Bull. Mater. Sci., Vol. 34, No. 5, August 2011, pp. 1053–1057. © Indian Academy of Sciences.

XRD spectra of new YBaCuO superconductors

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MS received 4 October 2010; revised 17 February 2011

Abstract. **XRD spectra of new YBaCuO superconductors were studied. There were 2 phases found in our samples, the superconducting phase and the non-superconducting phase. The more non-superconducting phase, the more anisotropy parameters were found. The amount of impurities have no effect on the value of *c*-axis which has a linear relation to the number of Cu-atoms. So the new formula of YBaCuO are the new types of superconductor in this family that have higher *c*-axis than the Y123.**

Keywords. **YBaCuO superconductor; solid state reaction.**

1. Introduction

Recently, Udomsamuthirun *et al* (2010) synthesized the new superconductors of YBaCuO materials by solid state reaction. They used the assumption that the number of Ba-atoms plus Y-atoms is equal to the number of Cu-atoms. The new formula of YBaCuO superconductors were Y5–6–11, Y7–9–16, Y5–8–13, Y7–11–18, Y156, Y3–8–11, and Y13–20–23. The XRD spectra and critical temperatures are shown to be the same as that of Y123. However, there are some impurity peaks in their XRD spectra.

The Y123 or $YBa_2Cu_3O_7$ was first discovered by Chu and coworkers in 1987 (Wu *et al* 1987) with $T_c = 92$ K. The other formula in the YBaCuO family compound such as $YBa_2Cu_4O_8$ (Y124), and $Y_2Ba_4Cu_7O_{15}$ (Y247) were found with a critical temperature at 80 K (Marsh *et al* 1988) and 40 K (Bordet *et al* 1988), respectively. The Y247 exhibits a superconducting transition with T_c ranging from 30 to 95 K, depending on the oxygen content (Karpinski *et al* 1989; Genoud *et al* 1992). The $Y_3Ba_5Cu_8O_{18}$ (Y358) (www.superconductors.org; Aliabadi *et al* 2009) becoming superconductor at 102 K was discovered in 2009. The Y358's band structure was calculated (Tavana and Akhavan 2010) which showed similar features with other YBaCuO superconductors.

In this paper, we study on the XRD spectra of the new YBaCuO superconductors of Udomsamuthirun *et al* (2010) samples that were synthesized by solid state reaction. We find an error in their calculations and some new properties have been found.

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2. Samples preparation

The new superconductors of Udomsamuthirun *et al* (2010) samples were synthesized by solid state reaction using raw materials Y_2O_3, $BaCO_3$ and CuO of high purity (99·9%) in the desired atomic ratio. The corresponding weight ratios were mixed, ground and reacted in air at 950°C for 24 h, and cooled to 100°C. The calcinations process in air was repeated twice with intermediate grinding. The powders were regrounded, pressed and sintered at 950°C for 48 h.

The XRD spectra of YBaCuO superconductors as Y123, Y358, Y5–8–13, Y7–11–18, Y156, Y3–8–11, and Y13–20–23 were investigated. Here, a Bruker X-ray diffractometer (D8) with CuKα radiation ($\lambda = 1{\cdot}5406$ Å) and FULLPROF program were used and the refinements were done by using the orthorhombic space group.

3. XRD spectra and discussion

The measured and calculated XRD spectra of our samples i.e. Y123, Y156, Y358, Y3–8–11, Y5–8–13, Y7–11–18 and Y13–20–23 are shown in figure 1. XRD spectra are measured from 10 to 90°. The main peaks are the ones which exist in Y123 sample. The FullProf (Rodriguez-Carvajal 2008) software program is used to determine the crystal structures. We find that the *Pmmm* space group can fit well on the superconducting phase and the lattice parameters are calculated and shown in table 1. However, these results do not agree with our calculations (Udomsamuthirun *et al* 2010). And we find that our former results are not correct

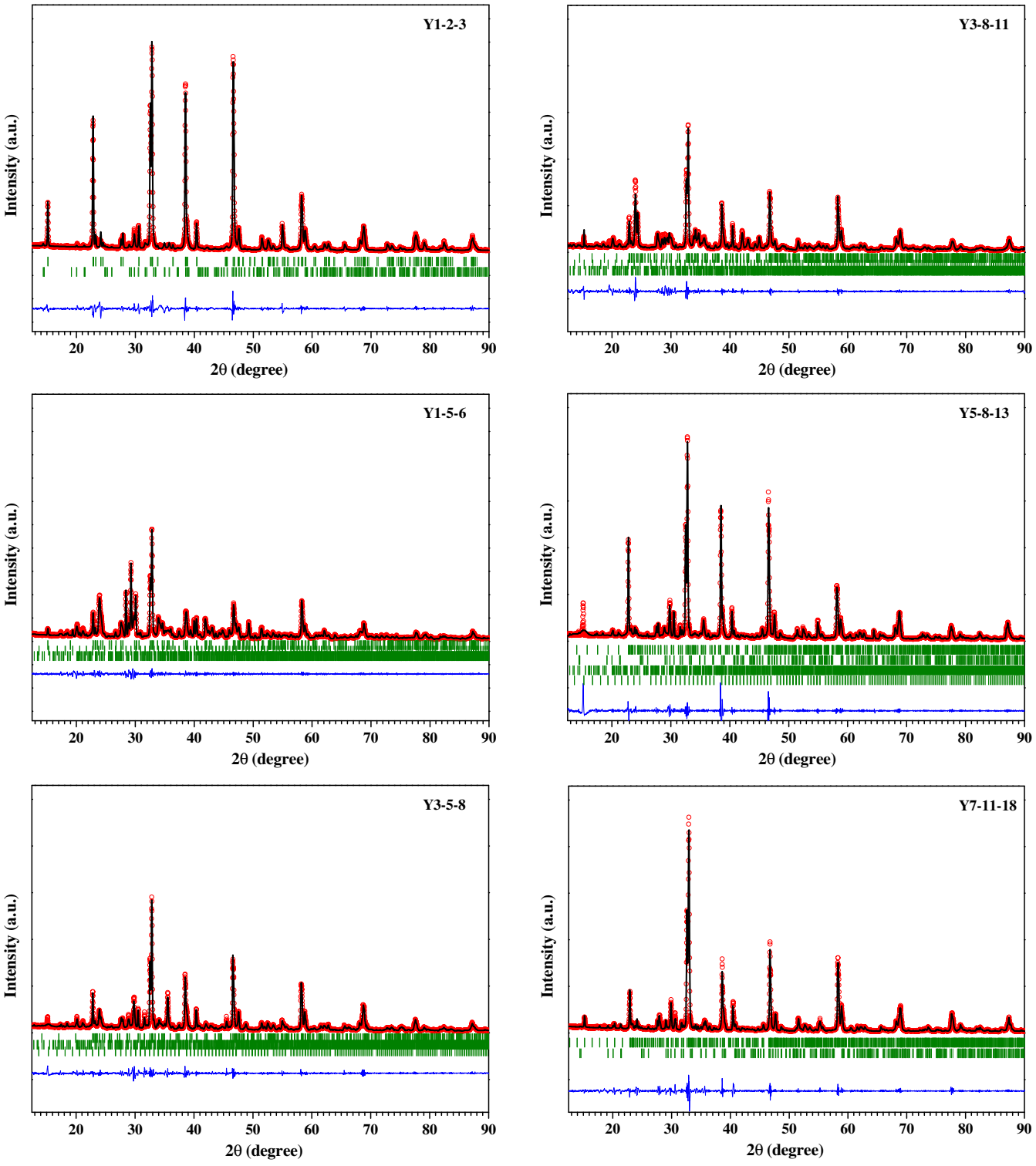

Figure 1. Various XRD patterns of YBaCuO superconductors (Experimental (o), calculated (solid line) and vertical tics below curve indicate Bragg positions).

because we focussed on the peak at 15° which is an important peak in this family. After calculating more accurately, we found that the peak at 15° is not the only main peak of this family but some materials can fit the peak at 15° well and some did not. We also found that the Y358[7]'s result being correct although they showed the spectra only at 20 to 80 degree.

In our samples, two phases were found, the superconducting phase and the non-superconducting phase. The lattice parameters of superconducting and non-superconducting

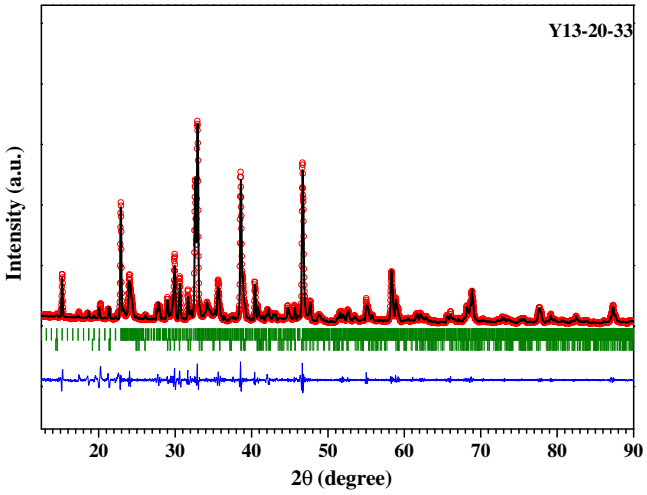

Figure 1. (*continued*).

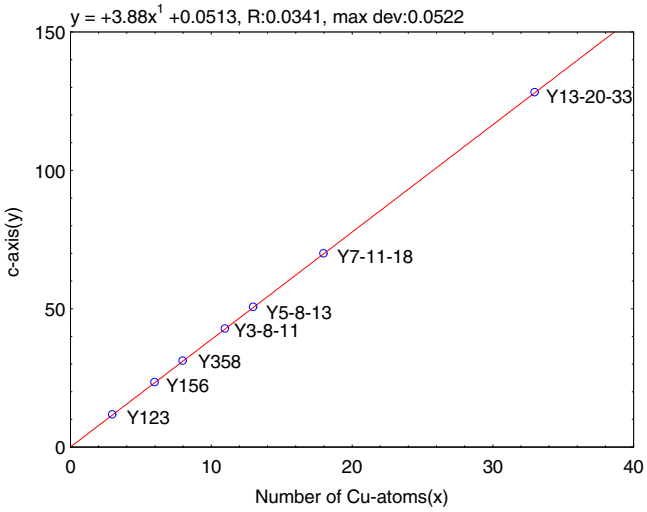

Figure 2. Number of Cu-atoms in our sample versus *c*-axis value from XRD spectra is shown here. Linear relation is found.

Table 1. Lattice parameters of superconducting phase in *Pmmm* space group.

Sample	T_c middle from Udomsamuthirun *et al* (2010)	Lattice parameter a(Å)	b(Å)	c(Å)	c/a ratio	Anis $= \frac{100(b-a)}{0{\cdot}5(b+a)}$
Y123	91·2	3·82192	3·88448	11·68625	3·06	1·62
		0·00007	0·00008	0·00015		
Y156	89·0	3·82175	3·88864	23·35624	6·11	1·74
		0·00013	0·00008	0·00068		
Y358	91·2	3·81914	3·88671	31·16624	8·16	1·75
		0·00009	0·00010	0·00051		
Y3–8–11	91·0	3·81432	3·88471	42·69924	11·20	1·83
		0·00009	0·00007	0·00065		
Y5–8–13	90·8	3·81909	3·89788	50·46070	13·21	2·04
		0·00007	0·00006	0·00088		
Y7–11–18	90·8	3·82378	3·88007	69·87022	18·27	1·46
		0·00006	0·00009	0·00118		
Y13–20–33	89·4	3·81547	3·87768	128·11636	33·58	1·62
		0·00007	0·00007	0·00216		

phases are shown in tables 1 and 3, respectively. The *a*- and *b*-axes lattice parameters of superconducting phases are in the same order of Y123 but *c* axis shows the linear relation with a number of Cu-atoms in the samples that are shown in figure 2. The linear relation is given by

$$c\text{-axis} = 3{\cdot}88\,(\text{number of Cu atoms}) + 0{\cdot}0513. \quad (1)$$

Our slope of '3·88' corresponds to the values of *a*- and *b*-axes of this system. This equation is very important for predicting the value of *c*-axis in the YBaCuO superconductor.

The percentage of phase composition of superconducting phase to non-superconducting phase are shown in table 2. And the lattice parameters of all non-superconducting phases are shown in table 3. There are 3 types of impurities in our samples, Y211, $BaCuO_2$ and $Ba_2Cu_3O_6$. The Y5–8–13 has all of these impurities that agree with a high anisotropy, 2·04%.

According to the percentage of superconducting phase, the anisotropy and the value of *c*-axis of our calculation, we find that our samples can be divided into 2 groups: firstly, the higher superconducting phase compounds that are Y123, Y7–11–18 and Y13–20–33 and secondly, the lower superconducting phase compounds that are Y156, Y358, Y3–8–11 and Y5–8–13. The higher superconducting phase compounds

Table 2. Percentage of phase composition of different samples.

Sample	Superconducting phase	Non-superconducting phase		
		Y2–1–1 *Pbnm*, *Pnma*	$BaCuO_2$ *Im*-3*m*	$Ba_2Cu_3O_6$ *Pccm*
Y123	94	6	-	-
Y156	17	-	19	64
Y358	22	-	20	59
Y3–8–11	21	-	2	77
Y5–8–13	28	12	12	48
Y7–11–18	66	34	-	-
Y13–20–33	74	26	-	-

Table 3. Lattice parameters of non-superconducting phase of our samples.

Sample	Non-superconducting phase								
	Y2–1–1 *Pbnm*, *Pnma*			$BaCuO_2$ *Im*-3*m*			$Ba_2Cu_3O_6$ *Pccm*		
	a(Å)	*b*(Å)	*c*(Å)	*a*(Å)	*b*(Å)	*c*(Å)	*a*(Å)	*b*(Å)	*c*(Å)
Y123	7·14030	12·19212	5·65228	-	-	-	-	-	-
	0·00070	0·00114	0·00055						
Y156	-	-	-	18·30958	18·30958	18·30958	13·04129	20·61419	11·42767
				0·00027	0·00027	0·00027	0·00029	0·00049	0·00030
Y358	-	-	-	18·29320	18·29320	18·29320	13·04490	20·65844	11·43265
				0·00000	0·00000	0·00000	0·00030	0·00045	0·00024
Y3–8–11	-	-	-	18·34700	18·34700	18·34700	13·02698	20·57860	11·41451
				0·00000	0·00000	0·00000	0·00024	0·00039	0·00019
Y5–8–13	12·18664	5·66623	7·12762	18·36461	18·36461	18·36461	13·05099	20·66645	11·43439
	0·00033	0·00019	0·00018	0·00377	0·00377	0·00377	0·00014	0·00024	0·00018
Y7–11–18	12·15761	5·64962	7·12308	-	-	-	-	-	-
	0·00040	0·00017	0·00013						
Y13–20–33	12·16495	5·64337	7·12744	-	-	-	-	-	-
	0·00027	0·00017	0·00013						

have lower anisotropy parameters than the lower superconducting phase compounds. The more non-superconducting phase, the more anisotropy parameters are found. And there is no relation between amount of superconducting phase on the value of *c*-axis. As the *c*-axis is increased, both higher and lower superconducting phases are found. We can conclude that the amount of impurities have no effect on the value of *c*-axis and (1) does not depend on the amount of impurities so that the new formula of YBaCuO is the new type of superconductor found in this family.

4. Conclusions

We study on the XRD spectra of the new YBaCuO superconductors of Udomsamuthirun *et al* (2010) synthesized by solid state reaction. We found some errors in their calculation. Two phases were found in our samples, the superconducting phase and the non-superconducting phase. The more non-superconducting phase, the more anisotropy parameters are found. The amount of impurities have no effect on the value of *c*-axis that show linear relation to the number of Cu-atoms. So the new formula of YBaCuO is the new type of superconductor found in this family which has higher *c*-axis than the Y123.

Acknowledgements

The author would like to thank Prof. Suthat Yoksan for useful suggestion. The financial support of the Office of the Higher Education Commission, Srinakhariwirout University and ThEP Centre, are acknowledged.

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