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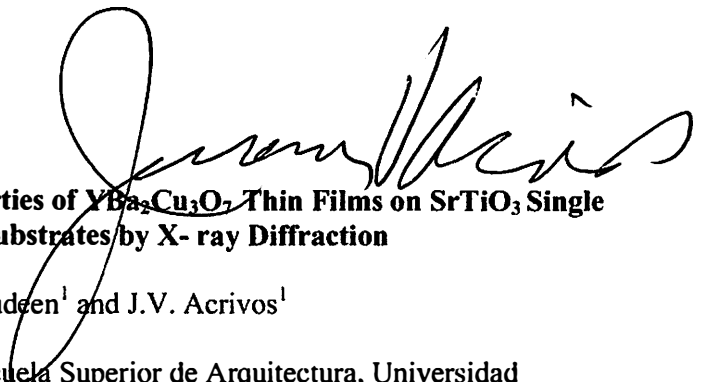
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Comparative Study of Structural Properties of YBa$_2$Cu$_3$O$_7$ Thin Films on SrTiO$_3$ Single Crystal and Bicrystal Substrates by X- ray Diffraction

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ABSTRACT

We present a comparative study in terms of structural properties deduced from X - ray diffraction diagrams between YBa$_2$Cu$_3$O$_7$ (YBCO) thin films fabricated on SrTiO$_3$ (STO) single crystal substrates and bicrystallines substrates with a symmetrical tilt angle of 24 degrees. Periodic Lattice Distortions (PLD) have been found around several Bragg peaks in YBCO thin films deposited on STO bicrystals while only diffraction peaks appear in the diagrams corresponding to the YBCO thin films deposited on STO single crystal substrates. Only in regions far away from the grain boundary the PDL have been investigated. Scans along different (h, k, l) directions allow us conclude that the q_{PLD} vector associated to the distortion is along the (h,-k,0) direction. However, we found that the amplitude of the components of the q_{PLD} vector are depending of the Bragg peak chosen. Such result indicated we have not a PDL with a simple q_{PLD} vector. In this line, other (h, k, l) directions must be investigated to deduce the exact origin of the PLD distortion. Independent on the q_{PLD} vector associated to the PLD, we believe such distortion is consequence of the stress field induced by the grain boundary in the YBCO thin film on the bricrystal.

INTRODUCTION

A major research effort in high-temperature oxide superconductors is the growth of high – quality thin films, in particular those based in YBa$_2$Cu$_3$O$_7$ (YBCO). Special interest has the fabrication of YBCO Josephson junctions, because of their application potential such as the fabrication of Superconducting Quantum Interference Devices (SQUIDs) [1]. The most widely used technique for the fabrication of Josephson junctions is the epitaxial growth of YBCO thin films on bicrystalline substrates with one tilt grain boundary: the grain boundary Josephson junctions (GBJJs). For those applications a good understanding of the precise microstructure of the material deposited on the bicrystal is required. At present, although some structural analyses using techniques like transmission electron microscopy (TEM) have been performed [2], most valuable information has been mainly derived from the transport and electromagnetic parameters associated to this kind of structures. In fact, we have an extensive previous experience in the study of such parameters of YBCO Josephson junctions fabricated on bicrystals with different tilt disorientation angles [3-5].

At this stage, we do not unequivocally understand the precise microstructure of YBCO thin films deposited on bicrystals. Previous studies using the TEM technique have been mainly focused in a detailed analysis of the facet topography and grain boundary dislocation content of the crystallographic grain boundaries because is the region where the most distortion is produced. However, no detailed studies have been performed in the two grains far away from the crystallographic grain boundary. Then, we believe that chemical and structural information of these systems may be obtained by means X- ray diffraction. This technique could bring new data to complete previous studies and be sensible to some distortions difficult to detect by other techniques. In this sense, we report a comparative study in terms of structural properties derived from the analysis of X - ray diffraction diagrams between YBCO thin films fabricated on SrTiO$_3$ (STO) single crystal substrates and bicrystallines substrates with a symmetrical tilt angle of 24° degrees. Side bands have been measured in the Bragg peaks with h and k index different from cero of the YBCO thin films deposited on STO bicrystals while only the diffraction peaks have been observed in the diagrams corresponding to the YBCO thin films deposited on STO single crystal substrates. Such side-bands reveals a PLD in the structure of the YBCO thin film deposited on the bicrystal. The PLD usually appear in low dimensional solids near a phase transition, e.g., metal to insulator transitions. In this case, we believe the distortion induced by the grain boundary in the YBCO thin film is the responsible of the presence of the side bands in the X-ray diagrams.

EXPERIMENTAL

YBCO films having 50 nm thickness and c- axis orientation were epitaxially grown in a high pressure pure oxygen dc sputtering system on single crystal substrates and bicrytalline substrates of STO oriented (100). The symmetrical tilt angle of STO bicrystals were 24 degrees, geometry used in our previous experiments on the analysis of transport and electromagnetic properties of grain boundary Josephson junctions. During the deposition process the substrate temperature was 900 ° C. The accurate control of film growth process with our sputtering system has been previously demonstrated [6]. Transition temperatures (T_C) are in the range of 89.5-91 K, transitions widths smaller than 0.2 K and critical current densities higher that 10^6 A/cm^2 at 77 K.

At this stage of our study, only regions far from the grain boundary have been investigated in the YBCO thin films deposited on the STO bicrystal. The data were collected using a four-circle diffractometer at beam line 7-2 at Stanford Synchrotron Laboratory. The X-ray beam line was conditioned by a focusing mirror and adjustable slits providing a focus spot 1 mm wide and 1 mm high at the sample. A monochromatic X – ray beam was obtained from the wiggler spectrum via a Si (111) double-crystal monochromator and an X – ray energy of 8048 eV was selected.

Most diffraction studies published in the literature have been performed on YBCO single crystal and no side bands have been detected. We believe it is the first time a detailed diffraction study have been performed on YBCO thin films on bicrystals. Although the structure of the YBCO thin films is also depending on the technique used for the deposition procedure, the stress induced in the thin film by the grain boundary have to be considered. In the sense, a study of the origin of the PLD observed in these YBCO thin films is of great interest because of the technological applications of the Josephson junctions fabricated using bicrystalline substrates.
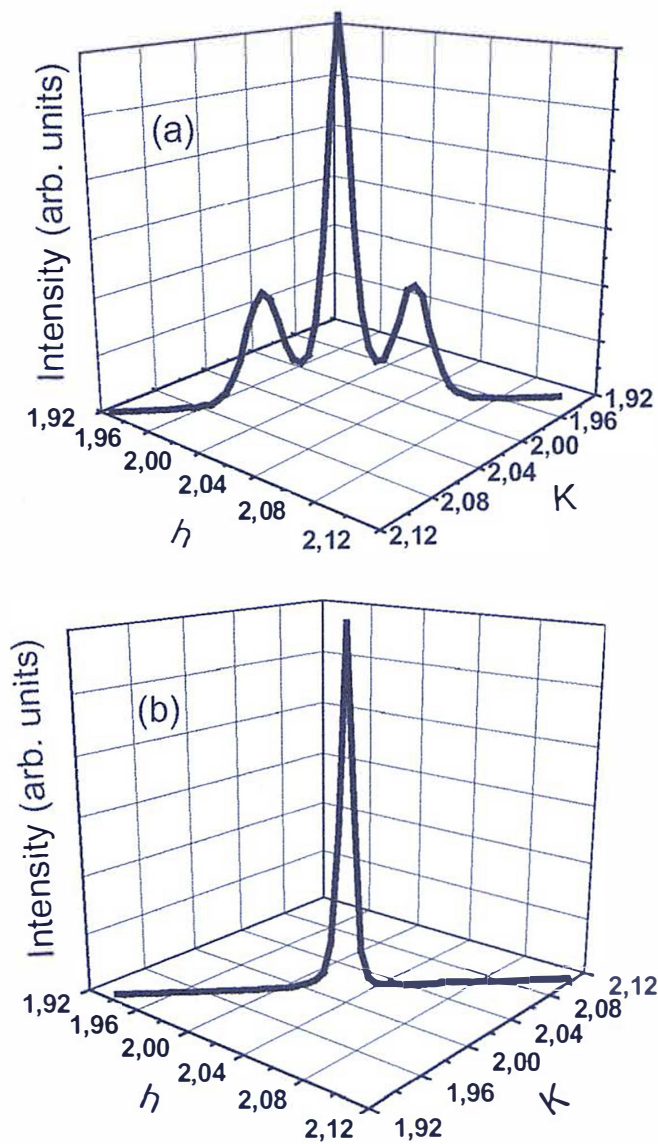

Figure 2. (a) h,-k scan and (b) h, k scan corresponding to the (222) Bragg peak.

RESULTS AND DISCUSSION

In figure1 we have plotted the diffraction scans around (112) peak measured for one YBCO thin film deposited on one STO bicrystalline substrate and on one STO single crystal substrate. While only the Bragg peak is observed in the case of YBCO thin films deposited on single crystal substrate, side-bands associated to a PLD are measured around the Bragg peak of YBCO thin films deposited on bicrystalline substrates. The side-bands have been observed in the Bragg peaks of all the YBCO thin films deposited on bicrystalline substrates [7] (by the high pressure technique) we have studied.
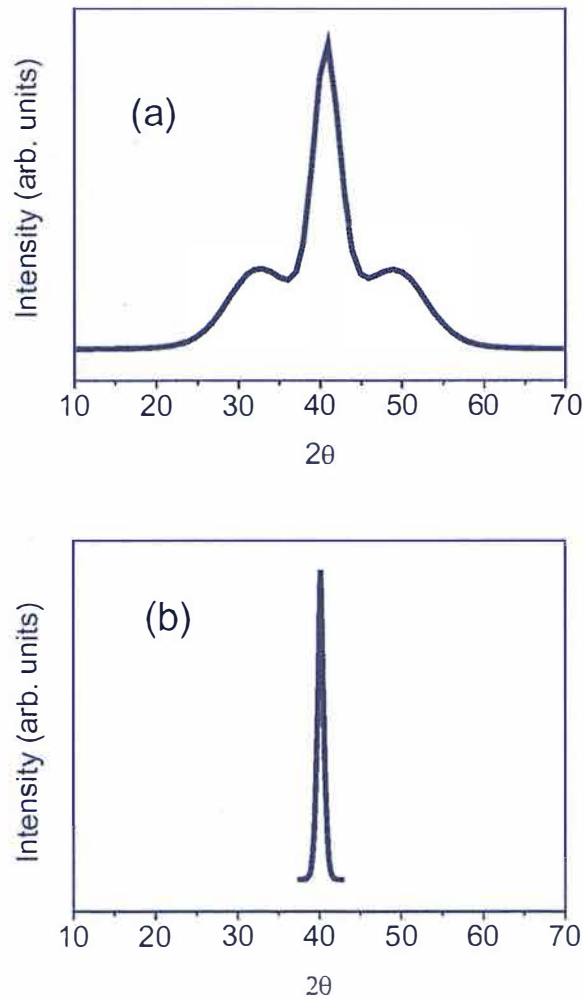

Figure 1. X- ray diffraction diagrams around (112) diffraction peak corresponding to one YBCO thin film deposited on: (a) one STO bicrystalline substrate with a symmetrical tilt angle of 24° and (b) one STO single crystal.

The side-bands presence is an indication a distortion is present in the YBCO thin film deposited on bicrystal. The direction of the distortion is described by the components of the q_{PLD} vector in the reciprocal space deduced from the position of such side bands. The side bands have not been detected in the Bragg peaks with index (001). That points to the q_{PLD} vector is in the a-b plane of the thin-film. Considering such result, and in order to bring more information on the direction of the q_{PLD} vector, scans along the (h, -k,0) and (h, k,0) directions have been performed in the Bragg peaks where the PLD distortions are detected. In figure 2 the scans corresponding to the (222) Bragg peak have been plotted. The results give evidence that the distortion is along the (h,-k,0) direction. The (h,-k,0) components of the q_{PLD} vector can be deduced from these scans just subtracting the (h k l) index of the Bragg peak from the (h k l) index of the side band. However, we found, the amplitude of the distortion in the reciprocal space is depending on the Bragg peak considered. This means that the side-bands peaks are not coming from a "simple" periodic lattice distortion with only a q_{PLD} vector. In Table I we show the components of q_{PLD} vector deduced from the side-bands position in different Bragg peaks.

(h k l) Bragg	q_{PLD}
3 2 2	(0.038, 0.038,0)
2 3 2	(0.038, 0.038,0)
2 2 1	(0.03, 0.03,0)
2 2 2	(0.03, 0.03,0)
2 2 4	(0.03, 0.03,0)
1 1 4	(0.016, 0.016,0)

Table I. Components of the q_{PLD} vector deduced from different Bragg peaks analyzed.

In this line, new experiments have to be designed to bring new data on the precise nature of the distortion observed. However, at this first stage of our study, other important question to answer is, independing on the direction of the q_{PLD} vector, if the observed PLD is intrinsic to the YBCO material in the thin film geometry (the stress induced in the YBCO thin film because of the lattice mismatch existing between YBCO and STO) or it is due to the particular substrate geometry, so to the possible distortion induced by the grain boundary. The comparison to the properties measured for the YBCO thin films deposited on STO single crystal allow us to discard the first possibility. The fact that the PLD are not measured in the diffraction scans of the YBCO thin film deposited on the single crystal substrate points to the PLD are not a consequence of the 2% lattice mismatch existing between the YBCO and STO substrate. In other case, the side-bands must be observed in the YBCO thin film independent on the type of STO substrate chosen.

To fabricate the bicristalline substrate two single crystals are cut at different angles, polished and fused together. A tilt grain boundary is formed at the interface of the two single crystals. The grain boundary is transferred to the thin film deposited on the bicrystalline substrate and the grain boundary is the barrier of the junction. Transmission electron microscopy (TEM) measurements [2] show that interatomic distances and relative positions of atoms, are changed by strain in the vicinity of the grain boundary. This results in a change of the bond lengths, valence atoms and the number of charge carrier present in the grain boundary. The maximal displacements are in the atomic plane next to the geometric plane of the grain boundary and it is

not clear how that changes away from this plane. A small amount of twinning could be necessary to reduce the elastic energy associated to the grain boundary. In this sense, q_{PLD} would be associated to a long-range modulation induced in the YBCO thin film by the grain boundary and the small value of q_{PLD} suggests it may not be detectable in TEM experiments.

On the other hand, it has been deduced that the superconducting transport properties depend strongly on the disorientation angle between the adjoining grains. In this sense, the structural properties must be depending as well on the disorientation angles between single crystals then it could be interesting to check if the distortion observed is depending on the disorientation angle or on the tilt direction of grain boundary, [100] or [001]. Previous studies some that the transport properties are depending on the tilt directions. In this sense, to complete this work in the future it would be very interesting to study YBCO thin films deposited on different kind of bicrystalline substrates. Such studies could reveal if some dependence exists between the magnitude of the distortion and the tilt angle of disorientation and bring new data about the nature of the distortion as well.

ACKNOWLEDGMENTS

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