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First principle energy calculation of YBCO superconductor

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Abstract

Background/Objectives: The crystal structure of YBCO Superconductor has fascinated the material science research group. The calculation of elastic constants, enthalpy and final energy of YBCO superconductor under pressure up to 30 GPa are further investigated in this research study. **Methods:** The pressure dependence of the elastic constants of the $\text{YBa}_2\text{Cu}_3\text{O}_7$ (YBCO) is investigated using the first principle calculations based on the density functional theory (DFT). The only input required is the lattice parameters at corresponding pressure of materials which are predicted using first principle computational methods at desired high-pressure state. **Findings:** The elastic constants, enthalpy and final energy of the YBCO Superconductor has been calculated by using ab-initio calculations. The enthalpy formation is the first value considered from the Density Functional Theory (DFT). **Applications:** This will explain elastic constants accurately as a function of composition. This enables the use of material optimization techniques to develop new materials that are systematically adapted to specific components.

Keywords: YBCO superconductor; density functional theory (DFT); elastic constants; pressure; enthalpy

1 Introduction

The discovery of the Ba-La-Cu-O system by Muller and Bednortz⁽¹⁾ with a T_{sc} of 30K has generated and further research has led Wu et al to the discovery of T_{sc} of 90 K. In 1964, Schooley and coworkers first reported superconductivity in SrTiO_3 , an oxide with perovskite crystal structure, with a quite low transition temperature, $T_c = 0.3\text{K}$. In 1975, Coworkers and Sleight found high transition temperature at 13K in $\text{BaPb}_{1-x}\text{Bi}_x\text{O}_3$. In 1986, Bednortz and Muller reported a remarkable superconducting transition at 30 K in LaBaCuO_3 (LBCO). Almost one year later, Wu and colleagues reported superconductivity in $\text{YBa}_2\text{Cu}_3\text{O}_7$ (YBCO), with $T_c = 90\text{K}$. The discovery of the Ba-La-Cu-O system by Bednortz and Muller with a superconducting transition temperature of 30K has generated a great deal of tremendous interest among physicists⁽²⁾. In 1964, Schooley and coworkers first reported superconductivity in SrTiO_3 , an oxide with perovskite crystal structure, with a quite low transition temperature, $T_c = 0.3\text{K}$. In 1975, Coworkers and Sleight found high transition temperature at 13K in $\text{BaPb}_{1-x}\text{Bi}_x\text{O}_3$. In 1986, Bednortz and Muller reported a remarkable superconducting transition at

30 K in LaBaCuO₃ (LBCO). Almost one year later, Wu and colleagues reported superconductivity in YBa₂Cu₃O₇, with T_c= 90 K⁽³⁾. The pressure dependence on sound velocities and elastic moduli⁽⁴⁾, pressure dependence of specific heat and Debye temperature of internal friction and linear thermal expansivity. The anomalous stiffening below critical temperature observed in poly crystals was also reported in single crystals. As for the mono crystalline elastic constants, only one set of complete C_{ij} derived from the phonon frequencies of an elastic scattering for a tetragonal structure was reported⁽⁵⁾. Using sound velocity measurements, Saint Paul and coworkers⁽⁶⁾ estimated C₃₃ and C₄₄. Also, from sound velocities, Golding and coworkers calculated the pseudo tetragonal elastic constants C₁₁ and C₃₃. Baumgart and coworkers⁽⁷⁾ determined C₁₁, C₃₃ and C₄₄. The elastic properties of YBCO superconductor were studied by Vetebskii and coworkers. Starting from the mean field energy, Millis and Rabe derived expressions for the singularity's behavior of the elastic constants and sound velocities near T_c. Calculation of Elastic constants, enthalpy and final energy values at different pressures for YBa₂Cu₃O₇ (YBCO) Superconductor is the main focus in the present study.

2 Theory and computational details

Furthermore, one can also directly obtain some useful information on the characteristics of bonding and the structural stability of a crystal. The elastic constants C_{ijkl} with respect to the finite strain variables is defined as⁽⁸⁾

$$C_{ij} = \left(\frac{\partial \sigma_{ij}(X)}{\partial e_{kl}} \right)_x$$

Where σ_{ij} and e_{kl} are the applied stress and Eulerian strain tensors and X and x are the coordinates before and after the deformation. For the isotropic stress, we have⁽⁹⁾

$$C_{ijkl} = c_{ijkl} + \frac{P}{2}(2\delta_{ij}\delta_{kl} - \delta_{il}\delta_{jk} - \delta_{ik}\delta_{jl})$$

$$C_{ijkl} = \left(\frac{1}{V(X)} \frac{\partial^2 E(X)}{\partial e_{ij} \partial e_{kl}} \right)_x$$

Where C_{ijkl} denotes the second-order derivatives. The Strain energy – strain curve has been used for calculation of elastic constants purpose. All the elastic constants increase with pressure. For orthorhombic crystal the mechanical stability is represented by the following condition⁽¹⁰⁾.

$$C_{11} > 0, C_{22} > 0, C_{33} > 0, C_{44} > 0, C_{55} > 0$$

$$C_{66} > 0 [C_{11} + C_{22} + C_{33} + 2(C_{12} + C_{13} + C_{23})] > 0$$

$$(C_{11} + C_{22} - 2C_{12}) > 0$$

$$(C_{11} + C_{33} - 2C_{13}) > 0$$

$$(C_{22} + C_{33} - 2C_{23}) > 0$$

The superconductor having tetragonal symmetry considered here comes under the second category and the six nonzero elastic constants for it are C₁₁, C₃₃, C₄₄, C₆₆, C₁₂ and C₁₃. The equations for the wave propagation in the tetragonal crystal are very easily obtained from the equations for the orthorhombic crystal by making the substitutions C₁₁=C₂₂, C₄₄=C₅₅ and C₁₃=C₂₃. Enthalpy of formation was assessed from GGA+U ab- initio Density Functional Theory (DFT) based calculations. The electronic structure and total energies of YBa₂Cu₃O₇ and the constituent oxides, YO₅, Ba₂O, and Cu₃O, were calculated by means MedeA-VASP⁽¹¹⁾ program using projector augmented plane waves basis set and generalized gradient approximation (GGA-PBE)⁽¹²⁾ to exchange-correlation functional combined with additional local orbital specific coulomb potential U = 3eV acting on Cu-3d states. The first value considered from Density Functional Theory (DFT) is Enthalpy formation. The final energy of the YBCO Superconductor has been calculated by using ab- initio calculations.

3 Results and Discussion

Knowledge of elastic constants are significant for understanding of the structural stability and properties of the crystal. The elastic constants under different pressures obey these stability criteria, implying that the orthorhombic $\text{YBa}_2\text{Cu}_3\text{O}_7$ is mechanically stable. The present results at ground state $C_{11}=1580\text{GPa}$, $C_{12}=713\text{GPa}$, $C_{13}=278\text{GPa}$, $C_{22}=-385\text{GPa}$, $C_{23}=-1177\text{GPa}$, $C_{33}=1355\text{GPa}$, $C_{44}=449\text{GPa}$, $C_{55}=328\text{GPa}$, $C_{66}=668\text{GPa}$ and at 20GPa $C_{11}=5348$, $C_{12}=2409\text{GPa}$, $C_{13}=1888\text{GPa}$, $C_{22}=5804\text{GPa}$, $C_{23}=1729\text{GPa}$, $C_{33}=4813\text{GPa}$, $C_{44}=1021\text{GPa}$, $C_{55}=1090\text{GPa}$, $C_{66}=1331\text{GPa}$. C_{11} , C_{22} , and C_{33} represent the resistance to linear compression, and the other elastic constants are mainly associated with the elasticity in shape. In the entire pressure range of our calculations, $C_{11}=5384\text{GPa}$, $C_{22}=5804\text{GPa}$ and $C_{33}=4813\text{GPa}$, were much larger than those of the other elastic constants. Further, the relationship $c_{22} > c_{11} > c_{33}$ under different pressures implied that the strength of the bonding along the [010] direction was stronger than those along the [001] and [100] directions. The calculated values of Elastic constants at different pressures are given in Table 1 and corresponding values versus pressure for YBCO superconductor is shown in Figure 1.

As can be seen from Table 1, all the elastic constants increase with pressure. The anisotropy factor A was obtained from the relation $A=2C_{44}/C_{11}-C_{12}$. The difference between single crystalline elastic constants, $C_{12}-C_{44}$ is well-known as the Cauchy pressure. A positive value of $C_{12}-C_{44}$ indicates the metallic bonding, whereas negative value significances covalent bonding. The Cauchy pressures positive value always indicates ductile nature, while a negative value corresponds to brittleness. The calculated values of enthalpy and final energy up to 30GPa are given in Table 2. The enthalpy and final energy versus pressure for YBCO superconductor is shown in Figure 2. The minimum enthalpy and final energy is $-2086.638\text{KJ mol}^{-1}$ and -2086.65 at ground state and $-2084.43\text{KJ mol}^{-1}$ and -2086.60 at 30GPa. From these results it is clear that the enthalpy and final energy of YBCO superconductor increases with pressure.

Table 1. Calculated Values of elastic constants C_{ij} (GPa) of $\text{YBa}_2\text{Cu}_3\text{O}_7$ under pressure

Pressure	C11	C12	C13	C22	C23	C33	C44	C55	C66
0	1,580	713	278	-385	-1,177	1,355	449	328	668
10	4,345	1,974	1,413	4,726	1,377	3,877	889	886	1,152
20	5,348	2,409	1,888	5,804	1,729	4,813	1,021	1,090	1,331

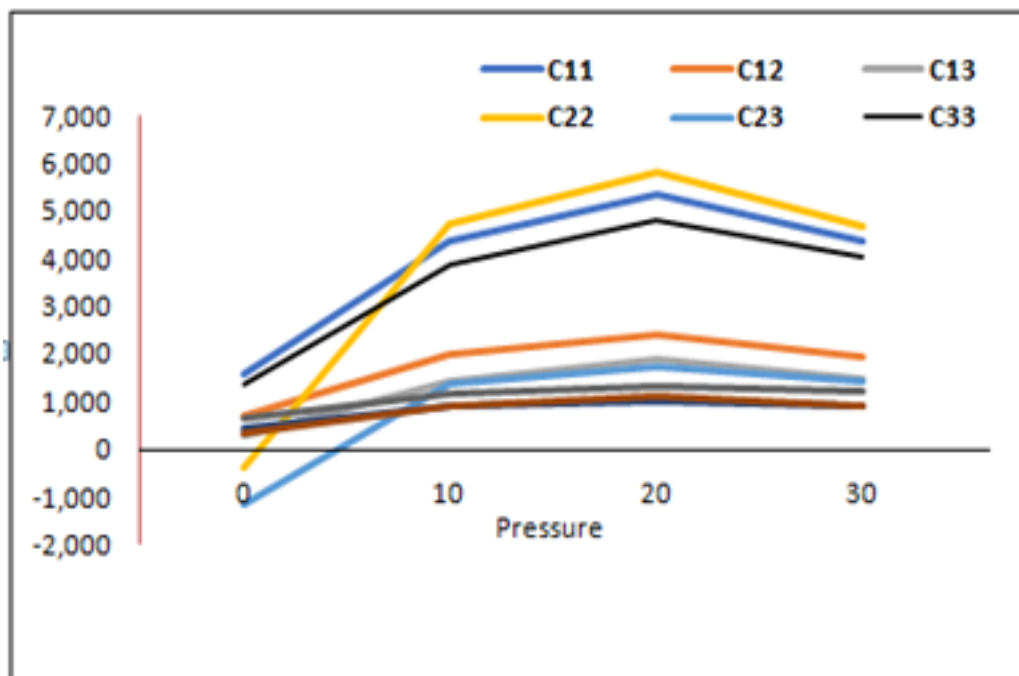
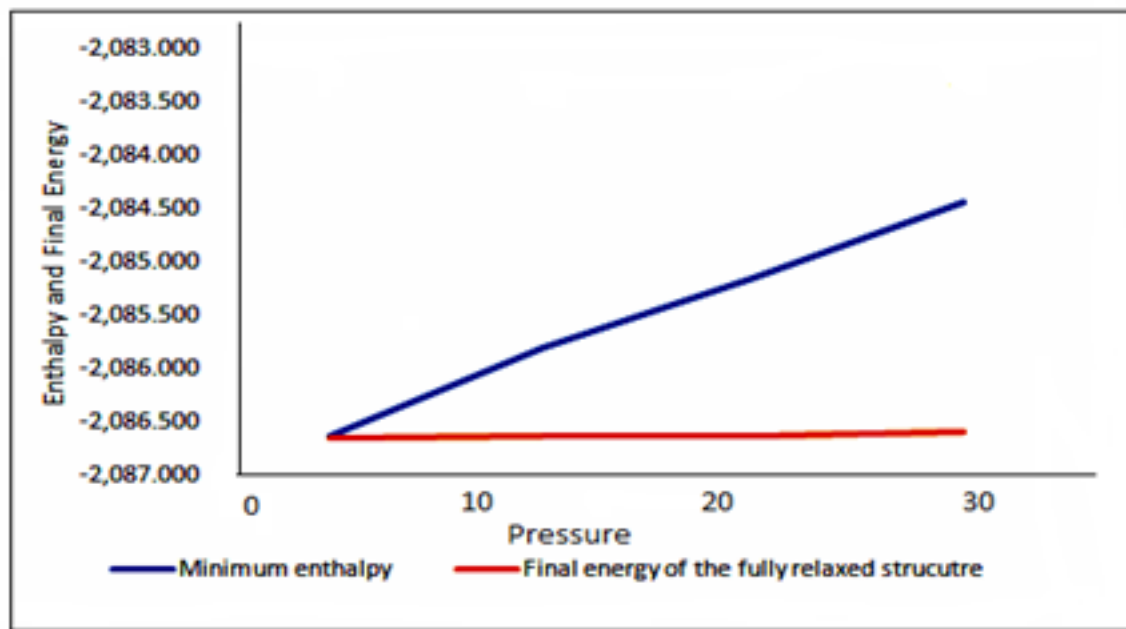


Fig 1. Elastic constants versus pressure for YBCO superconductor

Table 2. Calculated values of enthalpy and Final energy at different Pressures

Pressure (GPa)	Minimum enthalpy (KJ mol ⁻¹)	Final energy of the fully relaxed structure
0	-2,086.638	-2,086.65
10	-2,085.81	-2,086.64
20	-2085.156659	-2086.630299
30	-2,084.43	-2,086.60

**Fig 2.** Enthalpy and final energy versus pressure for YBCO Superconductor

4 Summary/Conclusion

In summary, the pressure dependence of the elastic constants of the $\text{YBa}_2\text{Cu}_3\text{O}_{7-x}$ (YBCO) is investigated using the first principle calculations based on the density functional theory (DFT). The elastic constants C_{11} , C_{22} , C_{33} , C_{44} , C_{55} , C_{66} , C_{12} , C_{13} and C_{23} are calculated at different pressures. In the entire pressure range of our calculations, $C_{11} = 5384 \text{ GPa}$, $C_{22} = 5804 \text{ GPa}$ and $C_{33} = 4813 \text{ GPa}$, were much larger than those of the other elastic constants, indicating that the deformation resistances of $\text{YBa}_2\text{Cu}_3\text{O}_7$ along the axial directions were stronger than those of the non-axial directions. The elastic constants C_{11} , C_{12} and C_{44} represent the elasticity in length and shape. All the elastic constants increase with pressure. The Enthalpy and final energy of the YBCO Superconductor has also been calculated by using GGA+U ab-initio calculations up to 30 GPa. The enthalpy and final energy of YBCO superconductor increases monotonically with pressure.

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