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The Conductivity Parameters of $YBa_2Cu_3O_{6.5+\delta}$ Superconductor Compound

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Abstract

The high-temperature superconductor like $YBa_2Cu_3O_{6.5+\delta}$ was prepared by solid-state reaction method at calcination temperatures (900 °C). The crystal structure was confirmed using X-ray diffraction, and it was found that $YBa_2Cu_3O_{6.5+\delta}$ showed orthorhombic phase with lattice parameters (a = 3.82030, b = 3.88548, and c = 11.6835 Å) with space group (Pmmm). The sample was sintered at sintering temperatures (900 °C) for (24 hr). The oxygen excess (δ) was nearly (0.36), which was effective in the appearing superconducting properties. The sample $YBa_2Cu_3O_{6.86}$ had a critical temperature of about (92 K). The simulation on the XRD-pattern was necessary to predicate the shape of the unit cell and the position of atoms in the unit cell. The last is very important to find some theoretical date, which are benefit in the predication the conductivity parameters through the sequence's unit cells, which are useful in the conductivity mechanism. This mechanism is depending on the concept of interlayer coupling, so the number of the layers including the unit cell is effective parameter in the conductivity mechanism through the normal resistivity created.

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1. Introduction

The main feature of superconducting materials is representing by the zero resistance at a certain temperature called critical temperature T_c. Since the discovery of superconductivity by Onnes in 1911, the theoretical development is still limited especially at high temperature superconductor. It is well known that BCS-theory is comfortable with low-temperature superconductors during the creation of Cooper pairs [1]. It was given a quite definition of the superconductivity mechanism and their related parameters. That is making the scientists are discovering different models giving more details on the conductivity mechanism. The appearance of different families of high temperature superconductor will making the difficulties on predicting the preferable mechanism related to the conductivity in high temperature superconductor. Since 1990, there are many theoretical models were appeared to classify the conductivity mechanism. One of these models are interlayer coupling model [2,3], which is classified in the like BCS-theory category. Then the number of Cu-O layers including is very important in the specification of conductivity mechanism. The definition of these layer is requiring the position of each atoms in the unit cell. So, it is necessary to simulate the crystal structure and predicating a required unit cell. There is a similar study was published previously [4]. It was concentrated on the conductivity mechanism in Hg–Ba–Ca–Cu–O system. The effect of Miller indices is useful as a coupling planes between the main layers in the unit cell if it is tetragonal or orthorhombic phase as discussed previously [5]. Then the analysis of XRD-pattern is representing the first step in the simulation of unit cell and the positions of atoms including. The resistivity behavior as a function of temperature is applying to conclude the normal resistivity because the normal resistivity is a function on how many layers including with the unit cell [6]. The correlation between the outputs of XRD-analysis and resistivity measurements are considering the inputs for the simulation of unit cell shape and conductivity mechanism. The main parameter in the distinguishing between the low temperature superconductor and high temperature superconductor is the coherence length $\xi(T)$, which is a function to wavelength of bosonic particles created by like BCS-theory. This parameter is comparing with the penetration depth $\lambda_L(T)$, which is a function to extension the magnetic field including. The principle equations those were dependent in the determination the coherence length and penetration depth are the following:

$$\xi = \frac{h v_f}{2\pi^2 K_\beta T_c} \quad (1)$$

$$v_f{}^2 = \frac{\hbar^2}{m^2}[3\pi^2 N_e]^{2/3} \quad (2)$$

$$\lambda = \lambda_{(0)}\left[1 - \left(\frac{T}{T_c}\right)^4\right]^{-\frac{1}{2}} \quad (3)$$

$$\lambda_{(0)} = \sqrt{\frac{m_e}{\mu_\circ N_e e^2}} \quad (4)$$

$$\mathbb{K} = \frac{\lambda}{\xi} \quad (5)$$

The parameter $\mathbb{K}$, is defining the order parameter, it is a factor to classify whether the superconductor is type I or

type II superconductor. The last one is a function to high temperature superconductor. When the system scale is so small that the electronic level spacing exceeds the bulk superconducting energy gap (Δ), a total instability of superconducting order is expected. As a result of the so-called Anderson criteria [7], superconductivity might theoretically survive at length scales much smaller than ξ.

2. Experimental Procedure

The samples of the superconducting compound $YBa_2Cu_3O_{6.5+\delta}$ were prepared by the solid-state reaction method. The principal materials were used must be high purity and imported from the Merck industry, they were Y_2O_3, $BaCO_3$, and CuO. The using of suitable weight for above compounds by the ratio 1-2-3, and mixing many times to make the homogeneity. The mixture was crushed using an agate slurry with the addition of some drops of propanol-2. The powder was calcined at temperature (900 °C) for (24 hr) in air and sintered as a pellet at temperature (900 °C) for (24 hr). The sintering process is happening under flow of oxygen to produce non-stoichiometric sample $YBa_2Cu_3O_{6.5+\delta}$ through the parameter δ. The sample had been examined by Iodmetric titration, it showed the value of δ = 0.36. Then the oxygen content is shown in the chemical composition $YBa_2Cu_3O_{6.86}$. The XRD-analysis and resistivity measurement are suitable to make this simulation of YBCO compound. The refinement of XRD pattern and the simulation on the unit cell shape was investigated by using the software CrysDiff, and Endeavour respectively.

3. Results and Discussion

The XRD analysis was performed to investigate a creation of the required structural phase in comparison to the database mentioned by COD1000030. The analysis of XRD-chart had been done by using a certain software called CrystDiff. The aim of this analysis is making a simulation on X-ray pattern to conclude a structural phase obtained for Y-Ba-Cu-O family. The output results are showing a lattice constants *a*, *b* and *c*, the space group, atomic positions, crystallite size, and a possible strain. A software CrystDiff and Endever were used to investigate the above features. The simulated output results of crystal structure were showed orthorhombic phase for sample $YBa_2Cu_3O_{6.86}$ with lattice constants of a = 3.8203, b = 3.8855 and c = 11.6835 Å. The calculated volume of unit cell is about V = 173.4 Å^3, space group (P/mmm), a density is about (6.378 gm/cm$^{3)}$, and its molecular weight of the compound is (666.19). The open crystal database was a source in the refinement of XRD pattern through a data sheet COD-1000030. It was found that there are eight peaks belonging to Miller indices (010), (102), (103), (104), (113), (020), (200), (123), (213), (220), (130), (310) at (2θ = 20-80), as shown in Figure 1. The most probable peak was mentioned by (103), that was a compatible with Duzgun [8], he exhibited the most peaks were predicated in our chart. There are four peaks with low intensity created in a pattern, they are belonging to (102), (200), (213), (220), (130), (310), which are belong to tetragonal phase. So, their appearance in low intensity is considering a sign on the stability of orthorhombic phase. The main feature is the splitting in the peaks (020), (200) and the peaks (123), (213). This is a good sign on the presenting an orthorhombic phase. Whereas the merging of above peaks is a sign on tetragonal phase. The orthorhombicity ratio is about 81.1% for the sample under study. This is a proof on the agreement of the refinement results with the standard data. The application of the output in the second software is giving a simulated orthorhombic unit cell and atomic position related, as shown in Figure 2. The simulation on the phase formation was showed the orthorhombic unit cell with atomic position as mentioned in Table 1.

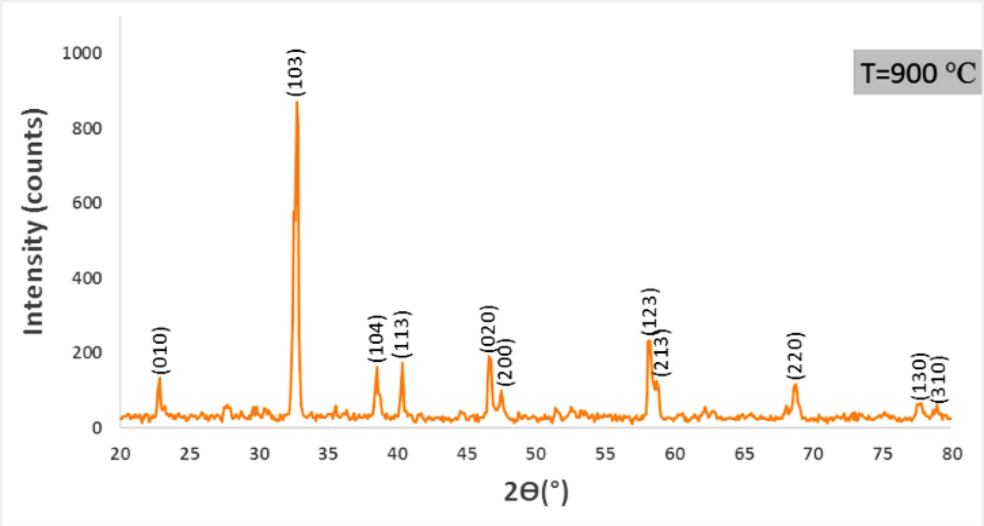

Figure 1. X-ray Diffraction spectrum of sample $YBa_2Cu_3O_{6.86}$ calcined at 900°.

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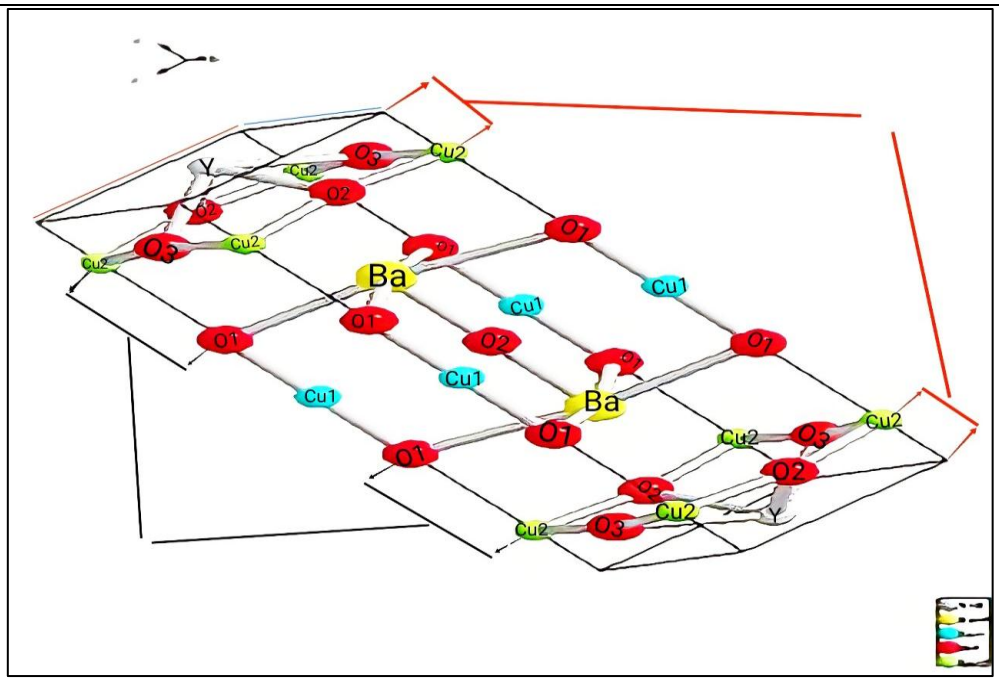

Figure 2. Explain the simulated unit cell of superconductor compound $YBa_2Cu_3O_{6.86}$.

Table 1. Indicate the atomic positions in the orthorhombic unit cell of $YBa_2Cu_3O_{6.86}$.

Atoms	X	Y	Z
Y1	0.5	0.5	0.5
Ba1	0.5	0.5	0.1839
Cu1	0	0	0
Cu2	0	0	0.3550
O1	0	0.5	0
O2	0.5	0	0.3782
O3	0	0.5	0.3769
O4	0	0	0.1584

The crystal structure of the $YBa_2Cu_3O_{6.86}$ was affected with the length of CuO chains toward c-axis, and the number of CuO_2 layer. It had a direct effect on various physical properties. It contains a single chain of CuO and two CuO_2 layer. The bending or extension of the bonds in the chain or planes had direct effect on structural properties appeared on the charge formation in the conductivity mechanism. So, the decreasing in the c-axes is a result of that bending, as discussed before [9]. They showed the Cu-O bond was the origin of charges inside a unit cell. Regarding the concept of interlayer coupling between the layers inside the unit cell and the results of unit cell simulation will help us to conclude some results functional to the conductivity mechanism at high-temperature superconductor. There are some simple equations used to calculate some parameters will useful in the conductivity mechanism, as mentioned in Tables 2 and 3. The critical temperature is useful to complete this calculation through the energy gap calculation.

In general, the extra oxygen in the superconducting compound play an important role to understand their effect on the superconducting behavior. The YBCO system, the electrical properties are significantly changed by the influence of oxygen content and the arrangement of oxygen ions in the CuO chain sites. The extra oxygen δ is well known the oxygen dopant atoms used to improve the conductivity of superconducting compounds. That is affecting the doping level, the conduction mechanism, through a creation of tetrahedron in the unit cell. The last is the main reason to accelerate the charge moving. In general, the superconducting compound $YBa_2Cu_3O_{6.5+\delta}$ has the parameter δ is very important to record the nature of superconducting compound if it is stiochmetric or not. So, if $\delta = 0$ the superconducting compound is stiochmetric and it is non superconducting. That means there is no extra oxygen insertion inside the unit cell. If $\delta \leq 0.5$, there is extra oxygen takes the maximum value and its effect on probability of motion like cooper pairs within the unit cell, and both values become less stable. The sample had been examined by Iodmetric titration; it showed the value of $\delta = 0.36$. So, the compound $YBa_2Cu_3O_{6.86}$ contains two plain of CuO_2 and one chain of CuO and both has direct effect on producing tetrahedron structure in the orthorhombic unit cell.

The resistivity curve as a function of temperature in the compound $YBa_2Cu_3O_{6.86}$ is appearing Figure 3. The critical temperature of compound $YBa_2Cu_3O_{6.86}$ reaches to (92 K) as appeared through the abrupt decreasing in the resistivity curve. It is better than that measured by Howe [10], he calculated the value of critical temperature of about (86 K) for $YBa_2Cu_3O_7$ because he concluded the ratio 69% of superconducting phase appeared, which is lower than the

predicated value 81.1% in this research. The normal resistivity is beneficial in the mechanism definition through the conclusion of how many modes are included in the unit cell. It is well known that the high-temperature superconductor like YBCO-system was composed of multi perovskite unit cells having a high normal resistivity. It was returned to a series resistance produced from a sequence of multilayers including as mentioned in Figure 2, for the Y-123 HTSc compound. The effective layers were mentioned by CuO_2 layers and the distance between them is considering the seed for orbital sharing to strengthen their coupling.

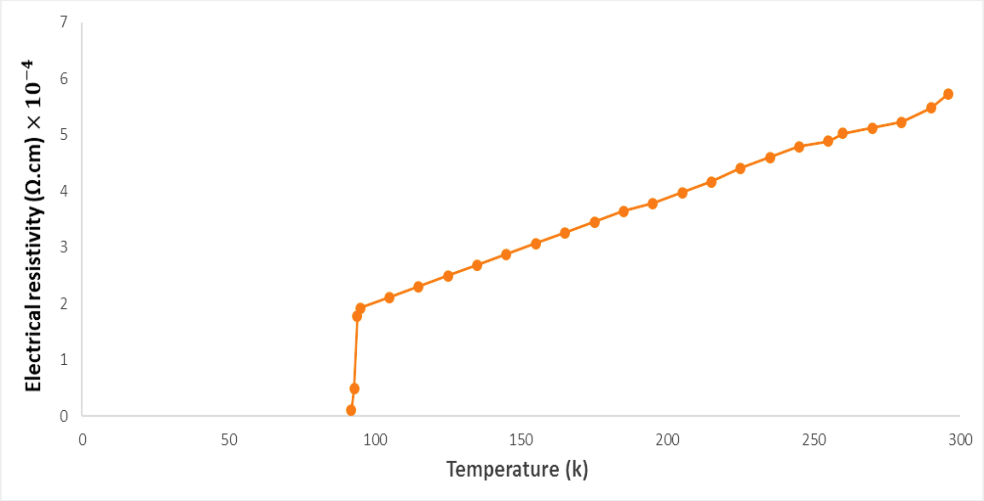

Figure 3. The electrical resistivity for $YBa_2Cu_3O_{6.86}$ compound.

Regarding YBCO-system, it has an orthorhombic unit cell structure with two CuO_2 layers per unit cell. The position of atoms was the way to define the parameter H_1, and H_2, which is the distance between CuO_2 layers and the distance between the CuO_2 layer and the sequence layer respectively [4]. Both H_1 and H_2 are measured along the *c*-axis, so that the distance H_1 was calculated with respect to *c*-axes related to the position of CuO_2 layer mentioned by the following equation

$P(CuO_2\text{-layer}) = 0.11576 \times 11.68 = 1.3520$ Å

Then the multiplication of the last result by two is representing the value of H_1 that is relating to the distance between CuO_2 layers. The elongation of this distance is a sign on the activity between these layers, during the interlayer coupling. It is a sign on the coupling of Cu(2) with the next atom in the chain coupling.

$H_1 = 1.3520 \times 2 = 2.702$ Å

Regarding to the next layer mentioned BaO, it is the next layer with respect CuO_2 layer. It is useful for providing more information about the position of oxygen atoms on the *c*-axis. On the other hand, the correlation between Cu(2)-ion and O(1)-ion is calculating, which are very important in the definition the long of the chain on the c-axis.

$P(\text{BaO-layer}) = 0.3364 \times 11.68 = 3.92915$ Å

The net in position of Cu(2), and O(1) on the chain axis is the difference between the position of above atoms.

$\Delta P = 3.92915 - 1.352 = 2.57715$ Å

The last one is multiplying by the factor two to define the parameter H_2, which means the overall distance between BaO-layer during the whole unit cell. The long of H_2 is a sign on the activity of the layers within the unit cell. The value of H_2 must be greater than H_1, or at least equal to H_1 ($H_2 \geq H_1$). As H_2 increased, it is a sign on the strength of the conductivity in the superconductor unit cell.

$H_2 = 2.57715 \times 2 = 5.1543$ Å

Then the summation between H-values is a function to H_{tot}. It is corresponding to effective of chain length along *c*-axis. On the other hand, it is remarking to the strength of the coupling between the orbitals of Cu(2), and O(1).

$H_{tot} = H_1 + H_2 = 2.702 + 5.1543 = 7.8563$ Å $= c$

The dimensions of the basal plane are measuring during the simulation on the X-ray diffraction. The basal plane is considering the origin of the charge carriers including in the unit cell. These charge carriers are the source to like Cooper pairs including. Then the parameters (*a* and *b*-axis) are mentioned to (L_{sc}, and W_{sc}) respectively. The subscript (*sc*) is a sign to the origin of superconductivity in the orthorhombic unit cell. Where $a = L_{sc} = 3.8203$ Å, and $b = W_{sc} = 3.88548$ Å. Now, there is a layer mentioned by the basal plane dimensions and a chain mentioned by *c*-value. Then the multiplicity of the two parameters W_{sc} and c is remarking to a superconducting channel in the unit cell. It is considering a cross section area for the motion of charge carriers in the unit cell.

$A_{sc} = b \times c$, $A_{sc} = 3.88548 \times 7.8563 = 30.5254$ Å^2

The cross section area is useful to calculate the charge carries including, but the charge density is a function to the number of charges per unit volume. So it is necessary to calculate the density of the charges created in the active region in the unit cell. The active region is a function to the interaction between CuO_2-layers and Cu(2)-O(1) chain, so the volume of the active region is dependent. The volume of active region is:

$V_{sc} = A_{sc} \times L_{sc} = W_{sc} \times c \times L_{sc} = 116.6165$ Å^3

This volume is considering a container for the charge reservation with in the unit cell, so the active charge density are applying to create a like Cooper pairs within the unit cell which is dependent on the following relation

$$N_D = {}^{1}/_{V_{sc}} \rightarrow N_D = {}^{1}/_{116 \cdot 6165} = 8.575111 \times 10^{-3}\ \text{Å}^{-3}$$

$N_D = 8.575 \times 10^{27}\ m^{-3}$

Regarding to the duplicate presences of the active region in the unit cell, it is necessary to multiply the last result by the factor two. Then the total charge density within the unit cell restricted between two basal planes is determining by the parameter N_e.

$$N_e = 2N_D = 17.150222 \times 10^{-3}\ \text{Å}^{-3} = 17.150222 \times 10^{27} m^{-3}$$

These charges density as calculated are electing to produce a carrier pairs during the layers coupling. They are responsible on the normal resistivity created in the superconductor sample. In addition to that, the value of charge density in the range of metallic form. The mean free time for the active charge density is a function to the normal resistivity that was measured practically from the resistivity measurements. The presences of superconductivity is a function to mean free time.

$$\tau = \frac{m_e}{N_e e^2 \rho} = 10.3633 \times 10^{-16}\ \text{sec}$$

A very short mean free time is a function to very long mean free bath, which is a main feature for superconducting concept. The mobility of charge carries is important parameter because it is related to the motivation of the charges and producing like Cooper pairs with the unit cell during the layers coupling in the active region.

$$\mu = \frac{\tau e}{m_e} = 18.2211 \times 10^{-5}\ \text{m}^2\text{V}^{-1}\text{s}^{-1}$$

Normally, the resistivity is a function to the material type. It does not relate to the dimension of the disc sample. Whereas the resistance of the disc sample is depending on its dimension. There is a difference between the resistance of the sample and resistance of the unit cell. Now, backing to Figure 2, the resistance of unit cell is a function of the dimension of active region mentioned by $\left[\frac{H_1 H_2}{c}\right]$. The parameter (2) is relating to duplicate in the resistivity regarding to the symmetry of both sides of unit cell, upper and lower region of unit cell. The parameter $\left[\frac{H_1 H_2}{H_{1+} H_2}\right]$, is a function to equivalent resistance of parallel layers with the unit cell. So the resistance function is relating to unit cell, and it is a function to the number of CuO_2 layers including.

$$\rho(\text{exp}) = \frac{f(R)}{2}\left[\frac{H_1 H_2}{c}\right]$$

$$f(R) = \frac{2 \times 10^{-6} \Omega m}{0{\cdot}8863 \times 10^{-10} m} = 2.25657 \times 10^4 \Omega$$

Actually, the resistance function is relating to the multi-perovskite unit cell, which is function to orthorhombic unit cell. In general, if there is a single perovskite unit cell there is a constant resistance function appeared. It can be represented by single mode resistance function which is about ($1.2906 \times 10^4\ \Omega$) [6]. Then the resistance function of the multi-perovskite orthorhombic unit cell is a function to a single-mode conductor mentioned by resistance function (R_{sm}). A single-mode conductor resistance is the resistance of a ballistic waveguide, which is independent of its length. The contact resistance of a multimode ballistic conductor with $N_{mode} = 1.2.3. ...$, so it is necessary to predicate how many modes including within the unit cell. If $N_{mod} = 2$, is applying then R_{mm} is multimode resistance equal to

$$R_{mm} = \frac{R_{sm}}{N_{mod}} = \frac{2{\cdot}25657 \times 10^4}{2} = 1.12828 \times 10^{\ 4}\Omega = R_{tot}$$

R_{tot} is the predicated total resistivity produced by a active region in a superconducting unit cell.

The last result is approaching to ($R_{sm} = 1.2906 \times 10^4\ \Omega$). That is attributing to the presence of a double perovskite structure including in the orthorhombic unit cell. It is a total resistance related to parallel resistance regarding to parallel active layers including. The proofing of $N_{mod} = 2$ is considering a sign on the number of CuO_2 layers including which is 2-layers. In general $N_{mod} = n_1 \times n_2$, where n_1 is the number of CuO_2 planes/chemical formula which is equal to 2. On the other side, n_2 is the number of chemical formulas/unit cell, which is equal 1 [6].

$$\lambda_{(0)} = \sqrt{\frac{\text{m}_\text{e}}{\mu_\circ \text{N}_\text{e} \text{e}^2}} = 406.2289\ \text{Å}$$

This is the penetration depth at zero temperature, which is the minimum value of the magnetic field inserted. Then the penetration depth at Tc-value is:

$$\lambda = \lambda_{(0)}\left[1 - \left(\frac{T}{T_c}\right)^4\right]^{-\frac{1}{2}} = 779.9125\ \text{Å}$$

The superconducting energy gap is a function to a like Cooper pairs created as a function to coupling energy is:

$$\Delta_{(0)} = \pi K_B T_C = 24.8927\ meV$$

The coherence length is the excitation of the wave function like Cooper pairs (ξ).

$$v_f{}^2 = \frac{\hbar^2}{\text{m}^2}[3\pi^2 \text{N}_\text{e}]^{2/3} = 92.1907 \times 10^4 \text{m/s}$$

$$\xi = \frac{h v_f}{2\pi^2 K_\beta T_c} 243 \cdot 89338422683 \times 10^{-10}\text{m}$$

$$\mathbb{K} = \frac{\lambda}{\xi} = 3.19775 > \frac{1}{\sqrt{2}}$$

The last result is indicting the presence type II superconductor. This is a proof on the exhibiting a high temperature superconductor mentioned by YBCO-system. In addition to that, this is a sing on the successful the conductivity mechanism in YBCO-system during the layers coupling within the unit cell.

Table 2. Indicate the output results related to the structure simulation.

The compound	Crystal structure [Å]	Tc (K)	Conductivity	Resistivity $[10^{-6}\Omega m]$	Resistance function $[10^{4}\Omega]$	N_{mod}	n_1	n_2
$YBa_2Cu_3O_{7-\delta}$	a = 3.8203 b = 3.8855 c = 11.683	92	$\frac{f(R)}{2}\left[\frac{H_1H_2}{c}\right]$	2	2.2565	2	2	1

Table 3. Indicate the output results due to conductivity mechanism.

The compound	N_D $10^{26}m^{-3}$	N_e $10^{26}m^{-3}$	τ $[10^{-16}s]$	μ $10^{-5}m^2V^{-1}s^{-1}$	$\lambda_{(°)}$ $[10^{-10}m]$	λ $[10^{-10}m]$	$\Delta_{(0)}$ [meV]	ξ $[10^{-10}m]$	Order parameter
$YBa_2Cu_3O_{7-\delta}$	85.75	171.50	10.3633	18.2211	406.228	779.912	24.89	243.89	3.1977

4. Conclusion

It has been noticed the simulation XRD-pattern is very important in the predicating the shape of unit cell. The reason of simulation on Y123 superconductor is return to appearing Y123 compound in two phases whether if it is tetragonal or orthorhombic phase. The results of simulation are depending on the experimental data mentioned by Ioddmetric titration, resistivity measurement, and XRD analysis. The important conclusion is considering the success of output results related to conductivity mechanism through the obtaining many important data. These data are very important to prove the presence of type II high-temperature superconductor. They are taken from the x-ray simulation and resistivity measurement. This method is so simple but it is useful in understanding the mechanism of conductivity.

Conflicts of Interest

The authors declare that there is no conflict of interest.

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