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ABSTRACT

Elastic properties of the low-pressure structure of the magnesium orthosilicate Mg_2SiO_4, (forsterite) are determined using a thermo dynamical method for the pressure range (0-24GPa). The geologically important quantities: second order elastic constants (SOE) and seismic wave velocity (V_p& V_s) are computed with the help of derived theory. The computed values of bulk moduli (B), and its pressure derivative (B') of Mg_2SiO_4in i.e. forsterite is tested by analyzing the compression in volume with increase of pressure with the help of phenomenological theory and other based on ab-initio molecular dynamic simulation equation of states (EOS). The results of C_{ij} agree well with the available experimental data in case of Mg_2SiO_4 (forsterite). Therefore, the results for the Mg_2SiO_4 (forsterite) may be important in geophysical study of these solids in earth's upper mantle.

Keywords:*Elasticity; Forsterite; High pressure; ab-initio, EOS.*

INTRODUCTION

The study of the elasticity of Earth materials has become increasingly important over the last decade, as contributions from global seismic tomography, seismological investigations of geographically and radially localized regions, mantle discontinuities, analysis of normal modes of oscillations, and other types of studies have revealed the Earth's mantle in unprecedented detail [1-6]. Moreover the elastic constants of Earth's materials at high pressure provide fruitful ground for an exploration of the foundations of material behavior in the relationship between structure and bonding. The fourth ranked elastic constant tensor is unusually rich in this regard and reflects the symmetry of the underlying structure. For example, the contrast between periodic and nonperiodic condensed matter is immediately apparent in the elastic anisotropy, a distinction that is not as clear in tensorial properties of lower rank such as the index of refraction, which is isotropic for cubic and nonperiodic materials a like [7]

The magnesium orthosilicate Mg_2SiO_4 (forsterite), is one of the main constituents of the middle and lower crust as well as upper mantle of middle and lower crust as well as upper mantle of the Earth [8,9]. The Mg_2SiO_4 forms several structures at ambient pressure, but in the Earth's interior it forms a sequence of phase from ortho-rhombic forsterite phase.

In this paper we present the calculation of the com plete elastic tensor of low symmetry Pbnm, which, is t he low-pressure structure of the magnesium orthosilic ate Mg_2SiO_4 (forsterite) as a functional of pressure de pendence of several important mechanical properties. A more serious limitation has been a lack of knowled ge of the relevant material properties at the extreme c onditions of the Earth's interior. Therefore we tried to through some information by analyzing the elastic beh avior of Mg_2SiO_4.

METHODOLOGY

The Anderson-Gruneisen δ_T parameter is defined

$$\delta_T = -\frac{1}{\alpha B}\left(\frac{\partial B}{\partial T}\right)_P \text{--------(1)}$$

where α is the coefficient of volume thermal expantion and B is isothermal bulk modulus.
Using definition of thermal expensivity

$$\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P \text{--------(2)}$$

in eq. (1) gives

$$\delta_T = -\frac{V}{B}\left(\frac{\partial B}{\partial V}\right)_P \text{--------(3)}$$

The first order pressure derivative of bulk modulus is defined as

$$B' = \frac{dB}{dP} \text{--------(4)}$$

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Considering , Kumar approximation[16] as

$$B' = (Constant)\frac{V}{V_0} - 1 \text{--------(5)}$$

where A is material- dependent constant

At P=0, $V = V_0$, $B' = B'_0$ then $= B'_0 + 1$, Thus Eq. (5) can be written as

$$\frac{dB}{dP} = (B'_0 + 1)\frac{V}{V_0} - 1 \text{--------(6)}$$

or

$$-\frac{V}{B}\frac{dB}{dV} = (B'_0 + 1)\frac{V}{V_0} - 1 \text{--------(7)}$$

$$-\frac{dB}{B} = (B'_0 + 1)\frac{dV}{V_0} - \frac{dV}{V} \text{--------(8)}$$

IntergratingEq.(8) we get

$$\frac{B}{B_0} = \left(\frac{V}{V_0}\right) exp(B'_0 + 1)\left(1 - \frac{V}{V_0}\right) \text{--------(9)}$$

Using the definition of the isothermal bulk modulus B in the above equation,

$$\frac{1}{B_0}\left(-V\frac{dP}{dV}\right) = \left(\frac{V}{V_0}\right) exp(B'_0 + 1)\left(1 - \frac{V}{V_0}\right) \text{--------(10)}$$

On intergrating Eq.(10) we get

$$1 + \frac{(B'_0+1)P}{B_0} = exp(B'_0 + 1)\left(1 - \frac{V}{V_0}\right) \text{--------(11)}$$

$$\frac{V}{V_0} = 1 - \frac{1}{A} In\left[1 + \frac{AP}{B_0}\right] \text{--------(12)}$$

Using the definition of the isothermal bulk modulus B in the above equation, we get,

$$\frac{B}{B_0} = \left[1 - \frac{1}{A} In\left\{1 + \frac{AP}{B_0}\right\}\right]\left\{1 + \frac{AP}{B_0}\right\} \text{--------(13)}$$

Equation (13) may be generalized as follows, where M represents any of elastic moduli.

$$\frac{M}{M_O} = \left[1 - \frac{1}{A} In\left\{1 + \frac{AP}{M_O}\right\}\right]\left\{1 + \frac{AP}{M_O}\right\} \text{-------(14)}$$

The collective expressions for the pressure dependence of elastic constants may be written as

$$\frac{C_{ij}}{C^O_{ij}} = \left[1 - \frac{1}{A_{ij}} In\left\{1 + \frac{A_{ij}P}{C^O_{ij}}\right\}\right]\left\{1 + \frac{A_{ij}P}{C^O_{ij}}\right\} \text{-----(15)}$$

Where

$A_{ij} = \left[(C'_{ij})_0 + 1\right]$ and $C'_{ij} = \left(\frac{\partial C_{ij}}{\partial P}\right)$.

Theory of Elasticity

According to Hook's law [7], the stress (σ) and strain (ε) for the crystal

$\sigma_{ij} = C_{ijkl}\varepsilon_{kl}$ where ($ijkl = 1,2,3,4$)

where the fourth rank tensor Cijkl is the elastic tensor .Thus elastic constant can be determined directly from the computation of the stress generalized by the small strains [17]. The unit cell symmetry determine nine independent elastic constants: C11, C12, C33, C44, C55, C66, C12, C13, C23.

The elastic constant completely specify, the elastic properties for the purpose of comparing with seismological data [18] .

The bulk moduli is related to the elastic constants

$$B = \frac{(C_{11}+C_{22}+C_{33})+2(C_{12}+C_{23}+C_{13})}{9} \text{--------(16)}$$

The shear moduli

$$C_s = \frac{(C_{11}+C_{22}+C_{33})}{15} - \frac{(C_{12}+C_{23}+C_{13})-3(C_{44}+C_{55}+C_{66})}{15} \text{--------(17)}$$

The speed of compressional Vp and shear waves Vs

Pure longitudinal and shear polarizations are found only in isotropic materials or along special high-symmetry propagation directions in anisotropic materials. For an isotropic, homogeneous material, the P and S wave velocities are related to the elastic moduli by

$$V_P = \sqrt{\frac{(3K+4C_s)}{3\rho}};\ V_S = \sqrt{\frac{C_S}{\rho}} \text{------(18)}$$

From which the bulk sound velocity

$$V_B = \sqrt{K/\rho} = \sqrt{V_P^2 - 4/3 Vs^2} \text{--------(19)}$$

where, the density ρ is derived and molecular mass of the forsterite. The Vp and Vs characterize an isotropic polycrystalline material.

Equation of State (EOS)

An isothermal EOS provides useful information about the relationship between pressure (P), volume (V) that helps to understand the behaviour of materials under the effect of high pressure. Up to now a number of workers have endeavoured to search for a simple form of the EOS, which has a small number of parameters. Moreover, the derivative form is much better than the integral forms because the error at large compressions is much exaggerated in the integral forms than in the derivative forms. The widely used EOS Birch-Murnaghan (BM) is expressed as

$$P_{BM} = \frac{3B_o}{2}\left[\eta^{-7/3} - \eta^{-5/3}\right]\left[1 + \frac{3}{4}(B'_o - 4)(\eta^{-2/3} - 1)\right] \text{--------(20)}$$

Recently Misra and Goyal [19] have reported an EOS using the *ab-initio* pseudopotential approach to the total crystal energy calculation. Using this approach the expression for the EOS is derived from the variationally determined valence electron eigenvalues and charge densities. The large and geometry-insensitive core contributions are explicitly projected out by using a pseudopotential formalism. The

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Density Functional (DF) formalism for the exchange and correlation potential is self consistently employed in the derivation.

Following the conventional DF formalism [20,21] the total crystal energy (E) is given by:

$$E = T_e + V_{e-e} + V_{e-ion} + V_{ion-ion} + E_{XC} \quad (21)$$

The individual contributions on the RHS of Eq. (8) are interpreted as the kinetic energy of electrons, the Coulomb part of the electron-electron interaction (the Hartree energy), the energy due to electron-ion interaction, the Coulomb part of the ion-ion interaction (the Ewald energy [22])and the electronic exchange-correlation energy. Since the effect of core electrons is included in the pseudopotential, the term "electrons" used in this paper refers to the valence electrons only.

Now the total crystal energy (E) as a function of the Seitz-Wigner radius (R) can be written as:

$$E = \frac{N}{R^2} - \frac{M}{R} + \frac{C}{R^3} - DR^2 - \frac{f}{gR+h} \quad \text{--------(22)}$$

where $M = (3/2\pi)(9\pi/4)^{1/3} Z^{4/3} + F_S Z^2 \approx 0.9163 Z^{4/3} + F_S Z^2$ with F_S being the structure dependent Ewald constant and for diamond structure $F_S = 1.671$, $N = (3/5)(9\pi/4)^{2/3} Z^{5/3} \approx 2.2099 Z^{5/3}$, $C = (3/4\pi) Z U_{PS}(\overline{G} = \overline{0}) \approx 0.2387 Z U_{PS}(\overline{G} = \overline{0})$ and $D \propto |V(\overline{G})|^2$ is a positive number, with $V(\overline{G})$ being the screened pseudopotential form factor.The last term is the correlation term with f = 0.88Z, g = $Z^{-1/3}$ and h = 7.80.

The pressure $P(\eta)$ as a function of the compression $\eta = V/V_o$ can readily be calculated using the following relation:

$$P(\eta) = -E' = \frac{1}{3V_o}\left[\frac{2B_0}{\xi^2 V_o^{2/3}}\left(\eta^{-5/3} - \eta^{-1/3}\right) - \frac{A}{\xi V_o^{1/3}}\left(\eta^{-4/3} - \eta^{-1/3}\right) + \frac{3C}{\xi^3 V_o}\left(\eta^{-2} - \eta^{-1/3}\right)\right] \quad \text{--------(23)}$$

where $\xi = (3/4\pi)^{1/3}$ and prime denotes differentiation w.r.t. volume (V). As the derivative of the correlation term is very small compared to the derivatives of the other terms, therefore, its contribution to the pressure is neglected. The equilibrium isothermal bulk modulus K_o and its first and second pressure derivatives K'_o and K''_o respectively. The Eq. (23), then, gets transformed into:

$$P(\eta) = \frac{B_o}{20}\left[\alpha\left\{6\eta^{-2} - 15\eta^{-5/3} + 10\eta^{-4/3} - \eta^{-1/3}\right\} + \beta\left\{3\eta^{-2} - 5\eta^{-4/3} + 2\eta^{-1/3}\right\} + \gamma\left\{\eta^{-2} - \eta^{-1/3}\right\}\right] \quad \text{--------(24)}$$

with $\alpha = 6 + 9\mathbf{B}_o B_0'' + (3B'_o - 4)(3B'_0 - 7)$, $\beta = 2(3B'_0 - 7)$, $\gamma = 12$ and the compression $\eta = V/V_o$.

RESULTS AND DISCUSSIONS

The pressure dependence of the elastic constants of the forsterite are computed with the help of equ.(15) using the input data from Table(1).The values of lattice parameter are taken as a=4.756 A^0, b=10.195A^0 and c=5.981A^0. The results for Mg_2SiO_4 (forsterite) is shown in fig(1). The C_{ij} values increase smoothly and monotonically with increasing pressure, It is found that forsterite is an anisotropic crystal, having C_{11} 30% larger than C_{22} or C_{33}. The C_{11} and C_{33} elastic constants, which are involved in longitudinal sound waves along symmetry directions, are found to monotonically increase with pressure. The comparison with experimental results from the Brillouin scattering experiments [23, 24] and ultrasonic measurements [25] presented in fig (1).The computed results are in good agreement with the available data.

The elastic constants C_{12}, C_{13} and C_{23}, which, are involved in transverse sound waves along symmetry directions are very close in forsterite. Moreover, the shear moduli C_{44}, C_{55} and C_{66}, which, are involved in transverse sound waves along symmetry directions, are also increasing with increasing pressure. While, C_{55} and C_{66} are very close in forsterite. It is also interesting to note from figs (1) that the value of C_{44} in larger than C_{66} and the reverse is in forsterite.

We have reported the values of C'ij and $B`_o$ in the Table (1). It is encouraging to note that the present values of $B_o$ and $B`_o$ are in good agreement with the experimental value in case of forsterite is much better than earlier reported values.

With the help of present values of Cij, we have also computed the values of V_P and Vs in forsterite. The present values of the wave velocities (V_P and V_S) values are slightly less Fig.(2) with respect to experimental values [26] and the seismically derived wave velocities in the upper mantle of the earth [27-28]. In the high pressure limit the longitudinal and shear wave velocities for forsterite differ by few percent from the upper mantle seismic velocities. This small difference due to cause of first, the upper mantle is expected to be primarily composed of Mg-rich silicate perovskite which secondary magnesiowutite

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and second, magnesiowutite is expected to contain several tens of percent FeO and to be subjected to temperature of about 2000-3000 K. The effect of composition and temperature are expected to reduced the p-wave and s-wave velocities of forsterite relative to zero temperature pericles by few tens of percent. The values of wave velocities (V_P and V_S) are decreasing .The values of elastic wave velocities lie in between the value of V_P and Vs .

Further the computed values of B_0 and B_0" are tested by analyzing the compression in volume with the help of two EOS: first based on phenomenological method and second which is based on *ab-initio* local density approximation (LDA) method. The results are shown in fig (3). It is encouraging to note from this fig that the percentage of compression in volume obtained with the help of both EOS is almost the same in forsterite up to the pressure rang 0-24 GPa. The percentage of compression differs with increase of the pressure and the value of compression is larger at P=140 GPa. This may be due to the lower value of bulk moduli in case of forsterite. The good agreement of P-V curve for Mg_2SiO_4 (α-forsterite) obtained with the help of both EOS which, support the computed values of elastic constants and other related constants. In view good agreement of C_{ij} with the available experimental data. in case of Mg_2SiO_4 (forsterite,).The results for the Mg_2SiO_4 may be important in geophysical study of these solids in earth's upper mantle.

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Tablc1: Comparisons of elastic constants C_{ij} (M in GPa), their pressure derivative $C`_{ij}$ (M` in GPa), bulk modulus(B_0 in GPa), shear modulus (C_s), first order pressure derivative of bulk moduli ($B`_0$) and second order pressure derivative of bulk moduli ($B`_0$ in GPa^{-1}) among theoretical results at zero pressure of earth's mineral with (at T=0K) and experimental measurement (T=300K)

Mg_2SiO_4	C11	C22	C33	C44	C55	C66	C12	C13	C23	B_0	Cs
Forsterite											
M(Present)	330	200	235	68	81	81	68	69	72	133.77 101[29]	83.06
M`(Present)	5.25	4.25	3.57	0.95	0.9	0.99	3.75	3.95	3.95	4.07 5.4 [29]	------
M``(Present)	---	----	----	-----	---	----	----	----	---	-0.0464	------
M[30]	328	200	235	65	81	81	64	69	74	129	81
M`	7.22	5.42	5.57	2.01	1.46	2.16	3.59	3.62	2.94	4.12	1.4
M[31]	367	220	233	78	89	91	78	79	81	141	89
M`	7.68	5.30	5.61	1.53	1.34	1.69	3.38	3.46	3.54	4.32	1.44

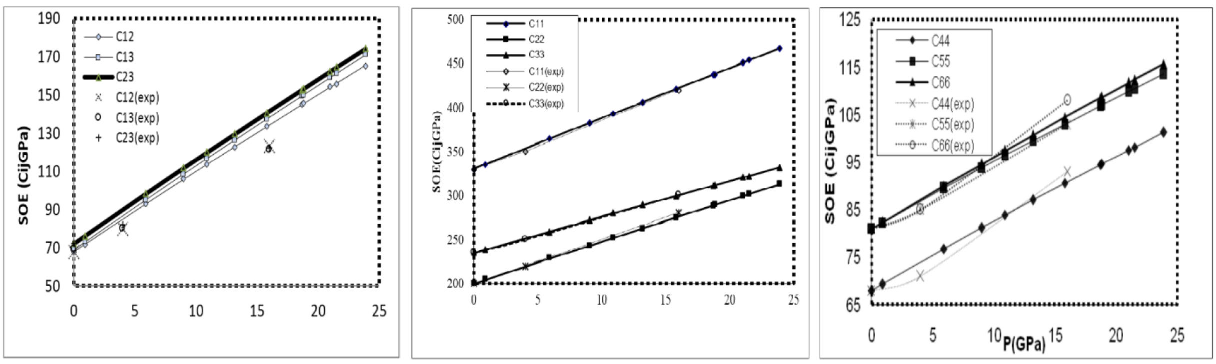

Fig.1: values of elastic constants (C_{ij} in GPa) with pressure (P=0-24) in GPa comparison with experimental valuesfor forsterite

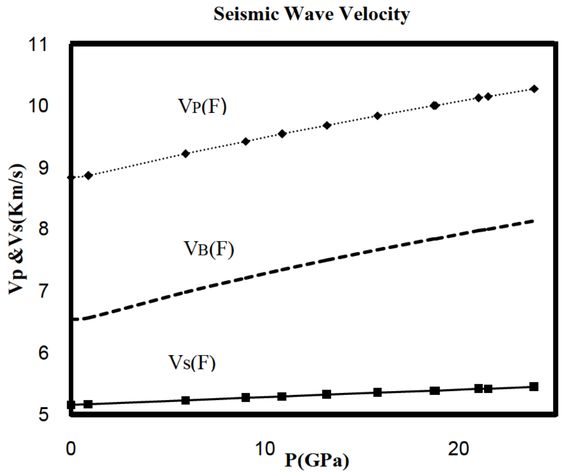

Fig. 2: Values of the P and S isotropic seismic wave velocities and sound wave velocities in Km/s with pressure in GPa.

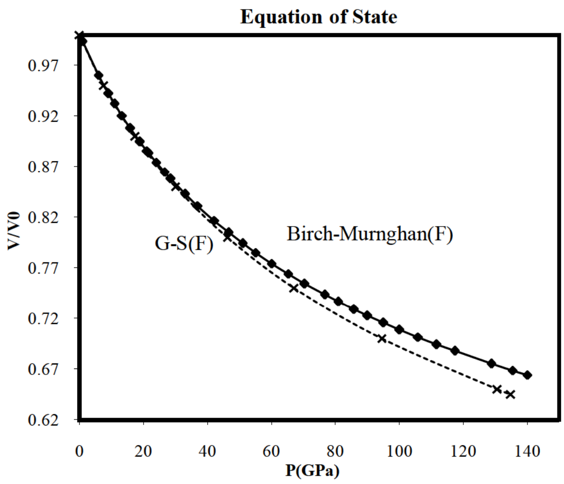

Fig. 3: values of the compression (V/V0) at different pressure (P in GPa)

REFERENCES

[1]. B.Romanowicz ,Seismic tomography of the Earth's mantle, Annu. Rev. Earth planet .Sci., 19 (1991) 77-99.

[2]. G.MastersS.Johnson,G.Laska and H.Bolton, A shear-velocity model of the mantle, Philos. Trans. R. Astron. Soc. A 354 (1996) 1385-1410.

[3]. J.B.Gaherty, T.H.Jordan and L.S. Gee., Seismic structure of the upper mantle in a central Pacific corridor, J. Geophys. Res.,101(1996) 22291-22309.

[4]. E.J. Garnero and D.V. Helmberger, Seismic detection of a thin laterally varying boundary layer at the base of the mantle beneath the central Pacific,Geophys. Res. Lett. 23 (1996) 977-980.

[5]. P.M.Shearer,Upper mantle seismic discontinuities, in Earth's Deep Interior: Mineral Physics and Tomography from the Atomic to the Global Scale, Geophys. Mo vol 117. pp .115-131 (2000).

[6]. M.Ishii and J.Tromp, Normal-mode and free-air gravity constraints on lateral variations in velocity and density of Earth's mantle,Science, 285 (1999) 1231-1236.

[7]. J.F.Nye,Physical Properties of Crystals:Their Representation by Tensor and Matrics, Oxford Univ, Press, New York, (1985).

[8]. C.B. Agrr,Phase transformations and seismic structure in the upper mantle and transition zone, in: R.J. Hemley (Ed.) Ultrahigh-Pressure Mineralogy: Physics and Chemistry of the Earth's Deep Interior. Minearalogical Society of America, Review in Mineralogy, 37 (1998) 165-203.

[9]. D.L. Anderson, Theory of the Earth, Blackwell Scientific Publications, 1998, pp 366.

[10]. D.L. Anderson and J.D. Bass, Transition region of the Earth's upper mantle, Nature , 320 (1986) 321-328.

[11]. T.S. Duffy and D.L. Anderson, Seismic velocities in mantle minerals and mineralogy of the upper mantle, J. Geophys. Res. B: Solid Earth Planets, 94 (1989) 1895-1912.

[12]. K.M. Fischer and D.A. Wiens, The depth distribution of mantle anisotropy beneath the Tonga subduction cone, Earth Planet.Sci. Lett., 142 (1996) 253-260.

[13]. S.I. Karato, Seismic anisotropy in the deep mantle, boundary layers and geometry of mantle convection, Pure Appl. Geophys., 151 (1998) 565-587.

[14]. B.Kiefer,L.Stixrude, R. M. Wentzovitch, Calculated elastic constants and anisotropy of Mg_2SiO_4 spinel at high pressure Geophys. Res. Lett. 24 (1997) 2841-2844.

[15]. Z. Wu and R. M. Wentzcovitch, Vibrational and thermodynamic properties of wadsleyite: A density functional study, J. Geophy. Res., 112 (2007) B12202, 11.

[16]. M. Kumar V. Pal B.R.K. Gupta,Phys.Chem. Minerals, 25 (1998) 27.

[17]. R.M.Wentzcovitch,,N .Ross and G.D.Price Earth Planet .Inter.,90,101-112 (1995).

[18]. M. Grimsditch, P. Loubeyre and Polian, Phys. Rev. B 33 (1986) 7192.

[19]. G. Misra and S.C. Goyal, P-V relation for cuprous halides :Pseudopential approach, Sol. Stat. Commun.136 (2003) 157-162.
[20]. P.Hohenberg and W.Kohn, Phys. Rev. 136, B864 (1964).
[21]. W.Kohn and L.J.Sham, Phys. Rev. 140, A1133 (1965) .
[22]. R.A.Coldwell-Horsfall and A.A.Maradudin, J.Math.Phys. 1, 395 (1960).
[23]. H. Shimizu,W.A. Bassett and E.M. Brody, J. Appl. Phys. 53 (1982) 620.
[24]. T.S. Duffy, C. Zha ,R.T. Downs, H. Mao, R.J. Hemley, Nature, 378 (1995) 170.
[25]. G. Chen, B. Li, R.C. Liebermann, Science, 272 (1996) 979.
[26]. B. Li, Compressional and shear wave velocities of ringwoodite gamma- Mg2SiO4 to 12 GPa, Am. Mineral, 88 (2003)1312-1317.
[27]. S.V.Sinogeikin, J.D. Bass, T. Katsura, Single-crystal elasticity of ringwoodite to high pressure and high temperature;implications for 520 km seismic discontinuity.,PEPI,136(1/2) (2003) 41-66.
[28]. J.M. Jackon,S.V.Sinogeikin, J.D. Bass, R.C. E. Liebermann,D.G.E. Isaak, Sound velocities and elastic properties of gamma Mg_2SiO_4 to 873 K Brillouin spectroscopy.,Am. Mineral 85 (2000) 296-303.
[29]. N.P. de Koker, L. Strixrude and B.B. Karki, Thermodynamics,structre, dynamics and freezing of Mg2SiO4 liquid at pressure, Geochimica et Cosmochimica Acta 72 (2008) 1427-1441.
[30]. C. da Silva, L. Stixrude, and R. M. Wentzcovitch, Elastic constants and anisotropy of fosterite at high pressure, Geophys.Res. Lett., 24, (1997) 1963–1966,.
[31]. A.Yoneda and M. Morioka, Pressure derivatives of elasticconstants of single crystal forsterite, in High Pressure Research:Applications to Earth and Planetary Sciences, Geophys. Monogr. Ser., vol. 67, edited by Y. Syono and M. H.Munghnani, pp. 207–214, AGU, Washington, D. C., (1992).