(IJAER) 2019, Vol. No. 18, Issue No. V, November **e-ISSN: 2231-5152, p-ISSN: 2454-1796**

BULK MODULUS OF $MGSIO_3$ POST-PEROVSKITE

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ABSTRACT

In this paper, $MgSiO_3$ post- perovskite is a regular material, in a single state. The effect of increasing pressure is to produce a linear relation between pressure and Bulk modulus at consents temperature. I have calculated the bulk modulus of $MgSiO_3$ post- perovskite at different pressure and volume at various constant temperatures, using an empirical model and found a better agreement with the experimental and theoretical data as compared to the values evaluated by the earlier researchers.

***Key words**: Bulk modulus, post-perovskites.*

I. INTRODUCTION

The term 'perovskite' is used to denote a category of inorganic crystalline solids with the general formula ABO3, where A and B are cations and O is an anion. A large number of perovskite-type oxides have been studied because of their interesting properties, including superconductivity, insulator–metal transition, ionic conduction characteristics, dielectric properties and ferro-elasticity [1–3]. Additionally, they have received great attention as high temperature proton conductors with the possibility of applications in fuel cells or hydrogen sensors and these solids are currently gaining considerable importance in the field of electrical ceramics, refractories, geophysics, astrophysics, particle accelerators, fission, fusion reactors, heterogeneous catalysis etc [4-7]. MgSiO3 is the most abundant mineral at great depths of Earth. The dynamical properties of MgSiO3 perovskite were studied very extensively [8]. The ab initio study of phonons and structural stabilities of the perovskite and other hypothetical phases of MgSiO3 which follow from soft modes of the cubic perovskite structure (Pmmm) shows that the Pmnb phase has the lowest ground state energy and other phases are unstable at zero-temperature. [9]. As is well known, silicate can transform to different dense phases with increasing temperature and pressure, and this leads us to expect that an undetermined solid phase may exist at the melting boundary, and thus may cast a potential constraint on deeper understanding of the melting of silicates. MgSiO3 perovskite is generally assumed to be abundant and stable phases existing in the lower mantle, but there are significant disagreements among the available experimental measurements on the melting of MgSiO3 perovskite determined by different investigators.

Recently, the authors [10-15] have been evaluated the mechanical and structural properties of perovskite solids. Therefore, we thought it would be of interest to give an alternative explanation for bulk modulus of MgSiO3 perovskite solid at different pressure and volume at various constant temperatures.

THEORY, RESULTS AND DISCUSSION

With increasing temperature, perovskite structures generally transform according to the following series: triclinic or monoclinic-rhombohedral-tetrahedral or orthorhombic-cubic perovskite structure [8]. Based on the recent in situ X-ray measurements, $MgSiO_3$ perovskite can transform to the cubic structure from the orthorhombic structure (P*bnm*) at 82.3 GPa and at temperature above 1180 K [16]. At higher temperatures, even though $MgSiO_3$ may decompose to MgO and SiO_2 phases, it is still very significant for us to employ those data to evaluate the melting at pressures lower than 82 GPa, and then it can allow us to discuss the fate of $MgSiO_3$ perovskite in much deeper lower mantle based on both the geophysical data and phase transformation information. Mg^{2+} occupies the 8-coordinated site (MgO_8) in the perovskite structure and due to the thermal expansion, it can transform to a cubic structure (Figure 1).

First, Anderson and Nafe [17] have proposed an empirical relationship between bulk modulus B at atmospheric pressure and specific volume V_0 of the form $B \sim V_0^{-x}$. They find it to hold for a particular class of compounds. The value of x depends on the class of compound. For alkali halide, fluorides, sulfides and telluride they find x to be 1 and oxide compounds x is close to 4. Recently Y. Al-Douri et al. [18] has studied the bulk modulus of IV, III-V and II-VI semiconductors and proposed an empirical relation for bulk modulus in terms of transition pressure (P_t). According to them bulk modulus of these semiconductors may be expressed as,

$$B = [99 - (\lambda + 79)] (10P_t)^{1/3} \qquad (1)$$

Where P_t is the transition pressure in GPa from ZB to β-Sn and λ is a parameter appropriate for the group-IV (λ = 1), III-V (λ = 5) and II-VI (λ = 8) semiconductors.

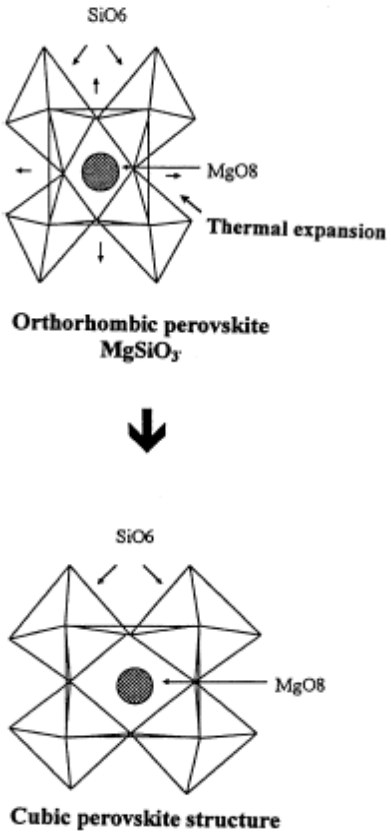

Figure 1. The axis of the ideal cubic structure and orthorhombic perovskite structure. It is clearly shown that the difference between two structures is due to the change of roughly 8-coordinated sites. As a result, $MgSiO_3$ should deviate from the cubic structure, and exists with an orthorhombic structure. In contrast, with increasing temperature, thermal expansion appears.

For getting better agreement with experimental and theoretical data for $MgSiO_3$ post-perovskite, previous concepts [17, 18], may be extend in terms of different pressure and volume at various constant temperatures by the following form,

$$\text{Bulk modulus} = (P/V)^{1/3}\, T' \qquad (2)$$

Where P (GPa) is pressure and V ($Å^3$) is volume. The value of T′ can be obtained by the following relation,

$$T' = 620 + (T/60) \qquad (3)$$

T is temperature in Kelvin.

The bulk modulus is an important mechanical property of a material and defines its resistance to volume change when compressed. Both experimental and theoretical results suggest that the bulk modulus is a critical single material property to indicate hardness. We have plotted B Vs (P/V)T′ curve for $MgSiO_3$ post-perovskite which is presented in the figure 2. We observe that in the plot of bulk modulus and pressure, volume and temperature, fall on a straight line. From the figure it is quite obvious that the bulk modulus trends in this compound decreases with increases volume and increases with increases pressure and fall on straight line according to the

different constant temperature of the compound. The proposed empirical relation (2) has been applied to evaluate bulk modulus values for $MgSiO_3$ post-perovskite. The values so obtained are presented in the table 1.

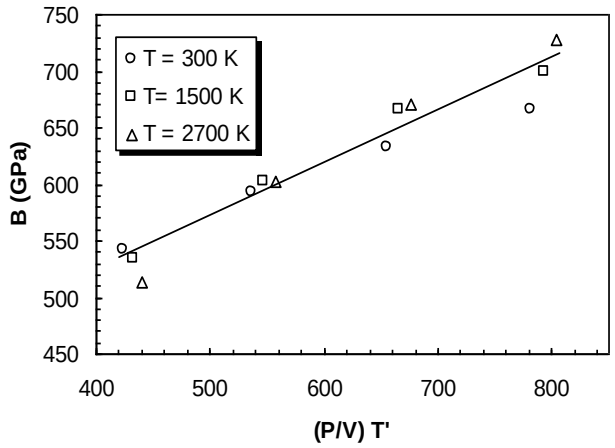

Figure 2. Plot of B (Bulk modulus) (GPa) against (P/V)T′ for $MgSiO_3$ post-perovskite. In this plot all experimental data are taken from reference [9].

Table: 1 In this table we have presented the values of bulk modulus B (GPa) for $MgSiO_3$ at T = 300 K.

Pressure (GPa)	Volume ($Å^3$)	B exp. [9]	B cal.
90	130.8	532.8	536.8
110	126.3	581.5	580.6
130	122.1	620.8	620.7
150	118.0	654.2	658.2

Table: 2 In this table we have presented the values of bulk modulus B (GPa) for $MgSiO_3$ at T = 1500 K.

Pressure (GPa)	Volume ($Å^3$)	B exp. [9]	B cal.
90	132.7	509.5	527.4
110	128.0	565.3	570.6
130	123.7	609.0	610.2
150	119.7	644.5	646.8

Table: 3 In this table we have presented the values of bulk modulus B (GPa) for $MgSiO_3$ at T = 2700 K.

Pressure (GPa)	Volume ($Å^3$)	B exp. [9]	B cal.
90	134.9	482.9	517.2
110	129.9	558.4	560.0
130	125.5	595.8	599.1
150	121.4	634.1	635.2

We note that the evaluated values of bulk modulus by our proposed relation are in close agreement with the experimental data as compared to the values reported by previous researchers so far.

CONCLUSIONS

From the above results and discussion obtained by using the proposed empirical relation, it is quite obvious that the parameter such as bulk modulus reflecting the mechanical property can be expressed in terms of pressure, volume and temperature of the material. Indeed, $MgSiO_3$ perovskite is only of orthorhombic structure (P*bnm*) at ambient temperature or lower temperature [19-23], and with increasing temperature, it transforms to a cubic structure [16], so it is possible that $MgSiO_3$ post-perovskite may have a cubic structure. For increasing pressure produces deviations from this simple behavior, due to a much larger reduction of the bulk modulus. This is definitely a surprising phenomenon and need further investigations of the reason. The values evaluated show a systematic trend and are consistent with the available data reported so far, which proves the validity of the approach. The calculated values are presented in table 1. It is also to be noteworthy that proposed empirical relations are simpler and widely applicable. The method presented in this work will be helpful to the material scientists for finding new materials with desired bulk modulus among series of structurally similar perovskite materials.

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