Electronic Structure and Structural Phase Stability of $BaFe_2As_2$ Compound under Pressure.

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Abstract—the electronic band structure and structural phase stability of $BaFe_2As_2$ compound has been studied using Quantum Espresso code. To study the structural stability and phase transition, the total energies of this compound have been computed as a function of reduced volumes and fitted with Brich Murnaghan equation. The estimated lattice parameters are in good agreement with available experimental data. The present calculations reveal that $BaFe_2As_2$ compound undergo structural phase transition from Tetragonal (T) into Collapsed Tetragonal (cT) phase under pressure. The calculated phase transition pressure is in good agreement with recent experimental data. The calculated valence charge density of collapsed tetragonal phase reveals that As-As interactions is becoming stronger under pressure.

Index Terms— Electronic Structure, Ab initio calculations, Structural phase transition, High pressure, Fe based superconductors.

1 INTRODUCTION

The discovery of iron- based superconductors has new and challenging ideas in the field of condensed matter physics by the exploration of theories and experimental data. The Fe based superconductors have layered crystal structures with FeAs layers and are found to undergo a structural phase transition and antiferromagnetic spin density wave transition. At normal conditions, the parent phases of the iron-pnictide $AEFe_2As_2$ (AE=Ca, Sr, Ba and Eu) (AE=Alkaline earth or rare earth) superconductors are paramagnetic with tetragonal cell structure, while at lower temperature these compounds undergo both magnetic and structural phase transition [1]. Superconductivity can be achieved in these compounds either by electron or hole doping or by applying pressure. Applied pressure has an advantage of introducing less disorder compared to chemical substitution. Isostructural transitions from tetragonal to collapsed tetragonal accompanied by negative compressibility axial properties have been reported for ternary phosphides under pressure [2], [3] and also in similar compounds [4]. These experimental observations of pressure induced isostructural phase transition accompanied by an increase in the a-axis and decrease in c-axis. The $CaFe_2As_2$, belongs to 122 family undergoes phase transition from a tetragonal to an orthorhombic phase at 172 K accompanied by a magnetic transition. At low temperatures, when the pressure is above 0.35 GPa, the orthorhombic structure of $CaFe_2As_2$ transforms to a collapsed tetragonal structure but there is no evidence of superconductivity [5], [6].

Goldman *et al* [7] using single crystal neutron and high energy X-ray diffraction measurements have identified the phase transitions among the ambient pressure paramagnetic tetragonal (T), the antiferromagnetic orthorhombic (O), and the nonmagnetic collapsed tetragonal phases of $CaFe_2As_2$. They have reported that $CaFe_2As_2$ undergoes structural phase transition from tetragonal to a collapsed tetragonal structure at 1.6 GPa, with a large volume reduction. The $EuFe_2As_2$ (122 layered structure) compound has been studied by Uhoya Walter *et al* [8] using designer diamond anvils at 300 K and tetragonal to collapsed tetragonal phase is observed at about 10.0 GPa. They found that anomalous compression of lattice parameters.

The structural distortions and pressure inhomogeneity resulting from different levels of hydrostaticity of a pressure transmitting medium have been widely studied in single crystalline $SrFe_2As_2$ [9]. Similarly, the appearance of superconductivity on suppression of SDW is possible either by applying pressure or by chemical substitution. The occurrence of structural or magnetic transitions and superconductivity under different hydrostatic or non hydrostatic conditions have been reported for $BaFe_2As_2$ single crystals [10], [11], [12]. Yu-Zhong Zhang *et al* utilized ab initio molecular dynamics to investigate the electronic and lattice structure of AFe_2As_2 (A= Ca, Sr, Ba) under pressure. They found that the structural phase transition from orthorhombic to tetragonal symmetry is always accompanied by a magnetic phase transition in all these compounds [13]. Gotsis *et al* [14] studied the structural, electronic and noncollinear magnetic properties of $BaFe_2As_2$ for low temperature orthorhombic phase as well as for high temperature tetragonal phase.

Walter O Uhoya *et al* [15] observed that $SrFe_2As_2$ undergoes structural phase transition from the tetragonal (T) phase to a collapsed tetragonal (cT) phase at about 10 GPa under nonhydrostatic conditions. They also found that T_c falls below 10K in the pressure range of 10-18 GPa. High pressure X-ray diffraction and electrical resistance measurements in $BaFe_2As_2$ compound have been carried out by Walter O Uhoya *et al* [16]. They found that at ambient conditions, a phase transition from tetragonal (T) phase to collapsed tetragonal (cT) phase is observed at 17 GPa under nonhydrostatic conditions which is

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comparable to 22 GPa under hydrostatic conditions.The common feature of 122 type Fe-pnictide superconductors is the presence of FeAs plane. The As atom in these superconductor lies above and below the centre of Fe square. Deepa Kasinathan *et al*. have reported that non-superconducting metallic state of $SrFe_2As_2$ and $SrFe_{1.8}Ru_{0.2}$ compounds undergo isostructural collapse from the ambient pressure tetragonal phase to a collapsed tetragonal phase [17]. Yildrium *et al* [18] have reported the structural and magnetic properties of Fe-pnictide system where the c axis collapses with the loss of Fe magnetism using density functional theory calculation.

Tomic *et al* [19] studied the uniaxial versus hydrostatic pressure-induced phase transitions in $CaFe_2As_2$ and $BaFe_2As_2$. Their investigations reveal that $CaFe_2As_2$ shows a unique phase transition from a magnetic orthorhombic phase to nonmagnetic collapsed tetragonal phase and no indication of a tetragonal phase was observed at intermediate uniaxial pressures. In contrast, $BaFe_2As_2$ shows two phase transitions from a magnetic orthorhombic to a collapsed tetragonal phase through an intermediate nonmagnetic tetragonal phase. Recently Hisao Kobayashi *et al* [20] have reported by the effective As-As hybridization along the c-axis appears at approximately 2.3 GPa in the tetragonal phase of $EuFe_2As_2$, along with a change in the electronic state of Fe. Because of these changes and the effective hybridization play key roles in the pressure induced superconductivity in the tetragonal phase of $AEFe_2As_2$.The above interesting reports have motivated the present study on $BaFe_2As_2$ compound using first-principles calculations. With the increase of computational power, *ab initio* calculations have become a powerful tool in understanding the electronic band structure and structural phase stability of materials. This paper deals with the theoretical investigation of high pressure phase transition of $BaFe_2As_2$ compound from tetragonal phase (I4/mmm) to collapsed Tetragonal (I4/mmm).The next section describes the method of calculation. The third section presents the crystal structure details. The fourth section describes the structural phase stability. The fifth section gives the result and discussion and the last section is devoted to conclusion.

2 Method of Calculation

QUANTUM ESPRESSO is an integrated suite of computer codes for electronic-structure calculations and materials modeling based on density-functional theory. It uses plane waves basis sets and pseudo potentials (PPs) to represent electron-ion interactions. QUANTUM ESPRESSO can thus be a very useful tool to study the properties of metals and insulators having different crystal structures. The atomic cores in this code are described by separable norm-conserving (NC) pseudo potentials, Ultra-Soft (US) pseudo potentials, and Projector-Augmented wave (PAW) sets [21]. Another very important feature of this code is high performance nature both in serial and parallel execution. The present calculations have been performed in a plane-wave pseudo potential representation using the PWSCF program within the generalized gradient approximation according to the Perdew-Burke-Ernzerhof (GGA-PBE) exchange correlation potential function [22].

In the present calculation, the valence states for Ba, Fe, and As atoms are taken as (6s), (3d, 4s, 4p) and (4s, 4p) respectively. The magnetic and non magnetic calculations are carried out with an energy cutoff of 40 Ryd for the wave functions and 340 Ryd for the charge densities. For the electronic-structure calculations, the Brillouin-zone integrations are performed by using the Gaussian smearing technique with a width of 0.04 Ryd. For k-point sampling a grid of 16x16x12 is used for non magnetic (NM), Ferromagnetic (FM) and antiferromagnetic (AFM) configuration of $BaFe_2As_2$ compound in I4/mmm structure.

3 Crystal Structure

At normal conditions, $BaFe_2As_2$ crystallises in the $ThCr_2Si_2$ type Tetragonal (T) structure (space group I4/mmm). The atomic positions for space group I4/mmm: Ba (2a) (0 0 0), Fe (4d) (1/2 0 1/4), and As (4e) (0 0 z_{As}), where z_{As} is the internal parameter. Present calculations reveal that variation of z_{As} as a function of pressure is not appreciable; hence the experimental value of internal atomic parameter z_{As} is used throughout the calculation. The high pressure phase of collapsed tetragonal structure (cT) is also having the same phase group but with larger **a** and smaller **c** lattice parameters under nonhydrostatic pressure conditions.

4 Structural Phase Stability

The occurrences of superconductivity in these types of compounds are due to structural or magnetic transitions under different hydrostatic or nonhydrostatic conditions [9], [10], [11], [12]. . High pressure X-ray diffraction and electrical resistance measurements in $BaFe_2As_2$ compound have been carried out by Walter O Uhoya *et al* [16]. They found that at ambient conditions, a phase transition from tetragonal (T) phase to collapsed tetragonal (cT) phase is observed at 17 GPa under nonhydrostatic conditions which is comparable to 22 GPa under hydrostatic conditions The calculated phase transition of about 16.8 GPa is in good agreement with the experimental value of 17 GPa under nonhydrostatic conditions [16]. In order to study the structural phase stability of this compound, the total energies are calculated in a similar manner to our early works [23], [24] by varying cell volume from 240 $Å^3$ to 120 $Å^3$. The estimated lattice parameters under hydrostatic pressure, are compared with that of experimental data under nonhydrostatic pressure conditions and are also presented in Table.1. The calculated total energies of different ordering namely, non magnetic (NM), Ferromagnetic (FM) and antiferromagnetic (AFM) are fitted with Birch–Murnaghan equation of state [25]. The fitted total energies of this compound reveal that antiferromagnetic ordering is stable when compared to non magnetic or ferromagnetic ordering. This is in agreement with the experimental results [26], [27].

TABLE .1

Estimated Lattice Parameters and P_T of $BaFe_2As_2$

Phase	Lattice parameter (Å)		Phase Transition Pressure P_T (GPa)
	a	c	
T	3.9594	13.007	
	(3.963)[a]	(13.02)[a]	16.8
cT	3.9321	10.452	(17)[a]
	(3.984)[a]	(10.59)[a]	

[a] [16]

The variation of total energies with molecular volume for antiferromagnetic ordering of this compound is shown in Fig. 1. From the graph, it can be clearly seen that the tetragonal structure is the most stable at ambient conditions for $BaFe_2As_2$ compound.

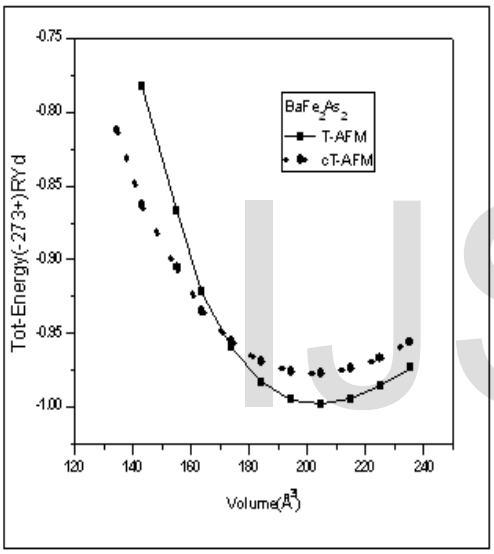

Fig.1 Calculated total energy vs molecular volume in normal and high pressure phases of $BaFe_2As_2$

The equilibrium volume (203.896 Å^3) of the Tetragonal phase is nearly equal to the experimental value (204.556 Å^3).The calculated lattice parameters of tetragonal as well as collapsed tetragonal phases are given in Table. 1. along with the experimental values. The pressure is obtained by taking the volume derivative of the total energy. The bulk modulus

$$B=-V_0\, dP/dV \qquad (1)$$

is also calculated from the P–V relation. The Equation of State (EOS) for this $BaFe_2As_2$ compound is showm in fig.2.The structural phase stability is determined by calculating Gibb's-free energy (*G*) [28] for tetragonal and collapsed tetragonal structures, which is

$$G=E_{tot}+PV-TS \qquad (2)$$

Since the theoretical calculations are performed at 0 K

$$H=E_{tot}+PV \qquad (3)$$

The structural phase transition pressure can be estimated by comparing the enthalpies of tetragonal phase to that of collapsed tetragonal phase. At a given pressure, a stable structure is one for which enthalpy has its lowest value and the transition pressures are calculated at which the enthalpies for the two phases are equal.

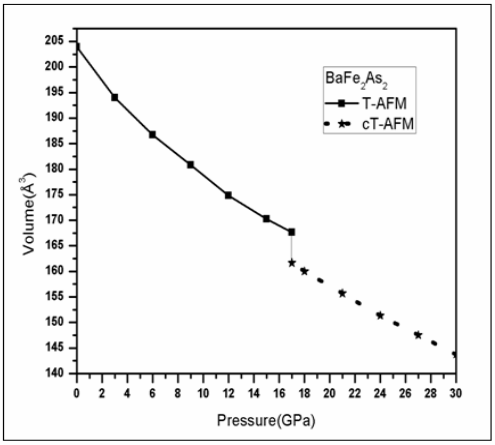

Fig. 2. Equation of State of $BaFe_2As_2$

The applied pressure has the advantage of introducing less disorder compared to chemical substitution. The antiferromagnetic ordering is strong against the applying pressure and it is more stable in the studied pressure range which is in agreement with the earlier reports [29]. The pressure dependence of Fe magnetic moments for the antiferromagnetic ordering in $BaFe_2As_2$ compound is shown in Fig. 3.

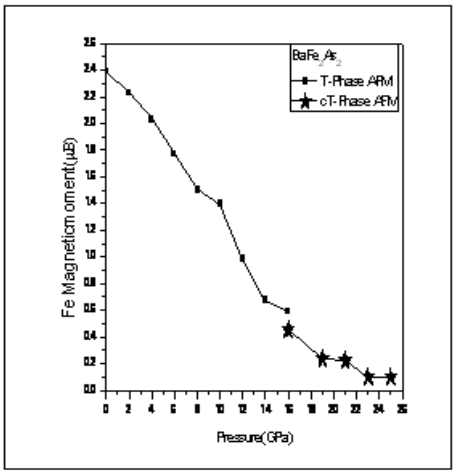

Fig.3. Calculated Fe magnetic moments for T and cT phase of $BaFe_2As_2$ under the pressures.

The Fe magnetic moment in the AFM ordering decreases linearly with applied pressure for $BaFe_2As_2$ compound. For both

the phases, Fe magnetic moment of cT phase is less when compared to tetragonal phase which is mainly due to As-As hybridization. Reducing the Fe-spin states reduces the Fe-As bonding and increases As-As interaction during the c-axis collapse. The present results are very similar to the earlier reported 122 type compound of $CaFe_2As_2$ [18].

5 Result and Discussion

The self consistent band structure calculations of $BaFe_2As_2$ compound is obtained at ambient as well as at high Pressures are shown in figures 4(a&b). From the electronic band structure and total energy calculations, one can understand the existence of cT phase under pressure. Due to c-axis collapse during structural phase transition, the comparable height decreases in the Fe-As, As-Ba-As planes indicating that the lattice parameters uniformly shrink. The calculated band profiles of $BaFe_2As_2$ of tetragonal phase as well as collapsed tetragonal phases are very similar. The main difference between them is band shift. There are several states are being above the Fermi level which crosses the E_F in the T-phase along the Z-Γ direction. Most of the bands are shifted towards lower energy in the cT-phase which is expected, since the cT-phase has the lower energy. The calculated band structure shows that appreciable As-p character in Fe centered bands, i.e. along Γ-X direction. As pressure increases, band crossing E_F along Γ-X direction is pushed at higher energy and completely above the Fermi level at 16.8 GPa in $BaFe_2As_2$ which is in agreement with earlier reported results [30]. The pressure-induced isostructural phase transition to a collapsed tetragonal at ambient temperature is not unique among arsenic compounds that have $ThCr_2Si_2$-type structure. This structural phase transition effect is found among the phosphides groups that are AT_2As_2 compounds, such as $EuCo_2P_2$, $SrNi_2P_2$ [31] and $EuFe_2P_2$ [32].

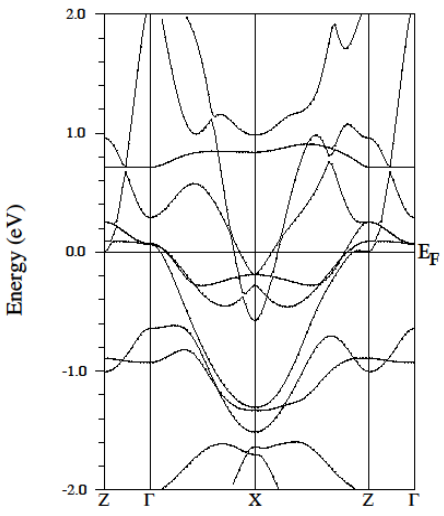

Fig 4 (a)

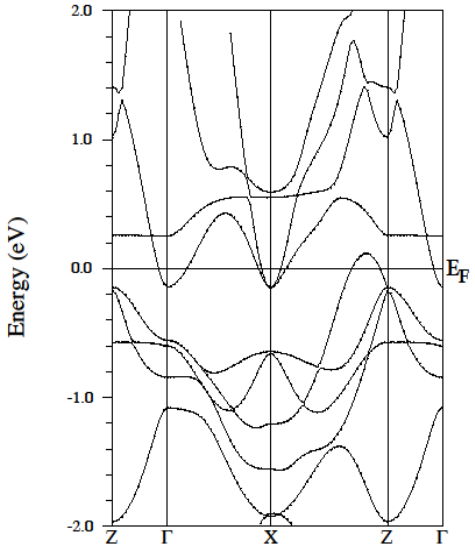

Fig 4 (b)

Figs .4 Band structure for T phase (a) and cT phase (b) of $BaFe_2As_2$

The study of phosphides compounds reveals that there is a rapid decrease in their c/a ratios in the collapsed tetragonal phase, associated with the formation of a P–P single bond between ions in adjacent planes along the *c* axis [33]. The recent report suggest that there is similar transition observed in the arsenic groups of compounds, with an enhancement of the As-As bonds across the Fe_2As_2 layer under pressure [34].

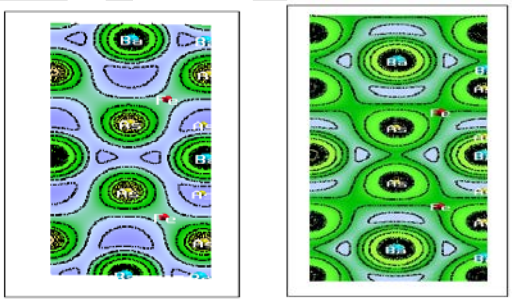

Fig 5(a) Fig 5(b)

Figs .5 valence charge density for T and cT phase of $BaFe_2As_2$

In order to demonstrate that there is a large hybridization between As ions in the $BaFe_2As_2$ compound, the valence electron charge density has been calculated for both the phases of $BaFe_2As_2$ compound. Figures 5 (a & b) show the valence electron charge density of Tetragonal and collapsed Tetragonal phase of $BaFe_2As_2$ compound. Figures 5 (a & b) clearly show that the As ion below the top Fe-plane makes a bond (or hybridizes) with the arsenic ion which is above the lower Fe-plane. According to valence electron charge density plots the As-As hybridization increased in the cT-phase. Due to close proximity of the As ions in adjacent Fe-layers, the observation of the As-As interaction is very obvious. What is interesting is

that there is almost same type of hybridization between two arsenic ions on the same Fe-plane as shown in Fig.5 b. The calculated valence charge density of $BaFe_2As_2$ also shows similar observations: in particular increased hybridization between As-As ions under pressure.

6 Conclusion

In the present study structural phase stability, high pressure behavior and electronic structure of $BaFe_2As_2$ compound is investigated using the Quantum espresso code. The calculated structural parameters obtained from the present results are in agreement with the experimental values. From the calculation, this compound undergoes a structural phase transition from Tetragonal into collapsed Tetragonal phase under pressure. The phase transition pressure obtained in this work agrees well with the recent experimental data. The present investigation also indicates that the Tetragonal structure $BaFe_2As_2$ is energetically more stable at ambient conditions. The valence charge density of collapsed tetragonal phase reveal that As-As interactions are stronger during the compression in c- axis. The strength of this interaction is mainly controlled by the Fe-As chemical bonding.

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