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Research paper

Debye temperature of CaO under high pressure up to 65.2 GPa

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Abstract

In the present work we used the experimental relative volume unit cell and the elastic stiffness constants measured by Speziale et al. (Journal of Geophysical Research, Vol. 111, (2006), pp. B02203 (12 pages)) using the Radial X-Ray Diffraction at high pressure from 5.6 up to 65.2 GPa to investigate the effect of high pressure on the bulk modulus, aggregate shear modulus, elastic wave velocities and Debye temperature of calcium oxide (CaO) ceramic material in cubic rock-salt (B1) phase. Our obtained values show that the bulk modulus increases monotonously with increasing pressure, while the aggregate shear modulus, the mean elastic wave velocity and the Debye temperature of CaO material varied non-linearly and non-monotonously with increasing pressure from 5.6 up to 65.2 GPa.

Keywords: *Calcium Oxide; Elastic Constants; High Pressure; Elastic Wave Speed; Debye Temperature.*

1. Introduction

IIA-VIA materials have been well known as classical thermionic and phosphors materials [1], they show suitability for different technological applications [1]. Using an ab initio plane-wave pseudopotential density functional theory method, Deng et al. [2] have investigated the structural B1–B2 phase transition and the elastic properties of the B1 phase of calcium oxide (CaO) material. They have also investigated the pressure dependence of the elastic properties and the Debye temperature of B1 phase up to 178 GPa.
Using full potential linear augmented plane wave (FP- LAPW) method, Labidi et al. [3] have investigated the structural, electronic, and optical properties of CaO, MgO and SrO binary compounds. They found that the band gaps of SrO and CaO compounds decrease quasi-linearly with increasing pressure, while that of MgO increases with increasing pressure.
Batra et al. [4] have performed a comparative investigation of the structures, stabilities, and properties of some alkaline earth metal oxides ((MgO), $(CaO)_n$, $(SrO)_n$, and $(BaO)_n$) nanoclusters using density functional theory, while Daoud and Rekab-Djabri [5] have investigated the pressure dependence of the bulk modulus of CaO material up to 65 GPa using semi-empirical approach.
Using both the powder X-ray diffraction (XRD) and the Brillouin spectroscopy (Single-crystal Brillouin scattering) techniques, Speziale et al. [6] have investigated the high pressure effect up to 65.2 GPa on the several mechanical properties of CaO material. They found a good general agreement between the results of the two methods. They found also that both the elastic constants C_{11} and C_{12} increase with rising pressure, while both the elastic constant C_{44} and the Zener anisotropy factor A decrease with increasing pressure.
Daoud [7] has studied the sound velocities and Debye temperature of BeSe material under high pressure up to 50 GPa, while several other works [8-26] have focalized on the investigation of structural, mechanical, thermal, electronic and optical properties of I-VII, II-VI, III-V and some other materials using different approaches.
The intent of this paper is to present and investigate the effect of high pressure up to 65.2 GPa on the bulk modulus, aggregate shear modulus, elastic wave velocities, and Debye temperature of CaO material using only the experimental data reported by Speziale et al. [6]. Our obtained results are analyzed and compared with other theoretical data [2, 5] of the literature.

2. Theory, results, and discussion

In object to study the effect of high pressure up to 65.2 GPa on the bulk modulus, elastic wave velocities and Debye temperature of CaO ionic material, we used the experimental relative volume unit cell and elastic constants reported by Speziale et al. [6]. Elastic constants of materials are essential physical quantities to describe their mechanical properties. Furthermore, these physical quantities can inform us about the structural stability of materials [27]. In cubic crystals, the bulk modulus B is related to the elastic constants C_{11} and C_{12} as follows: $B = (C_{11} + 2C_{12})/3$ [28]. For polycrystalline materials, the aggregate shear modulus G in Voigt-Reuss-Hill (VRH) approach is expressed as follows: $G = (G_V + G_R)/2$ [28], where G_V is the Voigt shear modulus and G_R is the Reuss shear modulus, which are expressed,

respectively as follows: $G_V = (C_{11} - C_{12} + C_{44})/5$, and $(5/G_R) = (4/(C_{11} - C_{12}))+ (3/C_{44})$ [28]. Our obtained values of the bulk modulus B and the shear moduli G_V, G_R, and G of CaO material are tabulated in Table 1, along the results reported in Ref. [5] found at equilibrium.

Table 1: Bulk Modulus and Shear Moduli Versus Pressure P Up to 65.2 GPa for Cao Compound in Cubic Rock-Salt Phase, * from Ref [5]

p (GPa)	0	5.6	14.3	22.1	36.6	49.7	57.8	65.2
B (GPa)	111.87 *	136.67	178.00	212.67	274.33	325.00	375.00	401.33
G_V (GPa)	80.26*	88.60	106.80	113.20	126.80	120.60	123.60	123.20
G_R (GPa)	80.26*	87.66	94.44	96.66	93.60	85.17	77.73	70.45
G (GPa)	80.26*	88.13	100.62	104.93	110.20	102.89	100.66	96.82

Our obtained values of the bulk modulus B are also traced in figure 1, along other data of the literature [2, 5]. We observe that the bulk modulus B of CaO compound increases with increasing pressure up to 65.2 GPa. The results are consistent with the values reported for CdSe, $Cd_{0.75}Cr_{0.25}Se$, ZnS, and $Zn_{0.75}Cr_{0.25}S$ materials [29]. Compared with the bulk modulus B at equilibrium, our obtained data of B using the experimental elastic constants measured by Speziale et al. [6] are somewhat larger than both the ab initio plane-wave pseudopotential DFT method [2] and semi-empirical approach [5] at high pressure.

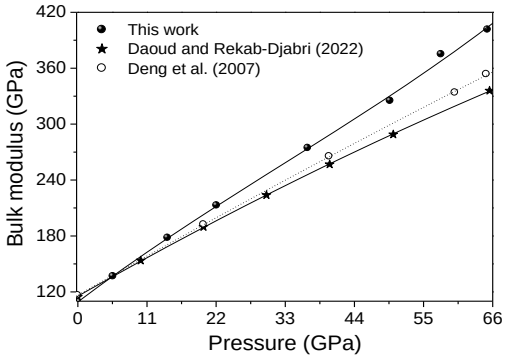

Fig. 1: Bulk Modulus B Versus Pressure for Cubic Rock-Salt CaO Compound, Along Data of Deng et al [2], and Daoud et al [5].

The knowledge of the sound velocity can play in important role in material science [30]. For polycrystalline materials, the mean value of the acoustic wave speed v_m is related to the longitudinal v_l and transverse v_t elastic wave velocities as follow: $v_m = ((1/3)(2v_t^{-3}+ v_l^{-3}))^{-1/3}$ [31-33]. The longitudinal wave speed v_l as well as the transverse wave speed v_t can be calculated from the elastic moduli (B, G) and the mass density ρ using these expressions: $v_l = ((3B+ 4G)/3\rho)^{1/2}$, and $v_t = (G/\rho)^{1/2}$[5], [31-33]. Our calculated data of v_l, v_t and v_m for CaO material are tabulated in Table 2, along the results reported in Ref. [5] determined at atmospheric pressure and room temperature.

Table 2: Longitudinal, Transverse and Mean Acoustic Wave Speeds Versus Pressure P Up to 65.2 GPa for Cao in Phase (B1), * from Ref [5]

p (GPa)	0	5.6	14.3	22.1	36.6	49.7	57.8	65.2
v_l (km/s)	8.090*	8.482	9.196	9.552	10.123	10.376	10.728	10.790
v_t (km/s)	4.899*	4.995	5.221	5.211	5.177	4.895	4.770	4.610
v_m (km/s)	5.415 *	5.535	5.804	5.812	5.800	5.509	5.382	5.210

The effect of high pressure up to 65.2 GPa on the longitudinal, transverse and mean acoustic wave speeds of CaO material is traced in figure 2. As shown in figure 2, both the transverse and mean acoustic wave speeds of CaO change non-linearly and non-monotonously with increasing pressure up to 65.2 GPa. Similar behavior for the acoustic wave speeds against pressure for cubic zinc-blende boron arsenide (BAs) semiconducting compound [34] was also observed. The second order polynomial fits of the acoustic wave speeds against pressure p for CaO are expressed as follows: $v_l = 8.19 + 0.70\ p - 4.69 \times 10^{-4} p^2$, $v_t = 4.94 + 0.02\ p - 4.04 \times 10^{-4} p^2$, and $v_m = 5.47 + 0.03\ p - 4.59 \times 10^{-4} p^2$, where v_l, v_t, and v_m are expressed in km/s, while p is expressed in GPa.

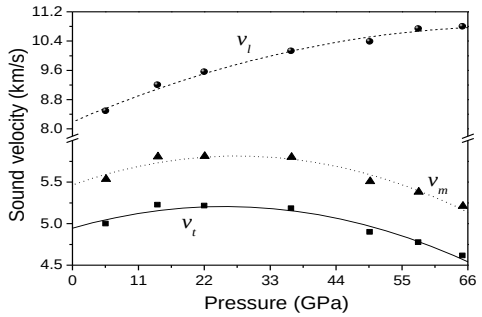

Fig. 2: Variation of the Elastic Wave Velocities as A Function of Pressure for Cubic Rock-Salt (B1) CaO Compound Up to 65.2 GPa.

The Debye temperature of material is an essential parameter in solid state physic [35-37], it is related to many other physical properties, such as the specific heat, the elastic constants, the melting temperature, thermal expansion and thermal conductivity [38-44]. It gives the knowledge about structural stability, density of solid, and strength of bonds between its constituent's atoms [45]. There are different expressions usually used to calculate the Debye temperature θ_D of crystal from the mean acoustic wave speed v_m [43-46], one of those formulas is expressed as follow [46]: $\theta_D = (\hbar/k_B)\left[(6\pi^2 n N_A \rho/M)\right]^{1/3} v_m$, where $\hbar = h/2\pi$, h is Planck's constant, n is the number of atoms of a molecule, N_A is the Avogadro's number, ρ is the mass density, k_B is Boltzmann's constant, and M is the molecular weight.
Our obtained values of the Debye temperature θ_D for CaO are tabulated in table 3, along the data determined at atmospheric pressure [5].

Table 3: Debye temperature θ_D Versus Pressure P Up to 65.2 GPa for CaO Compound in Cubic Rock-Salt Structure (B1), * from Ref [5]

p (GPa)	0	5.6	14.3	22.1	36.6	49.7	57.8	65.2
θ_D (K)	670.1*	697.7	742.4	754.8	769.0	741.0	731.3	714.8

Our obtained values of θ_D for CaO material are also traced in figure 3, along the data reported in Ref. [2].Similarly to the mean acoustic wave speed v_m, the Debye temperature θ_D of CaO material changes non-monotonously with increasing pressure from 5.6 up to 65.2 GPa.

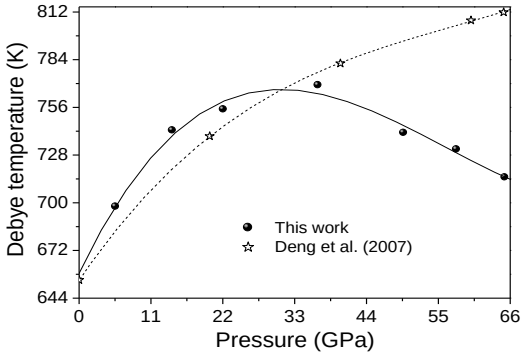

Fig. 3: Variation of the Debye Temperature θ_D As A Function of Pressure for Cubic Rock-Salt CaO Compound, Along Data of Deng et al. [2].

Similar behavior of θ_D against pressure for boron phosphide (BP) semiconducting material [47] was also observed. This behavior differs from that reported for CaO compound [2] (Figure 3), for cubic Cu_3N material [48, 49], and for cubic zinc-blende BN material [50] which indicates that the Debye temperature θ_D changes monotonously with increasing pressure.

3. Conclusion

Using the experimental relative volume unit cell and the elastic constants measured by Speziale et al. at high pressure from 5.6 up to 65.2 GPa, we have investigated the effect of high pressure on the bulk modulus, aggregate shear modulus, elastic wave velocities and Debye temperature of calcium oxide (CaO) ionic material. Our obtained data show that the bulk modulus increases monotonously with increasing pressure, while the quasi-isotropic shear modulus, the mean elastic wave velocity and the Debye temperature of CaO ceramic material change non-monotonously with increasing pressure from 5.6 up to 65.2 GPa. It should, however, be noted that at high pressure, the deviations between the different curves of the bulk modulus become more largely than those observed at low pressure.

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