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Physica C

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A new Y-based HTSC with T_c above 100 K

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ARTICLE INFO

Article history:

Received 16 March 2009

Received in revised form 28 June 2009

Accepted 2 September 2009

Available online xxxx

PACS:

61.05.–C

74.25.Fy

74.25.Ha

74.72.Bk

Keywords:

Y-based HTSC

XRD

Electrical properties

Magnetic properties

ABSTRACT

In search of finding the dominant mechanism in high temperature superconductivity phenomena, the $Y_3Ba_5Cu_8O_{18}$ compound was synthesized through the standard solid-state reaction technique. Characteristic XRD experiment was performed on the samples and was analyzed by the MAUD software refinement program. The analysis results indicate a 358 phase structure with the initial nominal stoichiometry. The electrical resistivity and its behavior under different magnetic field were measured. The electrical resistivity indicates the transition temperature $T_c^{onset} = 102$ K with transition width $\Delta T_c = 2.4$ K. This is the first observation of such a high transition temperature in the Y-based compound. Application of magnetic field leads the resistivity curve to spread out below transition region, and T_c ($\rho = 0$) shifts to lower temperatures. Also, a small broadening is observed by the application of high magnetic field in the T_c^{onset} region.

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1. Introduction

In 1986 Bednorz and Mueller, by substituting Sr in La–Cu–O (La214) compound, reached the superconducting transition temperature above 30 K [1]. On the basis of achieving higher T_c by the hydrostatic pressure applied on La214 [2], by replacing Y^{3+} – with ionic radius smaller than La^{3+} – in the $BaCuO_2$ perovskite, Chu and coworkers increased the transition temperature of $YBa_2Cu_3O_7$ (Y123) to around 92 K [3]. During the past two decades most research has been carried out on the YBCO-family compounds like Y123, $YBa_2Cu_4O_8$ (Y124), and $Y_2Ba_4Cu_7O_{15}$ (Y247) which are different by their number of CuO_2 planes and CuO chains or double chains and their relative positions. The electrons pair in the CuO_2 planes and the chains believed to be the carrier reservoirs. Doping of the carriers occurs by pumping oxygen into the chains. In the La214 compound there is one CuO_2 plane, but the Y123 structure has two CuO_2 planes and one chain. It is shown that by limited increase in the number of the CuO_2 planes in all high- T_c cuprate superconductors to three, the superconducting transition temperature increases [4].

A year after the discovery of superconductivity in the Y123 compound, compounds like Y124 was also synthesized. Y124 compound has one CuO double chain instead of the single chain in the Y123 compound, and becomes superconductor at 80 K [5]. Y247 is another compound based on Y that becomes a superconductor at 40 K [6]. This compound consists of alternative Y123 and Y124 structures with two inequivalent planes, one chain, and one double chain. Also, different Y-based compounds have been reported with different characteristic and structural properties [7].

In this paper, we will report a new compound of the Y-based high temperature superconductor with the highest transition temperature amongst this family of compounds. We will synthesize the samples by the solid-state reaction method and will evaluate its structural, electrical, and magnetic properties.

2. Experimental details

Five samples of $Y_3Ba_5Cu_8O_{18}$ (Y358) compound were synthesized by the standard solid-state reaction technique. Appropriate stoichiometric ratios of 3 N powders of Y_2O_3 , $BaCO_3$, and CuO were mixed, ground, and reacted in air at 840 °C for 12 h, and cooled to room temperature within 5 h. Calcination was repeated twice with intermediate grinding. The powders were reground, pressed into pellets 10 mm in diameter and 1 mm thickness under 10 ton/cm²

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pressure. The sintering temperature was determined by performing the TGA and DT analysis using a STA 16400 system. A single scan involved flowing N_2 gas through the sample chamber and ramping the temperature from 30 °C to 1000 °C at a rate of 20 °C per min. The samples were then synthesized at 890–930 °C for 24 h in an oxygen atmosphere. The samples were cooled to 500 °C and retained in oxygen flow for 10 h. Finally, the samples were furnace cooled to room temperature.

The crystal structure of the samples was investigated by the powder X-ray diffraction technique using Cu K_α radiation ($\lambda = 1.5406 \text{ \AA}$) Joel model JXA-840 diffractometer. The X-ray diffraction patterns were analyzed using the MAUD software refinement program, and the lattice parameters and orthorhombicity were determined.

A four-probe method was used for the resistivity and magneto-resistivity measurements of the samples within the temperature range 10–300 K and magnetic field 0–15 kOe. The size of the samples was $10 \times 3 \times 1 \text{ mm}^3$ and the electrical leads were attached on the long side of the samples by silver paste. The applied ac current was 10 mA with frequency 70 Hz, and the electrical resistance of the samples at room temperature was in the m Ω range. A Lake Shore 330 temperature controller, with a Pt resistor and GaAs diode, was respectively used for indicating and controlling the temperature.

3. Results and discussion

The measured and calculated XRD spectra of Y358 sample with designated Miller indices are shown in Fig. 1. To determine the crystal structure of the samples, the XRD spectrum was refined by the MAUD refinement software program. It is verified that predominantly single phase Y358 structure is formed with Pmm2 symmetry. However, small impurity peaks are observed and designated by (*) on the spectrum. The lattice parameters $a = 3.888 \text{ \AA}$, $b = 3.823 \text{ \AA}$, $c = 31.013 \text{ \AA}$, and unit cell volume $V = 460.971 \text{ \AA}^3$ are obtained from the refinement process. The difference between the experimental and the calculated patterns is shown in the bottom of Fig. 1. By comparing the Y358 sample lattice parameters with those of Y123 that are commonly presented in the literature, it is evident that the main peaks of the Y358 spectrum are the ones which also exist in Y123. The calculated values of a and b parameters of Y358 are very close to the a and b parameters of Y123, but the value of c parameter of Y358 is almost 3 times of the c parameter of Y123. Besides, the Y358 compound has three CuO chains and five CuO₂ planes from which one of the planes has no accompanying

apical oxygen. The twin peaks at 47° indicates an orthorhombic structure for Y358. The orthorhombicity of the sample is equal to $200(a - b)/(a + b) = 1.7\%$. The experimental mass density of the samples is about 4.3 g/cm³ and when compared with the theoretical value of 6.3 g/cm³, indicates some porosity in the samples.

Fig. 2 shows the electrical resistivity of Y358 compound versus temperature. The transition temperature $T_c (= T_c^{50\%}) = 100.1 \text{ K}$ and the transition width $\Delta T_c (= T_c^{90\%} - T_c^{10\%}) = 2.4 \text{ K}$ are evident from the figure. This is the first observation of such a high transition temperature in a Y-based compound. The electrical resistivity curve shows that for temperatures higher than T_c^{onset} , sample shows a metal-like characteristic with $d\rho/dT = 0.0036 \text{ (m}\Omega/\text{K)}$.

The temperature dependence of the electrical resistivity versus temperature for Y358 in the temperature range 95–105 K is depicted in Fig. 3. The values of $T_c^{\text{onset}} = 102 \text{ K}$, $T_c^{90\%} = 101 \text{ K}$, $T_c^{50\%} = 100.1 \text{ K}$, $T_c^{10\%} = 98.6 \text{ K}$, and $T_c(\rho = 0) = 98 \text{ K}$ are obtained from the curve. It is to be noted that the T_c related to Y358 is almost 10 K higher than the values commonly reported for typical Y123 compound. Of course, it is worth mentioning that T_c^{onset} as high as 116 K was observed in some of our samples.

To evaluate the effect of magnetic field on the transport properties, the electrical resistivity of the samples were measured with application of the magnetic field perpendicular to the larger surface of samples and the direction of current. The values of the applied field were 1, 2, 5, 8, 10, 12, and 15 kOe. A typical magnetic field dependence of resistivity of Y358 is shown in Fig. 4 in the range of 0–15 kOe. A very small change of the normal state resistivity and a noticeable broadening of the superconducting transition are observed in the resistivity curve with magnetic field. There are two parts in the mixed state of magnetoresistance curves: A steep part, associated with the onset of the superconductivity in the intragrain, and a transition tail parts due to the weak links coupling the grains. With the increase of the applied magnetic field, T_c^{onset} remains almost constant [8]. The change of resistivity in the mixed state region, due to the thermally activated flux creep, near T_c^{onset} is less sensitive to the magnetic field. The applied field should reach the intragranular critical field value before flux can penetrate the intragranular regions. Below T_c a branching phenomenon appears and $T_c(\rho = 0)$ decreases considerably by 22 K reaching 76 K. This effect is related to the inter-granular weak links of the superconducting material which is more sensitive to the applied magnetic field [9]. In our bulk samples due to the presence of defects and inhomogeneity, a minor broadening is observed near T_c . The effect of magnetic field on the electrical transport properties of Y358 is very similar to those of other 123 systems

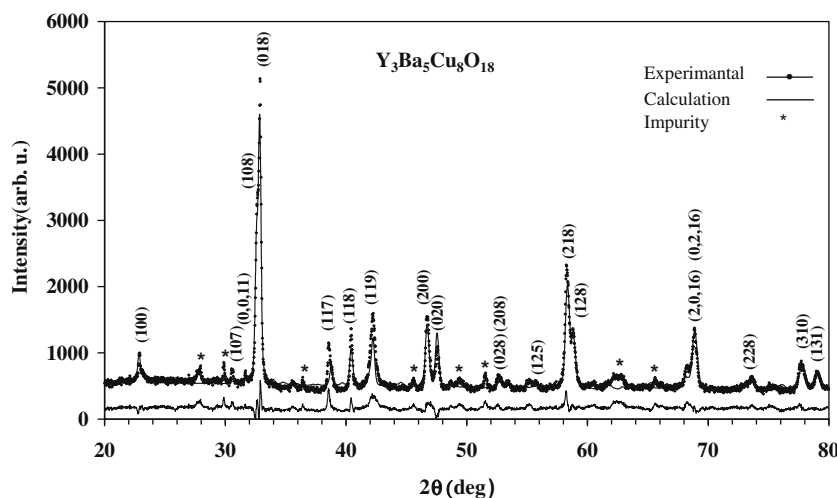


Fig. 1. XRD patterns of Y358 compound. The difference between the experimental points and the calculated line is shown in the bottom.

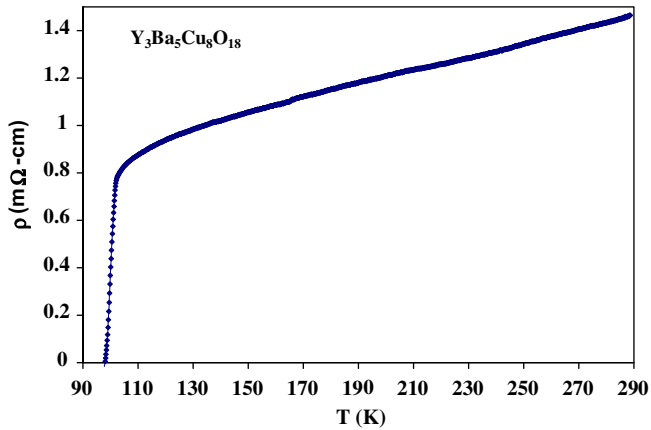


Fig. 2. Electrical resistivity of Y358 versus temperature showing T_c and ΔT_c .

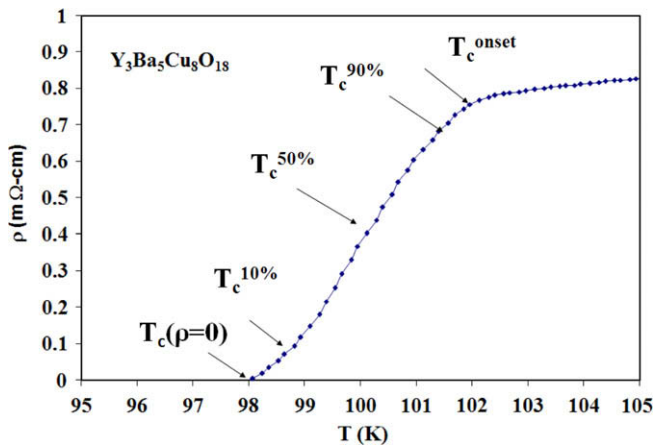


Fig. 3. Electrical resistivity of Y358 versus temperature showing various T_c 's.

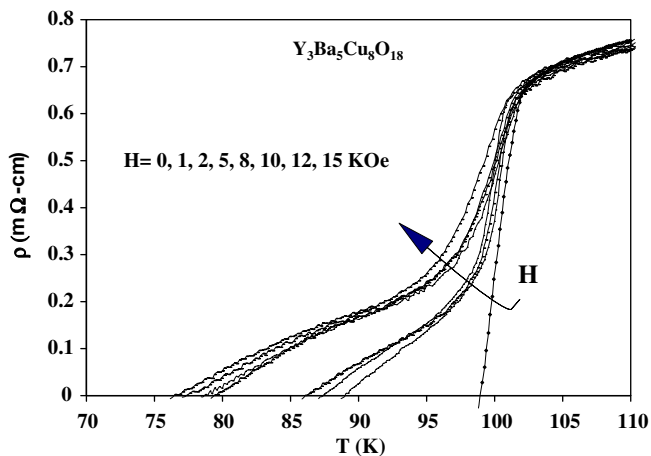


Fig. 4. Electrical resistivity of Y358 versus temperature under application of magnetic field $H = 1, 2, 5, 8, 10, 12,$ and 15 kOe.

[9]. This is expected due to the granular nature of the high- T_c cuprate superconductors.

There are many structural parameters such as the buckling angle, apical oxygen, and the number of CuO_2 planes, CuO chains, CuO double chains, and their relative orientation and placement which influence the electronic structure of the high- T_c cuprate superconductors, and thereby, enhancement of T_c . Recently, our DFT calculations [10] on the hole concentration in the planes and

the chains of different members of the YBCO family and the band structure of the Y358 compound has revealed that the hole content in four of the five planes in Y358 increases, and in the fifth plane, which has no apical oxygen, the hole content decreases. It is also worth noting that in one of the four planes, the content of hole increase puts this plane in the over-doping regime. Putting these all together, it is proposed that only three CuO_2 planes in the Y358 system are in the superconducting regime, which confirms the previous claim that the system with three copper oxide planes has the highest T_c in the cuprates [4].

In addition, it is concluded that in order to have a stronger superconductor with higher T_c in the YBCO-family one should pump more holes from the chains to the oxygen sites of the planes-tending to diagonal charge order; thereby, the apical oxygen which is often located between the two elements has an important role in the superconductivity mechanism.

Appearance of different Y-based compounds with different superconducting transition temperature and their different behaviors under the application of pressure and doping condition is indicative of the fact that chance for finding the optimum Y-based compound with still higher superconducting transition temperature is promising and search should be followed rigorously.

4. Conclusion

The Y123 superconductor compound has two CuO_2 planes and one CuO chain. The Y124 superconductor compound has one double chain instead of the single chain in Y123. The Y247 superconductor compound has one single, and one double CuO chain and one CuO_2 plane. In comparison, the highest T_c Y358 superconductor compound studied in this paper has crystal structure similar to Y123 with the exception of the number of CuO chains and CuO_2 planes, which exceed those in Y123. The Y358 has five CuO_2 planes and three CuO chains. It seems that increasing the number of the CuO_2 planes and also the position of the CuO chains have important effects on the value of the transition temperature in the Y358 compound. The Y358 compound synthesized by the solid-state reaction technique has $T_c^{\text{onset}} = 102$ K. Finally, it seems that Y123 compound is not the optimum compound, and for reaching a still higher transition temperature in the YBCO family, further combination of the components should be synthesized and studied.

Acknowledgments

The authors wish to thank S. Fallahi, M. Mazaheri, H. Hadipour, and A. Tavana for assistance and discussions. This work was supported in part by the National Centre of Excellence in Complex System and Condensed Matter (CSCM), Department of Physics, Sharif University of Technology <<http://cscm.ir>>.

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