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Physics

THERMODYNAMIC PROPERTIES OF OLIVINE UNDER THE EFFECT OF HIGH TEMPERATURES

KEY WORDS:

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ABSTRACT

The study of elasticity of the earth materials is of great interest for the geophysics. Earlier several attempts have been made to study the thermodynamic properties such as thermal expansivity and bulk modulus of solids under the effect of high temperatures. 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 analysed temperature dependence of isothermal bulk modulus and thermal expansivity in terms of Anderson-Gruneisen parameter and the thermal pressure for Olivine. The analysis is based on the thermodynamic and thermoelastic data reported by Anderson.

Introduction

The mineral olivine is a magnesium iron silicate. Chemical formula of Olivine is (Mg, Fe)2 SiO4. The ratio of magnesium and iron varies between the two ends members of the solid solution series: forsterite (Mg-end member) and fayalite (Fe- end member). Compositions of olivine are commonly expressed as molar percentages of forsterite (Fo) and fayalite (Fa) (e. g., Fo70Fa30). Forsterite has an unusually high melting temperature at atmospheric pressure, almost 1900 °C, but the melting temperature of fayalite is much lower (about 1200 °C). The melting temperature varies smoothly between the two end members, as do other properties. Olivine incorporates only minor amounts of elements other than oxygen, silicon magnesium and iron. Magnesium and nickel commonly are the additional elements present in highest concentrations.

Olivine gives its name to the group of minerals with a related structure, which includes tephroite (Mn2SiO4), monticellite (CaMgSiO4) and kirschsteinite (CaFeSiO4). Olivine named for its typically olive-green colour; through it may alter to a reddish colour from the oxidation of iron. Translucent Olivine sometimes used as a gemstone called peridot. Olivine is one of the weaker common minerals on the surface according to the Goldich dissolution series. It weathers to iddingsite (a combination of clay minerals, iron oxides and ferrihydrites) readily in the presence of water [1]. The presence of iddingsite on Mars would suggest that liquid water once existed there, and might enable scientists to determine when there was last liquid water on the planet [2].

The aluminium foundry industry uses olivine sand to cast objects in aluminium. Olivine sand requires less water than silicon based sand while providing the necessary strength to hold the mold together during handling and pouring of the metal. Less water means less gas (steam) to vent from the mold as metal poured into the mold [3].

Methodology and Formulation:

The equation of state EOS due to Singh and Gupta [4] used to study the thermo elastic properties of olivine, 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

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

Anderson Gruneisen parameter is a measurement of anharmonicity 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

$$\delta_T = \delta_T^0 x^k \tag{2}$$

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

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

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

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

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 [5]. 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
Olivine)	2.66	129.3	6.59

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 [5].

Temp.	V/V_0 Present	V/V_0 Exp	K_T Present	K_T Exp	α_T Present	α_T Exp
300	1	1	127.4	128	2.66	2.66
600	1.007	1.008	121.1	121.2	3.29	3.35
900	1.016	1.02	114.5	114.7	3.62	3.64
1200	1.025	1.03	107.2	107.8	3.81	3.86
1500	1.035	1.042	101.1	101.3	4.06	4.07

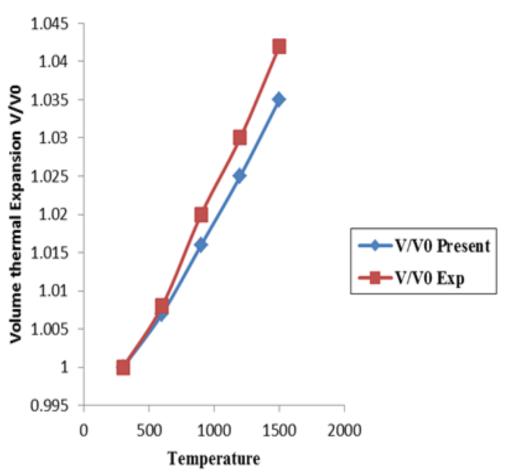

Figure 1. Volume thermal expansion of olivine at different temperatures

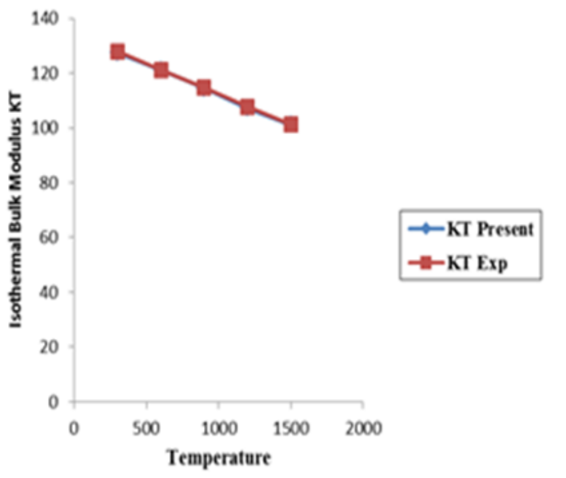

Figure 2 Isothermal bulk modulus (K_T) of olivine at different temperatures

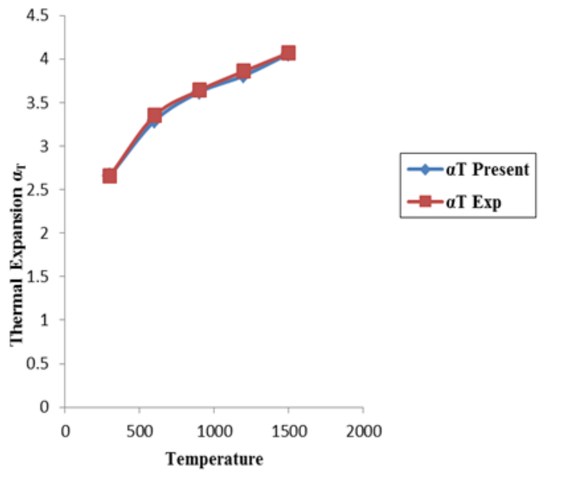

Figure 3 Thermal expansivity of Olivine at different temperatures

Result and Discussion

From the above observations, it is found that for Olivine 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. The experimental data for temperature dependence of thermodynamic quantities for olivine mineral reported by Anderson [5], which are considered to most accurate.

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