ION BEAM STUDY ON EPITAXIAL GROWTH FEATURES OF YBaCuO FILMS*

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ABSTRACT

The epitaxial growth features of $YBa_2Cu_3O_{7-x}$ (YBCO) films on (100) SrTiO₃ substrates have been studied by Rutherford backscattering spectrometry and axial channeling technique. A typical minimum yield value, X_{min} , of Ba yielded in channeling spectrum is 4.6 % for the film of 166 nm. Only (00L) peaks appeared in X ray diffraction patterns of the films. The results indicate that the YBCO films have good epitaxial growth quality with c- axis orientation perpendicular to the substrate surface. Simulation of RB process in films and substrates have also been performed using RUMP program, and analysis shows that compositions of the films are uniform with near (123) stoichiometry. The higher interface yields in the aligned spectrum reveal that there are extra defects in the interface layer owing to lattice mismatch and interface interaction.

Keywords: YBa₂Cu₃O_{7-x} films Epitaxial growth RBS Ion channel

1 INTRODUCTION

In recent years, various methods to prepare high T_c superconducting (HTS) films have been developed^[1,2]. YBa₂Cu₃O₇₋₂, (YBCO) films with T_c of above 90 K and the critical current density J_c of over 1.0×10^6 A/cm² (at 77 K) have been prepared on SrTiO₃ (STO) substrates by in situ pulsed laser deposition technique^[2-5]. Foi-YBCO films of high quality with the high T_c , J_c values and narrow transition widths, it is essential that the films have perfect epitaxial crystalline and highly c- axis direction perpendicular to substrate surface, and have (123) stoichiometry. In fact, the crystallographic lattice misfit of YBCO films with substrates will disturb epitaxial growth of the films, and the interface interactions, such as chemical reactions and interdiffusions at the interface, will destroy stoichiometry of the films. Therefore, in addition to in situ deposition parameters, the qualities of YBCO films grown

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epitaxially on the substrates as a template depend evidently on the lattice misfit, the interactions at interface, crystalline quality, orientation and surface polish of the substrates. Rutherford backscattering and ion channeling (RBS and IC) technique is an efficient tool for thin film studies^[6,7]. It is capable of revealing the crystalline features and stoichiometry of the HTS films, the composition variation with film- depth, and the crystal defects within the films. In practice, the information from RBS and IC measurements are often used to optimize in situ deposition conditions and examine the substrate surface processing techniques in preparation of HTS films.

In this paper we report the typical results of epitaxial growth features of HTS YBCO films on (100) STO substrates analyzed by RBS and IC with 2 MeV He ions. Discussions are given on the higher interface yields.

2 EXPERIMENTS

After polishing and ion etching, the STO substrates were annealed at 1200 °C for 24 h in order to improve the surface qualities. YBCO films were prepared on the annealed substrates by in situ pulsed laser deposition technique^[5] at the substrate temperature T_s of 780 °C with the oxygen partial pressure $P(O_2)$ of 26.7 Pa. The YBCO films showed superconductivity with $J_c = 2.0 \times 10^6 \text{ A/cm}^2$ at 77 K and $T_c = 92.4 \text{ K}$. The film deposition method was described in detail elsewhere^[6].

In order to study the epitaxial growth features and examine the effect of high temperature annealing on the surface quality of the STO substrates, RBS and IC measurement^[8] and X ray diffraction were performed. The spectra were taken on a three- axis goniometer with 2 MeV He ions of about 2 mm diameter in beam spot. Energies of the scattered ions were measured by the detector placed at 165° with respect to the beam incidence. The RBS system was calibrated with a Au- Ag- Ti film vacuum- deposited on a Si substrate. The calibration results were used for RBS simulation, in which we supposed that the compositions of YBCO films were constant throughout the films and the straggling value was negligible in such a thin film.

3 RESULTS AND DISCUSSION

Typical random and <100>- aligned channeling spectra of an STO substrate annealed at 1200 °C for 24 h are plotted in Fig.1. The best minimum yield value X_{min} of the aligned spectrum is 3 % for Sr, whereas for the substrates without annealing, the X_{min} values of Sr are about (24-40) %. Furthermore, the Sr surface peak and the yields of the entirely aligned spectrum of the non- annealed substrates are much larger than that in Fig.1. Obviously, the surface quality of STO substrates were significantly improved by high- temperature annealing.

A random and a <100> - aligned spectra of a YBCO film on (100) STO substrate

11



by high-temperature annealing are given in Fig.2. The solid line is a RBS simulation



Fig.2 Random, aligned and simulation spectra of a YBCO film on (100) STO annealed

Thickness of the film is 166 nm and the X_{\min} for Ba is 4.6 %. The solid line is a simulation of 166 nm YBCO/STO



Fig.3 The partial simulations of individual components of the YBCO film are added to Fig.2

of the specimen, which agrees well with the experimental results . The summed spectrum and the partial contributions of individual components obtained by the simulation are plotted in Fig.3. Analysis of the results indicates that compositions of the YBCO film are uniformly distributed with near (123) stoichiometry (Y:Ba:Cu:O =

No.2

1.0:2.0:3.3:7.0), and the film has a thickness of 166 nm. The front-edge and the back-edge of Ba yields are smooth and steep. This means that the surfaces of the film and the substrate are both mirror finish in atomic dimension.

The aligned spectrum provides information about crystalline characteristics of epitaxial films. From the aligned spectrum of Fig.2, a minimum yield value X_{min} of 4.6% can be obtained for Ba, indicating that the YBCO film has good epitaxial quality. The X ray diffraction pattern (Fig.4), in which only the (00L, L = 1, 2...7) peaks can be seen, shows that the film has a highly c-axis orientation perpendicular to the substrate surface.



In Fig.5 1,2 and 3 are the surface peaks of Ba, Y and Cu; 4, 5 and 6 are the interface peaks of Ba, Y and Cu

In order to further analyze the interface peaks in the aligned spectrum, the spectrum was plotted in Fig.5 together with simulated surface peaks. The three small peaks at 450, 420 and 390 ch. are obtained by RBS simulation for a surface layer of 1.45×10^{15} YBCO units/cm², corresponding respectively to the surface peaks of Ba, Y and Cu. The Ba surface peak almost equals to the result of RBS and IC measurement, but the Y and Cu peaks are much less. The Y and Cu surface peaks overlap with the Ba and Y interface peaks respectively, but obviously, the comparison can be made. Therefore, the Y and Cu contributions to the interface peaks in the aligned spectrum of Fig.3 are quite small. The high interface peaks of Ba, Y and Cu suggest extra defects in the interface layer. These defects are partly due to lattice mismatch at the interface, because epitaxial growth of YBCO films occurred immediately on the top of substrates. It is estimated that the lattice mismatch in b-axis of the YBCO films is about 0.5 % with respect to the (100) STO crystal, and the mismatch in a-axis is about 2%. In this case, extra defects such as mismatch dislocations or strain bowing would

No.2 Lai Chuxi et al.: Epitaxial growth features of YBaCuO films

be created in the interface layer. On the other hand, in the random spectrum of Fig.2 deviations between the RBS measurement and the simulation can be found in the vicinity of 410, 385 and 355 Ch., where the interface locates. The deviations imply that some components of the film and the substrate interdiffused across the interface and/or chemical reactions took place at the interface layer. We consider that the defects, which produced the high interface yields in the aligned spectrum, should partly come from the impurities introduced by the interface interactions.

4 SUMMARY

The results show that the high temperature annealing process improved significantly the surface quality of STO substrate, and YBCO films prepared on annealed (100) STO substrate by pulsed laser technique have good epitaxial quality with c-axis orientation perpendicular to the substrate surface and near (123) stoichiometry.

The results also reveal that extra defects existed in the interface layer between the film and substrate, though the YBCO films were deposited on (100) STO substrates which have perfect crystallinity and high surface quality. The defects in interface layer may be attributed partly to the lattice mismatch of the films with the substrates, and partly to the interactions at interface.

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