Research Article

Isobaric Study of the Elastic Properties for Alkaline Earth Oxides under High Temperature

Seema Gupta,^{1,2} S. P. Singh,² and S. C. Goyal^{1,2,3}

¹Department of Physics, Agra College, Agra 282002, India

²Department of Physics, Government Degree College, Sambhal, Moradabad, India

³K. P. Engineering College, N. H. 2, Etmadpur, Agra 283202, India

Correspondence should be addressed to Seema Gupta, seema_g_khushi@yahoo.co.in

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A simple and straightforward theoretical model is developed to investigate the elastic properties of alkaline earth oxides under the effect of temperature as well as pressure. The calculation is performed with the help of high pressure-high temperature equation of state based on thermodynamic analysis. The anharmonic term arising due to thermal expansion has been taken into account in the expansion of logarithmic series of the thermodynamic data. The results obtained for alkaline earth oxides are discussed and compared with experimental data under the combined effect of high temperature and high pressure. The results are found to be in good agreement with available experimental results.

1. Introduction

The equation of state (EOS) gives us valuable information about the change in bulk under the influence of temperature at a fixed pressure and is thus related to the compression of solids. The study of elasticity plays an important role in describing the high-temperature behaviour of solids. The studies based on the equation of state (EOS) are of importance in physics as well as in chemistry and in the earth sciences [1, 2]. The theoretical studies of EOS at high temperature and pressure are of fundamental interest because they permit interpolation and extrapolation into the regions in which the experimental data are sparse or lacking.

It is necessary to know the effects of the temperature and pressure on the elastic properties of alkaline earth oxides (AEOs) throughout the upper mantle of the Earth for better understanding about its structure, compositions, and mineralogy. The properties of alkaline earth oxides under varying conditions of temperature and pressure have attracted the attention of theoretical and experimental workers [3–9] because of their need in different branches of science [10].

The problem of evaluation of elastic moduli can be tackled in two different ways, for example, (i) by determining the constants or elastic moduli from temperature relationship, termed as equation of state [3–7] and (ii) by choosing suitable interionic potential and thereby evaluating elastic constants and elastic moduli [11–13]. Both methods help us to determine various properties of solids under varying conditions of pressure and temperature. It has been observed that the methods based on the theory of interionic potentials are very tedious [11–16] and involve a lot of computational work in addition to various approximations and it fails to evaluate the elastic constants or elastic moduli of complicated solids.

The purpose of the present study is to present a simple and straightforward method for evaluation of elastic constants of simple and complex solids at different temperatures. To determine the temperature dependence of elastic constants and their combination, different relations based on thermodynamic parameters have been proposed in the literature [17]. The well-known and widely used relations for predicting the temperature dependence of elastic constants are discussed by Suzuki et al. [18] and by

FIGURE 1: (a) Isobars of C_{11} at different temperatures for MgO, (b) isobars of C_{12} at different temperatures for MgO, (c) isobars of C_{44} at different temperature for MgO, and (d) isobars of K s at different temperatures for MgO.

Singh and Kumar [6]. The relation of Suzuki et al. [18] involves the complicated analytical form, and, hence, the complex computational work is required. Moreover, this relation predicts good results for the variation of volume but not for the elastic constants. This relation has further been simplified by Singh and Kumar [6] by considering the volume dependence of Anderson-Grüneisen parameter, though the methodology followed by these workers is too simple to explain the temperature dependence of elastic constants and the results are not good. It may be due to the reason that they have ignored the higher-order terms, that is, anharmonic terms, in the expansion of the logarithmic series of volume change.

In the present study, we have considered the anharmonic terms in the expansion of logarithmic series of volume change with temperature and probably first time investigated

the temperature dependence of elastic constants up to 2000 K of alkaline earth oxides at different pressures up to 100 GPa. The results predicted by the developed theory in case of alkaline earth oxides are critically discussed.

2. Theory

The theory is based on the sound thermodynamic analysis which includes properly the volume dependence of Anderson-Grüneisen parameter. Following Singh et al. [4], Singh and Kumar [6], Joshi and Gupta [7], and Kumar [5, 20–22], the relation for the change in volume to the volume is given by

$$\frac{V}{V_0} - 1 = -\frac{1}{A} \ln \left[1 + \frac{A}{K_0} \{P - \alpha_0 \beta_0 (T - T_0)\} \right]. \quad (1)$$

FIGURE 2: (a) Isobars of C_{11} at different temperatures for CaO, (b) isobars of C_{12} at different temperatures for CaO, (c) isobars of C_{44} at different temperatures for CaO, and (d) isobars of K at different temperatures for CaO.

Equation (1) can be written as follows

$$\frac{V}{V_0} - 1 = -\frac{1}{A} \ln \left[1 - \frac{A}{K_0} \{ \alpha_0 \beta_0 (T - T_0) - P \} \right], \quad (2)$$

where A is the parameter and is given by $A = (\delta^0 + 1) \approx (K'_0 + 1)$ as discussed in detail by Badi and Kumar [15], α_0 is the thermal expansion coefficient at T_0 , and K'_0 is the first-order pressure derivative of bulk modulus, which can be assumed nearly equal to δ_0 as mentioned elsewhere [4–7]. On expanding (2) and considering the terms up to third order, the high-order term, (2) becomes as follows:

$$\frac{V}{V_0} - 1 = \frac{1}{A} \left[e^{\alpha_0 A (T - T_0) - AP/K_0} - 1 + \frac{\{ \alpha_0 A (T - T_0) - PA/K_0 \}^3}{6} \right]. \quad (3)$$

Using the definition of the coefficient of volume thermal expansion α as $\alpha = (1/V)(dV/dT)_P$, (3) gives the following relation:

$$\frac{\alpha}{\alpha_0} = \frac{e^{\alpha_0 A (T - T_0) - AP/K_0} + \{ \alpha_0 A (T - T_0) - AP/K_0 \}^2 / 2}{1 + (1/A) \{ e^{\alpha_0 A (T - T_0) - AP/K_0} - 1 + \{ \alpha_0 A (T - T_0) - AP/K_0 \}^3 / 6 \}}. \quad (4)$$

Now, if we use the approximation that (αK) is independent of T , this gives

$$\alpha K = \alpha_0 K_0. \quad (5)$$

FIGURE 3: (a) Isobars of C_{11} at different temperatures for SrO, (b) isobars of C_{12} at different temperatures for SrO, (c) isobars of C_{44} at different temperatures for SrO, and (d) isobars of K at different temperatures for SrO.

Thus, (5) may be rewritten for B/B_0 as follows:

$$\frac{K}{K_0} = \frac{1 + (1/A) \left[e^{\alpha_0 A (T-T_0) - AP/K_0} - 1 + \{\alpha_0 A (T-T_0) - AP/K_0\}^3 / 6 \right]}{e^{\alpha_0 A (T-T_0) - AP/K_0} + \{\alpha_0 A (T-T_0) - AP/K_0\}^2 / 2} \quad (6)$$

We can generalize (6) as follows:

$$\frac{M}{M_0} = \frac{1 + (1/A) \left[e^{\alpha_0 A (T-T_0) - AP/K_0} - 1 + \{\alpha_0 A (T-T_0) - AP/K_0\}^3 / 6 \right]}{e^{\alpha_0 A (T-T_0) - AP/K_0} + \{\alpha_0 A (T-T_0) - AP/K_0\}^2 / 2} \quad (7)$$

From (7), the collective expressions for the temperature dependence of second-order elastic constants may be written as

$$\frac{C_{ij}}{C_{ij}^0} = \frac{1 + (1/A) \left[e^{\alpha_0 A (T-T_0) - AP/K_0} - 1 + \{\alpha_0 A (T-T_0) - AP/K_0\}^3 / 6 \right]}{e^{\alpha_0 A (T-T_0) - AP/K_0} + \{\alpha_0 A (T-T_0) - AP/K_0\}^2 / 2} \quad (8)$$

3. Results and Discussion

The values of temperature dependent of Second order elastic constants the bulk modulus of alkaline oxides at differnt pressure are computed with the help of above described

TABLE 1: Values of input data [5, 6, 9, 10, 13, 19] at room temperature. α (in 10^{-5} K^{-1}), δ^0 (dimensionless); elastic constants (C_{ij}) and bulk modulus (K) (in GPa); and first-order temperature derivatives ($(\partial C_{ij}/\partial T)_0$) (in 10^{-2} GPa).

Parameters	MgO	CaO	SrO
δ^0	5.3	5.6	5.4
α	3.12	3.04	4.20
C_{11}^0	298.906	220.53	173.00
C_{12}^0	96.4	57.60	45.0
C_{44}^0	157.13	80.03	56.0
K	159.67	111.96	86.0
$(\partial C_{11}/\partial T)_0$	-5.85	-4.90	-3.52
$(\partial C_{12}/\partial T)_0$	0.75	0.35	0.7
$(\partial C_{44}/\partial T)_0$	-1.26	-0.70	-0.56

theory using input data from Table 1. By using (6) and (8), we have thus calculated the values of the temperature dependence of second-order elastic constants and the bulk modulus of alkaline earth oxides at different pressure. The results are plotted in Figures 1, 2, and 3 from 300 K to 2000 K at different pressures for MgO, CaO, and SrO.

It is interesting to note from Figures 1(a), 2(a), and 3(a) that the values of C_{11} and C_{44} are decreasing with increase of temperature at 0 GPa, 10 GPa, 20 GPa, and 30 GPa isobars in all cases (MgO, CaO, and SrO). But the values of C_{12} are increasing with increase of temperature at all the pressure range. This clearly shows that there is a softening of the C_{11} and C_{44} elastic constants, while the values of C_{12} are slowly increasing with increase of temperature (Figures 1(b), 2(b), and 3(b)), at 0–30 GPa. It is also interesting to note that from Figures 1(c), 2(c), and 3(c) the values of C_{44} are decreasing with increase of temperature for 0–30 GPa. This is in good agreement with the experimental values at ambient condition. Thus, the behavior of C_{11} and C_{44} seems to be similar with increase of temperature at different pressure. If we draw our attention on Figures 1(d), 2(d), and 3(d) for the bulk modulus, we get the same pattern as that of C_{11} ; that is, the values of K are decreasing with increase of temperature at 0 GPa, 10 GPa, 20 GPa, and 30 GPa isobars in all cases (MgO, CaO, and SrO).

It is interesting to note from Figures 1, 2, and 3 that the softening of the bulk modulus increases with increase of pressure. Thus, the behavior of elastic constants with increase of temperature at low pressure (0–10 GPa) is different as compared to at high pressure (20–30 GPa). Such analysis regarding the behavior of elastic constants at different temperatures and pressures of alkaline earth oxides may be useful in explaining the physical properties like Debye temperature, elastic wave velocity, and so forth in geophysics.

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