) = \left(\frac{dK}{dr} \times \frac{dr}{dP} \right)$$

$$K' = \frac{dK/dr}{dP/dr} \dots\dots\dots (19)$$

Putting the values of $\frac{dK}{dr}$ and $\frac{dP}{dr}$ from equation (18) and (15) in equation (19) then we obtain the first pressure derivative of the isothermal bulk modulus K'.

$$K' = \frac{\frac{1}{r} \frac{f_1}{3f_2} \left(\frac{3}{dr^3} \frac{d^2 E}{dr^2} - \frac{3d^3 E}{dr^3} + \frac{4}{r^2} \frac{dE}{dr} \right)}{-\frac{1}{rf_2} \left(\frac{1}{r} \frac{d^2 E}{dr^2} - \frac{2}{r^2} \frac{dE}{dr} \right)}$$

$$K' = \frac{\frac{d^2 E}{dr^3} - \frac{3d^3 E}{r dr^2} + \frac{4}{r^2} \frac{dE}{dr}}{\frac{6}{r^2} \frac{dE}{dr} - \frac{3d^2 E}{r dr^2}} \dots\dots\dots (20)$$

A potential function of general form is required which obtained

$$E(r) = -A \left(\frac{a}{r} \right)^m + B \left(\frac{a}{r} \right)^n \dots\dots\dots (21)$$

We needed one or two of A and B to be positive in the energy dimension. The first term is commonly identified as attractive and the second as repulsive, but this is not always the case. [14,15]

Differentiating of equation (21) with respect to r then we get

$$\frac{dE}{dr} = \frac{Am}{a} \left(\frac{a}{r} \right)^{m+1} - \frac{Bn}{a} \left(\frac{a}{r} \right)^{n+1} \dots\dots\dots (22)$$

Now we have $B = \frac{Am}{n}$ so therefore $E'=0$ at $r=a$, the value of B putting in equation (21) then get

$$\frac{dE}{dr} = \frac{Am}{a} \left[\left(\frac{a}{r} \right)^{m+1} - \frac{Bn}{a} \left(\frac{a}{r} \right)^{n+1} \right] \dots\dots\dots (23)$$

Again differentiating of equation (23) with respect to r then we get

$$\frac{d^2 E}{dr^2} = \frac{Am}{a} \left[-\frac{(m+1)}{a} \left(\frac{a}{r} \right)^{m+2} + \frac{(n+1)}{a} \left(\frac{a}{r} \right)^{n+2} \right]$$



$$\frac{d^2E}{dr^2} = \frac{Am}{a^2} \left[- (n + 1) \left(\frac{a}{r}\right)^{n+2} + (m + 1) \left(\frac{a}{r}\right)^{m+2} \right] \text{----- (24)}$$

Again differentiating of equation (24) with respect to r then we

$$\begin{aligned} \frac{d^3E}{dr^3} &= \frac{Am}{a^2} \left[- \frac{(n + 1)(n + 2)}{a} \left(\frac{a}{r}\right)^{n+3} + \frac{(m + 1)(m + 2)}{a} \left(\frac{a}{r}\right)^{m+3} \right] \\ \frac{d^3E}{dr^3} &= \frac{Am}{a^3} \left[(m + 1)(m + 2) \left(\frac{a}{r}\right)^{m+3} - (n + 1)(n + 2) \left(\frac{a}{r}\right)^{n+3} \right] \text{----- (25)} \end{aligned}$$

Substituting the value of dE/dr from equation (23) in (14) and Equation (14) can be expressed as a pressure relationship

$$\begin{aligned} P &= - \frac{1}{r^2} \frac{f_1}{f_2} \frac{dE}{dr} \\ P &= - \frac{1}{r^2} \frac{Am f_1}{a f_2} \left[\left(\frac{a}{r}\right)^{m+1} - \left(\frac{a}{r}\right)^{n+1} \right] \text{----- (26)} \end{aligned}$$

Now substituting the value of dE/dr and d²E/dr² from equation (23) and (24) in (17) so therefore Equation (17) can be expressed as bulk modulus relation

$$\begin{aligned} K &= \frac{f_1}{3f_2} \left(\frac{1}{r} \frac{d^2E}{dr^2} - \frac{2}{r^2} \frac{dE}{dr} \right) \\ K &= \frac{f_1}{3f_2} \left(\frac{1}{r} \times \frac{Am}{a^2} \left[- (n + 1) \left(\frac{a}{r}\right)^{n+2} + (m + 1) \left(\frac{a}{r}\right)^{m+2} \right] - \frac{2}{r^2} \times \frac{Am}{a} \left[\left(\frac{a}{r}\right)^{m+1} - \left(\frac{a}{r}\right)^{n+1} \right] \right) \\ K &= \frac{f_1 Am}{3f_2 ar^2} \left[(n + 3) \left(\frac{a}{r}\right)^{n+1} - (m + 3) \left(\frac{a}{r}\right)^{m+1} \right] \text{----- (27)} \end{aligned}$$

Now substituting the value of dE/dr, d²E/dr² and d³E/dr³ from equation (23) (24) and (25) in (20) so therefore Equation (20) can be written as pressure derivative of bulk modulus relation

$$K' = \frac{(n+3)^2 \left(\frac{a}{r}\right)^{n-m} - (m+3)^2}{3(n+3) \left(\frac{a}{r}\right)^{n-m-3(m+3)}} \text{----- (28)}$$

Now applying the boundary conditions that at P=0, K=K₀ and r=a in equation (27) then we get

$$K_0 = \frac{f_1 Am}{3f_2 a^3} [n - m] \text{----- (29)}$$

So therefore

$$\frac{K_0}{[n - m]} = \frac{f_1 Am}{3f_2 a^3}$$

Substituting the value of $\frac{f_1 Am}{3f_2 a^3} = \frac{K_0}{[n-m]}$ from equation (29) in (26) and Equation (26) can be expressed as a pressure relationship

$$\begin{aligned} P &= - \frac{1}{r^2} \frac{Am f_1}{a f_2} \left[\left(\frac{a}{r}\right)^{m+1} - \left(\frac{a}{r}\right)^{n+1} \right] \\ &= - \frac{3K_0}{[n - m]} \left(\frac{a}{r}\right)^2 \left[\left(\frac{a}{r}\right)^{m+1} - \left(\frac{a}{r}\right)^{n+1} \right] \\ P &= \frac{3K_0}{[n-m]} \left[\left(\frac{a}{r}\right)^{n+3} - \left(\frac{a}{r}\right)^{m+3} \right] \text{----- (30)} \end{aligned}$$

Now we know that

$$\left(\frac{\rho}{\rho_0}\right) = \left(\frac{a}{r}\right)^3 \text{ or } \frac{a}{r} = \left(\frac{\rho}{\rho_0}\right)^{1/3} \text{ and } \left(\frac{\rho}{\rho_0}\right)^{1/3} = \left(\frac{V}{V_0}\right)^{-1/3}$$



Substituting the value of $\frac{a}{r} = \left(\frac{\rho}{\rho_0}\right)^{1/3}$ in equation (30), Equation (26) can be written as pressure relation

$$P = \frac{3K_0}{[n - m]} \left[\left(\frac{\rho}{\rho_0}\right)^{\left(\frac{n}{3}+1\right)} - \left(\frac{\rho}{\rho_0}\right)^{\left(\frac{m}{3}+1\right)} \right]$$

$$P = \frac{3K_0}{[n-m]} \left[\left(\frac{V}{V_0}\right)^{-\left(\frac{n}{3}+1\right)} - \left(\frac{V}{V_0}\right)^{-\left(\frac{m}{3}+1\right)} \right] \text{----- (31)}$$

Walzer et al [16] and Ulmann-Pan'kov [17] advocated an equation (26) restricted by the requirement $n = 2m$ so that $m = (K_0' - 2)$ and $n = 2(K_0' - 2)$ but with K_0' is not necessarily equal to 4. It is remarkable that we can obtain responsible results with such a wide of adjustable parameter.

$$P = \frac{3K_0}{[2(K_0' - 2) - (K_0' - 2)]} \left[\left(\frac{V}{V_0}\right)^{-\left(\frac{2(K_0'-2)}{3}+1\right)} - \left(\frac{V}{V_0}\right)^{-\left(\frac{(K_0'-2)}{3}+1\right)} \right]$$

$$P = \frac{3K_0}{[(K_0' - 2)]} \left[\left(\frac{V}{V_0}\right)^{-\left(\frac{2K_0'-1}{3}\right)} - \left(\frac{V}{V_0}\right)^{-\left(\frac{(K_0'-1)}{3}\right)} \right]$$

Substituting the value of $\frac{a}{r} = \left(\frac{\rho}{\rho_0}\right)^{1/3}$ and $\left(\frac{\rho}{\rho_0}\right)^{1/3} = \left(\frac{V}{V_0}\right)^{-1/3}$ in equation (28) and Equation (28) can be written as pressure derivative of bulk modulus.

$$K' = \frac{(n+3)^2 \left(\frac{a}{r}\right)^{n-m} - (m+3)^2}{3(n+3) \left(\frac{a}{r}\right)^{n-m-3(m+3)}}$$

$$= \frac{(n+3)^2 \left(\frac{\rho}{\rho_0}\right)^{(n-m)/3} - (m+3)^2}{3(n+3) \left(\frac{\rho}{\rho_0}\right)^{(n-m)/2} - 3(m+3)}$$

$$K' = \frac{(n+3)^2 \left(\frac{V}{V_0}\right)^{-(n-m)/3} - (m+3)^2}{3(n+3) \left(\frac{V}{V_0}\right)^{-(n-m)/2-3(m+3)}}$$

[C] Vinet - Redberg Equation of State

The relationship between the binding energy and the solid's intermolecular distance is stated in this equation of state. Vine and Redberg, who assumed that the interatomic interaction in solids was expressed by a form $A(1+ar)\exp(-br)$ with A, where a and b were the material constants, provided the basis for the derivation of this equation of state. Vinet et al. obtained the equation of state by employing the Redberg potential. The form of the potential is comparable to that described in the context of the Redberg potential. The binding energy function of Vinet and Redberg [18] can be represented as follows

$$U = -\Delta U(1 + a^*)e^{-a^*} \text{----- (32)}$$

Where $a^* = -\eta \left(1 - \frac{r}{a}\right)$ in which a is treated as an adjustable parameter

$$U = -\Delta U \left[1 - \eta \left(1 - \frac{r}{a}\right)\right] e^{\eta \left(1 - \frac{r}{a}\right)} \text{----- (33)}$$



Where $\eta = \left(\frac{a}{l}\right)$ is a dimensionless shape parameter whose value lies between 3 and 8 [19] and l is the scaling length that is treated as an adjustable parameter.

Now putting the value of $\frac{r}{a} = \left(\frac{V}{V_0}\right)^{1/3}$ in the equation (2) then we get

$$U = -\Delta U \left[1 - \eta \left(1 - \left(\frac{V}{V_0} \right)^{1/3} \right) \right] e^{\eta \left[1 - \left(\frac{V}{V_0} \right)^{1/3} \right]} \dots\dots\dots (34)$$

The Binding energy of solids could be calculated in the thermodynamics relation as follow

$$P = T \left(\frac{dP}{dT} \right)_V \\ = \left(\frac{dE}{dV} \right)_T = - \left(\frac{dU}{dV} \right)_T \dots\dots\dots (35)$$

In this relation the term $T \left(\frac{dP}{dT} \right)_V$ is the thermal pressure and uses the volume derivative of the binding energy to approximation the term $\left(\frac{dE}{dV} \right)_T$ which is called internal pressure. It should be mentioned that we have used the symbol U rather than the binding energy function of Vinet et al and indicate that is configurational potential energy .

Differentiating of equation (34) with respect to V then we get

$$\frac{dU}{dV} = -\Delta U \left[\left(1 - \eta \left\{ 1 - \left(\frac{V}{V_0} \right)^{1/3} \right\} \right) \cdot e^{\eta \left[1 - \left(\frac{V}{V_0} \right)^{1/3} \right]} \cdot -\eta \times \frac{1}{3} \left(\frac{V}{V_0} \right)^{\frac{1}{3}} \frac{1}{V_0} + e^{\eta \left[1 - \left(\frac{V}{V_0} \right)^{1/3} \right]} \times \eta \cdot \frac{1}{3} \left(\frac{V}{V_0} \right)^{-2/3} \frac{1}{V_0} \right] \\ \frac{dU}{dV} = -\frac{\Delta U \eta^2}{3V_0} \left(\frac{V}{V_0} \right)^{-2/3} \cdot e^{\eta \left[1 - \left(\frac{V}{V_0} \right)^{1/3} \right]} \left[1 - \left(\frac{V}{V_0} \right)^{1/3} \right] \dots\dots\dots (36)$$

Putting the values of $\frac{dU}{dV}$ from equation (36) in equation (35).Equation (35) can be written as

$$P = - \left(\frac{dU}{dV} \right)_T \\ P = \frac{\Delta U \eta^2}{3V_0} \left(\frac{V}{V_0} \right)^{-2/3} \cdot e^{\eta \left[1 - \left(\frac{V}{V_0} \right)^{1/3} \right]} \left[1 - \left(\frac{V}{V_0} \right)^{1/3} \right] \dots\dots\dots (37)$$

Putting the values of $\left(\frac{V}{V_0}\right)^{1/3} = x$, in equation (35) then we get

$$P = \frac{\Delta U \eta^2}{3V_0} [1 - x]x^{-2} e^{\eta[1-x]} \\ P = \frac{\Delta U \eta^2}{3V_0} \left[\frac{1-x}{x^2} \right] e^{\eta[1-x]} \dots\dots\dots (38)$$

The isothermal bulk modulus K which is the inverse of the isothermal compressibility is defined as

$$K = -V \left(\frac{dP}{dV} \right)_T \dots\dots\dots (39) \\ = -V \left(\frac{dP}{dx} \right) \left(\frac{dx}{dV} \right)$$

Now we know that $x = \left(\frac{V}{V_0}\right)^{1/3}$ and differentiating of equation with respect to V then we get

$$\frac{dx}{dV} = \frac{1}{3} \left(\frac{V}{V_0} \right)^{-2/3} \frac{1}{V_0} \\ = \frac{1}{3V_0} x^{-2} = \frac{1}{3V_0 x^2} \dots\dots\dots (40)$$



Therefore solved the equation (37) and differentiating of with respect to V then we get

$$P = \frac{\Delta U \eta^2}{3V_0} \left[\left(\frac{1-x}{x^2} \right) \frac{d}{dx} e^{\eta[1-x]} + e^{\eta[1-x]} \frac{d}{dx} \left(\frac{1}{x^2} - \frac{1}{x} \right) \right]$$

$$\frac{dP}{dx} = - \frac{\Delta U \eta^2}{3V_0 x^2} e^{\eta[1-x]} \left[\eta (1-x) + \frac{2}{x} - 1 \right]$$

$$\frac{dP}{dx} = - \frac{\Delta U \eta^2}{3V_0 x^3} e^{\eta[1-x]} [\eta x(1-x) + (2-x)] \text{ ----- (41)}$$

Putting the values of $\frac{dx}{dV}$ and $\frac{dP}{dx}$ from equation (40) and (41) in equation (39). Relation for the isothermal bulk modulus K can be written as

$$K = -V \left\{ - \frac{\Delta U \eta^2}{3V_0 x^3} e^{\eta[1-x]} [\eta x(1-x) + (2-x)] \cdot \frac{1}{3V_0 x^2} \right\}$$

$$K = \left(\frac{V}{V_0} \right) \frac{\Delta U \eta^2}{9V_0 x^5} [\eta x(1-x) + (2-x)] e^{\eta[1-x]} \text{ ----- (42)}$$

Putting the values of $\frac{V}{V_0} = x^3$, in equation (42) then we get

$$K = x^3 \frac{\Delta U \eta^2}{9V_0 x^5} [\eta x(1-x) + (2-x)] e^{\eta[1-x]}$$

$$K = \frac{\Delta U \eta^2}{9V_0 x^2} [\eta x(1-x) + (2-x)] e^{\eta[1-x]} \text{ ----- (43)}$$

Now applying the boundary condition at P=0, x=1 and K=K₀ in equation (41) then we get

$$K_0 = \frac{\Delta U \eta^2}{9V_0} \text{ or } 3K_0 = \frac{\Delta U \eta^2}{3V_0}$$

Putting the values of $\frac{\Delta U \eta^2}{3V_0} = 3K_0$, in equation (38) then we get

$$P = 3K_0 \left[\frac{1-x}{x^2} \right] e^{\eta[1-x]} \text{ ----- (44)}$$

$$P = 3K_0 x^{-2} (1-x) e^{\eta[1-x]} \text{ ----- (45)}$$

Putting the values of $K_0 = \frac{\Delta U \eta^2}{9V_0}$, in equation (43) then we get

$$K = \frac{K}{x^2} [\eta x(1-x) + (2-x)] e^{\eta[1-x]}$$

$$K = K_0 x^{-2} [\eta x(1-x) + (1-x) + 1] e^{\eta[1-x]} \text{ ----- (46)}$$

$$K = K_0 \left[\frac{\eta(1-x)}{x} + \frac{(2-x)}{x^2} \right] e^{\eta[1-x]} \text{ ----- (47)}$$

Equation (46) can be written as

$$K = K_0 x^{-2} [(\eta x + 1)(1-x) + 1] e^{\eta[1-x]} \text{ ----- (48)}$$

The first pressure derivative of isothermal bulk modulus K'

$$K' = \left(\frac{dK}{dP} \right)$$

$$= \left(\frac{dK}{dx} \right) / \left(\frac{dP}{dx} \right) \text{ ----- (49)}$$

Therefore solved the equation (48) and differentiating of with respect to x then we get

$$K = K_0 [x^{-2} + (\eta x + 1)(1-x)x^{-2}] e^{\eta[1-x]}$$

$$K = K_0 [2x^{-2} + \eta x^{-1} - x^{-1} - \eta] e^{\eta[1-x]} \text{ ----- (50)}$$

$$= \frac{-K_0 e^{\eta[1-x]}}{x^3} [3\eta x + \eta^2 x^2 - \eta x^2 - \eta^2 x^3 + 4 - 1]$$

$$\frac{dK}{dx} = \frac{-K_0 e^{\eta[1-x]}}{x^3} [\eta^2 x^2 (1-x) + \eta x (3-x) + 4 - x] \text{----- (51)}$$

Differentiating of equation (44) with respect to x then we get

$$\frac{dP}{dx} = 3K_0 \left[\left(\frac{1-x}{x^2} \right) \times -\eta e^{\eta[1-x]} + e^{\eta[1-x]} \times \left(-\frac{2}{x^3} + \frac{1}{x^2} \right) \right]$$

$$\frac{dP}{dx} = \frac{-3K_0 e^{\eta[1-x]}}{x^3} [1 + (\eta x + 1)(1-x)] \text{----- (52)}$$

Putting the values of $\frac{dK}{dx}$ and $\frac{dP}{dx}$ from equation (51) and (52) in equation (49). Relation for the first pressure derivative of isothermal bulk modulus K' [20,21] can be expressed as ss

$$K' = \left(\frac{dK}{dx} \right) / \left(\frac{dP}{dx} \right)$$

$$K' = \frac{1}{3} \left[\frac{\eta^2 x^2 (1-x) + \eta x (3-x) + 4 - x}{1 + (\eta x + 1)(1-x)} \right] \text{----- (53)}$$

Equation (53) can be written as

$$K' = \frac{1}{3} \left[\frac{x(1-x) + 2\eta x^2}{1 + (\eta x + 1)(1-x)} + \eta x + 2 \right] \text{----- (54)}$$

The value of parameter η can be determined in term of K'_0 by the boundary condition, $P=0$, $x=1$ and $K' = K'_0$ and in equation (54) then we get

$$K' = \frac{1}{3} [2\eta + 3] \text{ or } K' = \frac{2\eta + 3}{3}$$

and the value of $\eta = \frac{3}{2} (K'_0 - 1)$

III. RESULTS AND DISCUSSION

There are three equations of state for the analysis of the isothermal bulk modulus (K) and first pressure derivative (K') for MgO and CaO ionic solids that have been compared. In this work, Vinet et al, the first pressure derivative of the isothermal bulk modulus satisfy the Brennan-Stacey equation of state and the Walzer-Ullmann-Pan'kov work. Results and accessible experimental data have been compared. Figures 1, 2, and 3 and Figure 4 display the outcomes.

V/V ₀	Isothermal Bulk Modulus K for MgO			First pressure Derivative of Isothermal Bulk Modulus K' for MgO			Isothermal Bulk Modulus K for CaO			First pressure Derivative of Isothermal Bulk Modulus K' for CaO		
	(a)	(b)	(c)	(a)	(b)	(c)	(a)	(b)	(c)	(a)	(b)	(c)
1.00	162	162	162	4.13	4.13	4.13	114	114	114	4.05	4.05	4.05
0.95	199	199	199	3.84	3.94	3.85	139	140	139	3.77	3.86	3.78
0.90	243	245	243	3.59	3.77	3.61	170	171	170	3.52	3.70	3.54
0.85	296	303	298	3.36	3.63	3.39	206	211	207	3.30	3.56	3.33
0.80	361	376	364	3.16	3.50	3.19	250	261	253	3.10	3.44	3.14
0.75	440	470	447	2.97	3.38	3.02	304	324	309	2.92	3.33	2.97
0.70	536	591	549	2.80	3.28	2.85	370	406	379	2.75	3.23	2.81



0.65	656	751	679	2.64	3.19	2.70	451	514	466	2.60	3.14	2.65
0.60	805	966	844	2.50	3.11	2.55	552	659	578	2.45	3.05	2.51
0.55	994	1262	1057	2.35	3.03	2.41	679	857	721	2.32	2.98	2.37
0.50	1236	1679	1338	2.22	2.96	2.274	841	1134	909	2.19	2.90	2.24

Table-1: Values of Isothermal Bulk Modulus K and Values of First Pressure Derivative of Isothermal Bulk Modulus K' for MgO and CaO at different Compressions. Calculated from: (a) Bernan-Stacy EOS (b)Ullmann-Pankov EOS (c) Vinet EOS

Graphical Analysis:

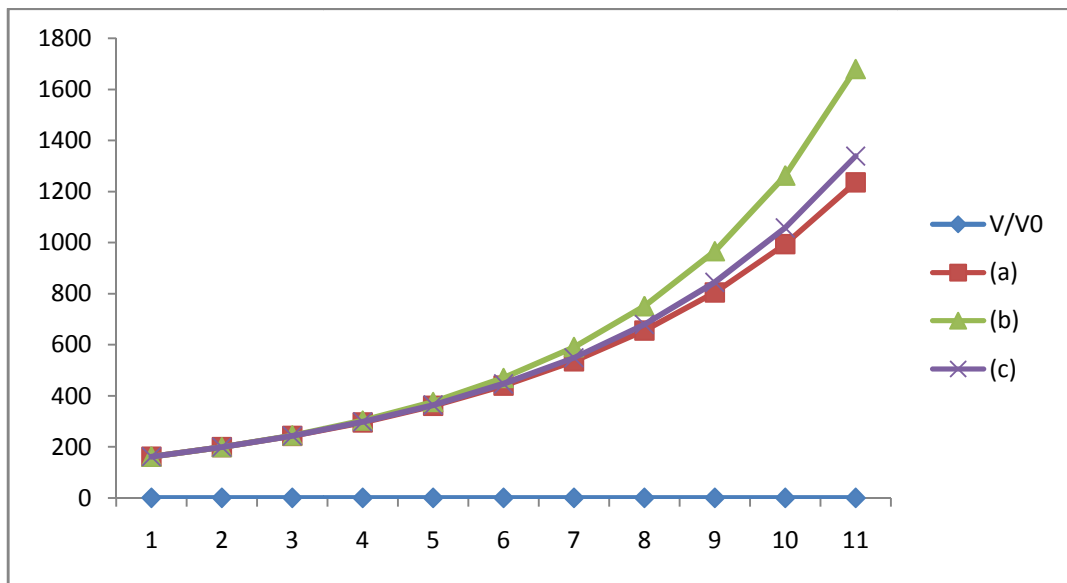


Figure (1) Isothermal Bulk Modulus K for MgO Calculated from (A) Bernan-Stacy EOS (B)Ullmann-Pankov EOS (C) Vinet EOS

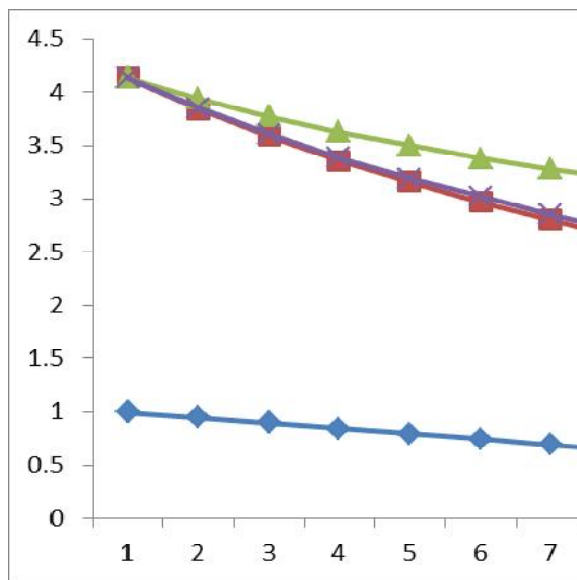


Figure (2) First pressure derivative of isothermal bulk modulus K' for MgO Calculated from (A) Bernan-Stacy EOS (B)Ullmann-Pankov EOS (C) Vinet EOS

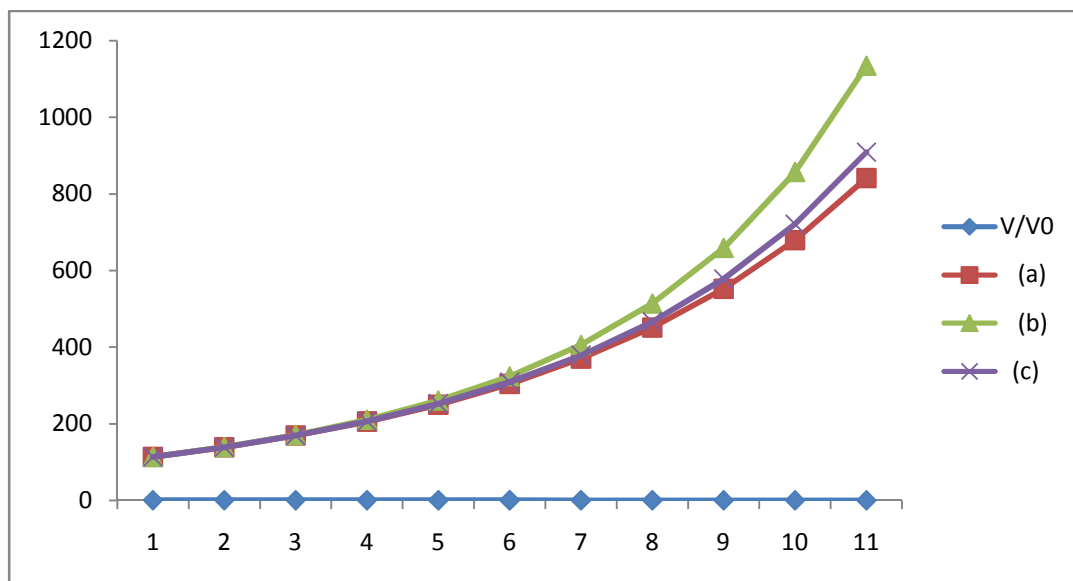


Figure (3) Isothermal bulk modulus K for CaO Calculated from (A) Bernan-Stacy EOS (B)Ulmann-Pankov EOS (C) Vinet EOS

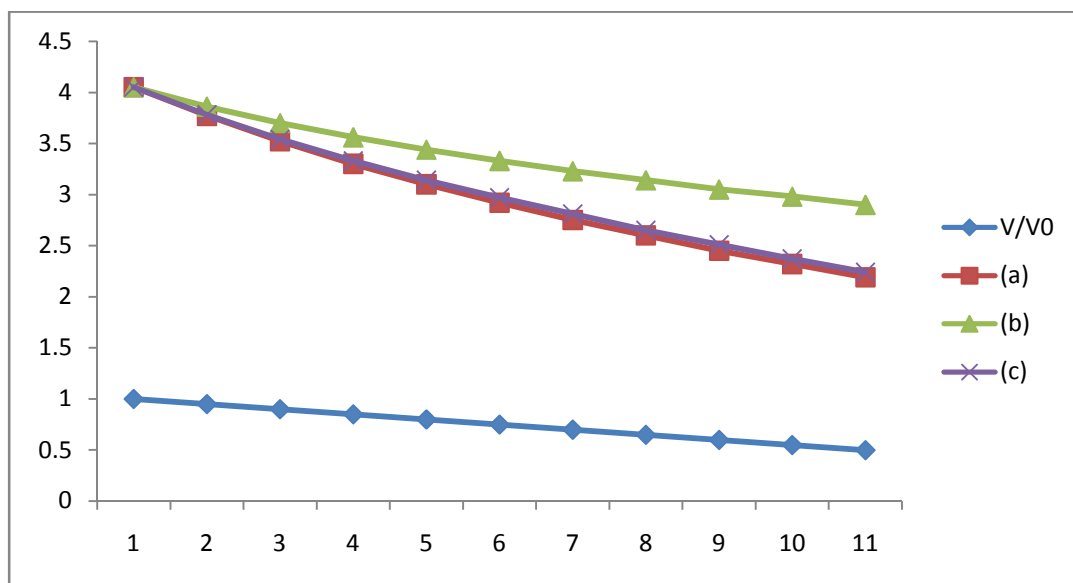


Figure (4) First pressure derivative of isothermal bulk modulus K' for CaO Calculated from: (A) Bernan-Stacy EOS (B)Ulmann-Pankov EOS (C) Vinet EOS

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