STUDY OF THERMAL EXPANSION OF IRON AND GEOPHYSICAL MINERALS

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ABSTRACT

The Coefficient of thermal expansion α for iron is studied at extreme P,T condition and presented in regular intervals of P and T. The preferred approach constrains α via the thermal pressure equation of state is more secure than those calculated from thermodynamic simplifications.

*Keywords: Iron, Thermal Expansivity, Equation of State.

INTRODUCTION

The thermal-chemical state of the Earth's core requires knowledge of iron rich alloys at Mega bar pressures and high temperatures. The Earth's core makes up nearly one third of the planets mass. Its composition property and dynamics are fundamental issues in the study of the Earth's interior. Deeply buried in the center of the planet, the core has kept its chemical composition a long-standing mystery. Cosmo chemical studies of meteorites and geochemical analysis of samples from shallower portions of the Earth suggest that the core is made of iron alloys containing nickel (Ni) and one or more lighter elements [1]. On the basis of observing seismic rays penetrating the deep interior of the Earth and the orbital dynamics of the Earth as a planet in the solar system, models have been constructed to describe the physical state, density profile and velocity profiles of the Earth's interior. By the knowledge of thermal state of the core and the equation-of-state (EOS) of various iron alloys at the pressure and temperature conditions of the core, the thermal state of the core can be deduced from the freezing point of core composition at the pressure of inner-outer core boundary and the adiabatic temperature gradient of the core composition under core pressures. Uncertainties in the core composition directly lead to uncertainties in the thermal state. By iteration, a self-consistent model of the thermal-chemical state of the core may be found.

Thermal expansion is a fundamental aspect of EOS. Various parameters have been introduced to characterize thermal expansion under elevated pressures. They fall into two general categories, one focusing on macroscopic thermodynamic quantities and derivatives, and the other based on lattice vibration theories and microscopic view of solids. [2, 3] In the first category, P–V–T data are grouped into isothermal, isobaric, or isochoric sets. A basic approach is to calculate the thermal expansion coefficient from isobaric data according

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to its definition. One can also calculate temperature-dependent bulk modulus by fitting isothermal data to the high-temperature Birch-Murnaghan EOS. Isochoric data allow the calculation of thermal pressure at constant volume, which is related to thermal expansion coefficient and isothermal bulk modulus. In the second category, the Mie-Gruneisen-Debye EOS is widely used to extract a number of thermoelastic parameters from P-V-T data, including the isothermal bulk modulus at ambient pressure ($K_{T,0}$), its pressure derivative ($K_{T,0}$), the Debye temperature at ambient pressure and temperature θ_0, the Gruneisen parameter γ_0 (which describes the volume dependence of the Debye temperature), and q (which is a parameter describing the volume dependence of the Gruneisen parameter). Jackson and Rigden [4] carried out a systematic analysis of P-V-T data of mantle minerals and found excellent agreements between different methods.

The volume – temperature relationship and thermal expansivity data are required for investigating the equation of state and predicting the compression data of solids at high temperatures [5, 6].

Specific thermodynamic properties :

Let a homogeneous system with pressure P, volume V, absolute temperature T and entropy S be in a state of equilibrium. This equilibrium state of the system can be described by any two of the above coordinates. The first order partial derivatives of these coordinates can be used to define several experimentally measurable thermodynamic properties. Following relations are important among them.

i) The coefficient of volume thermal expansion

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

ii) The pressure coefficient

$$\beta = \frac{1}{P}\left(\frac{\partial P}{\partial T}\right)_V \tag{2}$$

iii) The isothermal bulkmodulus

$$K_T = -V \left(\frac{\partial P}{\partial V} \right)_T \qquad (3)$$

iv) The adiabatic bulkmodulus

$$K_S = -V \left(\frac{\partial P}{\partial V} \right)_S \qquad (4)$$

v) The constant pressure specific heat

$$C_P = T \left(\frac{\partial S}{\partial T} \right)_P \qquad (5)$$

vi) The constant volume specific heat

$$C_V = T \left(\frac{\partial S}{\partial T} \right)_V \qquad (6)$$

Some well known direct relations which prove useful in the analysis are

i) The ratio of two specific heats and also of the two bulkmoduli

$$\frac{C_P}{C_V} = \frac{K_S}{K_T} = 1 + T\alpha\gamma \qquad (7)$$

ii) The differences of two specific heats

$$C_P - C_V = TV\alpha^2 K_T \qquad (8)$$

iii) The product of the volume thermal expansion coefficient and the isothermal bulkmodulus

$$\alpha K_T = (\partial P / \partial T)_V = \beta P \qquad (9)$$

iv) The difference of two bulkmoduli

$$K_S - K_T = \frac{T\gamma^2 C_V}{V} \qquad (10)$$

v) The Gruneisen parameter directly defined by the Mie-Grueneisen equation

$$\gamma = \frac{V\alpha K_T}{C_V} = \frac{V\alpha K_S}{C_P} = \frac{-V}{T}\left(\frac{\partial T}{\partial V}\right)_S = \frac{K_S}{T}\left(\frac{\partial T}{\partial P}\right)_S \qquad (11)$$

Empirical Relationships :

The original Murnaghan's equation was formulated [7] to predict P-V data for a solid at a fixed temperature. It did not contain any terms showing the variation of volume with temperature. More recently attempts have been made [5, 8, 9, 10] to incorporate the thermal effects so as to estimate the volumes at simultaneously elevated temperature and pressure. According to Akaogi and Navrotsky [8] we can write.

$$V / V_0 = 1 + \alpha_0 (T - T_0) + \alpha'_0 (T - T_0)^2 \qquad (12)$$

$$\alpha = (V / V_0)^{-1} \left[\alpha_0 + 2\alpha'_0 (T - T_0)\right] \qquad (13)$$

Where α_0 is the thermal expansion, V_0 the volume and α'_0 the temperature derivative of α at T = T_0 and P = 0. It should be mentioned that equations (12) and (13) are consistent with each other and are based on the standard definition of α given us.

$$\alpha = \frac{1}{V} \left(\frac{dV}{dT} \right)_P \qquad (14)$$

Fie and Saxena [9] have used an expression which can correctly be expressed as follows :

$$V / V_0 = 1 + \alpha_0 (T - T_0) + \tfrac{1}{2}\alpha'_0 (T - T_0)^2 - \Pi\alpha_0 (T - T_0)^{-1} \qquad (15)$$

Where Π is a constant having the units of T^2 and value equal to 1. We have introduced the constant Π in the last term to make it consistent with the other terms in equation (15) with respect to units. An expression of α corresponding to (15) is then obtained as follows:

$$\alpha = (V / V_0)^{-1}\left[\alpha_0 + \alpha'_0 (T - T_0) + \Pi\alpha_0 (T - T_0)^{-2}\right] \qquad (16)$$

Guillermet and Gustafson [10] considered an exponential dependence of V/V_0 on temperature as given below.

$$\frac{V}{V_0} = exp\left[\alpha_0 (T - T_0) + \frac{\alpha'_0 (T - T_0)^2}{2}\right] \qquad (17)$$

Equations (14) and (17) yield a linear dependence of α on temperature as follows:

$$\alpha = \alpha_0 + \alpha' (T - T_0) \qquad (18)$$

Plymate and Stout [5] have presented a more involved expression for the temperature dependence of (V/V_0) by taking into account the variation of thermal bulkmodulus (K) with temperature and pressure. The expression given Plymate and Stout is

$$\frac{V}{V_0} = \left[1 + \left(\frac{dK}{dT}\right)\left(\frac{T - T_0}{K_0}\right)\right]^{-1/K'_0}$$

$$exp\left[\left[\alpha_0 + \left(\frac{dK}{dT}\right)\frac{1}{K_0 K'_0}\right](T - T_0) + \left[\alpha'_0 - \left(\frac{dK}{dT}\right)^2 \frac{1}{K_0^2 K'_0}\right]\frac{(T - T_0)^2}{2}\right] \qquad (19)$$

Where dK/dT is the temperature derivative of isothermal bulkmodulus at constant pressure. K_0 and K'_0 are the values of the bulkmodulus and its first pressure derivative at atmospheric pressure. The expression of α corresponding to eq. (19) obtained as

$$\alpha = \alpha_0 + \frac{1}{K_0 K'_0}\left(\frac{dK}{dT}\right) - \frac{1}{K'_0}\left(\frac{dK}{dT}\right)\left[K_0 + \left(\frac{dK}{dT}\right)(T - T_0)\right]^+ \qquad (20)$$

$$+ \left[\alpha'_0 - \frac{1}{K_0^2 K'_0}\left(\frac{dK}{dT}\right)^2\right](T - T_0)$$

In deriving (19) and (20) the bulkmodulus has been assumed to vary linearly the temperature. This implies that dK/dT is constant and its value is taken at room temperature and atmospheric pressure. An expression for the temperature dependence of α has been obtained by Anderson et al [11] which can be expressed as follows:

$$\alpha = \alpha_0 \left[1 - \alpha_0 \delta_T \left(T - T_0 \right) \right]^{-T} \qquad (21)$$

Where $\delta_T = - \dfrac{1}{\alpha K} \left(\dfrac{dK}{dT} \right)_P \qquad (22)$

Equation (21) has been derived by integrating the following relationship and taking δ_T to remain constant

$$\frac{1}{\alpha^2} \left(\frac{d\alpha}{dT} \right)_P = \delta_T \qquad (23)$$

The expression for the temperature dependence of V/V_0 corresponding to (21) is been obtained as

$$V/V_0 = \left[1 - \alpha_0 \delta_T \left(T - T_0 \right) \right]^{-1/\delta_T} \qquad (24)$$

Some useful thermodynamic relationships for predicting the temperature dependence of α and K_T can be obtained by the use of the definition of the Anderson-Gruneisen parameter δ_T with certain physically plausible approximations. We define δ_T in two alternative ways as follows [12, 13].

$$\delta_T = - \frac{1}{\alpha K_T} \left(\frac{\partial K_T}{\partial T} \right)_P = - \frac{V}{K_T} \left(\frac{\partial K_T}{\partial V} \right) - \frac{1}{\alpha K_T} \left(\frac{\partial K_T}{\partial T} \right)_V \quad (25)$$

and $\delta_T = \dfrac{V}{\alpha} \left(\dfrac{\partial \alpha}{\partial V} \right)_T = \dfrac{1}{\alpha^2} \left[\left(\dfrac{\partial \alpha}{\partial T} \right)_P - \left(\dfrac{\partial \alpha}{\partial T} \right)_V \right] \qquad (26)$

Where P, V and T have their usual definitions of pressure, volume and temperature respectively. One of the most widely used thermodynamic approximations [13, 14, 15] is that the product.

$$\alpha K_T = \xi \qquad (27)$$

is assumed to remain constant ξ for a given solid. If this assumption holds good, then the integration of the first part of equation (25) considering to δ_T to be independent of temperature yields.

$$K_T - K_T^0 = -\alpha K_T \delta_T \left(T - T_0 \right) \qquad (28)$$

Where K_T^0 is the value of K_T at $T = T_0$

The volume derivative of equation (27) at constant temperature, treating ξ as constant gives

$$\alpha \left(\frac{\partial K_T}{\partial V} \right)_T + K_T \left(\frac{\partial \alpha}{\partial V} \right)_T = 0 \qquad (29)$$

So that equations (26) and (29) yield

$$\frac{V}{K_T} \left(\frac{\partial K_T}{\partial V} \right)_T = \frac{V}{\alpha} \left(\frac{\partial \alpha}{\partial V} \right)_T = \delta_T \qquad (30)$$

The integration of equation (30) gives the following two relationships

$$\left(\frac{K_T}{K_T^0} \right) = \left(\frac{V}{V_0} \right)^{-\delta_T} \qquad (31)$$

and

$$\left(\frac{\alpha}{\alpha_0} \right) = \left(\frac{V}{V_0} \right)^{\delta_T} \qquad (32)$$

Where α_0 and V_0 are the initial values of α and V. The relationship (31) and (32) yield the volume dependence of K_T and α at constant temperature under the effect of pressure. In order to determine the variation with temperature we rewrite equation : (25) in the following form.

$$\delta_T = - \frac{1}{\alpha K_T} \left(\frac{\partial K_T}{\partial T} \right)_P = - \frac{V}{K_T} \left(\frac{\partial K_T}{\partial V} \right)_P \qquad (33)$$

Equation (33) is obtained by substituting for $\alpha = (1/V)(\partial V / \partial T)_P$. The integration of equation (33) at constant pressure yields the same relationship as given by (31). Thus the equation (31) is applicable for studying the pressure dependence as well as the temperature dependence of K_T. The volume derivative of equation (27) at constant pressure, treating ξ as a constant gives.

$$\alpha \left(\frac{\partial K_T}{\partial V} \right)_P + K_T \left(\frac{\partial \alpha}{\partial V} \right)_P = 0 \qquad (34)$$

In view of equations (33) and (34) we can write

$$\delta_T = \frac{V}{\alpha} \left(\frac{\partial \alpha}{\partial V} \right)_P \qquad (35)$$

The integration of equation (35) at constant pressure yields a relationship similar to that given by equation (36). From the derivations given above it is clear that equation (31) under the effect of changing temperature and equation (32) under the effect of changing pressure are based on only one assumption, namely that δ_T remains constant the effect of changing pressure and temperature. On the other hand, equation (31) for changing pressure and equation (32) for changing temperature are valid under an additional assumption given by equation (27). At constant pressure treating ξ as constant,

$$\alpha \left(\frac{\partial K_T}{\partial T} \right)_P + K_T \left(\frac{\partial \alpha}{\partial T} \right)_P = 0 \qquad (36)$$

so that

$$\delta_T = -\frac{1}{\alpha K_T}\left(\frac{\partial K_T}{\partial T}\right)_P = \frac{1}{\alpha^2}\left(\frac{\partial \alpha}{\partial T}\right)_P \qquad (37)$$

Equations (25) (26) (30) and (37) together give

$$\left(\frac{\partial K_T}{\partial T}\right)_V = 0 \ and \ \left(\frac{\partial \alpha}{\partial T}\right)_V = 0$$

The integration of equation (37) yields another useful relationship for studying the temperature dependence of α. This is expressed as

$$(\alpha/\alpha_0) = [1-\alpha_0\delta_T(T-T_0)]^{-1} \qquad (38)$$

The variation of δ_T with temperature has been taken into consideration analytically in the model developed by Tallon [14]. The modified Gruneisen parameters g_{MT} and g_{MP} defined by Tallon are expressed as

$$g_{MT} = -V_0 \left(\frac{\partial \ln M}{\partial V}\right)_T \qquad (39)$$

$$g_{MP} = -V_0 \left(\frac{\partial \ln M}{\partial V}\right)_P \qquad (40)$$

Where V_0 is the volume V at atmospheric pressure and room temperature. M represents any of the elastic constants or moduli. If we put isothermal bulk modulus in place of M equations (39) and (40) then we obtain.

$$(g_{KT}) = -\frac{V}{K_T}\left(\frac{\partial K_T}{\partial V}\right)_T = \left(\frac{\partial K_T}{\partial P}\right)_T \qquad (41)$$

and

$$(g_{KP}) = -\frac{V}{K_T}\left(\frac{\partial K_T}{\partial P}\right)_P = -\frac{1}{\alpha K_T}\left(\frac{\partial K_T}{\partial P}\right)_T \qquad (42)$$

Thus at $V=V_0$, $g_{KT} = \partial K_T/\alpha_P$ and $g_{KP} = \delta T$ [the Anderson Gruneisen parameter equation (25)]. Using the definitions (eqations (39) and (40) and taking the assumption given by equation (27) Tallon [14] obained the following expression for the temperature dependence of α and K_T.

$$(T,P) = \alpha(T_0,P)exp\left[g_{KP}\left[\frac{V(T,P)-V(T_0,P)}{V_0}\right]\right] \qquad (43)$$

$$(T,P) = K_T(T_0,P)exp\left[-g_{KP}\left[\frac{V(T,P)-V(T_0,P)}{V_0}\right]\right] \qquad (44)$$

One can calculate the values of α and K_T at different temperature with the help of equations (43) and (44).

Thermal Expansivity of Iron at Very High Pressure And Temperature :

The thermal-pressure equation of state can be written as

$$P(V,T) = P_0(V,300K) + P_{TH}(T) \qquad (45)$$

where P_0 is the cold (300 K) pressure. One uses the 300 K P_0, V data for iron tabulated by Anderson et al. [15]. These data are consistent with the Mao et al. [16] data in the pressure range 0-300 GPa common to both data sets. In eq. (45) P_{TH} is the thermal pressure, the pressure in addition to P_0 resulting from increased temperature with constant volume.

By a thermodynamic identity, we have

$$\left(\frac{\partial P_{TH}}{\partial T}\right)_V = \alpha K_T \qquad (46)$$

Where K_T is the isothermal bulk modulus. A good approximation often used in high-temperature equations of state for nonmetals is that αK_T is independent of temperature. In this approximation, P_{TH} is proportional to $\Delta T = T - T_0$ (T_0, the reference temperature, is often 300 K), with αK_T being the proportionality constant. However, for metals, one must consider effects due to the thermal excitation of electrons [17, 18] and include a higher-order term. In other words, αK_T, not P_{TH}, is a linear function of T [19, 20, 21]. The integration of eq. (46) gives.

$$P_{TH}(\Delta T) = a(\Delta T) + \frac{1}{2}b(\Delta T)^2 \qquad (47)$$

or

$$P_{TH}(T) = a(T-T_0) + \frac{1}{2}b(T-T_0)^2 \qquad (48)$$

where a and b represent $(\alpha K_T)_{300K}$ and $\left(\frac{\partial \alpha K_T}{\partial T}\right)_V$ respectively.

One is guided by theory [20] for the value of the anharmonic coefficient, b in eq. (48), using $7.8 \times 10-7$ kPa K^{-2}. The effect of this nonlinear term in the calculated equation of state is small, but noticeable at very high temperature. In using equations (45) and (48) to get the complete equation of state, one has implicitly assumed that a and b in equation (48) are not dependent on volume (or pressure). The primary concern in justifying this assumption is with a since b already is a much smaller higher order term. The validity of assuming α is independent of volume is supported from experiment. The 300K isotherm values for αK_T [22] do not change systematically with volume; the standard deviation of αK_T determined over the full volume range. Furthermore, recent theoretical studies suggest that αK_T is insensitive to volume over a wide temperature range [19, 20, 23]. When comparing the work of Wasserman et al [19] and Stixrude et al [20] with that a Alfe et al. [21], there is some difference in the computed value of αK_T, especially at low temperatures. Regardless of the exact numbers for αK_T that emerge from

these theoretical studies, they show αK_T to be insensitive to volume (or pressure on an isotherm). At the highest temperature (6000 K) illustrated, however, the Alfe et al. [21] report shows some deviation from this general trend.

Resulting values of α (P,T) along with selected isobars and isotherms are listed in Table 1 and illustrated in Figs. 1-4. The results illustrated in Fig. 1 include some smoothing, especially at lower pressure, of the primary values listed in Table 1.

P(GPa)	T(K)							
	300K	1000K	2000K	3000K	4000K	5000K	6000K	7000K
40	3.47	3.85	5.30					
60	2.83	3.00	3.98	4.78	7.17			
80	2.32	2.51	3.14	3.55	4.97	6.56		
100	1.94	2.10	2.54	2.90	3.72	4.48	6.50	
120	1.65	1.79	2.10	2.42	2.96	3.62	4.65	6.53
140	1.41	1.56	1.77	2.02	2.42	2.92	3.60	4.80
160	1.23	1.38	1.52	1.71	2.04	2.45	2.96	3.90
180	1.09	1.23	1.34	1.49	1.78	2.10	2.52	3.28
200	0.99	1.10	1.21	1.37	1.56	1.86	2.22	2.80
220	0.91	1.00	1.11	1.28	1.42	1.70	1.96	2.48
240	0.84	0.95	1.04	1.20	1.32	1.56	1.80	2.22
260	0.80	0.90	0.98	1.12	1.23	1.47	1.67	2.00
280	0.76	0.85	0.93	1.06	1.17	1.39	1.57	1.84
300	0.74	0.81	0.89	1.00	1.11	1.31	1.48	1.70
330	0.69	0.77	0.86	0.98	1.07	1.25	1.38	1.52
360	0.68	0.75	0.84	0.96	1.04	1.19	1.30	1.42

Table 1: Values of $\square$ $\square$ (P,T) (ɨ $10^{-5}K^{-1}$) for iron along selected isotherms and isobars (GPa) determined from the equation – of state.
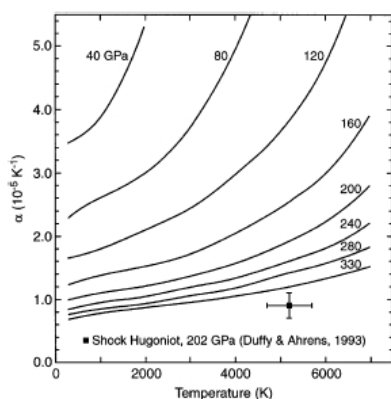

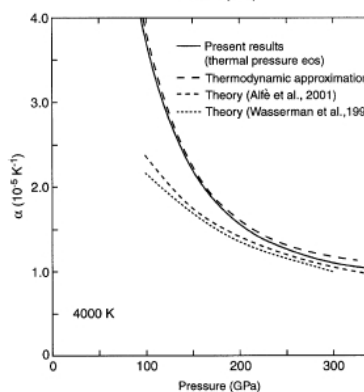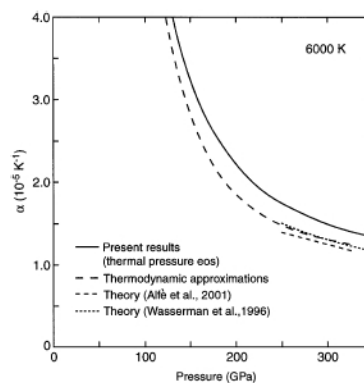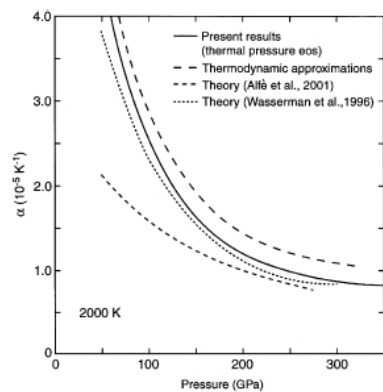Figure 1 : α(T) along selected isobars. The Shock Hugoniot value was reported at 202 GPa and 5200 K [33]

Figure 2, 3 and 4 : α(P) for iron determined from our present equaiton of state method on 2000K, 4000K and 6000K isotherm respectively, Comparisons are made with results from simplifying thermodynamic

assumptions discussed here and with results from theoretical studies.

THERMAL EXPANSIVITY AND BULK MODULUS FOR MINERALS:

One of the most widely used thermodynamic approximations [13, 14, 15, 24] for studying the high temperature high pressure behaviour of solids is that the product of volume thermal expansion coefficient, i.e., the thermal expansivity and the isothermal bulk modulus K_T remains constant. Thus we can write

$$\alpha K_T = \xi \qquad (49)$$

where the product has ξ has been assumed to remain constant under the variation of pressure or temperature. If this assumption does not hold, then equation (49) yields the following relationship for the isobaric variation αK_T and ξ with the change in volume under the effect of temperature;

$$\frac{V}{\alpha}\left(\frac{d\alpha}{dV}\right)_P + \frac{V}{K_T}\left(\frac{dK_T}{dV}\right)_P = \frac{V}{\xi}\left(\frac{d\xi}{dV}\right)_P \qquad (50)$$

The data reported by Anderson et al [25] for two minerals at high temperatures are used in the present study to access the validity of basic assumptions regarding the variations of α, K_T and ξ with temperature. In particular, one studies the variation of α and volume with temperature using the thermodynamic model due to Xia and Xiao[26].

Taking the high temperature data from Anderson et al [25] one made an attempt to plot αK_T and ξ each as function of V/V_0, where V_0 is the volume at 300K. Values of V/V_0 corresponding to different temperatures were estimated from the data on density [25]. Systematic linear relationship are obtained only for ln K_T, versus ln V/V_0 for Mgo and Mg_2SiO_4 [Figures: 5, 6]. Plots for ln α or ln ξ versus lnV/V_0 are found to be unsystemaic and non-linear. The validity of this assumption has been demonstrated by Xia and Xiao by calculating the thermal expansivity of MgO up to 1800K in good agreement with experimental data. The minerals under study remain in the solid phase for the temperature range considered here.

Temperature (K)	V/V_0		α	
	Calculated from present study	Experimental Value Ref. [32]	Calculated from present study	Experimental Value Ref. [32]
300	1.000	1.000	31.2	31.2
400	1.0033	1.0033	34.9	35.7
500	1.0070	1.0073	37.7	38.4
600	1.0109	1.0112	40.0	40.2
700	1.0150	1.0153	41.8	41.4
800	1.0194	1.0196	43.4	42.6
900	1.0239	1.0240	44.7	43.8
1000	1.0285	1.0284	45.9	44.7
1100	1.0333	1.0331	46.9	45.6
1200	1.0382	1.0379	47.8	46.5
1300	1.0432	1.0427	48.6	47.1
1400	1.0484	1.0476	49.3	48.0
1500	1.0536	1.0528	49.9	48.9
1600	1.0589	1.0581	50.5	49.8
1700	1.0643	1.0635	51.0	50.4
1800	1.0697	1.0688	51.5	51.3

Table 2: Values of V/V_0 and thermal expansivity $\alpha(10^{-6}K^{-1})$ for MgO $V=V_0$ at T=300K

Temperature (K)	V/V_0		α	
	Calculated from present study	Experimental Value Ref. [32]	Calculated from present study	Experimental Value Ref. [32]
300	1.000	1.000	27.2	27.2
400	1.0029	1.0028	30.4	30.3
500	1.0061	1.0059	32.9	32.2
600	1.0095	1.0094	34.8	33.6
700	1.0131	1.0129	36.5	34.8
800	1.0169	1.0164	37.8	35.9
900	1.0208	1.0199	39.0	37.0
1000	1.0248	1.0238	40.1	38.1
1100	1.0290	1.0277	41.0	39.2
1200	1.0333	1.0320	41.8	40.5
1300	1.0376	1.0363	42.5	41.6
1400	1.0421	1.0407	43.1	42.7
1500	1.0466	1.0451	43.7	43.9
1600	1.05512	1.0498	44.2	45.0
1700	1.0559	1.0547	44.7	46.2

Table 3: Values of V/V_0 and thermal expansivity $\alpha(10^{-6}K^{-1})$ for Mg_2SiO_4 $V=V_0$ at T=300K

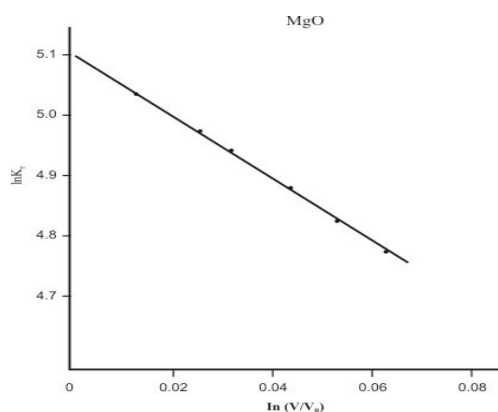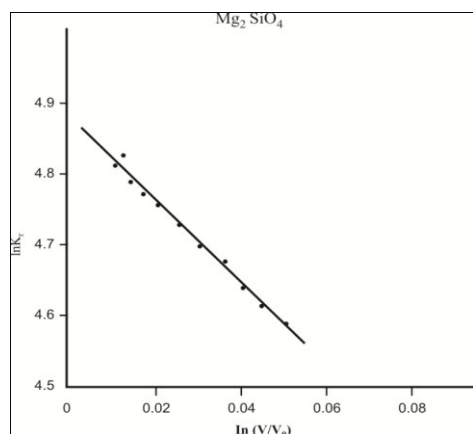Figure -5

Figure -6

RESULT AND CONCLUSION

One's result indicate that the value for α at 202 Gpa and 5200K should be about $1.8 \times 10^{-5} K^{-1}$ for iron. Results from theory favour a little lower value at this pressure and temperature, but are also significantly higher than the value of $0.91+0.20 \times 10^{-5} K^{-1}$ [27] reported from shock experiments. The good agreement between the calculated and experimental values of α and V/V_0 support the validity of assumption used for minerals under study.

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