Available online at http://www.journalijdr.com

International Journal of DEVELOPMENT RESEARCH

ISSN: 2230-9926

International Journal of Development Research
Vol. 4, Issue, 12, pp. 2663-2668, December, 2014

Full Length Research Article

THEORETICAL INVESTIGATIONS ON THE ELASTIC PROPERTIES OF $CaSiO_3$ BY EOS

Singh, R. S. and *Deepti Sahrawat

Department of Physics, Faculty of Science, J. N. V. University, Jodhpur (Rajasthan)

ARTICLE INFO

Article History:
Received 11th September, 2014
Received in revised form
03rd October, 2014
Accepted 08th November, 2014
Published online 27th December, 2014

Key words:
Phase transition,
Equation of state,
Elastic properties.

ABSTRACT

The elastic properties of $CaSiO_3$ are calculated as a function of temperature using different equations of state (EOS). Equations of state have been used to study pressure as a function of volume compression at a given temperature. The EOS's for solids under low compression by evaluating the pressure-volume derivative properties viz., isothermal bulk modulus and its pressure derivatives calculated for $CaSiO_3$. The elastic moduli such as Bulk modulus, Shear modulus, Young's modulus and Poisson's ratio have been calculated as a function of pressure. The values of elastic moduli have been obtained using compressional wave velocity and shear wave velocity. It is emphasized that all EOS's give satisfactory results which is in good agreement with Stacey EOS.

INTRODUCTION

Equation of State (EOS) of solids describes the relationships amoung thermodynamic variables such as pressure, volume and temperature (P, V, T). This information can only be obtained by using sophisticated theoretical models. It provides numerous information of non-linear compression of a material at high pressure and has been widely applied to engineering and other scientific researches. The behavior of metals and materials at normal pressure and temperature is much different than that at high pressure and high temperature. The EOS is of considerable interest for basic research and numerous important applications.The equation of state (EOS) of condensed matter is very important in many fields of basic and applied sciences including physics and geophysics. The EOS is fundamentally important in studying the properties of materials at different pressure and at high temperature. The knowledge of the P-V-T EOS of relevant standard materials is one of the most basic information needed for pressure calibration. Various EOS are intended to account for the volumetric properties of solid whose structural configurations vary with pressure and temperature. For performing calculations with the help of an EOS for a material at high pressures, we need the parameters K_0 , K_0' , all at zero pressure. EOS can be made by studying the variation of $K'=dK/dP$ with pressure or compression (V/Vo). The P-V relationships reveal that the volume decreases continuously with the increase in pressure. The bulk modulus also increases with increase in pressure but its pressure derivatives K' decreases with the increase in pressure. The purpose of the present study is to assess the validity of some important EOS's. A comparison of the result for P-V relationships, bulk modulus and its pressure derivative has been presented with various EOS's. In this paper, the EOS has been extended to calculate the theoretical values of both compressional and shear velocities of $CaSiO_3$ using isothermal EOS. The other different elastic parameters viz., young's modulus, shear modulus, and poison's ratio are also determined by using pressure–density relationship for $CaSiO_3$.

***Corresponding author: Deepti Sahrawat**
Department of Physics, Faculty of Science, J. N. V. University, Jodhpur (Rajasthan)

Variation of pressure with compression at room temperature

The values of P, K and K' has been obtained as a function of compression V/V_0 from EOS's for $CaSiO_3$ with input parameters as (K_0 = 232 GPa and K_0' = 4.8 GPa for $CaSiO_3$). We have used four EOS`s (a) Modified Rydberg EOS, (b) Birch Murnaghan EOS, (c) Stacey reciprocal K-primed EOS, (d) Kushwah logarithmic EOS for calculating the pressure, bulk modulus and its pressure derivatives are as follows:

a. Modified Rydberg EOS

$$P = 3K_0 x^{-K'_\infty}\left(1-x^{1/3}\right)\exp\left[t\left(1-x^{1/3}\right)\right]$$

$$K = 3K_0 x^{-K'_\infty}\exp\left[t\left(1-x^{1/3}\right)\right]\left\{K'_\infty\left(1-x^{1/3}\right)+\frac{t}{3}\left[x^{1/3}\left(1-x^{1/3}\right)\right]+\frac{x^{1/3}}{3}\right\}$$

$$K' = K'_\infty + t\frac{x^{1/3}}{3} + \frac{x^{1/3}}{3\left(1-x^{1/3}\right)} - \frac{P}{9K}tx^{1/3} + \frac{1}{1-x^{1/3}} + \frac{x^{1/3}}{\left(1-x^{1/3}\right)^2}$$

Where

$$x = V/V_0$$

$$t = \frac{3}{2}K'_0 - 3K'_\infty + \frac{1}{2}$$

$$t = -3K_0K''_0 - \frac{3}{4}K'^2_0 + \frac{1}{12}$$

Here K_0, K'_0 and K''_0 are respectively zero pressure values of K, K', K'' and K'_∞ is the value of K' at $P \to \infty$.

b. Birch Murnaghan EOS

$$P = \frac{3}{4}K_0\left(x^{-7}-x^{-5}\right)\left[1+\frac{3}{4}A_1\left(x^{-2}-1\right)\right]$$

$$K = \frac{1}{2}K_0\left(7x^{-7}-5x^{-5}\right)+\frac{3}{8}K_0A_1\left(9x^{-9}-14x^{-7}-5x^{-5}\right)$$

$$K' = \frac{K_0}{8K}\left[\left(K'_0-4\right)\left(81x^{-9}-98x^{-7}-25x^{-5}\right)+\frac{4}{3}\left(49x^{-7}-25x^{-5}\right)\right]$$

Where

$$x = \left(V/V_0\right)^{1/3} \text{ and}$$

$$A_1 = \left(K'_0 - 4\right)$$

c. Stacey Reciprocal k-primed EOS

$$\ln\frac{V}{V_0} = \frac{K'_0}{K'^2_\infty}\ln\left(1-K'_\infty\frac{P}{K}\right)+\left(\frac{K'_0}{K'_\infty}-1\right)\frac{P}{K}$$

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

$$\frac{1}{K'} = \frac{1}{K'_0} + \left(1-\frac{K'_\infty}{K'_0}\right)\frac{P}{K}$$

d. Kushwah Logarithmic EOS

$$Px^{K'_\infty} = B_1\ln\left(2-x\right) B_2\left[\ln\left(2-x\right)\right]^2 + B_3\left[\ln\left(2-x\right)\right]^3$$

$$K = K'_\infty P + \frac{x^{1-K'_\infty}}{2-x}\left[B_1 + 2B_2\ln\left(2-x\right)+3B_3\left\{\ln\left(2-x\right)^2\right\}\right]$$

$$K' = 2K'_\infty - \frac{K'^2_\infty P}{K} + \frac{2}{2-x}\left[\frac{K'_\infty P}{K} + \frac{x^{2-K'_\infty}}{K\left(2-x\right)}\left\{B_2 + 3B_3\ln\left(2-x\right)\right\}-1\right]$$

Where $x = V/V_0$

$$B_1 = K_0$$

$$B_2 = \left(\frac{K_0}{2}\right)\left(K'_0 - 2K'_\infty + 2\right)$$

$$B_3 = \left(\frac{K_0}{6}\right)\left(K_0K''_0 + K'^2_0 + 3K'^2_\infty - 3K'_0K'_\infty - 12K'_\infty + 6K'_0 + 6\right)$$

The results for P, K and K' as function of V/Vo down to 0.915 are given in table1-3. The results obtained from various EOS are found to present in general fair agreement with each other.

ELASTIC MODULI OF $CaSiO_3$

There are mainly two types of sound velocities V_P and V_S i.e. for compressional or longitudinal and shear or transverse waves, respectively. These are related to bulk modulus (K), shear modulus (G) and density (ρ) as :

$$V_P = \left(\frac{K+\frac{4}{3}G}{\rho}\right)^{1/2}$$

$$V_S = \left(\frac{G}{\rho}\right)^{1/2}$$

The Shear modulus (G), Young's modulus (Y) and Poisson's ratio are as follows:

$$G = \frac{3}{5}\left(K - 2P\right)$$

$$Y = \left(\frac{9KG}{3K-G}\right)$$

$$\sigma = \left(\frac{3K+4P}{12K-4P}\right)$$

We make use of these equations for calculating shear modulus, Young's modulus and Poisson's ratio with help of K and P as a function of density .The results for these elastic moduli and sound velocities from various EOS's at different compression for $CaSiO_3$ at different compression are presented in table 4-7 respectively. [(ρ_0 = 4.321 Kg/m^3) for $CaSiO_3$]

RESULTS AND CONCLUSION

For determining the values of pressure, isothermal bulk modulus and its derivatives, equations of state have been used exclusively. We have theoretically determined the variation of different elastic parameters viz., young's modulus, shear modulus, and poison's ratio of $CaSiO_3$ with compression. In this study we have employed the equations to calculate the young's modulus, shear modulus, poison's ratio and have been reported in table 4-7. It has been observed that the pressure increases with decrease in compression of the material as depicted in Fig. 1. The pressures calculated are found to be in good agreement with Stacey EOS. Bulk modulus also increases with decrease in compression as depicted in Fig. 2, but pressure derivative of bulk modulus decreases with decrease in compression as depicted in Fig. 3. It is also observed that the elastic moduli increase with increase in pressure and density.

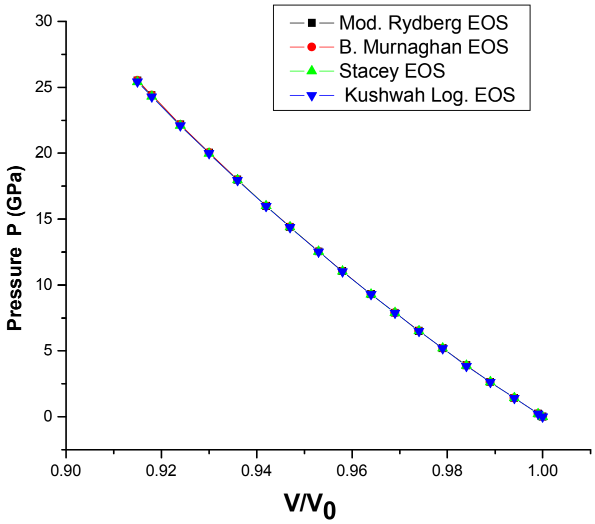

Fig. 1. Pressure P (GPa) versus Compression (V/V_0) for $CaSiO_3$

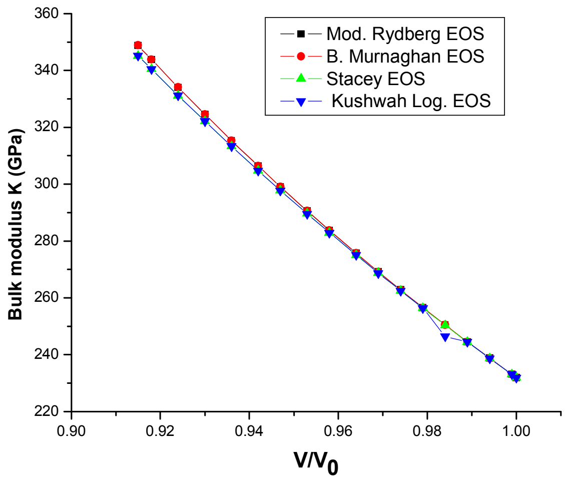

Fig. 2. Bulk modulus (GPa) versus Compression (V/V_0) for $CaSiO_3$

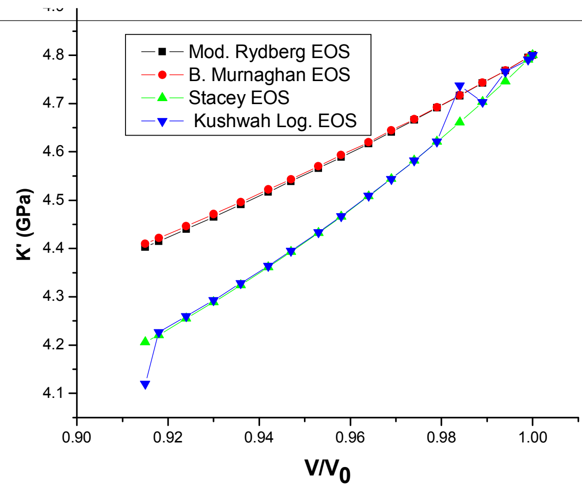

Fig. 3. Pressure derivative bulk modulus (GPa) versus Compression (V/V_0) for $CaSiO_3$

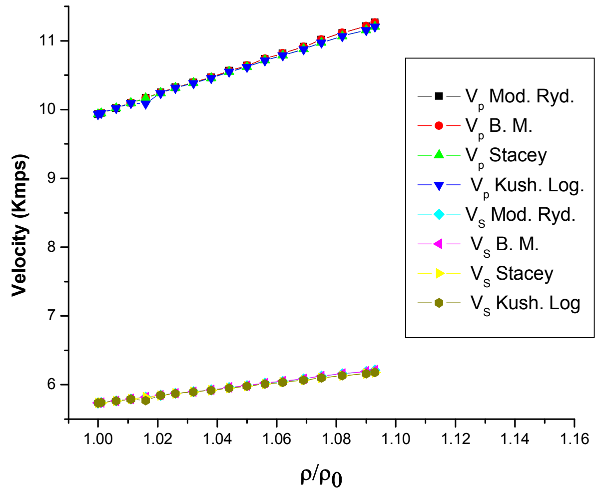

Fig. 4. Reduced velocities versus normalized density for $CaSiO_3$

Table 1. Values of pressure for $CaSiO_3$ calculated from (a) Modified Rydberg EOS, (b) Birch Murnaghan EOS, (c) Stacey reciprocal K-primed EOS, (d) Kushwah logarithmic EOS.

	P			
V/V_0	(a)	(b)	(c)	(d)
1.000	0.000	0.000	0.000	0.000
0.999	0.233	0.233	0.221	0.233
0.994	1.417	1.417	1.415	1.416
0.989	2.635	2.635	2.631	2.635
0.984	3.890	3.890	3.879	3.858
0.979	5.181	5.181	5.182	5.180
0.974	6.511	6.511	6.507	6.508
0.969	7.880	7.880	7.882	7.875
0.964	9.289	9.289	9.269	9.282
0.958	11.035	11.036	11.032	11.024
0.953	12.538	12.539	12.535	12.522
0.947	14.400	14.401	14.383	14.376
0.942	16.003	16.004	15.987	15.971
0.936	17.989	17.990	17.959	17.946
0.930	20.046	20.047	19.973	19.989
0.924	22.176	22.179	22.090	22.103
0.918	24.384	24.387	24.307	24.291
0.915	25.517	25.521	25.408	25.413

Table 2. Values of bulk modulus (K) for $CaSiO_3$ calculated from (a) Modified Rydberg EOS, (b) Birch Murnaghan EOS, (c) Stacey reciprocal K-primed EOS, (d) Kushwah logarithmic EOS

	K			
V/V_0	(a)	(b)	(c)	(d)
1.000	232.00	232.00	232.00	232.00
0.999	233.12	233.12	233.06	233.12
0.994	238.78	238.78	238.76	238.76
0.989	244.57	244.57	244.50	244.51
0.984	250.50	250.51	250.34	246.51
0.979	256.58	256.58	256.39	256.38
0.974	262.80	262.81	262.49	262.49
0.969	269.17	269.18	268.76	268.73
0.964	275.69	275.71	275.03	275.10
0.958	283.73	283.75	282.95	282.91
0.953	290.61	290.64	289.63	289.58
0.947	299.09	299.12	297.79	297.77
0.942	306.34	306.39	304.81	304.75
0.936	315.28	315.34	313.36	313.33
0.930	324.49	324.57	322.04	322.14
0.924	333.98	334.07	331.09	331.18
0.918	343.76	343.86	340.48	340.46
0.915	348.75	348.86	345.12	345.19

Table 3. Values of pressure derivative of bulk modulus (K') for $CaSiO_3$ calculated from (a) Modified Rydberg EOS, (b) Birch Murnaghan EOS, (c) Stacey reciprocal K-primed EOS, (d) Kushwah logarithmic EOS

	K'			
V/V_0	(a)	(b)	(c)	(d)
1.000	4.800	4.800	4.800	4.800
0.999	4.795	4.795	4.791	4.791
0.994	4.768	4.768	4.746	4.766
0.989	4.742	4.743	4.703	4.703
0.984	4.716	4.717	4.661	4.737
0.979	4.691	4.692	4.621	4.621
0.974	4.666	4.668	4.582	4.582
0.969	4.641	4.644	4.544	4.544
0.964	4.617	4.620	4.508	4.509
0.958	4.589	4.593	4.466	4.467
0.953	4.566	4.570	4.432	4.434
0.947	4.539	4.543	4.393	4.395
0.942	4.517	4.522	4.361	4.364
0.936	4.491	4.496	4.324	4.328
0.930	4.465	4.471	4.289	4.293
0.924	4.440	4.446	4.255	4.260
0.918	4.415	4.422	4.221	4.227
0.915	4.403	4.410	4.206	4.120

Table 4. Values of elastic moduli calculated from (a) Modified Rydberg EOS with different compression for $CaSiO_3$

V/V_0	ρ/ρ_0	ρ(g/cc)	G(GPa)	Y(GPa)	σ	V_P	V_S
1.000	1.000	4.231	139.200	348.000	0.250	9.935	5.736
0.999	1.001	4.235	139.591	349.092	0.250	9.949	5.741
0.994	1.006	4.256	141.566	354.616	0.252	10.022	5.767
0.989	1.011	4.278	143.580	360.244	0.255	10.096	5.794
0.984	1.016	4.299	145.634	365.980	0.257	10.171	5.821
0.979	1.021	4.320	147.729	371.825	0.258	10.247	5.848
0.974	1.026	4.341	149.865	377.783	0.260	10.323	5.876
0.969	1.032	4.366	152.045	383.857	0.262	10.396	5.901
0.964	1.038	4.392	154.268	390.050	0.264	10.469	5.927
0.958	1.044	4.417	156.995	397.644	0.266	10.565	5.962
0.953	1.050	4.443	159.319	404.110	0.268	10.641	5.988
0.947	1.056	4.468	162.171	412.040	0.270	10.739	6.025
0.942	1.062	4.493	164.601	418.795	0.272	10.818	6.052
0.936	1.069	4.523	167.584	427.083	0.274	10.914	6.087
0.930	1.075	4.548	170.642	435.575	0.276	11.017	6.125
0.924	1.082	4.578	173.777	444.277	0.278	11.116	6.161
0.918	1.090	4.612	176.993	453.197	0.280	11.212	6.195
0.915	1.093	4.624	178.631	457.741	0.281	11.266	6.215

Table 5. Values of elastic moduli calculated from (b) Birch Murnaghan EOS with different compression for $CaSiO_3$

V/V_0	ρ/ρ_0	ρ (g/cc)	G(GPa)	Y(GPa)	σ	V_P	V_S
1.000	1.000	4.231	139.200	348.000	0.250	9.935	5.736
0.999	1.001	4.235	139.591	349.092	0.250	9.949	5.741
0.994	1.006	4.256	141.566	354.617	0.252	10.022	5.767
0.989	1.011	4.278	143.581	360.246	0.255	10.096	5.794
0.984	1.016	4.299	145.636	365.984	0.257	10.171	5.821
0.979	1.021	4.320	147.722	371.832	0.258	10.247	5.848
0.974	1.026	4.341	149.870	377.795	0.260	10.323	5.876
0.969	1.032	4.366	152.051	383.874	0.262	10.396	5.901
0.964	1.038	4.392	154.277	390.074	0.264	10.470	5.927
0.958	1.044	4.417	157.008	397.676	0.266	10.566	5.962
0.953	1.050	4.443	159.336	404.151	0.268	10.642	5.989
0.947	1.056	4.468	162.192	412.094	0.270	10.740	6.025
0.942	1.062	4.493	164.628	418.862	0.272	10.818	6.053
0.936	1.069	4.523	167.617	427.166	0.274	10.915	6.088
0.930	1.075	4.548	170.683	435.677	0.276	11.018	6.126
0.924	1.082	4.578	173.826	444.401	0.278	11.118	6.162
0.918	1.090	4.612	177.051	453.345	0.280	11.214	6.196
0.915	1.093	4.624	178.694	457.902	0.281	11.268	6.215

Table 6. Values of elastic moduli calculated from (c) Stacey reciprocal K-primed EOS with different compression for $CaSiO_3$

V/V_0	ρ/ρ_0	ρ (g/cc)	G(GPa)	Y(GPa)	σ	V_P	V_S
1.000	1.000	4.231	139.200	348.000	0.250	9.935	5.736
0.999	1.001	4.235	139.571	349.039	0.250	9.948	5.741
0.994	1.006	4.256	141.555	354.589	0.252	10.022	5.767
0.989	1.011	4.278	143.541	360.145	0.254	10.095	5.793
0.984	1.016	4.299	145.549	365.764	0.256	10.168	5.819
0.979	1.021	4.320	147.614	371.537	0.258	10.243	5.846
0.974	1.026	4.341	149.683	377.325	0.260	10.317	5.872
0.969	1.032	4.366	151.798	383.241	0.262	10.388	5.896
0.964	1.038	4.392	153.898	389.116	0.264	10.457	5.920
0.958	1.044	4.417	156.529	396.476	0.266	10.550	5.953
0.953	1.050	4.443	158.738	402.653	0.268	10.623	5.978
0.947	1.056	4.468	161.412	410.132	0.270	10.715	6.011
0.942	1.062	4.493	163.699	416.530	0.272	10.789	6.036
0.936	1.069	4.523	166.471	424.281	0.274	10.879	6.067
0.930	1.075	4.548	169.258	432.076	0.276	10.974	6.100
0.924	1.082	4.578	172.143	440.147	0.278	11.066	6.132
0.918	1.090	4.612	175.120	448.472	0.280	11.156	6.162
0.915	1.093	4.624	176.582	452.560	0.281	11.205	6.179

Table 7. Values of elastic moduli calculated from (d) Kushwah logarithmic EOS with different compression for $CaSiO_3$

V/V_0	ρ/ρ_0	ρ (g/cc)	G(GPa)	Y(GPa)	σ	V_P	V_S
1.000	1.000	4.231	139.200	348.000	0.250	9.935	5.736
0.999	1.001	4.235	139.590	349.092	0.250	9.949	5.741
0.994	1.006	4.256	141.556	354.592	0.252	10.022	5.767
0.989	1.011	4.278	143.548	360.164	0.255	10.095	5.793
0.984	1.016	4.299	145.549	365.764	0.256	10.168	5.819
0.979	1.021	4.320	147.611	371.530	0.258	10.243	5.846
0.974	1.026	4.341	149.684	377.330	0.260	10.317	5.872
0.969	1.032	4.366	151.787	383.211	0.262	10.388	5.896
0.964	1.038	4.392	153.919	389.175	0.264	10.458	5.920
0.958	1.044	4.417	156.519	396.447	0.266	10.550	5.953
0.953	1.050	4.443	158.721	402.606	0.268	10.622	5.977
0.947	1.056	4.468	161.407	410.119	0.270	10.715	6.011
0.942	1.062	4.493	163.684	416.485	0.272	10.789	6.036
0.936	1.069	4.523	166.463	424.257	0.274	10.879	6.067
0.930	1.075	4.548	169.295	432.176	0.276	10.975	6.101
0.924	1.082	4.578	172.182	440.249	0.278	11.068	6.133
0.918	1.090	4.612	175.127	448.483	0.280	11.156	6.163
0.915	1.093	4.624	176.621	452.661	0.281	11.206	6.180

Moreover the density determined from the above calculations increases linearly with the calculated pressures. The nature of young's modulus, shear modulus, poisson's ratio with compression have been predicted and tabulated. The dependence of sound velocities has been determined using the pressure-density relationship. Furthermore we have predicted the variation of shear and compression wave velocity with different pressures as depicted in Fig-4. Our theoretical investigations are in accordance with existing literature and few evidences. The calculated Poisson's ratio is in agreement with current studies. Most practical materials typically have poisson's ratio σ values between 0 and 0.5. Metal oxides usually have σ values around 0.25. The shear sound velocity has agreed with previous literature. The rate of increase of compression velocity with pressure is faster than shear velocity. The present work has predicted various parameters for low pressures. The EOS's employed in our study are found to be in accordance with each other over the whole analysis including all elastic parameters.

Acknowledgment

We are thankful to UGC, New Delhi for the financial assistance.

REFERENCES

Anderson , O.L., 1995. Equation of state for Geophysical and Ceramic Science , Oxford University Press, New York.

Birch, F., 1968. *J. Geophys. Res*., 7, pp- 817.

Dunn, M.L., Ledbetter, H., 1995. *J. Mater. Res*., 10, pp- 2715–2722.

Elizer, S. "High Pressure Equation of State, Theory and Applications", Ed. Elizer, S. and Ricci, R.A., 1991, (North-Holland Amsterdam).

Ferroelectric and Multiferroic Materials, Proceedings Materials Research Society Symposium 2011 November.

Ghiorso, M.S., 2004. *American J. Sci*., 304, pp- 752.

Hama, J., Suito, K., 2004. *J. Phys. Chem. Solids*, 65, pp-1581.

Kumar M., Subramanian, S.S., Gaurav, S., 2014. *Int. J. Enh. Res. Sci. Tech. & Eng*., 3, pp- 536-541.

Kumar, M., 1994. *Solid State Communication* 92, pp- 463.

Lautrup, B., 2005. Physics of Continuous Matter. Institute of Physics: Bristol, pp- 135–144.

Prieto, F.E., Renero, C., 1992. *J. Phys. Chem. Solids* 53, pp-485.

Schlosser, H., Ferrante, J., 1995, 1995. *J. Phys. Rev. B* 18, pp-6646.

Shanker, J., Dulari, P., Singh, P.K., 2009. *Physica B*, 40, pp-4083.
Shrivastava, H.C., 2009. *Physica B*, 404, pp- 251- 254.
Singh, B.P., Gajendra, S., 2011. *Int. J. of Pure & Appl. Phys*., 49, pp- 467.
Stacey, F.D., 2000. *Geophys. J. Int*., 143, pp- 621. Nanoscape, 2008, 5(1), Fall.
Stacey, F.D., 2005. *Rep. Prog. Physics*, 68, pp- 341.
Wang, Y., Weidner, D.J., Guyot, F., 1996. *J. Geophy. Res*., 101(B1), pp- 661-672.
Wani, T.A., Singh, P. 2010. *Int. J. Phy. and App*. 2, pp- 9-12.

****