THEORETICAL PREDICTION OF GRUNEISEN PARAMETER & DEBYE TEMPERATURE FOR $BiFeO_3$

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ABSTRACT

In the present work have calculated Gruniesen parameter (γ) at different up to the compression range 0.92 using B-M and Stacey EOS for Bismuth ferrite (BiFeO3) and Debye temperature (θ_D) up to the pressure of 11 GPa. Result obtained by Birch-Murnghan EOS shows that γ vs V/V_0 is straight line and having slight variation with compression than the computed results obtained from Stacey EOS, which strongly supports the validity of Birch-Murnghan EOS for calculating Gruneisen parameter for Bismuth ferrite up to the compression range of the order of 0.92. The effective values of Debye temperature (θ_D) obtained from B-M EOS strongly suggest its validity for Bismuth ferrite.

Keywords: Gruniesen parameter, Bismuth ferrite, Debye temperature Equation of state.

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I INTRODUCTION

Room temperature multiferroic BiFeO3 is one of the most intensively studied materials of the moment. Among multiferroics Bismuth ferrite BiFeO3 (BFO) commonly considered as a model system and is perhaps the only material that is both magnetic and ferroelectric with a strong electric polarization at ambient conditions. Bismuth Ferrite BiFeO3 is commonly considered to be a model system [1,2] for multiferroic especially for ABO_3 perovskites where the ferroelectricity is driven by an A cation with $6s^2$ lone pair electrons. The perovskites BFO is one of the very few robust multiferroics with ferroelectric and antiferromagnetic order well above room temperature. The effect of high pressure and perovskite is more complex. In this paper the equation of state has been extended to calculate the theoretical values of both Gruniesen parameter and Debye temperature using isothermal EOS. We present the analysis for the variation of Gruniesen parameter with compression and variation of Debye temperature with pressure. The Debye characteristic temperature is one of the important characteristics of substance, which reflects its structure stability, the strength of bonds between its separate elements, structure defects availability and

its density. The Debye temperature θ_D has slightly different meanings and different numerical values, depending on the type of data from which it has been computed, and depending on how the computations have been made. In the present work we have evaluated the Debye temperature at different pressure for $BiFeO_3$.

The Gruneisen parameter (γ) has considerable appeal to geophysists because it is an approximately constant, dimensionless parameter that varies slowly as a function of pressure [3]. Unfortunately, the experimental determination of Gruneisen parameter (γ) is extremely difficult [3]. As the result of difficulty associated with obtaining an accurate value for Gruneisen parameter (γ) experimentally, many scientists related Gruneisen parameter (γ) at atmospheric pressure (P=0) to the first derivative of the bulk modulus with respect to pressure K_T' via $\gamma = (1/2)K_T'-X$, where X is constant . These relations may be expanded to take into account the variation of Gruneisen parameter (γ) with pressure. In these more general cases Gruneisen parameter γ is a function of the equation of state. Despite the intrinsic relationship between Gruneisen parameter and equation of state, it is frequently the case that the choice of the functional form of both the Gruneisen parameter and the equation of state to which it should be related are made independently of each other, and somewhat arbitrarily, this has resulted in a literature in which there is a wide range of value of Gruneisen parameter for many geologically relevant materials.

II THEORY

The Grüneisen parameter (γ) is of considerable importance to Earth scientists because it sets limitations on the thermoelastic properties of the lower mantle and core. Borton and Stacey [4,5], find correlation for Gruneisen parameter (γ) leading to-

$$\gamma = \frac{\frac{1}{2}K_T' - \frac{1}{6} - \frac{f}{3}\left(1 - \frac{P}{3K_T}\right)}{\left(1 - \frac{4}{3}\frac{P}{K_T}\right)}$$

Where, f =2.35 a constant, K_T is isothermal bulk modulus and K_T' is the first pressure derivative of isothermal bulk modulus.The Debye temperature is closely related to many physical properties of solids, such as elastic constants, specific heat and melting temperature. One of the method to calculate the Debye temperature is from elastic constant data. The Debye temperature may be estimated from the average sound velocity Vm [6] ;

$$\theta_D = \frac{\hbar}{K}\left[\frac{3n}{4\pi}\left(\frac{N_A\rho}{M}\right)\right]^{\frac{1}{3}} v_m$$

Where, symbols have their usual meaning viz. h is Plank's constants, N_A is Avogadro's number, n is no. of atoms per formula unit, M is the molecular mass per formula unit, ρ is the density & Vm is given as;

$$V_m = \left[\frac{1}{3} \left(\frac{2}{V_S^3} + \frac{1}{V_P^3} \right) \right]^{-\frac{1}{3}}$$

Where Vp and Vs are the compressional velocity & shear wave velocity respectively which are obtained from Navier's equation[7] as follows;

$$V_P = \sqrt{\left(K + \frac{4}{3} G \right)} \frac{1}{\rho} \qquad \text{and} \qquad V_s = \sqrt{\frac{G}{\rho}}$$

K is the Bulk modulus & The isotropic shear modulus (G) within the voigt limit[6,8] is as follows;

$$G = \frac{3}{5}(K - 2P)$$

In terms of Bulk and Shear Modulus, the Young's modulus [8] can be written as

$$Y = \frac{9KG}{3K + G}$$

III RESULT AND DISCUSSION

In the present work we have made an attempt for the theoretical prediction of Gruneisen Parameter γ and Debye temperature θ_D by using above expressions and input data at different compressions [V/V_0 = 1 to 0.915]. The input values are taken from reference [9]. The graph plotted between γ Vs. V/V_0 and P vs θ_D are shown in Fig.1 and Fig. 2 respectively. It is clear from graph Fig.1 that the value of γ as calculated by using equation (1) with reference to input data corresponding to two different EOS (Birch-Murnghan & Stacey EOS), gives close agreement with each other. The graph plotted between γ and V/V0 for BiFeO3 is straight line. For better approximation Fang and Rong [10] and also A. K. Pandey et.al. [5] has suggested that γ vs V/V_0 curve must be straight line and having slight variation with compression values which strongly supports the Birch-Murnghan EOS for calculating Gruneisen parameter both at high as well as low pressure ranges.

Fig.2 shows the predicted pressure dependence of agreegate Debye temperature. At zero pressure we have calculated θ_D= 51.12K. From Fig. 2 it is also clear that the Debye temperature θ_D monotonically increases with the increasing pressure. As the pressure increases all elastic wave velocities gradually increases. Due to increase in the elastic wave velocities v_m increases which directly affect the Debye temperature effective change in the Debye temperature is observed in the computed results obtained by B-M EOS. Thus the validity of B-M EOS is justified in case of

Bismuth ferrite. At low temperatures the vibrational excitations arise solely from acoustic vibrations and thus θ_D determines phonon frequency and specific heat.

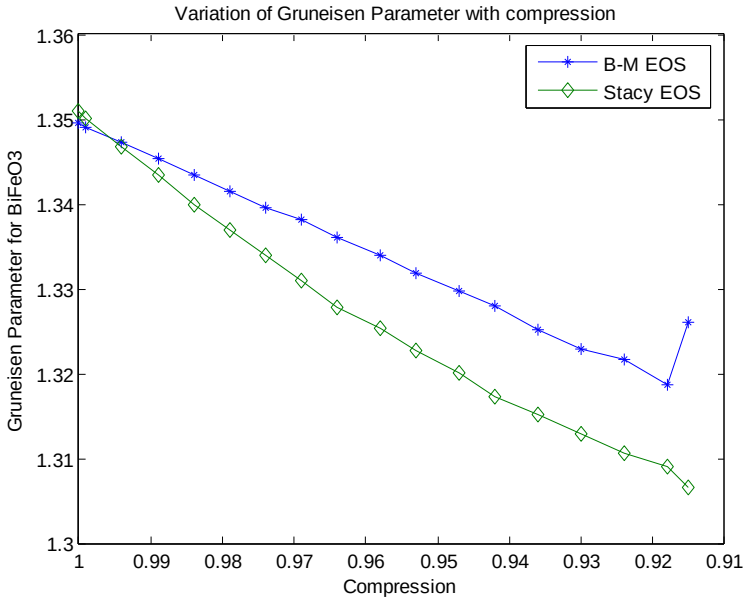

Figure-1: Variation of Gruneisen Parameter with compression for $BiFeO_3$

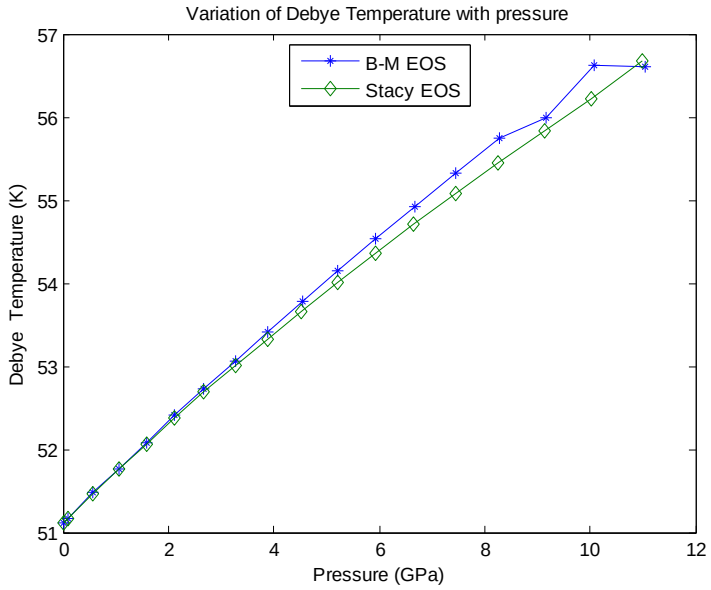

Figure-2: Variation of Debye Temperature Θ_D (K) with Pressure for $BiFeO_3$

Table-1-Calculated values of Gruneisen Parameter and Debye Temperature

V/V0	P(B-M)	P(Stcy)	γ (B-M)	γ (Stcy)	θD(B-M)	θD(Stcy)
1	0	0	1.350	1.351	51.117	51.117
0.999	0.098	0.098	1.349	1.350	51.174	51.175
0.994	0.569	0.569	1.347	1.347	51.479	51.461
0.989	1.062	1.062	1.345	1.343	51.768	51.766
0.984	1.577	1.577	1.344	1.340	52.079	52.059
0.979	2.116	2.116	1.342	1.337	52.409	52.371
0.974	2.679	2.679	1.340	1.334	52.727	52.687
0.969	3.269	3.268	1.338	1.331	53.065	53.007
0.964	3.887	3.885	1.336	1.328	53.410	53.332
0.958	4.535	4.531	1.334	1.325	53.773	53.657
0.953	5.214	5.208	1.331	1.323	54.142	54.006
0.947	5.927	5.918	1.330	1.320	54.535	54.360
0.942	6.675	6.663	1.328	1.317	54.913	54.717
0.936	7.46	7.444	1.325	1.315	55.333	55.079
0.93	8.287	8.265	1.323	1.313	55.739	55.445
0.924	9.158	9.127	1.322	1.311	56	55.835
0.918	10.07	10.034	1.319	1.309	56.620	56.228
0.915	11.034	10.988	1.326	1.307	56.598	56.675

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