------ Raf. Jour. Sci., Vol. 16, No. 1 Physics, Special Issue, pp. 65-74, 2005 ------

Determination of the Relative Directions of YBCO HTS thin Films with Respect to ZrO_2 Single Crystal Substrate

Bassam M. Mustafa
Department of Physics
College of Science
Mosul University

(Received 24/10/2001 ; Accepted 15/2/2003)

ABSTRACT

In this research a method is proposed to determine the direction of the axis of YBCO HTS (high temperature superconductor) thin films epitaxially grown on ZrO_2 single crystals, with respect to the directions of axis of crystals of ZrO_2 of the substrate, using the data from Laue and osillating crystal methods. .After making calculations on Laue and vibrating crystal difraction pictures by projecting them on computer screen, the lattice parameters was determined by drawing the reciprocal lattice picture.The angle between the YBCO and substrate crystals was found to be 45 degree. This method can be equally applied to determine the direction of any epitaxially grown thin film with respect to the crystals of the substrate.

تحديد الاتجاهات النسبية لأغشية YBCO الفائقة التوصيل ذات الدرجة الحرارية العالية بالنسبة لبلورات ZrO_2 الاحادية والتي تمثل الارضية

الملخص

في هذا البحث اقترحت طريقة, لتحديد اتجاهات المحاور البلورية للأغشية الرقيقة من نوع YBCO الفائقة التوصيل ذات الدرجة الحرارية العالية,وذلك بالنسبة لاتجاهات محاور بلورات الارضية ZrO_2 وذلك باستخدام البيانات التي حصل عليها بطريقة لاوي وطريقة تذبذب البلورة. وبعد اجراء الحسابات على صور لاوي وطريقة تذبذب البلورة من خلال اسقاطها على شاشة الحاسوب تم تحدبد الأبعاد البلورية من خلال رسم صورة الشبيكة المقلوبة لبلورات اغشية YBCO وتلك التى للأرضية. وقد وجدنا ان الزاوية بين اتجاه بلورات YBCO وبلورات الارضية تساوي 45 درجة. علما انه يمكن تعميم هذه الطريقة لتحديد اتجاه اية اغشية بلورية منماة على ارضيات من بلورات احادية.

INTRODUCTION

Soon after the discovery of the high temperature superconductivity HTS (Bednorze and Muller, 1986), the YBCO superconductor was found to have very interesting properties. (Sharp, 1990), on the other hand YBCO thin film epitaxially grown on different crystal substrates was found to reveal further fascinating properties, which may bring various devices like superconducting cables, motors, generators, into application (Lynn and Muller, 1990). One of the best applications of YBCO thin films was to use them as a natural Josephson Junctions (Ovsyannikov et al., 1994; Song et al., 1997). So good informations must exist about the situation of YBCO crystals with respect to their substrate and about their lattice parameters to cover the ever-increasing .revolution in micro electronic (Mustafa, 2001).

In this paper an x-ray method was designed based on the analysis of the data from Laue, and vibrating crystal methods, for finding the relative directions of YBCO thin film crystals (or any other epitaxially grown films) relative to the single crystal of the substrate, this is done by comparing the principle and the first order reflections in the diffraction pattern pictures of the vibrating crystal with the reflection predicted by a computer model of the reciprocal lattice R. L.

EXPERIMENTAL

The data used in this paper (Laue and vibrating crystal diffractograms on which I depend in this paper, is shown in figs.1,2,3,6,7,9 in a form of computer images which greatly simplifies the measurement) which comes from an experiment which I did at the solid state department at Moscow State University on a sample consists of a single crystal of YBCO epitaxially grown on ZrO_2 substrate with its flat surface perpendicular to (100) direction .The samples were prepared in the geological dept. at Moscow State University. The aim of the experiment was to direct the sample with respect to the x-ray direction and to make a preliminarily estimation of the lattice parameters. The YBCO thin film was grown with its c-parameter along the (100) direction of the substrate. In reality the direction of growth is some what deviated from the (100) direction of the substrate (within few degrees) due to the way of cutting the crystal or small error in the horizontallity during the preparation of YBCO films, for this reason the four fold axis of symmetry is somewhat deviated from the x-ray direction, as shown in (fig. 1), (which is a Laue diffraction pattern, taken with the x-ray perpendicular to the surface of the sample).

By projecting the poles on the Wolf net the four-fold axis of symmetry is corrected to coincide with the x-ray direction as shown in (figs.2, 3).

The figure shows two kinds of diffraction spots, which is due to the diffraction from the thin film and the form the substrate. The next step is to align the sample such that one of the base-axis a or b will be horizontal as shown in (fig. 3), so if we consider the ray direction as z-axis then the c-axis of YBCO crystal and 100 direction of the substrate will coincide, therefor a or b will be along the x-axis as in (fig 4).

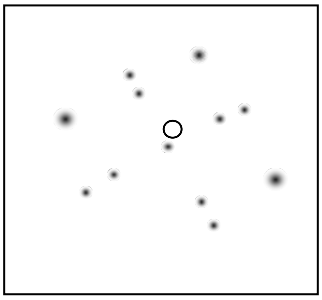

Fig. 1

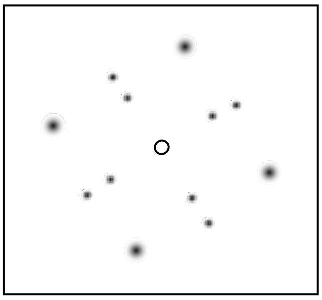

Fig. 2

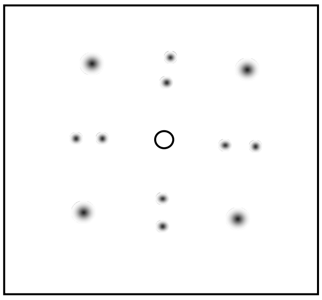

Fig. 3

Fig.1 undirected sample.
Fig. 2 partially directed sample.
Fig.3 totally directed sample.

Fig. 1,2 ,3 showing Laue diffraction patterns of YBCO thin film

To determine the structure of any crystal one of the favorable methods is to us one of the rotating crystal methods and we chose the vibrating crystal methods for its simplicity and by using the same Laue CAMERA.

The vibrating crystal experiment is done with a device which consist as in fig. 5 from Lane Camera in which the goniometer can be rotated within limited angle such that the diffracted x-ray spots is totally full on the cassette of the Laue camera, the speed of rotation can have different values depends on the pattern which we want.

For example from our experience and in order to have good pattern the crystal must vibrate within its angular range for half an hour. In contrast to Laue method vibrating crystal uses monochromatic x-ray and we use Cu radiation.

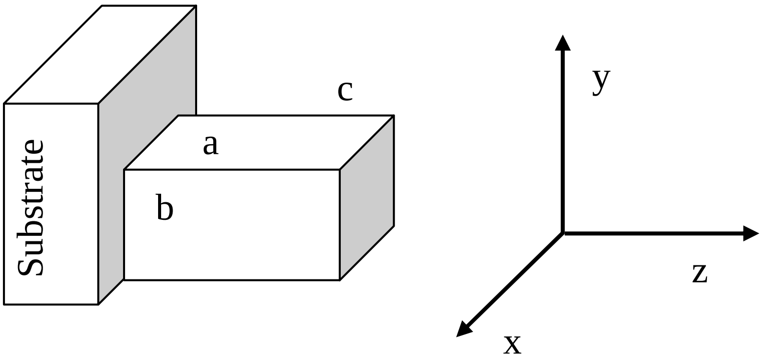

Fig.4:Schematic representation of position of YBCO crystal with respect to substrate referance frame.

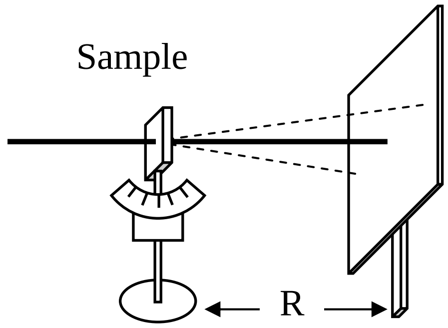

Fig.5: Experimental setting of the vibrating crystal method of measurment.

THEORY

If we look to the diffractograms of the vibrating crystal (Fig 9,10,11) we see that the diffraction pattern is consisting of a principle horizontal pattern in the middle and two curved first order patterns above and below the principal one .the principle horizontal line can can easily interpreted on Bragg law directly and for the geometry of the YBCO film and that of the substrate i.e.:

$$2d \sin \theta=\lambda \quad .... \quad (1)$$

$$\frac{1}{d^2}=\frac{h^2}{a^2}+\frac{k^2}{b^2}+\frac{l^2}{c^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots \quad (2)$$

Sense h = 0 ; k = 0 then

$$\frac{1}{d^2}=\frac{l^2}{c^2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.. \quad (3)$$

the wavelength of Cu –K α line of the x-ray used is :

λ=1.54 A^o

from the former discussion the c lattice parameter can be identified . The problem is with first order patterns which can not interpreted as in the former procedure .For this reason the reciprocal lattice picture for YBCO and ZrO_2must be drawn

In order to draw reciprocal lattice picture, we muse find the reciprocal lattice vectors A,B, and C. This can be done by using lattice parameters a, b and c for YBCO whose values are 3.82 ,3.88,11.7 A respectively then the reciprocal lattice vectors $\overline{A},\overline{B},\overline{C}$ of YBCO will be;

$$\overline{A}=2\pi\frac{\overline{b}\times\overline{c}}{\overline{a}\,.\,\overline{b}\times\overline{c}} \qquad \overline{B}=2\pi\frac{\overline{c}\times\overline{a}}{\overline{a}\,.\,\overline{b}\times\overline{c}} \qquad \overline{C}=2\pi\frac{\overline{a}\times\overline{b}}{\overline{a}\,.\,\overline{b}\times\overline{c}} \quad \ldots\ldots\ldots\ldots(4)$$

after substitution by the values of the lattice parameters

A= 1.8 A^{-1} B= 1.8 A^{-1} C= 0.6 A^{-1}

The drawing of the three dimensional reciprocal lattice is not an easy job. Fig. 6 shows the three dimensional reciprocal lattice for YBCO.A thorough study of this picture shows that in the direction of the C-axis we have the reflections (001), (002),(003), (004)…….etc from the planes which is perpendicular to the along the direction of the arrow and can be calculated using eq.(3) .These reflections comes from the planes (001), (002),(003), (004)……..etc which is perpendicular to the lattice direction c.

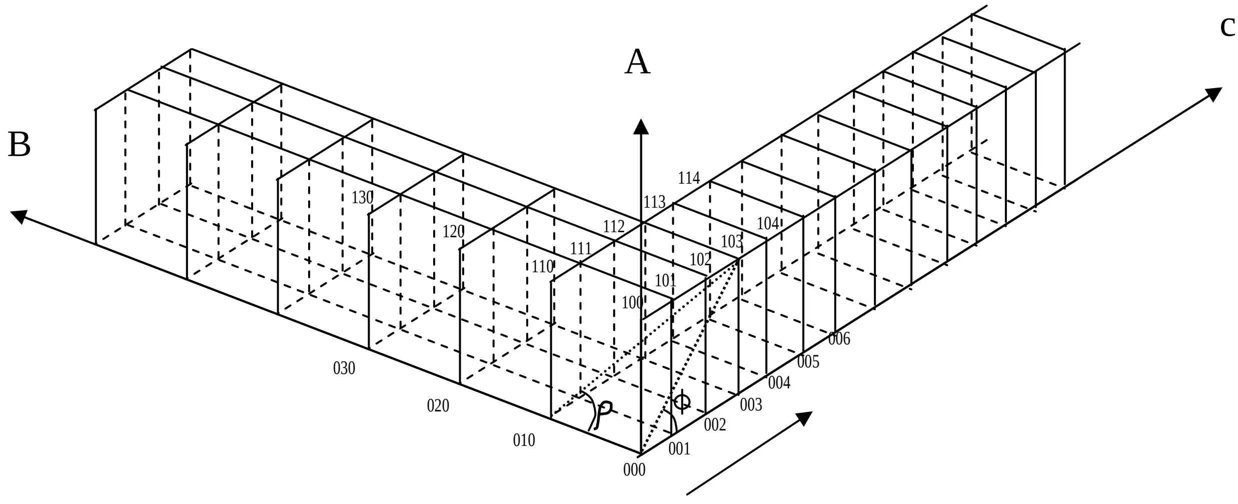

Fig.6: Three dimensional diagram for the reciprocal lattice for YBCO.

Along the upper edge of the same reciprocal lattice and in the direction of the C-axis along the direction of the arrow we see the reflections 101, 102, 103, 104 …….etc, these reflections happens at the the planes (101) ,(102) , (103),(104)……etc ,which are inclined planes in which two lattice parameters are shared, the (c) and the (a) lattice parameters. this enable us to determine the lattice parameter (a) , the values of the L.P (a) can be calculated according to the formula:

$$a \text{ or b} = \frac{\lambda}{\mathrm{m_n}}\sqrt{R^2 + r_n^2} \qquad \text{……………………………………….(5)}$$

where R represents the distance of the film from the sample λ wavelength of monochromatic x-ray and m_n and r_n are shown in (fig. 7) which is one of the first order vibrating crystal pattern. By turning the sample by 90 degrees around the c-axis of the YBCO, we will the reflections 011, 012, 013, 014………etc. Which comes from reflections from the planes (011), (012), (013), (014)………etc. which are inclined planes in which two lattice parameters are shared , the (c) and the (b) lattice parameters . this enable us to determine the lattice parameter (b), the values of the L.P (a) can be calculated according to the formula (5).

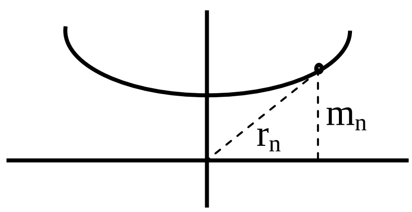

Fig. 7: Geometrical representation of the method for measuring the lattice parameters from vibrating crystal diffraction data.

Till now we have distinguished the directions of YBCO crystals with respect to the x-ray. the values of the L.P. of YBCO. these two physical quantities are essential for obtaining a clear concept of the problem of finding the relative directions of the YBCO and ZrO_2 with respect to each other.
The same procedure can be repeated for ZrO_2crystals taking into account that ZrO_2 crystals are of cubic structure with L.P. a = b = c = 5.07 A .The R.L. for ZrO_2 is shown in fig 9. The values of the L. P. can be found according to eq 3. Fig 8 shows the V.C. pattern which will be interpreted below as belongs to ZrO_2, from which the L .P. for it can be found according to eq 5.

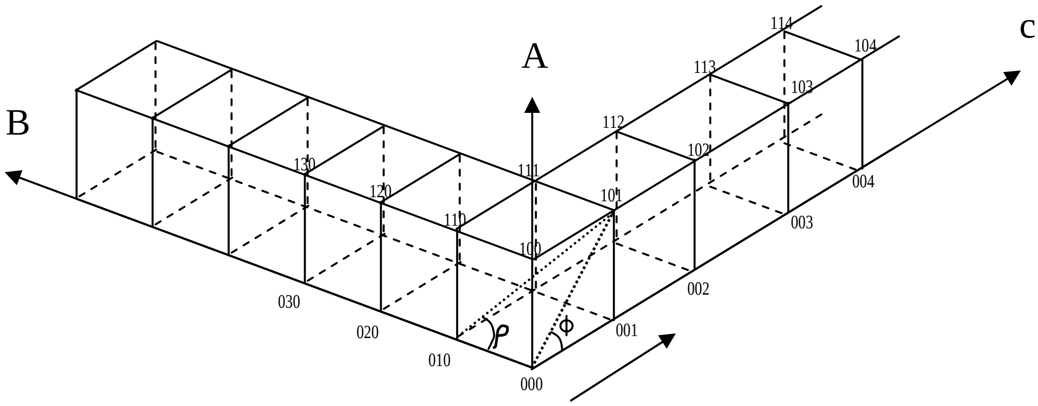

Fig. 8 Three dimensional diagram for reciprocal lattice of ZrO_2 substrate .

Having found the directions of YBCO and ZrO_2crystals with respect to the reference frame which concides with x-ray direction ,we can determine the relative direction of each crystal with respect to the other which we will consider in the next section.

CALCULATIONS AND RESULTS

The central principle line contains many spots ,from the R. L. (fig 9) we see that along the C-axis we have reflection from the planes (l00) . table 1 contains the hkl values and the corresponding values of diffraction angles 2θ. Using eq 3, the L.P.of the c- planes of the thin film and the substrate can be determined. The results of measurement are:

For the thin film c = 11.7 A ; For the substrate c = 5.1 A .Which is in good agreement with the real values .Which means that the c –axis of the sample concides very well with the direction of x –ray .

The upper and lower patterns in (Fig. 9) is due to reflection h0l or 0kl (because the a or b parameters may be along the x–axis) This clear from (Fig.9) Which is a drawing of the reciprocal lattice of the YBCO. Therefor the upper and lower patterns are due to reflections h0l or 0kl, Therefor if the lattice parameter (a) of the film are parallel to that of the substrate, therefor h0l or 0kl of both will exist simultaneous. But if there are some angle between them each will reveal its own pattern when we align at the correct angle.

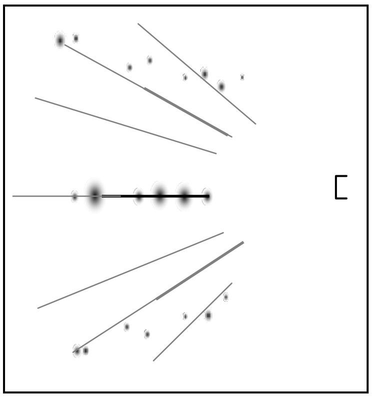

Fig.9: Vibrating crystal diffraction pattern showing principle and first order diffraction points.

Table 1: Principle diffraction Data.

Hkl	2q
002	15.17
003	22.86
004	30.65
002 sub	35.27
005	38.58

Results of analysis of the pattern of (fig. 9) using eq. (5) is shown in table 2:

Table 2:Diffraction data for the (a) lattice parameter.

m_n/mm	**r_n/mm**	**a A^o**	**Hkl**
18.9	25.4	3.86	103
20.4	31.7	3.85	104
22.75	40.2	3.84	105
26.1	51.8	3.86	106

R: equals 40 mm

The average value of a is equal to 3.85 A^o which is close to the value of a parameter of YBCO which is equal to 3.82A^o.

Fig.10 shows diffraction pattern when the sample was turned by 90^o around the c-axis (z-axis) or x-ray direction, the diffraction pattern is similar to that of (fig.9) the result of measurement is shown in table 3.

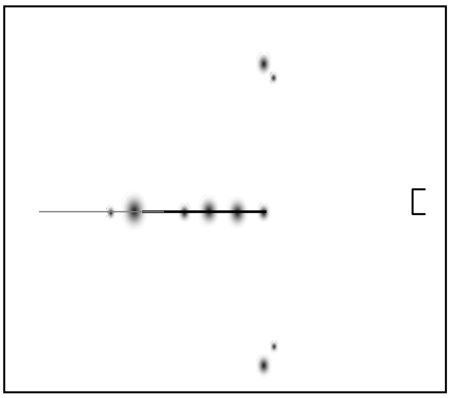

Fig.11: Vibrating iffraction pattern of the substrate after 45 degree rotation.

Table 3: Data for the determination of the (b) Lattice parameter.

M_n	r_n	(b) A	Hkl
18	25	4.04	103
20	31.3	3.91	104
22.25	39.5	3.89	105
25.5	51	3.91	106

The average value of the lattice parameter is 3.94 A, which is close to the lattice parameter b of the YBCO, which is about 3.88 A^o. Thus it is clear that for the studied directions of both the (a) and (b) for the YBCO crystal, and from figures 6 and 9, and tables 2 and 3, we can not find any reflection which is related to the substrate in the upper and the lower first order patterns .Whereas reflection 002 of the substrate exists in the central pattern of both, and in table 1, if we return to the Laue diagrams of figures 1, 2 and 3, we found that we have two kinds of four fold axis within 45^o from one another so when the sample was turned by 45^o around the z-axis and starting from the situation of (fig.9) and taking a vibration crystal picture of this new situation a diffraction pattern similar to that of (fig. 9) and (fig. 10) is shown, which contains the first order reflections 102 of the substrate as shown in (fig. 11). The result are written in table 4.

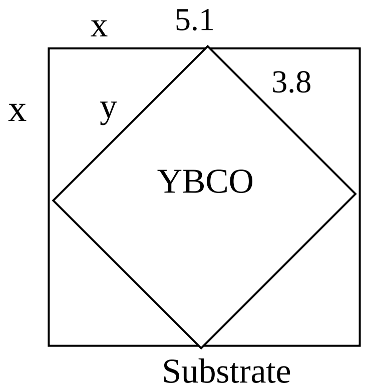

Fig.12: Schematic diagram of the position of of YBCO crystal with Respect to the sustrate crystal.

Table 4 : Diffracion data for the Substrate.

r_n	M_n	Hkl	(a)A
24	13.75	102	5.16

As shown in the table, the lattice parameter of that crystal is equal to 5.16 which is the lattice parameter of the ZrO_2 crystal. When the sample wasturned another 90^o from the final situation we get a diffraction pattern like that of fig. 10 so the situation of YBCO crystal with respect to that of ZrO_2 substrate is as shown in (fig. 12). By simple geometry we can find that the situation fulfill that $y^2 = x^2 + x^2$.

CONCLUSIONS

1- Relative orientation of single crystal YBCO HTS thin films can be measured successfully using a method of mixing Laue and vibrating crystal methods with a comparison with reciprocal lattice picture.
2- The a direction of the YBCO crystals is inclined by 45^o with respect to 010 direction of ZrO_2.
3- This method is a general method which can be used generally to any epitaxially grown thin film of a single crystal substrate.

REFERENCES

Bednorz, J.G. and Muller, K.A.,1986. Possible High Tc Superconductivity in Ba-La-CuO System, Z. Phys. B. Vol. 46, pp.189-193.

Gilbert, A.M.G.; Medici, A. H.; Schuller, I.K.; Schmidl, F. and Seidel, P., 1999. Photodoping of YBaCuO Grain Boundary Joseohson Junctions, Journal of Superconductivity, Vol. 12, No. 1,pp.121-123.

Lynn, J.W., 1990. High Temperature Superconductivity, Springer, New York.

Mustafa, B.M., 2002. Theoretical Study of a Signal Generator in GHz Using High temperature Superconductors, Raf. Jour. Sci, Vol.13,No.4,pp.105-117 .

Ovsyannikov, G.A.; Ivanov, Z.G.; Mygind, J. and Pederson, N.F.,1994. Microwave radiation from 2-D array Josephson Junction, Physica, B, 194-196, pp.107-108.

Sharp, J.H., 1990. A review of crystal chemistry o mixed oxides superconductors ,Br. Ceram. Trans. J., 89, pp1-7.

Song,I.;Eam,Y.;Park,G.;Lee,E.H. and Park,S.J.,1997. Microwave coupling for frequency-locked Josephson Junction arrays, Appl. Phys. Lett.Vol 70,No.24 ,pp.3290-3292 .