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Modeling and Prediction investigation of the resistivity of the Perovskite $La_{0.57}Y_{0.10}Ba_{0.23}Ca_{0.10}MnO_3$ compound

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Abstract

Based on the mathematical model, the electrical resistivity of $La_{0.67-x}Y_xBa_{0.23}Ca_{0.1}MnO_3$ composites was investigated. The model reproduces the essential characteristics of the experimental results and also gives a description of many curves for different magnetic fields between 0 Tesla and 10 Tesla. The simulated results give many interestingfeatures of this composite, the resistivity as afunction of temperature changes due to different electrical fields. For the best mathematic model obtained in this investigation, the best Mean Relative Error (MRE) between experimental and theoretical results is reached at 0.29% for $LY_{0.1}$BCMO.

Simulations results show the prediction of the resistivity versus temperature of $LY_{0.1}$BCMO from different applied magnetic between 5T and 10T, without any experiment using the mathematicalmodel.

Key Words: *Manganite; Metal–insulator transition; Prediction mathematical model; Perovskite*

1. Introduction

Perovskite is calcium titanate natural mineral $CaTiO_3$, a relatively rare mineral having an orthorhombic crystal structure (cubic pseudo). $CaTiO_3$ was discovered for the first time in the roller coaster by Gustav Rose in 1839 and named by reference to the mineralogist L.A.Perovski (1792-1856). The perovskite term was generalized for all the structures described by the formula ABO_3. Most of the compounds which crystallize in this structure have ionic bonds, we mention here perovskites $LnMO_3$ or Ln is a rare earth (Ln = Pr, La, Nd, Sm, Gd, Y ... ..) and M a metal transition (M = Mn, Co, Cr, Ni ... ..). Perovskites are a real treasure chest for materials science. They are functional materials with tailored properties [1-2-3]. Indeed, the richness of their phase diagrams and their ability to absorb strong non-stoichiometry effects for modulating within very wide limits their electronic and magnetic properties. Also, according to their compositions and structures, these materials can be superconducting at relatively high temperatures, transforming the mechanical pressure or heat into electricity, accelerate chemical reactions or experience reduced electrical resistance under the action of a magnetic field. Accordingly, perovskites have many applications in areas as diverse as modern electronics (memories, capacitors, ultrafast electronics ...) [4-5-6-7], automotive pollution control [8-9], photovoltaic cells [10-11] or batteries fuel [12] and transparent ceramics [13-14].

Manganese perovskites have especially been a renewed interest in the discovery of the magneto-called "colossal" in 1993 in thin films of $La_{2/3}Ba_{1/3}MnO_3$[15]. This property, as evidenced by Jonker and Van Santen in 1950 [16], consists of a radical change in electrical resistivity when a magnetic field is applied to these materials. This characteristic makes them interesting for applications such as new read heads in order to increase the storage capacity of hard drives. These manganite perovskite structure adopted for general formulation $RE_{1-x}AE_xMnO_3$ or RE is a cation trivalent rare earth (La^{3+}, Pr^{3+}, Nd^{3+}, Sm^{3+}, Y^{3+}, etc.) and AE is a divalent alkaline earth (Ca^{2+}, Ba^{2+}, Sr^{2+}, etc. .). It is thus possible to obtain complete solid solutions ($0 \leq x \leq 1$) as in the case of $La_{1-x}Ca_xMnO_3$[17] or $La_{1-x}Sr_xMnO_3$ (under certain conditions of synthesis). If stoichiometric compounds of undoped or $REMnO_3$ $AEMnO_3$ respectively type does contain manganese in the trivalent state and tetravalent, any substitution of RE by AE (or vice versa) will result in a doping with holes (or electrons) and thus stabilize a valence mixed Mn^{3+} / Mn^{4+} originally, for example, the exceptional properties of magnetoresistance. One of the fundamental characteristics of these manganitesrespect the strong correlations between structure, electronic properties, and magnetic properties. Also, after recalling some generalities about the structure of these materials and the nature of magnetic interactions in the origin of the observed behavior, we will put forward the important role played by the mixed valence Mn^{3+} / Mn^{4+}.

PerovskiteManganites which we can sum interested crystallize in the perovskite structure of theABO_3 generic formula. In this structure, the Bravais lattice

site B is simple cubic. The oxygen ions occupy the edges of the circles and the cation A occupies the center of the cube. The A site can be occupied by an alkaline earth Ca, Sr, Ba or Pband/or a trivalent element such as La, Pr, Nd ... Site B meanwhile, hosts a transition element such as manganese in if manganites. The transition metal is 6-coordinate octahedral and the coordination sphere of the atom A may vary from IV to XII. Perovskite, in its ideal form cubic, is shown in figure 1. By its ability to be deformed, this structure accommodates a wide variety of atoms in various valencies. It, therefore, enables a wide variety of compositions. This composition is the result of an insertion of an $AMnO_3$ parent compound with an alkaline earth atom has two vacant spaces in its electronic structure, which allows us to write the balance loads the doping reaction is given as follow:

$$A^{3+}Mn^{3+}O_3^{2-} \Rightarrow A_{1-x}^{3+}A_x^{2+}Mn_{1-x}^{3+}Mn_x^{4+}O_3^{2-} \qquad (eq1)$$

Where x is the percentage of substitution

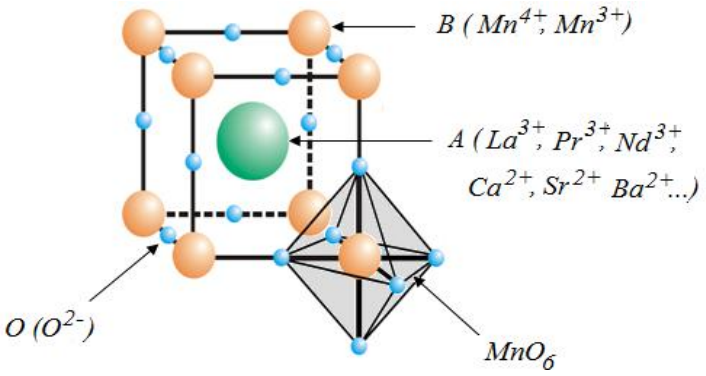

Figure 1. Perovskite structure ideal of $AMnO_3$[18]

It is obvious (in cases where there is no oxygen vacancies or gaps in the site A), according to the charge balance equation, the percentage x control the ionization level manganese ion. Indeed, the introduction of a divalent atom in the parent compound generates ions additional percentages of Mn^{4+} and Mn^{3+}. These ions have two different electronic structures that will play a key role in the study of mechanisms of structural and magnetic transitions through the double exchange mechanism and distortion Jahn -Teller respectively.

On the one hand, the substitutions at the site A were the subject of much research. The principle is to change the average ionic radius of the site A. It does so directly on the structural distortion. The angle of the Mn-O-Mn bond is changed. Thus modifies the orbital overlap of the manganese and oxygen. The double exchange theory provides a ferromagnetic coupling and electrical conductivity maximized for a linear configuration of the Mn-O-Mn bond.

On the other hand, according to Perovskit emanganites of type $R_{1-x}A_xMnO_3$, the electrical conductivity is influenced by the charge transfer when the element R is doped,the Mn^{4+} change to $Mn^{3+}$and creating the holes in the e_g band(band gap energy) by the effect ofHund's rule.This modification of charge between $Mn^{4+}$and Mn^{3+} produces a ferromagnetic coupling which plays a fundamental and a basic element on the electrical conductivity [19].

Here Hund's law states that when several degenerate atomic orbitals (and energy) are free, electrons are placed so as to occupy the greatest possible number. The electrons occupy these degenerate orbitals with identical spins (or parallel) before placing with opposing spins. In a perovskite structure and how to place the valence electrons, one must know the energy gap between the two levels $e_g$and t_{2g} as shown in figure 2. In the case of manganites, the energy gap between these two levels is around 1.5 eV[20]. The four ion Mn^{3+} valence electrons will populate the three levels and a level t_{2g}withe$_g$ under the law of Hund. The presence of the electron on a level e_g is explained by lower energy balance of the system by comparing the energy gap (1.5 eV) between t_{2g} levels and e_g.The interaction energy between two opposite spin electrons on the same level which is about 2 eV[21].

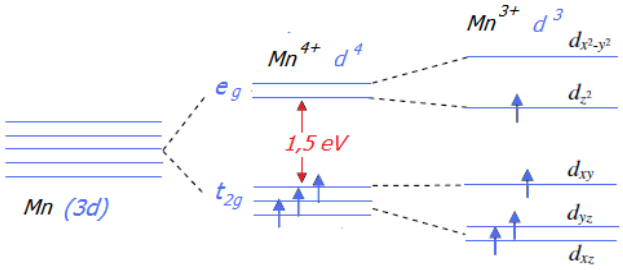

Figure 2. Transfer charge for the structure of $AMnO_3$

In this paper, we study the electrical resistivity of the Perovskite $La_{0.67-x}Y_xBa_{0.23}Ca_{0.1}MnO_3$ based on amathematical model in order to reproduce experimental results and give prediction results at different electrical fields between5 Tesla and 10 Tesla. Section II presents the experimental study of this Perovskite which was prepared at different series of electrical measurements under several magnetic fields from 0 to 5T. In section III, on the one hand a description of themathematical model of resistivity versus temperature at magnetic fields from 0 to 5T is presented. On the other hand, a several comparison withmathematical study is given by indicating the best Mean Relative Error (MRE)equal to 0.29 %. In section IV, Simulations results are given to confirm the prediction of the resistivity versus temperature of the Perovskite at different applied magnetic from 5T to 10T, by using the mathematical model and without any experiment.

2. Experimental study of the Perovskite$La_{0.57}Y_{0.10}Ba_{0.23}Ca_{0.1}MnO_3$

A polycrystalline sample of nominal composition $La_{0.67-x}Y_xBa_{0.23}Ca_{0.1}MnO_3$ was prepared according to the solid-state reaction method at high temperature until 1400 C°. In this work different series of Electrical measurements of this composite sample were carried at different temperature ranging from 240 to 350K under several magnetic fields rising from 0 to 5T.
In this work different series of polycrystalline $La_{0.67-x}Y_xBa_{0.23}Ca_{0.1}MnO_3$samples were synthesized by a conventional solid state reaction as shown in figure 3. It can be noticed that the resistivity decrease with increasing of the field. Also, T_{MI} values are nearly to thehigh-temperature side when the field rises.Where T_{MI} means thetemperature atMetal–Insulator (M–I) transition between ferromagnetic (FM) and paramagnetic (PM) at Curie temperature (T_C) which is usually accompanied by T_{MI}. This transition is specified by a peak in the resistivity appearing at the T_{MI} temperature, nearly the same as T_C[22].This decrease of the resistivity due to the presence of many electrons tunneling, and the increase of the conduction by the applied magnetic field between 0 and 5 T.

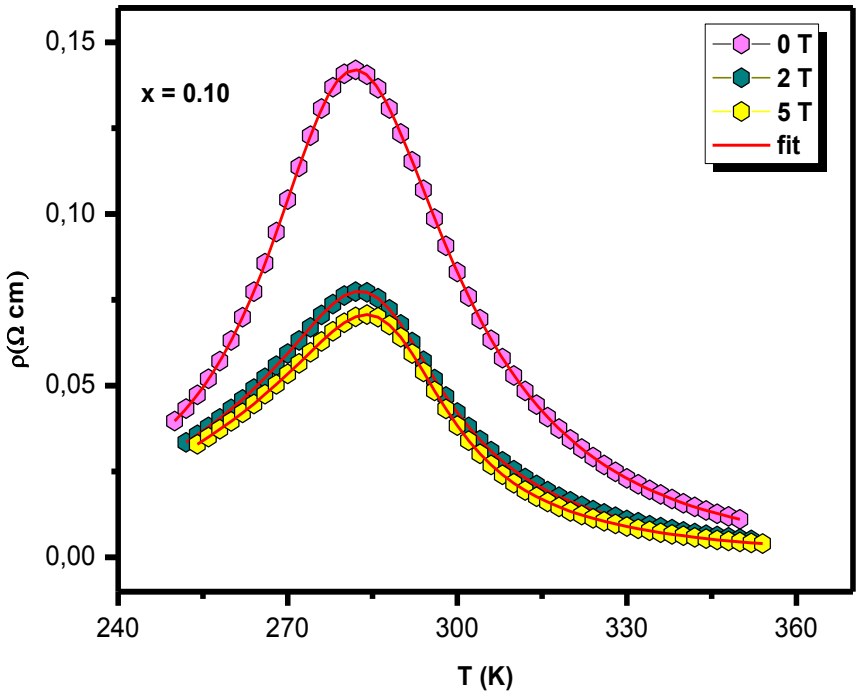

Figure3. Resistivity versus temperature of $LY_{0.1}BCMO$ under different applied magnetic field for0T, 2T, and 5T

Figure 3 illustrates the temperature dependence of the resistivity of the sample under different magnetic fields viz. 0 T, 2 T and 5 T. From this figure it's clear that the resistivity at a given temperature is found to decrease with increasing field. The decrease of the resistivity may be due to the fact that the applied magnetic field induces delocalization of charge carriers and increases the metallic phase fraction with the help of the external field leading to the large enhancement of conductivity. This behavior present an important characteristic in perovskite and the main of this work is to apply a mathematical model in order to find a new solution to predict the effect of the magnetic field in the resistivity.

3. Modeling of Resistivity versus temperature of LY0.1 BCMO under different fields

A mathematical model is a description of a system using mathematical concepts. The process of developing a mathematical model is termed mathematical modeling. Mathematical models are used to explain a system and to study the effects of different components, and to make predictions about behavior. In this paper,it is noticed that mathematical model is based on different equations in order to approach for experiment results. Hence to evaluate and make a comparison between mathematical model and experiment results it is necessary to specify the error. The error function to be minimized inour study is Mean Relative Error (MRE), and is given asfollow [23]:

Where Experimental output (Y_{Exp}) iscompared with the theoretical output (Y_{Theo}) providedby the user with mathematical method, and n is the number of experiments.

3.1. Modeling of Resistivity versus temperature of $LY_{0.1}$BCMO underField F=0 T

According to figure4, measurements were carried out in magnetic fields of 0 T. A typical plot of resistivity versustemperature in the case of $LY_{0.1}$BCMO.

$$MRE = \frac{1}{n} \times \sum_{i=1}^{n} \left| \frac{Y_{Exp} - Y_{Theo}}{Y_{Exp}} \right| \qquad (eq\ 2)$$

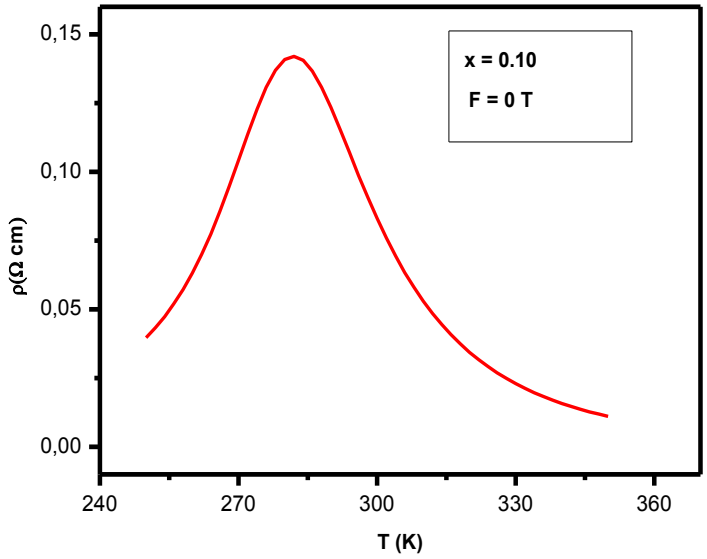

Figure4. Experimentalresistivity versus temperatureof LY0.1BCMOunder applied magnetic fieldF=0T

According to the mathematical method, theresistivity (R) on thevariationof temperature (T) and field (F) is presented by:

Wherea_2, a_3,b_1,b_2,b_3,c_1,c_2,$c_3$are constants given by table 1:

Table 1: different constants used for the resistivity (R) under applied magnetic field F=0T

a_2	a_3	b_1	b_2	b_3	c_1	c_2	c_3
0.06337	0.04153	281.1	283.6	282.9	13.1	24.36	57.77

And A is a function of the field F presented by:

$$A = (p_1 \times F^2 + p_2 \times F + p_3)$$

Where the constant p_1,p_2,$p_3$given by table 2:

$$R = A \times \exp\left(-((T-b_1)/c_1)^2\right) + a_2 \exp\left(-((T-b_2)/c_2)^2\right) + a_3 \exp\left(-((T-b_3)/c_3)^2\right) \quad (eq3)$$

Table 2: different constants to define a function A

p_1	p_2	p_3
0.002633	-0.0164	0.03748

According to figure5,figure6 and figure7, the minimum Mean Relative Errors (MRE) calculated from resistivity between 0 and 0.16 Ω.cm for test data using (eq2) is about 0.29%. Since the error values are low, therefore, it can be concluded that there is good consistency between the experimental and mathematical results for adifferent measurement. Hence, mathematical results can be applied to model the experiments precisely.

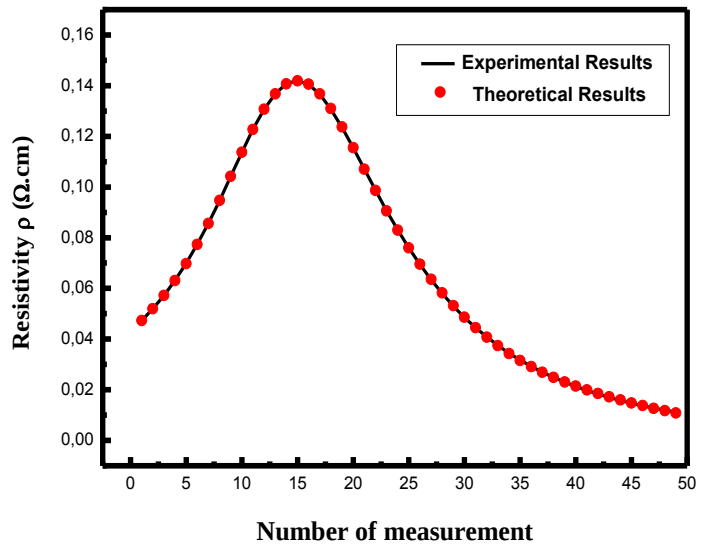

Figure5. Comparison between the experimental and mathematicalof $LY_{0.1}BCMO$values for different number of measurement of the Resistivity under applied magnetic field F=0T

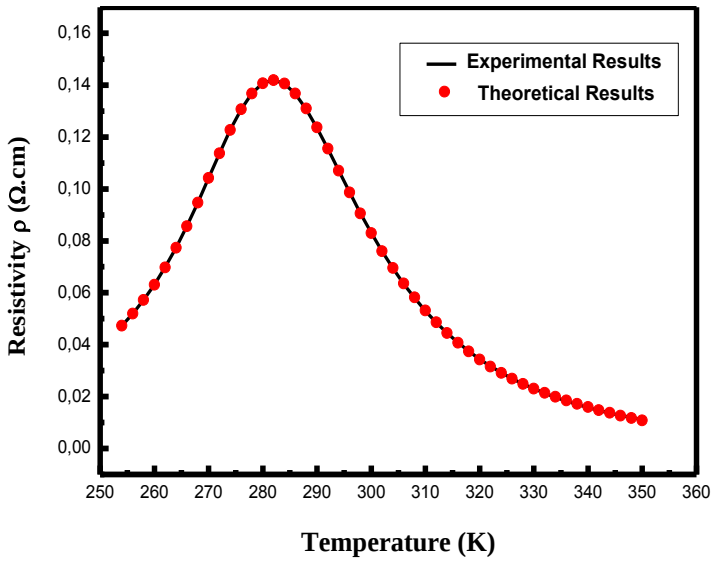

Figure6. Comparison between the Experimental and Theoretical valuesof$LY_{0.1}BCMO$ for different Temperatures under applied magnetic field F=0T

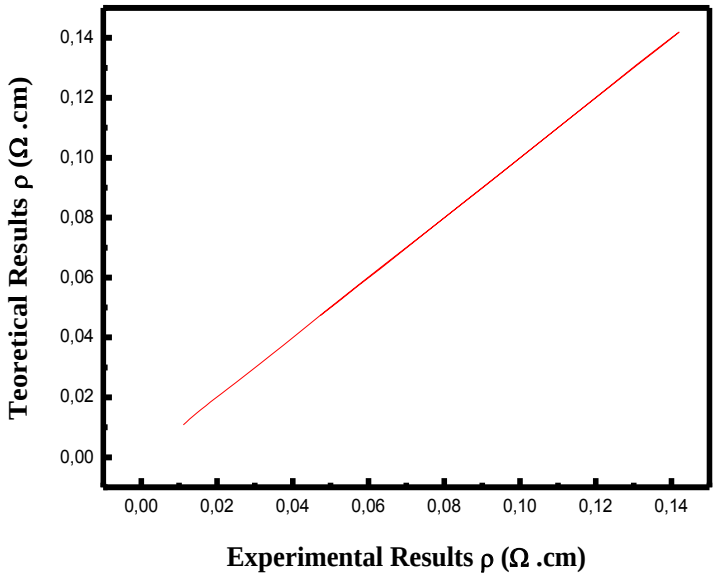

Figure7. Comparison between the experimental and mathematical values of the Resistivityof $LY_{0.1}BCMO$ under applied magnetic field F=0T

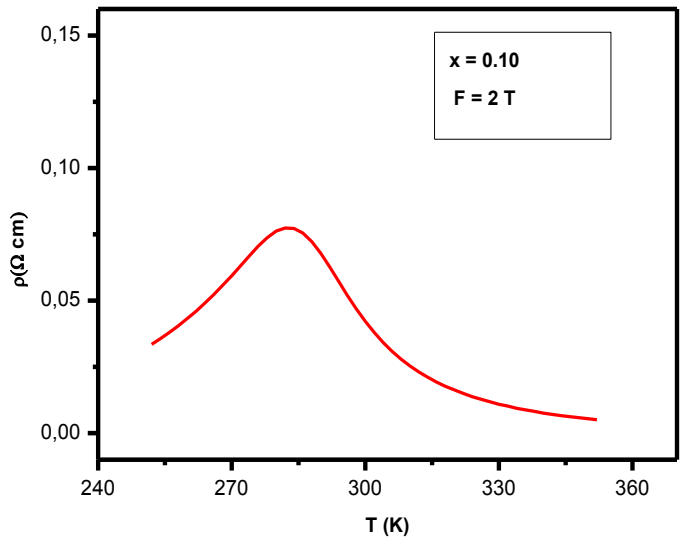

Figure8:Resistivity versus temperatureof$LY_{0.1}BCMO$under applied magnetic field F=2T

Table 3: different constants used for the resistivity (R) under applied magnetic field F=2T

a_2	a_3	b_1	b_2	b_3	c_1	c_2	c_3
0.03556	0.02886	284.4	281.4	266.6	11.34	22.57	63.57

3.2. Modeling of Resistivity versus temperature of $LY_{0.1}BCMO$ underFieldF=2 T

According to figure 8, measurements were carried out in magnetic fields of 2 T. A typical plot of resistivity versus temperature in the case of $LY_{0.1}BCMO$.

According to the mathematical method, the resistivity (R) on thevariationof temperature (T) and field (F) is presented by:

$$R = A \times \exp\left(-((T-b_1)/c_1)^2\right) + a_2 \exp\left(-((T-b_2)/c_2)^2\right) + a_3 \exp\left(-((T-b_3)/c_3)^2\right) \qquad (eq4)$$

Wherea_2,a_3,b_1,b_2,b_3,c_1,c_2,$c_3$are constants given by this table 3:

According to figure 9, figure10 and figure 11, the minimum Mean Relative Errors (MRE) calculated from resistivity between 0 and 0.16 Ω.cm for test

data using (eq2) is about 0.51%. Since the error values are low, therefore, it can be concluded that there is good consistency between the experimental and mathematical results for adifferent measurement. Hence, the mathematicalresults can be applied to model the experiments precisely.

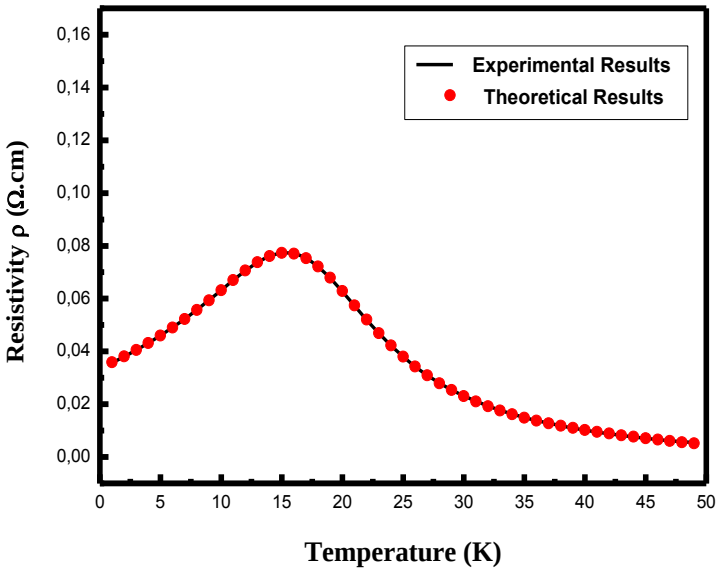

Figure 9. Comparison between the Experimental and Theoretical valuesof $LY_{0.1}BCMO$ for different number of measurement of the Resistivity under applied magnetic field F=2T

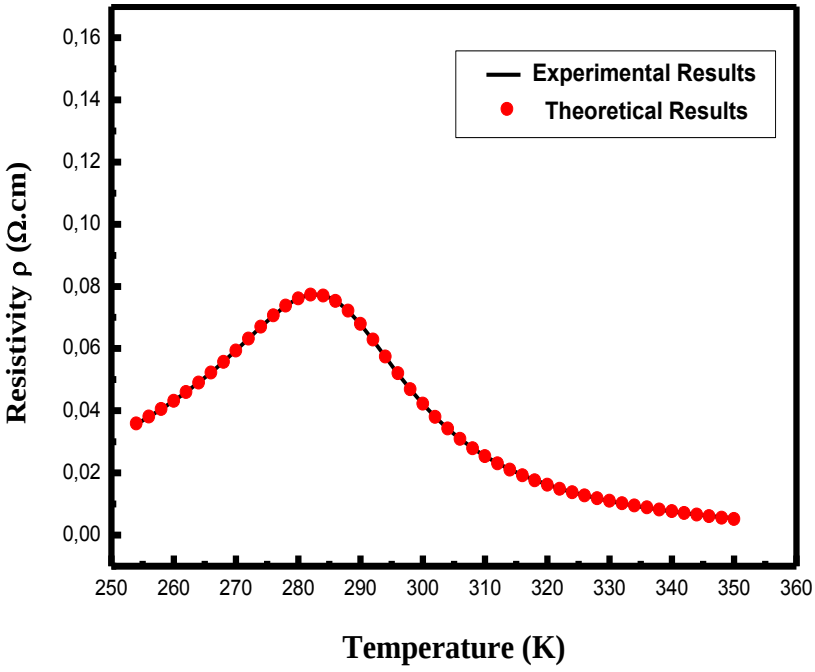

Figure 10. Comparison between the experimental and mathematical valuesof$LY_{0.1}BCMO$ for different Temperatures under applied magnetic field F=2T

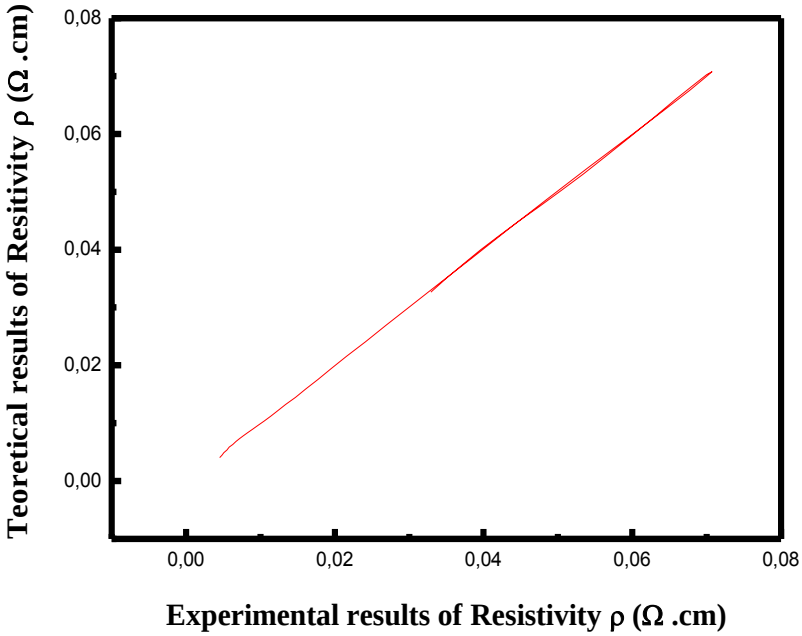

Figure 11. Comparison between the experimental and mathematical values of the ResistivityofLY$_{0.1}$BCMO under applied magnetic field F=2T

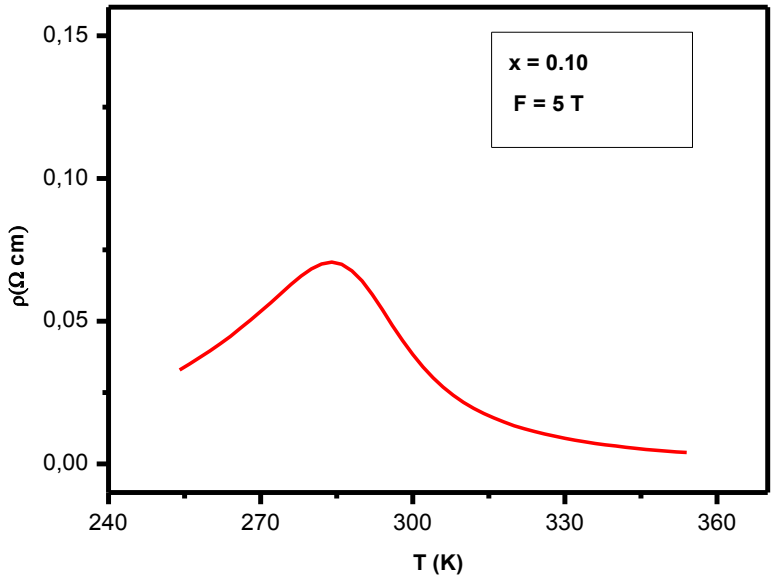

Figure 12. Resistivity versus temperatureof LY$_{0.1}$BCMOunder applied magnetic field F=5T

3.3. Modeling of Resistivity versus temperature of LY$_{0.1}$BCMO under Field F=5 T

According to figure 12, measurements were carried out in magnetic fields of 5T. A typical plot of resistivity versus temperature in the case of LY$_{0.1}$BCMO.

According to the mathematical method, the resistivity (R) on thevariationof temperature (T) and field (F) is presented by:

$$R = A \times \exp\left(-((T-b_1)/c_1)^2\right) + a_2 \exp\left(-((T-b_2)/c_2)^2\right) + a_3 \exp\left(-((T-b_3)/c_3)^2\right) \quad (eq5)$$

Wherea$_2$,a$_3$,b$_1$,b$_2$,b$_3$,c$_1$,c$_2$,c$_3$are constants given by this table 4:

Table 4: different constants used for the resistivity (R) under applied magnetic field F=5T

a$_2$	a$_3$	b$_1$	b$_2$	b$_3$	c$_1$	c$_2$	c$_3$
0.06323	-0.02557	285.7	287	306.5	12.224	41.211	27.444

According to figure13, figure 14 and figure15, the minimum Mean Relative Errors (MRE) calculated

from resistivity between 0 and 0.16 Ω.cm for test data using (eq2) is about 1%. Since the error values are low, therefore, it can be concluded that there is good consistency between the experimental and mathematical results for adifferent measurement. Hence, the theoretical or mathematical results can be applied to model the experiments precisely.

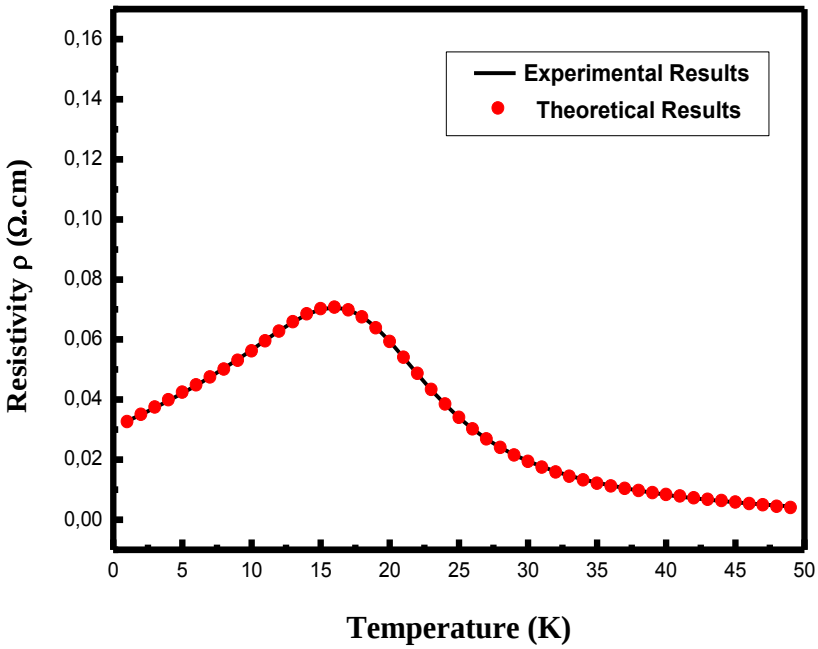

Figure 13. Comparison between the Experimental and Theoretical valuesof$LY_{0.1}$BCMO for different number of measurement of the Resistivity under applied magnetic field F=5T

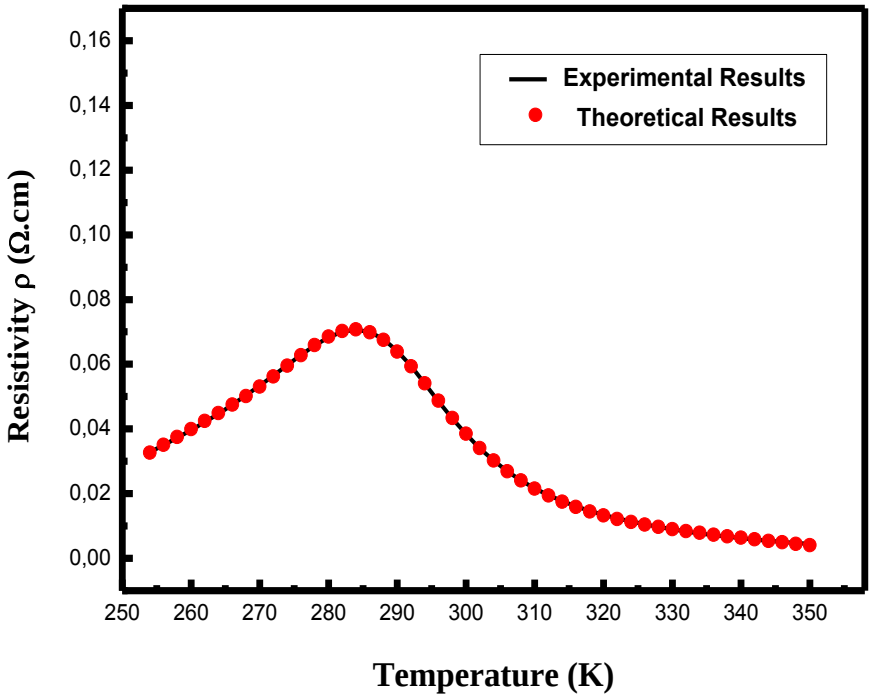

Figure 14. Comparison between the experimental and mathematical valuesof $LY_{0.1}$BCMO for different Temperatures under applied magnetic field F=5T

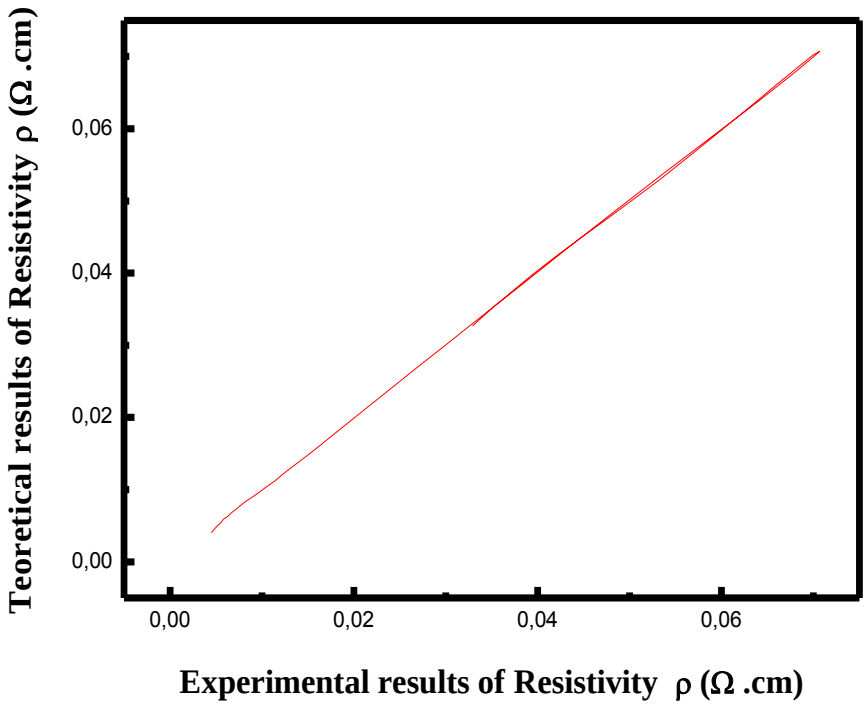

Figure 15. Comparison between the experimental and mathematicalvalues of the Resistivityof $LY_{0.1}BCMO$ under applied magnetic field F=5T

4. Modeling of Resistivity versus temperature of LY0.1 BCMO between Field F=5T and 10T

According to simulations result showing infigure 16, we have estimated the variation of the resistivity as afunction of temperature under different applied magnetic field until F=10T by using (eq 5). Finally, we have attempted to explain the resistivity change obtained from mathematical and experimental. From different curves of resistivity, when the field increased, the resistivity decreased.

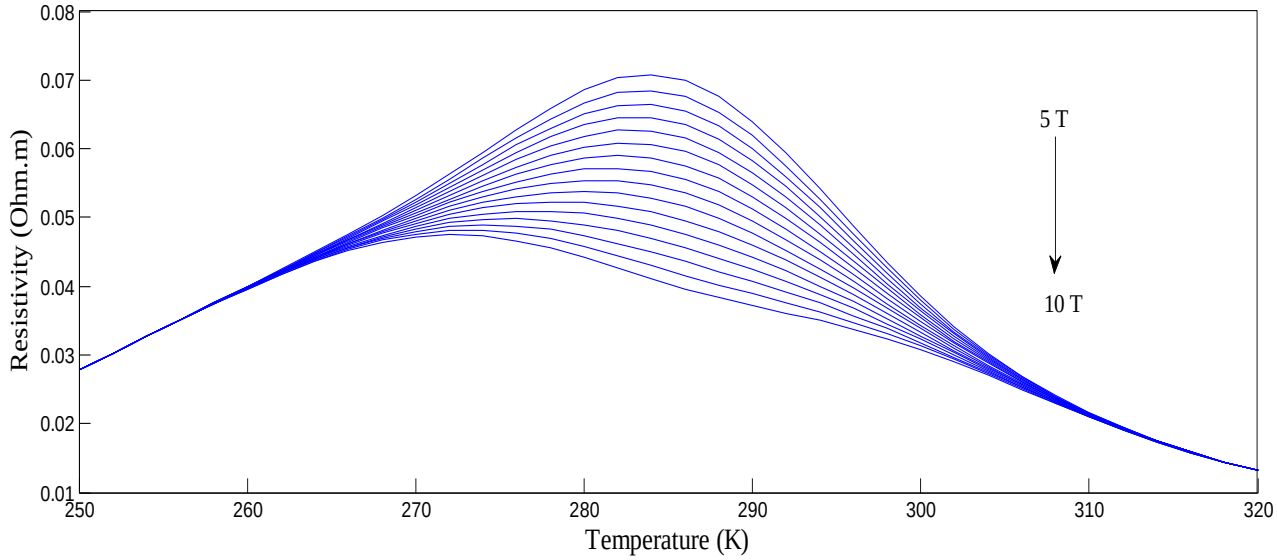

Figure 16:Simulations results of a prediction ofvariation of the resistivity as function of temperatureunder different applied magnetic field from F=5Tto 10T for $LY_{0.1}BCMO$ sample

5. Conclusion

In this work, a series of polycrystalline $La_{0.67-x}Y_xBa_{0.23}Ca_{0.1}MnO_3$ samples were synthesized by a conventional solid state reaction at a temperature between 240 K and 350 K under magnetic fields rising from 0 to 5T as shown in figure 3. On the one hand, we reproduced the experimental results of the resistivity versus temperature of $LY_{0.1}BCMO$ under different applied magnetic field for 0T, 2T, and 5T using the mathematical model. Table 5 shows comparison results between measured and predicted

valuesgiven by mathematical study using Mean Relative Error (MRE) for evaluation. From this table we cana deduced that the the best Mean Relative Error (MRE) is to 0.29 % when we apply a magnetic field F=0 T.

Table 5: The normalized errors of measured and predicted valuesfor different fields

Perovskite at percentage of substitution x=0.1	Field = 0T	Field = 2T	Field = 5T
Mean Relative Error (MRE)	0.29 %	0.51 %	1 %

On the other hand, by using (eq 5) an estimation of the variation of the resistivity as a function of temperature under different applied magnetic field until F=10 T is proposed. We achieved different mathematical curves of resistivity as function of temperature until 10 T of applied magnetic, without making experiment.

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