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Growth of simplified buffer template on flexible metallic substrates for $YBa_2Cu_3O_{7-\delta}$ coated conductors

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A much simplified buffer structure, including a three-layer stack of $LaMnO_3$/MgO/composite Y_2O_3–Al_2O_3, was proposed for high performance $YBa_2Cu_3O_{7-\delta}$ (YBCO) coated conductors. In this structure, biaxially textured MgO films were prepared on solution deposition planarized amorphous substrate through ion-beam-assisted deposition (IBAD) technology. By the use of *in situ* reflection high-energy electron diffraction monitor, X-ray diffraction and atomic force microscope, the influence of deposition parameters, such as film deposition rate, ion penetrate energy and ion beam flux, on crystalline orientation, texture, lattice parameter and surface morphology was systematically investigated. Moreover, stopping and range of ion in mater simulation was performed to study the effects of ion bombardment on MgO films. By optimizing IBAD process parameters, the best biaxial texture showed ω-scan of (002) MgO and Φ-scan of (220) MgO yield full width at half maximum values of 2.4° and 3.7°, indicating excellent biaxial texture. Subsequently, $LaMnO_3$ films were directly deposited on the IBAD-MgO template to improve the lattice mismatch between MgO and YBCO. Finally, YBCO films grown on this simplified buffer template exhibited a critical current density of 2.4 MA/cm^2 at 77 K and self-field, demonstrating the feasibility of this buffer structure.

1. Introduction

Due to their low production cost and high current carrying capability, second-generation high-temperature superconducting coated conductors (CCs) have been intensively investigated by researchers worldwide [1–3]. A typical CCs structure consists of $YBa_2Cu_3O_{7-\delta}$ (YBCO) functional films grown on inexpensive flexible metallic tape with intermediate buffer layers [4–6]. Normally, flexible substrates do not provide the single crystal structure (biaxial texture) required for YBCO thin films. To induce biaxial texture in buffer layers, two well established techniques have been explored to induce crystallographic alignment, i.e., incident substrate deposition [7,8] and ion-beam-assisted deposition (IBAD) [9–11]. In the IBAD approach, yttria-stabilized zirconia and $Gd_2Zr_2O_7$ are the mostly explored texturing materials [12,13]. Nevertheless, the slow evolution procedure of biaxial texture (with thickness >500 nm) for these fluorite-structured materials limits their application prospect. Alternatively, the rock-salt materials, such as MgO, have attracted much attention because this template uses a much thinner thickness (~10 nm) to obtain a sharp in-plane texture (7°) [14], showing the potential ability for high production efficiency in a continuous process.

Up to now, in the IBAD-MgO approach towards commercial application, a typical multi-layer stack, including $LaMnO_3$ (LMO)/homo-epitaxial (epi) MgO/IBAD-MgO/Y_2O_3/Al_2O_3/Hastelloy, is utilized to achieve high performance in YBCO functional layer [15]. In this structure, electrochemical or mechanical polishing technology is needed to obtain smooth surface on Hastelloy tapes. Al_2O_3 acts as a barrier to block the outward ionic species diffusion from substrate to YBCO films and Y_2O_3 is used as a seed layer for IBAD-MgO. 10 nm-thick IBAD-MgO film plays a role as the template layer and epi-MgO serves as a protection layer to continue the crystalline texture from IBAD-MgO. LMO is used as a cap layer to improve the lattice mismatch between MgO and YBCO. In order to decrease the production cost, significant and impressive methods have been made.

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For example, one way is to decrease the number of buffer layers from five layer to four layer [16]. The other way is to use chemical solution deposition approach instead of vacuum coating technology for Al_2O_3 and Y_2O_3 process [17].

In this study, we demonstrated a three-layer simplified buffer structure (LMO/IBAD-MgO/composite Y_2O_3–Al_2O_3) for YBCO CCs. The amorphous composite Y_2O_3–Al_2O_3 (YAlO) layer, prepared by a low-cost solution deposition planarization (SDP) technology, acted both roles as barrier and seed layer for IBAD-MgO films. Subsequently, biaxially textured IBAD-MgO films were deposited on this substrate. Meanwhile, the effects of deposition rate, ion energy and ion beam flux on the evolvement of crystalline orientation, texture and surface morphology were investigated. Lastly, LMO films were directly coated on IBAD-MgO template without epi-MgO layer and the performance of the buffer layer was evaluated by depositing YBCO functional layer on the surface.

2. Material and methods

10 mm-wide bare Hastelloy C-276 tape was used as a starting platform with root-mean-square (RMS) roughness of 50 nm over a 5 μm × 5 μm area. One micrometer thick YAlO layer was subsequently coated on the platform by SDP method. A detailed introduction of SDP technology could be found elsewhere [18]. After YAlO coatings, the RMS roughness value on the surface reached 0.2 nm, which was smoother than that of electrochemical and mechanical polishing technology [19].

Based on the smooth surface, 12 nm-thick MgO thin films were deposited on YAlO substrate by a reel-to-reel IBAD system at room temperature. The MgO source was provided by electron beam evaporation. The deposition rate, monitored by a quartz crystal microbalance, varied from 0.05 nm/s to 0.6 nm/s. During the deposition process, a Kaufman ion gun was utilized to generate a neutralized beam of Ar ions with 0–800 eV ion energy and 10–60 mA ion beam flux. Meanwhile, the development of biaxial texture on the surface was monitored *in situ* by reflection high energy electron diffraction (RHEED). As IBAD-MgO films were too thin to be detected by X-ray diffractometer (XRD), additional 80 nm-thick epi-MgO films were grown on IBAD-MgO without assisting ion beam around 600 °C. Then XRD analysis (Bede D1), including θ–2θ, ω-scans, Φ-scans, pole figure and reciprocal space measurements, was performed to characterize the crystalline quality, texture and lattice parameter. The surface morphology and roughness were investigated by atomic force microscope (AFM, Seiko SPA300HV). In addition, stopping and range of ions in matter (SRIM, 2013) simulation was utilized to investigate the effects of ion beam on IBAD-MgO [20]. Then LMO films were fabricated on IBAD-MgO layer with and without epi-MgO layer through radio-frequency magnetron sputtering. Finally, to testify the buffer layer quality, 500 nm-thick YBCO films were deposited on LMO/IBAD-MgO/SDP-YAlO template by metal organic chemical vapor deposition. The detailed experiment condition was shown elsewhere [21,22].

3. Results

3.1. Influence of deposition rate to the texture and crystal quality in MgO films during IBAD

Fig. 1 exhibits RHEED patterns of IBAD-MgO films deposited by varying deposition rate from 0.05 nm/s to 0.6 nm/s. The film shows a fiber texture (with out-of-plane texture and without in-plane texture) with the deposition rate of 0.05 nm/s. As deposition rate reaches 0.1 nm/s, a typical pattern of biaxial texture is shown in the RHEED image with highly defined spots and a similar pattern is observed with the deposition rate of 0.18 nm/s. However, when deposition rate increases to 0.3 nm/s, an unclear ring is observed on the surface, indicating that some residual polycrystalline MgO grains exist in MgO film. With the continuous increase of deposition rate, the diffraction ring gets clearer and the texture begins to deteriorate.

Additional 80 nm-thick epi-MgO layer was coated on IBAD-MgO to investigate the epitaxial nature of MgO films. The results of XRD θ–2θ scans with deposition rate from 0.1 nm/s to 0.4 nm/s are shown in Fig. 2. For all samples, there is only (002) reflection of MgO except for Ni alloy peaks from Hastelloy substrate. What's more, it is also found that the highest intensities could be achieved with the deposition rate of 0.15 nm/s and 0.18 nm/s. As long as increasing the deposition rate from 0.18 nm/s to 0.4 nm/s, the intensity of (002) peak decreases monotonically, indicative of the deterioration of crystal quality. These results demonstrate the deposition rate can significantly determine the crystalline quality in IBAD-MgO films.

It should be noted that the in-plane texture with high quality is critical in preventing the development of high-angle grain boundaries in the YBCO functional layer [23]. For this reason, it is important to investigate the full width at half maximum (FWHM) values of biaxial texture in IBAD-MgO films. The in-plane ($\Delta\Phi$) and out-of-plane ($\Delta\omega$) FWHM values are presented in Fig. 3 as a function of deposition rate. It can be seen that both the out-of-plane and in-plane texture exhibit a gradual improvement with increasing deposition rate from 0.1 nm/s to 0.18 nm/s. As deposition rate continues to increase, the biaxial texture starts to deteriorate. When the deposition rate increases to 0.4 nm/s, no in-plane texture is detected. According to RHEED image in Fig. 1e, in-plane texture still exists in this film. This result indicates that in-plane texture in MgO film is too weak to be detected by XRD analysis with the deposition rate of 0.4 nm/s. As deposition rate reaches 0.6 nm/s, both in-plane and out-of-plane texture can't be detected by XRD, which is consistent with RHEED results in Fig. 1.

The rocking curves of ω-scan and Φ-scan, as well as pole figure of epi-MgO deposited on the optimal IBAD-MgO template are shown in Fig. 4. The best texture is obtained with FWHM values of $\Delta\omega = 2.4°$ and $\Delta\Phi = 3.7°$, respectively, which is comparable to the results from other researchers [24–27]. From Fig. 4c, only four equally distributed points with the interval of 90° can be seen, indicating that epi-MgO layer is epitaxial growth on IBAD-MgO layer with high quality and good in-plane orientation.

3.2. Effect of ion beam to the texture and crystal quality in MgO films during IBAD

Fig. 5 shows the real-time development of biaxial texture in 12 nm-thick IBAD-MgO films at different ion energies by RHEED observations. When the ion energy is 0 eV, i.e., without assisted ion beam, the RHEED pattern shows a polycrystalline diffraction ring, suggesting that the film has no texture. With 400 eV assisted ion energy, the scattering spots indicate the development of texture from a random out-of-plane distribution to a fiber texture. Then the transition from scattering to diffraction spots begins at 550 eV ion energy. The spots are indistinct, indicating that cubic-phase MgO islands develop on the surface with poor in-plane alignment. As the ion energy increases to 800 eV, the in-plane texture improves prominently, as revealed by the appearance of bright spots in the RHEED pattern.

During IBAD, the interaction between ions and atoms influence the nucleation kinetics on MgO surface. Thus grain size and surface morphology is largely dependent on ion bombardment. AFM was employed to get a comprehensive picture about the surface morphology of IBAD-MgO. Fig. 6 presents the AFM images of IBAD-