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Analysis of the thermoelastic properties of nanocrystalline Foresterite using a thermodynamic equation of state

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ABSTRACT

A new potential independent equation of state is used in the present work to analyze the thermo-elastic properties of nanocrystalline Foresterite (nc- Fo) under varying temperature and pressure conditions. The newly developed EOS is found to be valid for explaining the elastic behavior of nanocrystalline forsterite satisfactorily over the temperature range from 300 K to 1573 K with a pressure variation from 0 to 9.6 GPa. The values calculated for the volume compression under varying temperature- pressure conditions are compared with the available experimental data and also with those obtained by using different approaches. It is found that the results obtained in the present study are more close to the experimental data in comparison to those reported earlier. The same model is further extended to study the variation in the bulk modulus and thermal expansion coefficient of Foresterite nano-mineral ver the temperature range from 300 K to 1573 K. The results show the same trend of expansion as observed in single nanocrystals at high temperature.

1. Introduction

The study of the thermo elastic behavior of minerals, ionic solids, metallic solids, alloys etc. under different pressure and temperature conditions is important for understanding the earth's deep interior and its evolution. It also provides vital information about the dynamics of the earth's lower mantle. A variation of the temperature-pressure conditions affects the atomic structure, stability and atomic interactions and thus modifies the physical properties, like the compressibility, electrical conductivity, elasticity, and thermal expansivity [1,2] of the material.

The physical and rheological properties of a material are greatly influenced by its size and shape, which in turns affects the geo-physical processes [3]. Despite of the limitation of the nanocrystalline forms of minerals in the earth's crust and mantle, its importance in geophysics cannot be neglected [4–6]. The effect of grain size on the elastic properties of nanocrystalline metal, alloys, ceramics, and oxides has been studied both experimentally [7,8] and theoretically [9,10] during the past years. Some of the experimental studies [11–13] on nanocrystalline materials have concluded that the elastic moduli of nanocrystalline materials decrease with a decrease in grain size. Though the olivine group of minerals are usually studied in bulk form [14–18], yet the nanostructured minerals in nano-form have been studied less under high pressure and high temperature.

The olivine group of minerals comprises of Foresterite and Fayalite. Foresterite (Mg_2SiO_4), commonly abbreviated as Fo, is the member of the olivine solid solution series rich in magnesium whereas Fayalite (Fe_2SiO_4) is the iron rich member. Fayalite has a high refractive index and is heavier than Foresterite. Foresterite is found to be the most abundant mineral in

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the earth's mantle under the depth of 400 km [19,20]. Foresterite is found mainly in igneous rocks having rich magnesium and iron content and also in meteorites [21–23]. It has exceptionally high toughness and superior mechanical properties. It has been found as a potential material for bone implants and also has wide biomedical applications [24]. So, it is important to study more about the thermo elastic behavior of nanocrystalline Foresterite.

Various potential dependent [25,26] and potential independent [27–30] model theories have been evolved and used to investigate the elastic properties of bulk materials and nanomaterials during the past decades. However, the results reported by these investigators show large variations, as compared to the experimental values. So, it becomes necessary to provide a model theory which could determine the thermo elastic properties of nanomaterials so as to explain the experimental results successfully. The main motive of the present study is to formulate a simple pressure and temperature dependent equation of state for studying the thermo elastic properties of nanocrystalline minerals. The method of formulation of the potential independent equation of state and its application is described in Section 2. The results obtained for Foresterite nanocrystal are discussed in Section 3.

2. Formulations and analysis

Under high pressure, the product of the volume thermal expansion coefficient (α_T) and the bulk modulus (B_T) can be considered as constant at constant tessmperature [31,32], i.e.

$$\alpha_o B_o = \alpha_T B_T \tag{1}$$

Differentiation of Eq. (1) w.r.t. volume V leads to the relation:

$$\alpha\left(\frac{dB}{dV}\right)_T + B\left(\frac{d\alpha}{dV}\right)_T = 0 \tag{2}$$

The Anderson-Gruneisen parameter δ_T at constant temperature T is given by

$$\delta_T = \frac{V}{\alpha}\left(\frac{d\alpha}{dV}\right)_T \tag{3}$$

Using Eqs. (2) and (3), δ_T can be defined as

$$\delta_T = \frac{V}{\alpha}\left(\frac{d\alpha}{dV}\right)_T = -\frac{V}{B}\left(\frac{dB}{dV}\right)_T \tag{4}$$

Considering δ_T to be independent of V, it becomes

$$\delta_T = \left(\frac{dB}{dP}\right)_T = B'_O. \tag{5}$$

The Anderson-Gruneisen parameter δ_T and η are related as follows [33,34]:$(\frac{\delta_T+1}{\eta}) = A$, where

$$\eta = V/V_o \tag{6}$$

where A is a constant.

Using Eq. (6) in Eq. (4), and upon integrating it, we get

$$\frac{B}{B_o} = \frac{V}{V_o}\ \exp\ A\left[1 - \frac{V}{V_o}\right] \tag{7}$$

where B is the bulk modulus and is defined as

$$B = -V\left(\frac{dP}{dV}\right)_T \tag{8}$$

In view of Eq. (8), the expression of the bulk modulus B can be expressed as follows:

$$\frac{B}{B_o}\ \exp\ A\left[1 - \frac{V}{V_o}\right]dV = -dP, \tag{9}$$

where B_o, V_0 are the bulk modulus and volume at zero pressure.

On integrating Eq. (9), the equation for pressure (P) can be written as

$$P = \frac{B_o}{A}\left[\exp\ A\left\{1 - \frac{V}{V_o}\right\} - 1\right], \tag{10}$$

where

$$A = B'_o + 1 \tag{11}$$

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