Thermo-Elastic Properties of Manganese (II) Oxideat High Temperature

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Abstract- *The equation of state EOS due to Singh and Gupta [5] has been used to study the thermo elastic properties of Manganese (II) oxide, because of its simple and straight forward applications in high temperature physics. This model is applicable under the assumption that A-G parameters δT is a temperature dependent parameter which remains constant even in high temperature range.It is found that for MnO α increases and KT decreases considerably at higher temperature.*

Keywords- EoS , A-G parameters, Bulk Modulus Manganese

I. INTRODUCTION

The behavior of minerals under extreme conditions of pressure temperature plays an important role in understanding the dynamics and evolution of the lower mantle of the earth. Due to the lack of direct samples from the lower mantle, seismic observations and laboratory measurements are the only available means to understand this region. Thus physical and chemical properties of minerals are crucial to understand the lower mantle of earth. The EOS plays a central role in the study of the earth's deep interior.. The behavior of thermo-elastic constant under the effect of temperature has attracted the attention of theoretical as well as experimental workers [1-4] because of their essential need in the study of technological problems. For different class of solids many equations of states are available. Among the number of isothermal and isobaric EOS described earlier [6-10], we prefer the EOS due to Singh & Gupta [5] because of its simple and straight forward assumptions in high temperature physics. In the past, several equations of state have been derived within the Mie-Gruneisen approximation in terms of low pressure, and temperature dependence is introduced into the E0S through some thermal pressure [11]. Vinetet al. [12] then developed the temperature EOS by modeling the variation of bulk modulus with temperature and a known experimental value of thermal expansion. This model is however, applicable under the assumption that Anderson Gruneisen parameter δ_T is a temperature dependent parameter which remains constant even in high temperature range.

Manganese (II) oxide

Manganese(II) oxide is the inorganic compound with formula MnO [13]. MnO is a basic oxide that is insoluble in water but dissolves in acids, forming manganese (II) salts [14].

Preparation and occurrence

MnO can be prepared by the reduction of any higher oxide with hydrogen [14] e.g.:

$$MnO_2 + H_2 \rightarrow MnO + H_2O$$

Commercially it is prepared by reduction of MnO_2 with hydrogen, carbon monoxide or methane [14]:

II. STRUCTURE AND PROPERTIES

MnO has the NaCl, rock salt structure, where cations and anions are both octahedrally coordinated [14]. MnO has the distinction of being one of the first compounds [15] to have its magnetic structure determined by neutron diffraction in 1951 [15]. This study showed that the Mn^{2+} ions form a face centered cubic magnetic sub-lattice where there are ferromagnetically coupled sheets which are anti-parallel with adjacent sheets.

III. APPLICATIONS

Together with manganese sulfate, MnO is a component of fertilizer and feed additives. Many thousands of tons are consumed annually for this purpose [16].

IV. METHODOLOGY

The equation of state EOS due to Singh and Gupta [5] has been used to study the thermo elastic properties of Manganese (II) oxide, The Anderson Gruneisen parameter δ_T may be defined as

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

Anderson Gruneisen parameter is basically a measurement of anharmonicity in a crystal. The temperature dependence of δ_T is given by the following empirical relationship

$$\delta_T = \delta_T^0 x^k$$
(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).

So the value of k is defined as

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

Using equation (1),

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

On integration it- thermal expansion coefficient (α_T),

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

where α_0 is the thermal expansion coefficient at T_0.
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, bulk modulus is given by

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

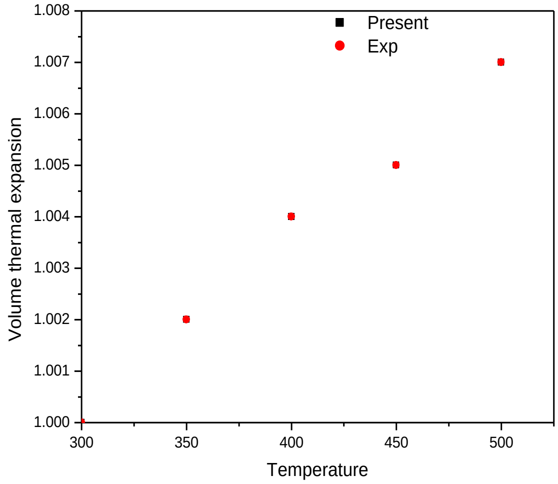
The expression for the volume thermal expansion can be written as follows

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

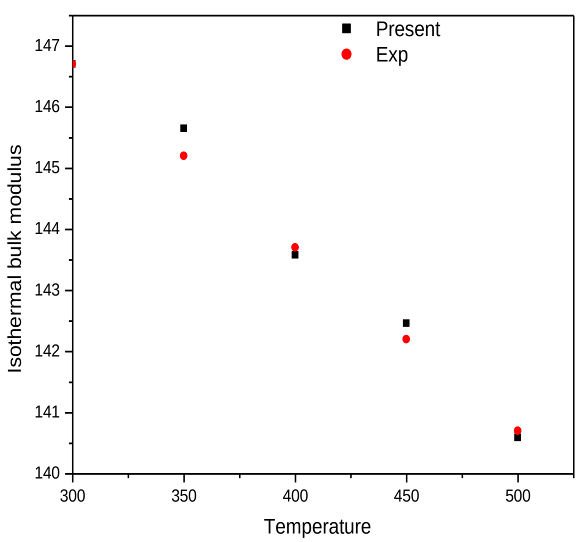
The values of thermal expansivity (α_T), isothermal bulk modulus (K_T) and volume thermal expansion (V/V0), at different temperatures and atmospheric pressure have been calculated using Eqs.(4), (5) and (6) respectively. These equations need only three input parameters such as Anderson Gruneisen parameter (δ_T^0), volume 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 have been taken directly from the graphs, which are based on the experimental results [4

Calculated Values of volume thermal expansion, bulk modulus and thermal expansion along with experimental data [4]

Temperature	**V/V_0 Present**	**V/V_0 Exp**	**α_T Present**	**α_T Exp**	**K_T Present**	**K_T Exp**
300	1	1	3.46	3.46	146.7	146.7
350	1.002	1.002	3.56	3.58	145.65	145.2
400	1.004	1.004	3.67	3.68	143.58	143.7
450	1.005	1.005	3.76	3.77	142.46	142.2
500	1.007	1.007	3.83	3.85	140.59	140.7



Volume thermal expansion of MnOat different temperatures



Isothermal bulk modulus (K_T) of MnO at different temperatures

V. RESULT

It is found that for MnO α increases and K_T decreases considerably at higher temperatures. Values of volume expansion have been calculated upto 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 many minerals have been reported by Anderson [4] which are considered to be most accurate.

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