

# Volume dependence of isothermal bulk modulus and thermal expansivity of MgO

K. Sushil

*Department of Physics, Institute of Basic Sciences, Khandari, Agra 282002, India*

Received 4 January 2005; received in revised form 16 May 2005; accepted 2 June 2005

## Abstract

A relationship between the isothermal bulk modulus and the isobaric volume expansion for MgO has been used to obtain values for the isothermal bulk modulus at different temperatures up to 3000 K along isobars at selected pressures up to 224 GPa. The volume dependence of the Anderson–Grüneisen parameter,  $\delta_T$ , has been taken into account under isobaric as well as isothermal conditions. The pressure dependence of thermal expansivity has also been studied along isotherms at selected temperatures up to 3000 K. The method presented here allows the prediction of thermal expansivity and isothermal bulk modulus in the pressure–temperature space, showing a behaviour that is consistent with the available experimental data and ab-initio results.

© 2005 Elsevier B.V. All rights reserved.

PACS: 62.20; 65.70

Keywords: Isothermal bulk modulus; Thermal expansivity; Anderson–Grüneisen parameter; MgO

## 1. Introduction

MgO (periclase) is an important ceramic material and geophysical mineral. The equation of state (EOS) and thermoelastic properties for this solid have been investigated in detail and reported in the recent literature [1–8]. In the present study, we concentrate our attention on the work due to Jacobs and Oonk [5], who have formulated an EOS for MgO following an earlier study made by

Grover et al. [9] which revealed a nearly precise linear relationship between the logarithm of the bulk modulus and the volume up to volume changes of 40%. Jacobs and Oonk have written this relationship as

$$V_m^0(T) = V_m^0(T_0) + b \ln \left( \frac{K^0(T)}{K^0(T_0)} \right), \quad (1)$$

where  $V_m^0$  denotes molar volume,  $K$  the isothermal bulk modulus,  $T_0$  a reference temperature (usually room temperature) and the superscript “0” refers to standard pressure (1bar).  $b$  is a constant

*E-mail address:* [k\\_sushil23@rediffmail.com](mailto:k_sushil23@rediffmail.com).

depending only on the material. The isothermal bulk modulus which is the inverse of the isothermal compressibility is defined as

$$K_T = -V \left( \frac{\partial P}{\partial V} \right)_T. \quad (2)$$

It should be emphasized that the relationship given by Grover et al. [9] has been shown to be valid for the isothermal volume compression in case of MgO [10], whereas Eq. (1) taken by Jacobs and Oonk represents the variation of bulk modulus with the change in volume under isobaric condition at room pressure.

The parameter  $b$  appearing in Eq. (1) has been found [11] to be related to the Anderson–Grüneisen parameter

$$\delta_T = -\frac{1}{\alpha K_T} \left( \frac{\partial K_T}{\partial T} \right)_P, \quad (3)$$

where  $\alpha$  is thermal expansivity or volume thermal expansion coefficient. Taking  $\delta_T$  to depend on volume as  $V(T, P)/V(T_0, P)$  along an isobar and as  $V(T, P)/V(T, 0)$  along an isotherm, we have used Eq. (1) at higher pressures for calculating  $K_T$  as a function of temperature. Values of thermal expansivity are also calculated at higher pressures along isotherms at selected temperatures. It should be mentioned that the model used in the present study is consistent with the recent work of Raju et al. [11] on temperature derivative and pressure derivative of bulk modulus.

## 2. The Anderson–Grüneisen parameter

The Anderson–Grüneisen parameter,  $\delta_T$ , is defined by Eq. (3). If we use the definition of thermal expansivity

$$\alpha = \frac{1}{V} \left( \frac{\partial V}{\partial T} \right)_P \quad (4)$$

in Eq. (3), we get

$$\delta_T = -\frac{V}{K_T} \left( \frac{\partial K_T}{\partial V} \right)_P. \quad (5)$$

If  $\delta_T$  is assumed to remain constant then Eq. (5), on integration, yields

$$\frac{K_T(T, P)}{K_T(T_0, P)} = \left[ \frac{V(T, P)}{V(T_0, P)} \right]^{-\delta_T}. \quad (6)$$

However, there is evidence that  $\delta_T$  changes with the variation in volume. The volume dependence of  $\delta_T$  has been explored by Chopelas and Boehler [12] and by Anderson and Isaak [13] using the following relations respectively:

$$\delta_T + 1 = (\delta_T^0 + 1) \frac{V}{V_0} \quad (7)$$

and

$$\frac{\delta_T}{\delta_T^0} = \left( \frac{V}{V_0} \right)^k, \quad (8)$$

where  $k$  is a dimensionless thermoelastic parameter. The value of  $k$  usually remains between 1.4 and 1.2 for MgO at different temperatures [2]. For the sake of simplicity one can take  $k = 1$  in Eq. (8). Tallon [14] performed a detailed study of solids under high pressures and high temperatures for the case that  $k = 1$ . The two basic assumptions considered by Tallon [14] for the volume dependence of the Anderson–Grüneisen parameter,  $\delta_T$ , are expressed as

$$\frac{\delta_T(T, P)}{\delta_T(T, 0)} = \frac{V(T, P)}{V(T, 0)} \quad (9)$$

and

$$\frac{\delta_T(T, P)}{\delta_T(T_0, P)} = \frac{V(T, P)}{V(T_0, P)}. \quad (10)$$

Eq. (9) holds for isothermal conditions at any temperature  $T$  and also at  $T = T_0$ , whereas Eq. (10) holds for isobaric conditions at any pressure  $P$  and also at  $P = 0$  [14,15]. Combining Eqs. (5) and (10), and then integrating along an isobar we get

$$K_T(T, P) = K_T(T_0, P) \times \exp \left\{ -\delta_T(T_0, P) \left[ \frac{V(T, P)}{V(T_0, P)} - 1 \right] \right\}. \quad (11)$$

Download English Version:

<https://daneshyari.com/en/article/9837435>

Download Persian Version:

<https://daneshyari.com/article/9837435>

[Daneshyari.com](https://daneshyari.com)