THEORETICAL PREDICTION OF ELASTIC CONSTANTS FOR MgO

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Abstract: Precise knowledge of the elastic properties of MgO periclase, under high-pressure condition is therefore crucial for constructing the accurate mineralogical model of the Earth's lower mantle. In present work an attempt has been done to calculate the pressure dependence elastic properties such as isothermal bulk modules (K_T), Young's modulus of elasticity Y and shearing stress G for geophysical MgO by using three deferent phenomenological EOS viz. the Born-Mayer EOS, Murnaghan EOS and Birch EOS. The result shows that the value of elastic parameter as calculated by using Murnughan EOS and Birch EOS shows close agreement with each other while Born-Mayer EOS shows deviation in calculated values.

Keywords: Geophysical Minerals; Elastic Properties; Youngs modulus; Isothermal EOS; Isothermal Bulk modulus.

1. Introduction

Geophysical minerals MgO is the major constituents of the Earth's lower mantle and core. Periclase (MgO) is a simple oxide with cubic NaCl structure. Thermo elastic properties like isothermal bulk modules (K_T), Young's modulus of elasticity and shearing stress of geophysical MgO, under high temperature and high pressure has been studied by using isothermal equations of states (EOS).

Elastic properties significantly influence fundamental properties of solids viz., interatomic potential, equations of state (EOS), specific heat, thermal expansion, Debye temperature, melting point and Gruneisen parameter via elastic constant. Thermo elastic behavior of solids at high temperature gives the knowledge of temperature dependence of elastic modulii. In present work Various isothermal equations of state (EOS) such as the Born-Mayer EOS [1], Murnaghan EOS [2] and Birch EOS [3,4] are used to study for

prediction of pressure dependent elastic properties such as isothermal bulk modulus (K_T), Young's modulus of elasticity and shearing stress of MgO.

2. Theory

An EOS can be derived from the volume derivative of lattice potential energy [5, 6] by using the relation

$$P = -\left(\frac{dW}{dV}\right)_T \quad (1)$$

where W for an ionic crystal can be written as the sum of electrostatic energy and short range overlap repulsive energy Φ .

By using an exponential function for Φ , we get an EOS known as Born-Mayer EOS [1] which can be written as

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

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

K_0 and K'_0 are the isothermal bulk modulus and its first pressure derivative at zero pressure respectively.

A simple EOS based on assumption according to which the isothermal bulk modulus depends linearly on pressure, Murnaghan EOS [2] can be written as;

$$P = \frac{K}{K'_0} \left[\left(\frac{V}{V_0} \right)^{-K'_0} - 1 \right] \quad (3)$$

On the basis of finite strain theory, Birch obtained an EOS [3, 4] which is as follows;

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

Expression for isothermal bulk modulus can be obtained by using the relation

$$K_T = -V \left(\frac{\partial P}{\partial V} \right)_T \quad (5)$$

Hence by using equation (5) in equations (2), (3) and (4) expression for K_T can be written as follows;

$$K_T = P \left[\frac{2}{3} + \frac{\eta}{3} \left(\frac{V}{V_0} \right)^{\frac{1}{3}} \right] + \frac{3K_0}{(\eta - 2)} \left(\frac{V}{V_0} \right)^{-\frac{4}{3}} \left[\frac{\eta}{3} \left(\frac{V}{V_0} \right)^{\frac{1}{3}} - \frac{2}{3} \right] \quad (6)$$

$$K_T = K_0 \left(\frac{V}{V_0} \right)^{-K'_0} \quad (7)$$

$$K_T = \frac{5}{3}P + K_0 \left(\frac{V}{V_0} \right)^{-\frac{7}{3}} \left[1 - \frac{3(4-K'_0)}{2} \left\{ \left(\frac{V}{V_0} \right)^{-\frac{2}{3}} - 1 \right\} \right] \quad (8)$$

The isotropic shear modulus (G) [7] within the voigt limit is as follows;

$$G = \frac{3}{5}(K - 2P) \quad (9)$$

In terms of Bulk and Shear Modulus, the Young's modulus [8] can be written as

$$Y = \frac{9KG}{3K + G} \quad (10)$$

We make use of above equations for calculating Bulk modulus, Shear modulus, Young's modulus.

3. Results and Discussion

In the present work we have made an attempt for the theoretical prediction of isothermal bulk modulus, shear modulus and Young's modulus of elasticity for mineral MgO at different compression ranges [$V/V_0 = 1$ to $V/V_0 = 0.6$]. In this calculation we have used three different isothermal EOS viz. Morn-Mayer EOS, Murnaghan EOS and Birch EOS. The Input values for K_0 and K'_0 are 157 GPa and 4.37 respectively taken from reference [8]. The calculated values of different parameters like K_T , G, and Y are given in Table (1-2). The graph plotted between compression ratio V/V_0 vs K_T , G, Y are shown in the Fig. (1-3). From these plots it is observed that results obtained by the use of Murnaghan EOS and Birch EOS shows close agreement with each other while Born-Mayer EOS shows some deviation. These results indicate that in the above said compression ranges Murnaghan EOS and Birch EOS are suitable for the prediction of elastic constant such as isothermal bulk modulus, shear modulus and Young's modulus of elasticity for mineral MgO.

Table 1: Calculated values of elastic constants K_T (GPa) by using Born-Mayer, Murnaghan and Birch EOS

V/V_0	$K_T(\text{B-M})$ (GPa)	$K_T(\text{Murn})$ (GPa)	$K_T(\text{Birch})$ (GPa)
1	157	157	157
0.9	373.11	219.76	213.13
0.8	1118.44	402.12	358.59
0.7	3607.88	797.73	619.13
0.6	12987.77	1759.11	1120.23

Table 2: Calculated values of elastic constants G(GPa) and Y (GPa) by using Born-Mayer, Murnaghan and Birch EOS

V/V ₀	G(B-M) (GPa)	G(Murn) (GPa)	G(Birch) (GPa)	Y(B-M) (GPa)	Y(Murn) (GPa)	Y(Birch) (GPa)
1	76.88	76.88	76.88	192	192	192
0.9	114.63	110.39	106.78	497.4	283.67	274.54
0.8	545.28	177.15	154.26	1407.17	463.4	404.75
0.7	1696.56	321.98	233.91	4400	851.39	623.25
0.6	5962.29	673.92	377.83	15513.04	1792.82	1018.92

Fig. 1. Variation of K_T Vs V/V_0 with different EOS

Fig. 2. Variation of G Vs V/V_0 with different EOS

Fig. 3. Variation of Y Vs V/V_0 with different EOS

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