Study the Phonon Properties of Multiferroic Materials by using the DAF Model

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Abstract

Multiferroic materials have special property of conversion of magnetic and electric fields so thatits magneto-electric polarization is changed. When external electric field applied on multiferroic material net magnetization is also changed. In the present investigation Di-Launay Angular Force (DAF) model has been used to study the $BiFeO_3$ multiferroic materials and its phonons properties to check the softening of phonons are present in their crystal symmetry directions and it is supposed to be connected to phase changes in the selected material.

1. Introduction

In a unique characteristic of solid-state compounds known as multiferroic materials, at least two order states, such as magnetic, electric, or piezo-elastic phases coexist. These materials are crucial for technological applications because the coupling between the ferro-phases and the piezo-elastic properties allows for direct control of the ferromagnetic and ferroelectric properties via externally applied mechanical stress. Ferromagnets, for example, are well known for displaying strong piezo-magnetic properties. Piezoferroelectrics are arguably a special class of magneto-elastic or electro-elastic coupled multiferroics. There are also opposite effects, whereby magnetic and electric fields that are provided externally can change the form of the material by causing a mechanical strain. In the figure 1 provides a visual representation of Optical Properties of Multiferroic $BiFeO_3$ and also represent the complicated interaction between electric polarisation, electric field, and strain; magnetization, magnetic field, and strain; and stress, strain, electric polarisation, and magnetization.In the table 1 shown the Position Coordinates and Wyckoff position of $BiFeO_3$ in Cubic Phase, while fascinating piezo-electric and piezo-

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magnetic couplings result from the coexistence of ferro-order and piezo-elastic features, there are two more multiferroic potential states that exhibit cross couplings between the order states. These more multiferroic kinds are listed below. There are two types of multiferroics: one is magneto-electric, in which the electric and magnetic order states coexist, and the other is elasto-magnetoelectric, in which all three order states are present. Any sort of ferroic ordering, such as ferromagnetic, anti-ferromagnetic, ferri-magnetic, paramagnetic, and super-paramagnetic, as well as their electrical counterparts, should be included. But rather than having numerous order states, multiferroic materials are exciting from a scientific and practical standpoint because of the cross coupling phenomena that can happen between the order levels. The conversion of energy held in magnetic and electric fields is made easier by the magneto-electric effect. Therefore, magneto-electric multiferroic materials have the special property that, when an applied external magnetic field is present, the electric polarisation is changed, and, conversely, when an applied external electric field is present, the multiferroic solid's net magnetization is changed. Multiferroics can therefore be electrically or magnetically [1-induced] to produce the magneto-electric effect, which is mathematically represented by the magneto-electric coupling coefficient. The change in the sample's magnetization (M) brought on by the introduction of an electric field (E) is known as the electrically induced magneto-electric effect.
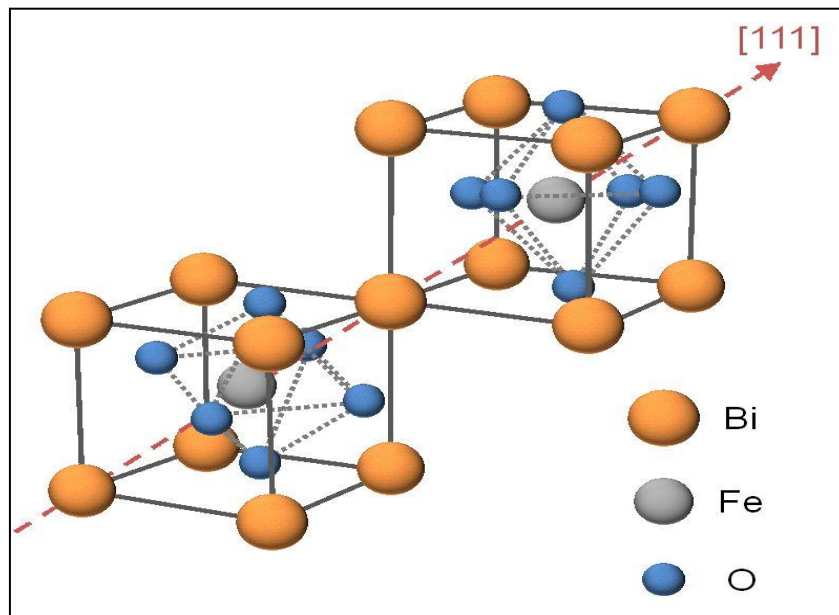
Fig 1:- Optical Properties of Multiferroic BiFeO$_3$

2. Methodology

In the present investigation Di-Launcy Angular Force (DAF) constant model, has been used to study the phonons in the to check whether softening of phonons are there or not in some crystal symmetry directions as it is supposed to be connected to phase changes in these compounds. In DAF model, the relative of the reference atom and one of the neighbours is considered. The magnitude of this component is $\hat{r}_i \times (\overrightarrow{S_o} - \overrightarrow{S_i})$, therefore the restoring De-Launey Angular Force is

$$F_{ai} = -a'[\hat{r}_i \times (\overrightarrow{S_o} - \overrightarrow{S_i})] \times \hat{r}_i$$

Where a' be the force constant associated with this type of force called angular force consant. The restoring force on the reference atom is taken to be proportional to the component of the relative displacement perpendicular to the line joining the two atoms at their equilibrium

positions. The forces due to all neighbours arc calculated separately and summed up together. In the different constants are used for the various categories and the net force on the reference atom obtained by summing over the contribution from all the neighours.

3. Results for phonon dispersion

The present calculation involves four central force constants α_1, α_2, α_3, α_4 and four angular force constants α_1', α_2', α_3' and α_4' between Fe-O, Bi-O, Bi-Fe and O-O atoms respectively up to third nearest neighbour. By using de lanuey angular force model a dynamical matrix of the order of 15×15 is obtained. This calculated dynamical matrix of (15x15) is reduced to three matrices of the order (5x5) at Zone Centre (ZC). Calculation of the cubic phase of BiFeO3 using a non-empirical model of an ionic crystal with dipole inclusion. In the present

calculation the inter-atomic force constants are obtained by fitting the calculated results is obtained by disregarding the long-range dipole interaction at the ZC mode of infrared active phonon frequencies. The force constants is calculated and taking as input parameters, the dynamical matrix is solved at the ZC as well as along three symmetric directions (k00), (kk0) and (kkk). The ZC phonons are obtained, phonon dispersion curves thus obtained in three symmetric directions for $BiFeO_3$. The phonon density of state has been calculated by using sampling method, firstly solves the dynamical matrix and derived cubic structure, for large number of uniformly distributed points of different values of wave vectors, to generate a large number of frequencies. To complete phonon density of state, the first brillouin zone is divided into 1000 points and secular determinant is solved. For accurate measurement of phonon density of state or frequency distribution, appropriate weights have been assigning to the frequencies corresponding to the points. The specific heat of a substance is defined as amount of heat required to raise the temperature of a unit mass of substance by a unit degree of temperature. Using Einstein's quantum theory of specific heat, calculate the value of specific heat equal to $\frac{hv}{kT}$. According to Einstein, the average energy of an oscillator vibrating with frequency v is given by $\frac{hv}{(e^x-1)}$

In this regards the energy of gram atom of the solid consisting of N atoms is

$$3N \frac{hv}{e^x - 1}$$

By using equation $Cv(v) \frac{dU}{dT} = 3R \frac{x^2 e^x}{e^x - 1}$

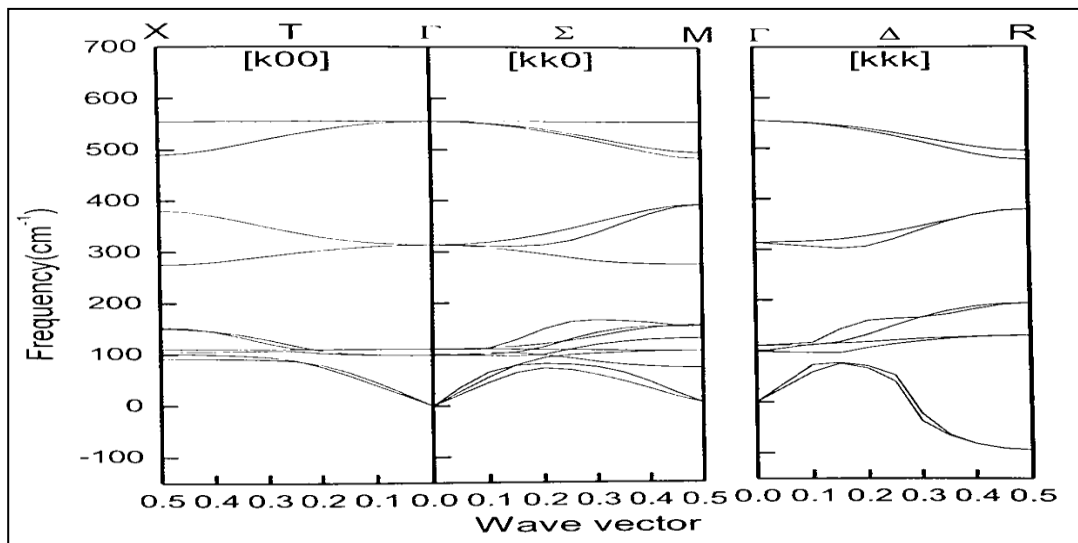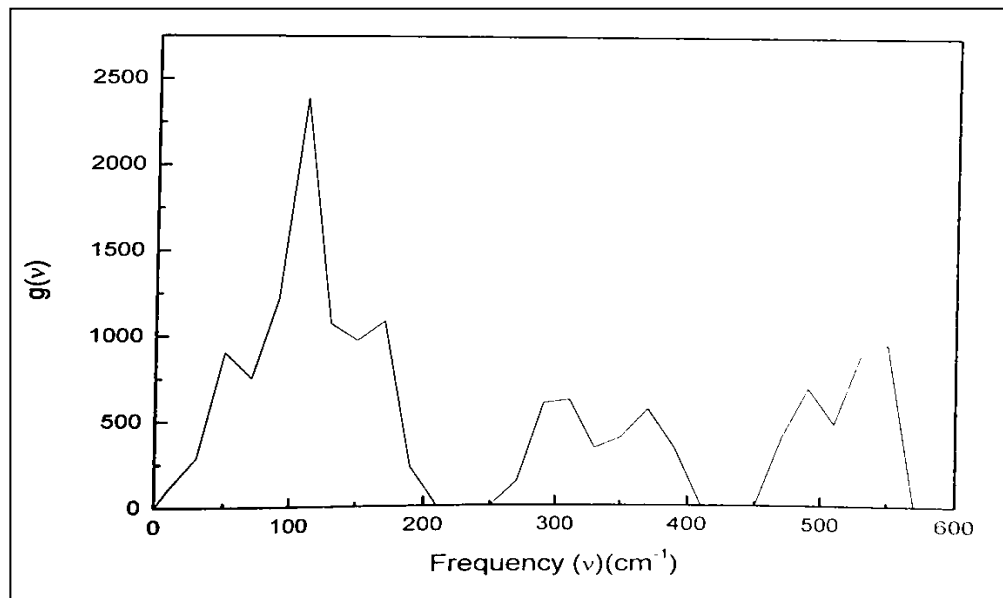The value of $Cv(v)$ is calculating for specific heat at constant volume $Cv(v)$

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Fig 2:-Phonon Dispersion Curve BiFeO₃

Fig 3:-Phonon Density of $BiFeO_3$

Table 1:- Position Coordinates and Wyckoff position of $BiFeO_3$ in Cubic Phase

Atom	Lattice Coordinates			Wyckoff Positions
	x	Y	Z	
Bi	0.5	0.5	0.5	1a
Fe	0	0	0	1b
O1	0.5	0	0	3c
O2	0	0.5	0	
O3	0	0	0	

Table 2:- Value of force Constants (10^3 dyne cm^{-1})

Compound	Force Constant							
$BiFeO_3$	α_1	α_1'	α_2	α_2'	α_3	α_3'	α_4	α_4'

73.0	9.0	-16.0	-19.0	77.0	6.5	-4.8	0.34

Table 3:- Calculated Zone Centre Phonon Frequencies in cm^{-1}

Modes	ZC Phonons of BiFeO$_3$			
	T$_{1u}$	T$_{1u}$	T$_{1u}$	T$_{2u}$
Present Work	656	412	97	120

4. Discussion

The computed inter-atomic force constants are displayed in the results, it is noted that the force constant between the Bi and O atoms has a substantial negative value, suggesting a significant coupling along the Bi-O chain that prevents the displacement of the Bi atom against the O atoms. Table 2 clearly shows that the force constant between Fe and O in BiFe03 is the greatest of all inter-atomic interactions. This indicates that the covalent connections between iron and oxygen are stronger than the covalent bonds between iron and (Bi-Fe). The matrix is solved at zone centre using the inter-atomic force constants listed in table2 input parameters. Table 3 contains a list of the zone centre phonons that were so collected.Table 3 makes it clear that the current computation of the cubic BiFeO$_3$ zone centre phonons does not produce an unstable TO mode. The zone centre phonons and other theoretically computed results correspond well. Unfortunately, the present computation cannot be compared to any experimental data. The whole phonon dispersion spectrum is obtained once the dynamical matrix is solved in the three symmetric directions, and it is displayed in figure 2. BiFe03's estimated phonon dispersion curves in figure 2 make it clear that phonon branches are spread very consistently over the whole structure in all symmetric orientations.According to the calculated eigen frequencies and eigen vectors, the top three branches of phonon dispersion curves, which are caused by the vibrations of the Fe atom, the middle three branches, which are located at about 315 cm-, and the lower nine branches, which are caused by the vibrations of the Bi and O atoms. The primary goal of the current computation is to confirm that modes soften along major symmetry at the Brillouin Zone (BZ) border directions. The characteristics that are anticipated to be present include softening of phonons and instability of modes.

In order to produce a vast number of frequencies, wave vectors were scattered at sites with various values. The initial Brillouin zone is split into 1000 points in order to have a complete phonon density of state, and the secular determinant is thus solved. Additionally, suitable weights have been assigned to the frequencies corresponding to the places (on the faces, the edges, in the interior, and at the corners) of the first Brillouin zone in order to facilitate more precise estimates of the phonon density of state or frequency distribution. For cubic

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structures, the 48 non-equivalent sites with the proper weights may be used to accurately determine the phonon density of state at the first Brillouin zone.The frequencies for all 1000 points in the first Brillouin zone are provided by the 48 non-equivalent points with weight factors, yielding 15000 frequencies for the cubic perovskite structure with 15x15 matrixes. These frequencies are separated into a limited number of 20cm-1 wide equal intervals. According to the phonon dispersion phenomenon, figure 3 has been produced to represent the estimated phonon density of state for BiFe03. The key peaks for BiFe03 in the current study are 50 cm-I, 110 cm-I, 170 cm-I, 310 cm-1, 370 cm-I, 490 cm-I, and 550 cm-I, with 110 cm-I being the most noticeable peak. The peaks at 110 cm-I are the acoustical phonons, whereas the peaks below and above 110 cm-I are caused by the optical phonons.

5. Conclusion

By using the DAF model, many phonon parameters for the cubic phase of BiFeO3 have been determined, including zone centre phonons, phonon dispersion, and density of state. The calculations show that the force constant 2 between the Bi and O atoms has a significant adverse value, including a significant coupling throughout the Bi-O chain that prevents the displacement of the Bi atom against the O atoms. The strongest interatomic contact in BiFeO3 is the force constant 1 between Fe and O. This indicates that the covalent link between iron and oxygen is the strongest of the four (Bi-Fe). The softening of modes is observed near the zone border according to estimations of phonon density.The characteristics that are thought to be related to phase transitions in these compounds include the softening of phonon instability of modes. The results of the current computation show that the cubic phase of BiFeO3 contains certain unstable modes with an imaging frequency at the zone border.As a result of its ability to concurrently exhibit adjustable mechanical, magnetic, electric/dielectric, thermal, and optical characteristics, multiferroic materials represent a significant source of technological applications. Additionally, these factors can couple to one another, resulting in intriguing cross-coupling phenomena that increase the applicability of multiferroics forinnovative uses.

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