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Research paper

Bulk modulus of CaO under high pressure up to 65 GPa

Salah Daoud [1]*, Hamza Rekab-Djabri [2, 3]

[1]Laboratory of Materials and Electronic Systems (LMSE), Faculty of Sciences and Technology, Bordj Bou Arreridj University, 34000 Bordj Bou Arreridj, Algeria
[2]Laboratory of Micro and Nanophysics (LaMiN), Oran ENP, BP 1523, El M'Naouer, 31000, Oran, Algeria
[3]Faculty of Nature and Life Sciences and Earth Sciences, Akli Mohand-Oulhadj University, 10000, Bouira, Algeria
**Corresponding author E-mail:salah_daoud07@yahoo.fr*

Abstract

In the present study we used some equilibrium experimental data reported by Mammon et al. (Geophysical Research Letters, Vol. 8, No. 2, pp. 140-142) to investigate the effect of high pressure up to 65 GPa on the bulk modulus of calcium oxide (CaO) material. We used the Vinet's equation of state (EOS) model. The fit of the bulk modulus as a function of pressure p obeys the 2nd order polynomial expression: $B = 115.37 + 3.84\ p - 7.25 \times 10^{-3}\ p^2$ (where both B and p are expressed in GPa). Our results are analyzed and compared with other theoretical data of the literature. Similar behavior for the bulk modulus versus pressure was observed for some other materials with different crystallographic structures from the literature, which commonly increases with increasing pressure.
We estimate also the Debye temperature θ_D of our material of interest using the experiential lattice parameter and elastic constants measured at normal conditions by Speziale et al. (Journal of Geophysical Research, Vol. 111, (2006), pp. B02203 (12 pages)). Our obtained value (670.1 K) is in good agreement with other data of the literature.

Keywords:*Calcium Oxide; High Pressure; Vinet's Equation of State (EOS); Bulk Modulus; Debye temperature.*

1. Introduction

Metal oxides are a class of materials, which are commonly used for the microelectronic and catalysis applications [1]. In several last years, particular attention was focused on ZnO semiconducting material due to its potential use in ultraviolet light-emitting diodes and laser diodes [1]. Calcium oxide (CaO) compound is one of the most basic materials for industrial; it is used as a base material for applications ranging from photographic and electroluminescent thin films to magneto-optical devices [2]. CaO is also considered as a prototype oxide from the theoretical point of view having a wide bandgap (7.1 eV) and a high dielectric constant (11.8) [1].
Using the radial X-ray diffraction technique, Speziale et al. [3] have investigated the high pressure effect up to 65.2 GPa on the elastic constants C_{ij} and anisotropy factor of CaO compound. They found that both the elastic constants C_{11} and C_{12} increase with increasing pressure, while C_{44} decreases with increasing pressure. Using full-potential linearized augmented plane-wave (FP-LAPW) approach within the density functional theory (DFT), Nguyen et al. [4] have studied the structural, electronic, magnetic, and optical properties of CaO, CaO_2 and CaO_3 binary materials. They mentioned that CaO is a paramagnetic material, showing the insulator nature with a band gap of 6.25 eV, while CaO_2 and CaO_3 materials have total magnetic moments of 2 and 4 μ_B, respectively.
Using different theoretical, semi-empirical and empirical approaches, several works [5-19] have successfully studied different physical properties of many materials with different crystallographic structures. Okba and Mezouar [20] have investigated some physical parameters of calcium chalcogenides at high pressures using semi-empirical approach, while Tsuchiya and Kawamura [21] have studied the elastic properties and their pressure dependence of four alkaline earth oxides (MgO, CaO, SrO, and BaO) binary compounds using the ab initio full-potential linear muffin-tin-orbital (FP-LMTO) method.
In the present work, we try to investigate the effect of high pressure up to 65 GPa on the bulk modulus of calcium oxide (CaO) material using only the equilibrium experimental data reported by Mammon et al [22]. Additionally, using the experiential lattice parameter and elastic constants measured by Speziale et al [3], we have calculated the Debye temperature θ_D of our material of interest. Our obtained results are analyzed and compared with other theoretical data of the literature.

2. Theory, results and discussion

In object to investigate the effect of high pressure on the bulk modulus of CaO material, we used the Vinet's equation of state (EOS) model. For more details on the relationships between pressure p, relative volume (V/V_0), equilibrium bulk modulus B and the first-order pressure derivative of the bulk modulus B'_0, please see Ref [20]. Using the experimental parameters ($V_0 = 27.83$ Å^3, $B_0 = 114.7$ GPa, and $B'_0 = 4.1$) reported by Mammon et al. [22], the obtained values of the bulk modulus B versus pressure p for CaO compound are reported in table 1 and traced in Fig. 1, along the results of Deng et al [23].

Table 1: Bulk Modulus B Versus Pressure p Up to 65 GPa for CaO Compound in Cubic Rock-Salt Structure (B1)

p (GPa)	0	10	20	30	40	50	60	65
B (GPa)	114.70	153.66	189.76	223.93	256.73	288.43	319.27	334.41

One can observe that the bulk modulus B of CaO increases with increasing pressure up to 65 GPa. Similar behavior for the bulk modulus versus pressure was observed for the two approaches. Similar behavior for the bulk modulus under pressure was observed for calcium-based chalcogenides CaX (X = S, Se, Te) [20], cubic zincblende (B3) aluminum phosphide (AlP) semiconducting compound [24], and cubic zincblende thallium - phosphide (TlP) material [25]. The fit of our data on the bulk modulus as a function of pressure p (where both B and p are expressed in GPa) obeys the 2nd order polynomial expression: $B = 115.37 + 3.84\ p - 7.25 \times 10^{-3}\ p^2$. As the pressure varied from 0 to 65 GPa, the bulk modulus of CaO changed from 114.7 to 334.41 GPa.

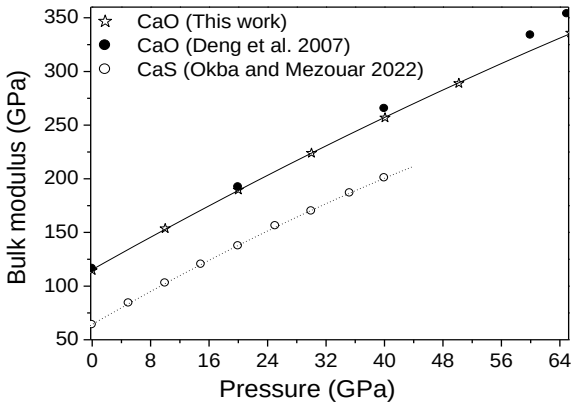

Fig. 1: Variation of the Bulk Modulus Ba Function of Pressure for Cubic Rock-Salt (B1) CaO Compound, Along Data of Deng et al. [23].

The Debye temperature θ_D is an important thermodynamical quantity describing various physical properties of solids that are related to lattice vibrations [6, 8, 26]. Debye temperature θ_D represents highest mode of vibration of the crystal, during phonon vibrations [27], it is usually calculated from the elastic constants C_{ij} [28-32]. To estimate the Debye temperature θ_D of cubic rock-salt CaO compound, we use the experiential structural parameters and elastic constants measured at normal conditions [3]. The values of the lattice parameter and the elastic constants C_{ij} used here are: a = 4.8115 Å, C_{11} = 219.4 GPa, C_{12} = 58.1 GPa, and C_{44} = 80 GPa, respectively [3]. For materials with cubic zincblende (B3) and cubic rock-salt (B1) structures, the Debye temperature θ_D can be obtained from the following simplified formula: $\theta_D \approx 595.467\ (v_m/a)$ [31], where v_m is the average sound velocity (given in km/s) and a is the lattice parameter (expressed in Å).
For aggregate polycrystalline solids, the mean value of the acoustic wave speed v_m is given as follows [28-31]:

$$v_m = \left[\frac{1}{3}\left(\frac{2}{v_t^3} + \frac{1}{v_l^3}\right)\right]^{-1/3} \quad (1)$$

Where $v_l$is the longitudinal wave velocity and v_t is the transverse elastic wave velocity, respectively. In general both the longitudinal v_l wave speed increases with increasing pressure [31]. They can be calculated from the elastic moduli as follows; $v_l = \left((3B + 4G)/3\rho\right)^{1/2}$ and $v_t = (G/\rho)^{1/2}$ [23], [29], where ρ is the mass density, B is the bulk modulus, and G is the shear modulus. The values of B and G for CaO compound are found to be 111.87 GPa (112 GPa [3]) and 80.26 GPa (80.05 GPa [3]), respectively. For more details on the relationships between the elastic constants C_{ij}, the bulk modulus B and the shear modulus G of the aggregate materials, please see for example the Refs [33, 34]. The mass density ρ can be calculated as follows: $\rho = ZM/N_AV$ [35-37], where Z is the number of molecules per unit cell (in a conventional unit cell of cubic rock-salt lattice, there are four molecules [38]), N_A is the Avogadro number, M is the molecular weight, and V is the unit cell volume. Our values of ρ, v_l, v_t, $v_m$and θ_D for cubic rock-salt CaO compound are found to be 3.344 g/cm^3, 8090.4 m/s, 4899.1 m/s, 5414.7 m/s, and 670.1 K, respectively. Our obtained value of the Debye temperature θ_D for CaO lies between the two theoretical values (654.66 K and 687.63 K) reported by Deng et al [23].

3. Conclusion

Using the equilibrium experimental parameters reported by Mammon et al., in the present work we investigate the effect of the high pressure up to 65 GPa on the bulk modulus for cubic rock-salt CaO compound. We found that the bulk modulus B and the pressure p are related by the following quadratic expression: $B = 115.37 + 3.84\ p - 7.25 \times 10^{-3}\ p^2$. Our results are analyzed and compared with other theoretical data of the literature. Similar behavior for the bulk modulus under pressure was observed for some other materials of the literature. The Debye temperature θ_D of our material of interest was also estimated at normal conditions using the lattice parameter and the elastic constants measured by Speziale et al. Our obtained value (670.1 K) of θ_D for CaO agrees well with other data of the literature.

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