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In-Plane Orientation and Coincidence Site Lattice Relation of $Bi_2Sr_2CaCu_2O_x$ Thin Films Formed on Highly Mismatched (001) YAG Substrates

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The in-plane orientation of (001) $Bi_2Sr_2CaCu_2O_x$ (2212) thin films on highly mismatched (001) YAG substrates is investigated with X-ray diffraction. The observed irregular in-plane orientation has coincidence site lattice (CSL) relation of 2212[510]//YAG[120]. The interface structure model based on near CSL theory reveals that the in-plane position of 19 Bi atoms regularly coincide well with those of the substrate surface atoms. Two other kinds of weak in-plane orientation are also observed.

1. Introduction

High temperature superconductor $Bi_2Sr_2CaCu_2O_x$ (2212) is epitaxially grown with irregular orientation on highly mismatched substrates. For example, we reported that 2212 thin films with vicinal (11n) surfaces (n= 7 or 9) were epitaxially grown on 5° off (110) $SrTiO_3$ substrates.[1-3] Bi-Sr-Ca-Cu-O thin films with (01n) surfaces were also fabricated on (110) MgO substrates by using CeO_2 buffer layers.[4] As for (001) 2212 thin films on (001) MgO substrates, the in-plane orientation is explained with near coincidence site lattice (NCSL) theory.[5] This paticular feature in the crystal growth of high temperature superconductors can be confirmed in other cases.

Artificial grain boundary junctions have been fabricated by using the orientation control of superconducting films.[6] Hence we have been investigating on the orientation control of the superconducting films. However the critical temperature (T_c) of the (11n) and (01n) Bi-Sr-Ca-Cu-O films has been lower than 70K.[1,3] The artificial grain boundaries between Bi-Sr-Ca-Cu-O films with (11n) and (01n) orientation showed comparatively low T_c of 25-30K.[7] On the other hand, Tc=105K was reported for (001) Bi-Sr-Ca-Cu-O films on (001) MgO substrates.[8] We also demonstrated that an artificial grainboundary junction between (001) Bi-Sr-Ca-Cu-O (BSCCO)films with in-plane orientation of BSCCO[100]//MgO[100]//$SrTiO_3$[100] and BSCCO[100]//$SrTiO_3$[100] showed microwave response up to 65K.[9] Therefore, the in-plane orientation control of (001) BSCCO films is important for constructing planer-type superconducting devices, in paticular constructing superconducting quantum interface devices.

Irregular in-plane orientation of (001) 2212 films can be realized by choosing suitable substrates. The lattice constants of substrates are calculated based on CSL theory.[10] According to CSL theory, in regard to (001) 2212 films formed on (001)substrates of cubic, tetragonal, and orthorhombic materials, the in-plane orientation of 2212[kl0]//substrate[mn0] necessitates the following condition:

$$\frac{(a_{2212})^2}{(a_{sub.})^2} = \frac{m^2+n^2}{k^2+l^2} \tag{1}$$

where a_{2212} and $a_{sub.}$ are the a-axis lengths of 2212 and substrate material. We assume that the cell dimensions of 2212 are a=5.396 Å, b=5.395Å, and c=30.643Å. According to eq. (1), the substrate a-axis lengths to realize irregular in-plane orientation are calculated as follows:

(i) In case of 2212[510]//Sub.[120], $a_{sub.}$= 12.30Å, which is close to the lattice constant of $Y_3Al_5O_{12}$(YAG) (12.066Å).
(ii) In case of 2212[210]//Sub.[200], $a_{sub.}$= 6.03Å, which is close to the lattice constant of RbO_2 (6.01Å).
(iii) In case of 2212[210]//Sub.[300], $a_{sub.}$= 4.02Å, which is close to the lattice constant of LiF (4.017Å).
(iv) In case of 2212[200]//Sub.[210], $a_{sub.}$= 4.83Å, which is close to the lattice constant of CaO (4.8105Å).

YAG is chemically and thermally stable. It does not show any phase transition up to the high melting point of about 1900°C, so that it can be used as substrates to fabricate 2212 films. LiF has comparatively low melting point of 848°C, and it is not suitable for a high temperature superconductor substrate. Fine single crystals of RbO_2 and CaO have not been obtained so far, and so we have not used them as the substrates. It has been reported that $Bi_2Sr_2CuO_x$ films can be fabricated on (001) (Nd,Y)AlO_3 substrates.[11] Therefore, we have choosed (001) YAG as the substrate, have fabricated 2212 films, and have studied the orientation with the multiple operations of X-ray diffraction.

2.Experimental

As-grown 2212 films were prepared on (001) YAG substrates at 660°C in O_2 atomosphere of 300mTorr by single-target sputtering. The target composition was $Bi_2Sr_2Ca_{1.1}Cu_2O_x$, the induced electric power was 100W, and the distance between the substrate and the target was 40mm. The fabrication time was about 120 minutes, and the film sickness was about 1200 Å. The growth rate of 10Å/min was comparatively small.

Bragg-Brentano (θ-2θ) method of X-ray diffraction was performed with a RIGAKU RAD-rC X-ray diffractometer using CuK_α radiation and equipped with a graphite monochromator in the scattering beam path.

The in-plane orientation was examined with χ scanning method of X-ray diffraction using 2212 (02160) reflection. We used a RIGAKU RINT-2000 X-ray diffractometer which utilized CrK_α radiation and equipped a vanadium filter in the scattering beam path. The (001) 2212 films were mounted as the c-axis was aligned to the X(chi)-axis of the diffractometer. The X-ray incident angle and the diffraction angle 2θ were set at 11.78° and 94.29°, and the X-ray intensity profiles were collected by scanning the in-plane rotation angle χ.

3.Results and Discussion

Figure 1 shows the X-ray intensity profile of a 2212 film fabricated on a (001) MgO substrate at 660°C as an example of the results measured with Bragg-Brentano method. In figure 1, only the (002n0) main peaks and the satellite peaks of (00131) and (00171) were observed, which shows that this film is a (001) 2212 film with the incommensurate modulated structure. All the 2212 films were determined to have (001) orientation by using the similar measurements.

The X-ray intensity profile measured with the χ scanning method is shown in figure 2. In fig.2 the position of 0° was chosen to align to the MgO substrate [100]. The four sharp peaks, indicated with symbol (C) in fig.2, were observed at χ = 38°, 52°, 128°, and 142°. These films are found to be

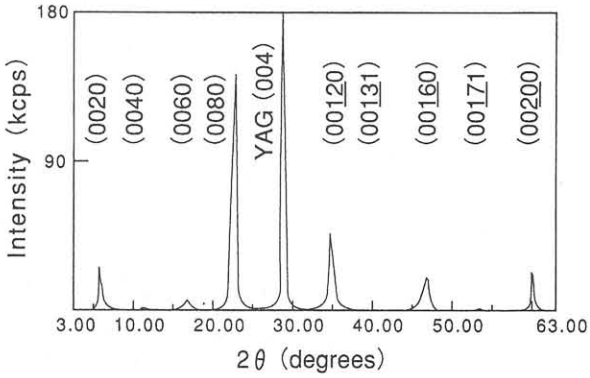

Fig.1: X-ray intensity profile of (001) $Bi_2Sr_2CaCu_2O_x$ thin film on (001) YAG substrate.

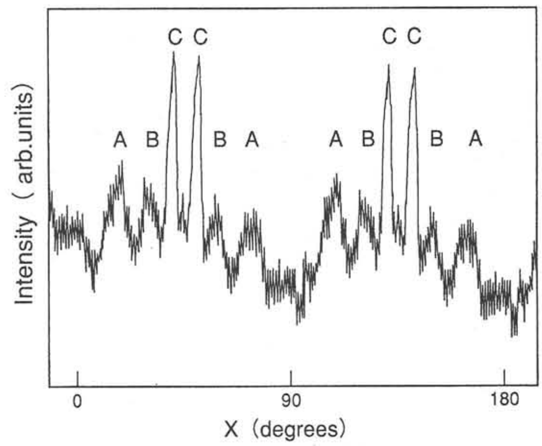

Fig.2: χ scanning profile of (001) $Bi_2Sr_2CaCu_2O_x$ thin film on (001) YAG substrate.

irregularly in-plane oriented. The observed angle 38° corresponds well to the calculated angle 38° between YAG [510] and [120]. Thus, the irregular in-plane orientation has CSL relation of 2212[510]//YAG[120]. Weak peaks indicated with symbol (A) are observed at 18°, 72°, 108°, and 162°. These peaks are caused by the 2212 (02160) and (20160) reflections from domains with in-plane orientation of 2212[100]//YAG[310]. Other weak peaks with symbol (B), which were observed at 31°, 59°, 121°, and 149°, are caused by the 2212 (02160) and (20160) reflections from the domains with in-plane orientation of 2212[100]//YAG[530]. There is no possibility to confound these 12 peaks with satellite reflections because of the use of (02160) reflections.[5] In fig.2, signals of the peaks over noise level were not observed at χ = 0°, 45°, 90°, et al.

The CSL condition (1) is so strict that 2212[100]//YAG[310] does not satisfy (1). Hence we analyze the CSL relation based on NCSL theory. Irregular in-plane orientation of 2212[kl0]//YAG[mn0] may occur when the reciprocal coincidence densities Σ_{2212} and Σ_{YAG} are not too large and the coincidence misfit f defined with eq.(2) is small:

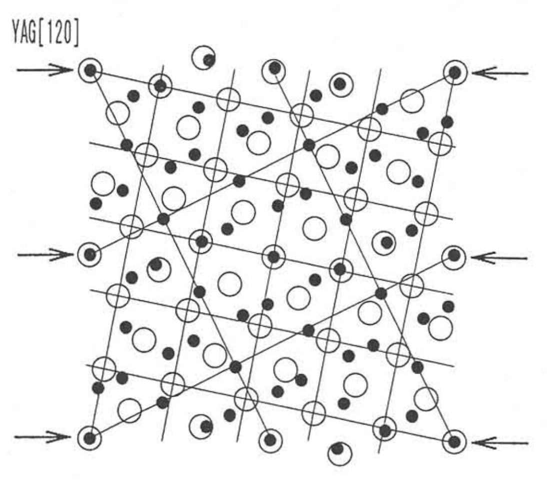

Fig.3: Coincidence site lattice model of (001) $Bi_2Sr_2CaCu_2O_x$ and (001) YAG interface.

$$f = \frac{2\,|\,(\Sigma_{2212})^{1/2}\cdot a_{2212} - (\Sigma_{YAG})^{1/2}\cdot a_{YAG}\,|}{(\Sigma_{2212})^{1/2}\cdot a_{2212} + (\Sigma_{YAG})^{1/2}\cdot a_{YAG}} \quad (2)$$

where a_{YAG} = 12.066Å, and $\Sigma_{2212}(=k^2+l^2)$ and $\Sigma_{YAG}(=m^2+n^2)$ are defined as the NCSL unit cell volume divided by the volume associated with each crystal lattice. In case of 2212[510]//YAG[120], Σ_{2212}=26, Σ_{YAG}=5, and f=0.02.

As for 2212[510]//YAG[120], based on NCSL theory, the interface structure model between (001) YAG substrate surface and the Bi layer is shown in figure 3. According to the NCSL model shown in fig.3, the in-plane positions of 19 Bi atoms, regularly aligned to the YAG [120] direction, coincide well with those of the substrate surface atoms in the NCSL unit area of 27Å×27Å. This phenomenal interface model is considered to support the occurrence of the in-plane orientation of 2212[510]//YAG [120]. The sharpness of the peaks at 38°, 52°, 128°, and 142° in fig.2 is supposed to result from the considerably regular coincidence of the in-plane atomic positions in the interface.

4.Conclusions

2212 films were fabricated on highly mismatched (001) YAG substrates by single-target sputtering. The in-plane orientation was investigated with θ-2θ and χ scanning methods of X-ray diffraction. The θ-2θ scanning profiles confirmed that the fabricated films were (001) oriented. In the χ scanning profiles the sharp peaks were observed at χ = 38°, 52°, 128°, and 142°, which indicates that these films are irregularly in-plane oriented and that the observed irregular in-plane orientation has CSL relation of 2212[510]//YAG[120]. The interface model based on near CSL theory reveals that the in-plane positions of 19 Bi atoms, which are regularly aligned in YAG [120] direction, coincide well with those of the substrate surface atoms. The sharpness of the 2212[510]//YAG[120] peaks is supposed to result from the considerably regular coincidence of the in-plane atomic positions in the interface. Two other kinds of weak in-plane orientation with CSL relations of 2212[100]//YAG[310] and 2212 [100]//YAG[530] were also observed.

Acknowledgement

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