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Applied Chemistry

Elixir Appl. Chem. 39C (2011) 5063-5065

ISSN: 2229-712X

Theoretical prediction of elastic properties of garnets

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ARTICLE INFO

Article history:
Received: 3 August 2011;
Received in revised form:
23 September 2011;
Accepted: 30 September 2011;

Keywords
Mantle minerals,
Seismic velocities,
Debye temperature,
Hills averaging method,
Pyrope garnet and Grossular garnet.

ABSTRACT

The elastic properties of mantle minerals are important for the interpretation of the structure and composition of the lower mantle and also in seismic studies. The elastic properties of minerals depend on its composition, crystal structure, temperature and the level of defect. In the present work we have calculated the elastic parameters such as bulk modulus, shear modulus, seismic velocities, and Debye temperatures of some garnets such as Pyrope garnet ($Mg_3Al_2Si_3O_{12}$) and Grossular garnet ($Ca_3Al_2Si_3O_{12}$) at different temperature ranges by using Hill's averaging method and other methods of thermodynamics.

Introduction

Elastic properties of mantle minerals are closely related to many fundamental properties such as equation of state (EOS), specific heat, thermal expansion, Debye temperature, Gruiensen parameter, melting point and interatomic potentials. Elastic constant and their variations with temperature provide useful knowledge about nature of interatomic forces [1].

The Debye temperature θ_d is an important quantity and closely related to many physical properties [2] of solids such as specific heat and melting temperature. Debye temperature gives the knowledge about structure stability, the strength of the bonds between its constituent atoms, structure defects stability and density of the materials.

Pyrope is red in color and chemically a magnesium aluminium silicate with the formula $Mg_3Al_2Si_3O_{12}$. The color the Pyrope varies from deep red to almost black. Transparent Pyrope is used as gemstones. Grossular is green in color and chemically calcium aluminium silicate with the formula $Ca_3Al_2Si_3O_{12}$. Other shades include cinnamon brown, red and yellow. Pure crystals of garnet are still used as gemstones. The gemstone verities occur in shades of green, red, yellow and orange.

In the present study, a simple and straight forward model theory Hills averaging method was used to analyze the elastic properties of Pyrope garnet and Grossular garnet. Theory: Debye derived an expression for the Debye temperature [2]; it may be defined as

$$\theta_d = \frac{h}{k}\left[\frac{9N}{4\pi V}\right]^{\frac{1}{3}}\left[\int\left(\frac{1}{c_1^3}+\frac{1}{c_2^3}+\frac{1}{c_3^3}\right)\frac{d\Omega}{d\pi}\right]^{-\frac{1}{3}}$$

(1)Where h is Planks constant, k is the Boltzmann constant, $d\Omega$ is the solid angle of the element, c is the velocity of sound, N is Avogadro number and Vis the volume. In terms of above parameter, the specific heat at low temperature(less than $\theta_d/12$) can be written as [2]

$$c_v = \frac{12\pi^4 Nk}{5}\left(\frac{T}{\theta_d}\right)^3 \qquad (2)$$

At higher temperature the above expression becomes difficult but is well defined. Binni [3] and independently Gilvary [4] were first to suggest that a Debye temperature (θ_d) can be calculated by averaging the elastic stiffness coefficient C_{ij}.

The Debye temperature is defined in terms of mean sound velocity as [5]

$$\theta_d = \frac{h}{k}\left(\frac{9N}{4\pi}\right)^{\frac{1}{3}}\left(\frac{\rho}{M/n}\right)^{\frac{1}{3}} v_m$$

$$\text{or } \theta_d = 251.2\left(\frac{\rho}{\mu}\right)^{\frac{1}{3}} v_m \qquad (3)$$

where v_m (km/s) is mean velocity and ρ (gm/cc) is density, M is the molecular mass, n is the number of atoms in the molecular formula, μ is the mean atomic mass, and k, h, and N are the usual atomic constant.

The mean velocity of sound can be calculated by [6]

$$\frac{3}{v_m^3} = \frac{2}{v_s^3} + \frac{1}{v_l^3} \qquad (4)$$

Where v_l and v_s are the longitudinal and transverse sound velocities.

The probable values of the average shear and longitudinal sound velocities can be calculated from Hills equation as follows [6]

$$v_s = \left(\frac{G}{\rho}\right)^{\frac{1}{2}}, v_l = \left[\frac{K+\frac{4}{3}G}{\rho}\right]^{\frac{1}{2}} \qquad (5)$$

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The adiabatic bulk modulus K_s for cubic crystal in terms of elastic stiffness constant (C_{ij}) can be given as [7]

$$K_s = \frac{1}{3}(C_{11} + C_{12}) \quad (6)$$

According to Hills averaging method [8] shear modulus G in the term of elastic stiffness constant (C_{ij}) can be written as

$$G = \left[\frac{C_{44}(C_{11} - C_{12})(C_{11} - C_{12} + 3C_{44})}{3(C_{11} - C_{12}) + 4C_{44}} \right]^{\frac{1}{2}} \quad (7)$$

Result and Discussion:

In present work the value of adiabatic bulk modulus K_s has been calculated by using equation (6). The value of input parameter C_{11} and C_{12} taken from literature [9] displayed in table (1). The value of shear modulus G has been calculated by using equation (7). Also the value of transverse sound velocity (v_s) and longitudinal sound velocity v_l has been calculated by using equation (5). Substituting the calculated value of v_s and v_l in equation (4) we obtained the value of mean sound velocity (v_m). Further substituting the value of v_m in equation (3) we can find the Debye temperature (θ_d). The calculated and experimental values of Debye temperature (θ_d) corresponding to different temperatures for Pyrope garnet and Grossular garnet has been displayed in the table (2) and table (3) respectively. The calculated value of mean sound velocity v_m, longitudinal velocity v_l, transverse velocity v_s, shear modulus G and adiabatic bulk modulus K_s along with their experimental values are displayed in table (2) and (3) for Pyrope garnet and Grossular garnet respectively. The graph has been plotted between experimental and calculated value of K_s with temperature T (K), shown in fig. (1). From fig (1) it is clear that the calculated and experimental value of K_s supports with each other in case of both Grossular garnet and Pyrope garnet. The graph has also been plotted between experimental and calculated value of G with temperature T (K), shown in fig. (2). From fig (2) it is clear that the calculated and experimental value of G supports with each other in case of both Grossular garnet and Pyrope garnet. Again the plotted graph between Debye temperature (θ_d) and temperature T (K), shown in fig. (3) indicate that the Debye temperature decreases with increasing temperature.

When we consider the critical analysis of Debye temperature as calculated by using Hills averaging method, it is found that the Debye temperature calculated in case of Grossular garnet support well having maximum deviation only upto 0.2% where as in case of Pyrope garnet the deviation with experimental value is upto 2%. From the graph (1-3) it is also clear that the calculated value of shear modulus (G) and Debye temperature (θ_d) has greater value for Grossular garnet than Pyrope garnet, but the adiabatic bulk modulus (Ks) for Grossular garnet is less than Pyrope rich garnet.

Fig. 1: Graph plotted between Ks and T for grossular garnet and pyrope garnet along with their experimental values

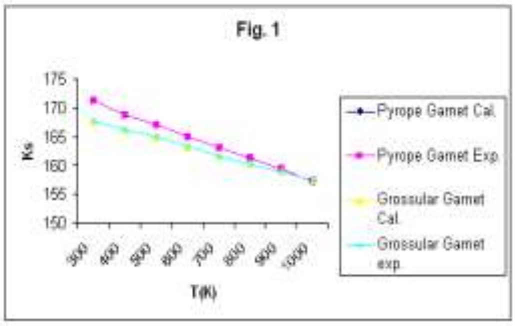

Fig. 2: Graph plotted between G and T for grossular garnet and pyrope garnet along with their experimental values

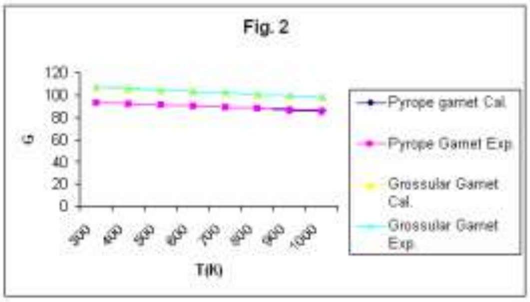

Fig. 3: Graph plotted between and T for grossular garnet and pyrope garnet along with their experimental values

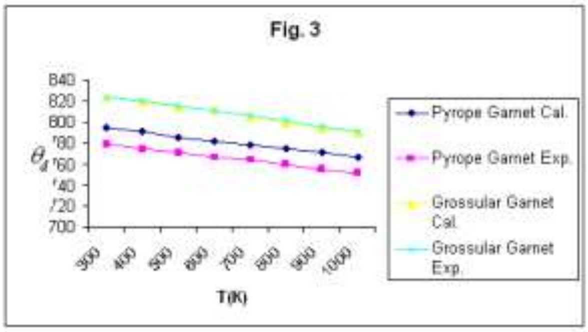

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Table1: Input values of temperature dependence of measured values elastic constant for Pyrope garnet ($Mg_3Al_2Si_3O_{12}$) and Grossular garnet ($Ca_3Al_2Si_3O_{12}$)

		Pyrope Garnet					Grossular	Garnet	
T(K)	C11	C22	C44	ρ(gm/cc)	T(K)	C11	C22	C44	ρ(gm/cc)
300	296.6	108.5	91.6	3.705	300	318.9	92.2	102.9	3.597
400	292.7	106.9	90.8	3.696	400	315.2	91.8	101.4	3.589
500	289.2	105.9	90	3.686	500	311.7	91.5	100.4	3.581
600	285.5	104.6	89.1	3.675	600	307.8	91.1	99.8	3.571
700	282.1	103.7	88.3	3.664	700	303.8	90.5	98.7	3.562
800	278.5	102.6	87.4	3.653	800	300.2	90.4	97.6	3.552
900	274.8	101.5	86.5	3.642	900	296.5	90.2	96.5	3.542
1000	271.2	100.3	85.5	3.631	1000	292.7	89.9	95.3	3.532

Table2: Calculated values of adiabatic bulk modulus (Ks), shear modulus (G), Longotudinal velocity (vl), transverse velocity (vs), mean velocity (vm) and Debye temperature (θd) along with their experimental values [9] at different temperature for Pyrope garnet (mass=403.13 gm)

T(K)	Ks cal	Ks exp.	Gcal	Gexp	Vlcal	vlexp	Vs cal	Vsexp	Vm	θd (cal.)	θd(exp.)	%deviation in θd
300	171.2	171.2	92.57	92.6	8.92	8.92	5	5	5.56	794.119	779	2
400	168.8	168.8	91.63	91.6	8.87	8.87	4.98	4.98	5.54	790.621	775	2
500	167	167	90.66	90.6	8.84	8.84	4.96	4.96	5.51	785.63	771	2
600	164.9	164.9	89.64	89.7	8.8	8.8	4.94	4.94	5.49	781.999	767	2
700	163.2	163.2	88.66	88.7	8.76	8.76	4.92	4.92	5.47	778.372	764	2
800	161.2	161.2	87.62	87.6	8.73	8.72	4.9	4.9	5.45	774.749	759	2
900	159.3	159.3	86.57	86.5	8.68	8.68	4.86	4.87	5.43	771.13	755	2
1000	157.3	157.3	85.98	85.5	8.64	8.64	4.85	4.85	5.4	766.097	751	2

Table 3 : Calculated values of adiabatic bulk modulus (Ks), shear modulus (G), Longotudinal velocity (vl), transverse velocity (vs), mean velocity (vm) and Debye temperature (θd) along with their experimental values [9] at different temperature for grossular garnet (mass=450.15 gm)

T(K)	Ks cal	Ks exp	Gcal	Gexp	Vlcal	vlexp	Vs cal	Vsexp	Vm	θd (cal.)	θd(exp.)	%deviation in θd
300	167.8	167.8	107	106.9	9.29	9.29	5.5	5.45	6.04	823.186	824	0.1
400	166.3	166.2	105.4	105.7	9.25	9.25	5.42	5.43	6.01	818.489	820	0.2
500	164.9	164.9	104.2	104.5	9.21	9.22	5.39	5.4	5.98	815	816	0.1
600	163.3	163.3	103.1	103.1	9.18	9.18	5.37	5.37	5.96	810.321	811	0.1
700	161.6	161.6	101.8	101.8	9.14	9.14	5.35	5.34	5.93	805.564	806	0.1
800	160.3	160.3	100.5	100.5	9.1	9.1	5.32	5.31	5.89	799.381	801	0.2
900	159	158.9	99.11	99.1	9.07	9.06	5.29	5.29	5.86	794.562	796	0.2
1000	157.5	157.5	97.69	97.7	9.03	9.03	5.26	5.26	5.83	789.75	791	0.2