Thermal Expansibility of Pyrope At Elevated Temperatures And Pressure

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Abstract- *Earlier several attempts have been made to study t properties such as thermal expansivity and bulk modulus of solids under the effect of high temperatures and pressure . Thermal expansivity and bulk modulus are important thermodynamic quantities for understanding the high temperature behaviour and the equation of state for solids. To understand the thermodynamic and thermoelastic behaviour of solids at high temperature, it is necessary to have reliable value of thermal expansivity and isothermal bulk modulus along with the value of Anderson-Gruneisen parameter and the thermal pressure for the range of temperatures from room temperature to the melting temperature. The present work shows temperature dependence of isothermal bulk modulus and thermal expansivity in terms of Anderson-Gruneisen parameter and the thermal pressure for Pyrope. The analysis is based on the thermodynamic and thermoelastic data reported by Anderson.*

Keywords- Equation of stste ,Thermal Expansivity, Bulk modulus

I. INTRODUCTION

The mineral pyrope is a member of the garnet group. Pyrope is the only member of the garnet family to always display red colouration in natural samples, and it is from this characteristic that it gets its name: from the Greek for fire and eye. Despite being less common than most garnets, it is a widely used gemstone with numerous alternative names, some of which are misnomers. Chrome pyrope, and Bohemian garnet are two alternative names, the usage of the later being discouraged by the Gemological Institute of America [1].

The composition of pure pyrope is $Mg_3Al_2(SiO_4)_3$, although typically other elements are present in at least minor proportions - these other elements include Ca, Cr, Fe and Mn. Pyrope forms a solid solution series with almandine and spessartine, which are collectively known as the pyralspite garnets (pyrope, almandine, **sp**essartine). Iron and manganese substitute for the magnesium in the pyrope structure. The resultant, mixed composition garnets are defined according to their pyrope-almandine ratio. The semi-precious stone rhodolite is a garnet of ~70% pyrope composition.

II. METHODOLOGY AND FORMULATION

The equation of state EOS due to Singh and Gupta [2] used to study the thermo elastic properties of Pyrope, because of its simple and straightforward applications in high temperature physics. This model is applicable under the assumption that A-G parameters δ_T is a temperature dependent parameter which remains constant even in high temperature range.

The Anderson Gruneisen parameter δ_T may be defined as

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

Anderson Gruneisen parameter is a measurement of an harmonicity in a crystal. Recent studies revealed that δ_T changes with temperature and it must be considered as a temperature dependent parameter. The temperature dependence of δ_T is given by the following empirical relationship

$$\delta_T = \delta_T^0 x^k \qquad (2)$$

Where $x=T/T_0$, T_0 is the reference temperature and δ_T^0 is the value of Anderson Gruneisen parameter at $T= T_0$ and k is new dimensionless thermo elastic parameter, whose value will be calculated by the slope of the graph plotted between log (δ_T), and log(T/T_0).

Therefore, the value of k defined as

$$k = \left(\frac{\partial \ln \delta_T}{\partial \ln x}\right) \quad (3)$$

Using equation (1),

$$\delta_T^0 \left(\frac{T}{T_0}\right)^k = \frac{1}{\alpha^2}\left(\frac{d\alpha}{dT}\right)_p$$

The integration of above equation gives the final expression for thermal expansion coefficient (α_T),

$$\alpha_T = \alpha_0 \left[1 - \frac{\delta_T^0 \alpha_0}{T_0^k (k+1)}\left(T^{k+1} - T_0^{k+1}\right)\right]^{-1} \quad (4)$$

Where α_0 is the thermal expansion coefficient at T_0.

Using the definition of A-G parameter, at p=0, we have,

$$-\left(\frac{dK_T}{dT}\right) = \alpha_0 K_0 \delta_T$$

Using (2)

$$-\left(\frac{dK_T}{K_0}\right) = \alpha_0 \delta_T^0 \left(\frac{T}{T_0}\right)^k dT$$

Integrating the above equation, the final expression for isothermal bulk modulus given by

$$K_T = K_0 \left[1 - \frac{\alpha_0 \delta_T^0}{T_0^k (k+1)}\left(T^{k+1} - T_0^{k+1}\right)\right] \quad (5)$$

The expression for the volume thermal expansion can written as follows

$$\frac{V}{V_0} = \exp\left[\int_{T_0}^{T} \frac{\alpha_0}{\left[1 - A\left(T^{k+1} - T_0^{k+1}\right)\right]} dT\right] \quad (6)$$

Where

$$A = (\alpha_0 \delta_T^0 / T_0^k (k+1))$$

The values of thermal expansivity (α_T), isothermal bulk modulus (K_T) and volume thermal expansion (V/V0), at different temperatures and atmospheric pressure have been calculated using equations (4), (5) and (6) respectively. These equations need only three input parameters such as Anderson Gruneisen parameter (δ_T^0), thermal expansion coefficient (α_0) at zero pressure along with reference temperature and the dimensionless thermoelastic parameter (k). The dimensionless thermoelastic parameter (k) have been calculated from slope of the graph, log (δ_T) versus log (T/T_0), which comes out in the form of a straight line. The variation of δ_T^0 with temperature have been calculated from Eq. (2) using the values of thermal expansivity (α). The input parameters of thermal expansion coefficients at zero pressure and reference temperature taken directly from the graphs, which are based on the experimental results [3]. The calculated values of thermal expansivity (α_T) and volume thermal expansion (V/V0) for various minerals are plotted with temperature and compared to the previous studies.

Table 1. Input parameters at zero pressure and room temperature.

Mineral	α_0 ($10^{-5}K^{-1}$)	K_0 (GPa)	δ_T^0
Pyrope	2.36	171.2	6.27

Table 2: Calculated values of volume thermal expansion (V/V_0) , Isothermal Bulk modulus (K_T) and thermal expansion coefficient (α_T) at different temperatures along with experimental data [3].

Temp.	V/V_0 Pres.	V/V_0 Exp.	α_T Pres.	α_T Exp.	K_T Pres.	K_T Exp.
200	1	1	2.32	2.36	169.89	169.4
400	1.003	1.002	2.61	2.64	167.18	166.5
600	1.007	1.008	2.69	2.9	162.23	161.4
800	1.012	1.014	3.01	3.03	156.67	156.6
1000	1.015	1.017	3.01	3.07	153.37	154.1

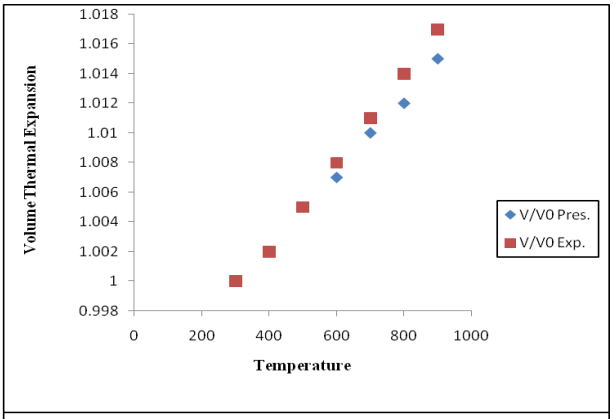

Fig.1 Volume Thrmal Expasivity of Pyrope at different Temperatures

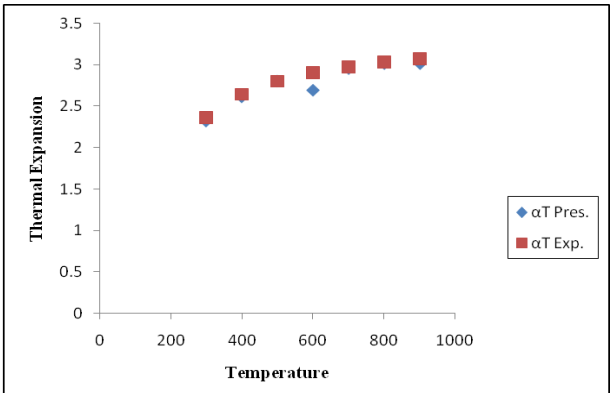

Fig.2 Thermal Expansion of Pyrope at different Temperatures

III. RESULT AND DISCUSSION

From the above observations, it is found that for pyrope α_T (Thermal Expansion) increases and K_T (Isothermal bulk modulus) decreases considerably at higher temperatures. Values of volume expansion have calculated up to the temperatures close to their melting temperatures. The results are in good agreement with the available experimental data based on density measurements.

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