Atomic-Scale Modeling of Heterointerfaces in Superconducting Thin Film Multilayers

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High-temperature superconductors are typically prepared as multilayer films by deposition on oxide substrates such as MgO, LaMnO3 and CeO2 [1]. In the case of the former, better adhesion and superconducting properties can be obtained by introducing a BaZrO3 buffer layer [2], while CeO2 is often deposited on LaMnO3 substrates for the same purpose.

In this study, first-principles calculations based on density functional theory are combined with empirical potential models to probe the structures and energetics of ideal BaZrO3(001)[001]/MgO(001)[001], CeO2(100)[110]/LaMnO3(110)c[001] and CeO2(110)[001]/LaMnO3(110)c[001] heterointerfaces in an effort to understand the effect of lattice misfit, interface adhesion (chemical bonding) and crystal alignment on epitaxial growth of 123 cuprate superconductors. Small misfit parameters between the component lattices in both cases result in coherent interfaces of low excess energy and high stability. In the case of BaZrO3(001) on MgO(001), the BaZrO3 crystal is most stable when terminated by a ZrO2 layer [3]. Band gaps at the interfaces are also found to be significantly different to those of the component crystals on account of the different bonding environments and contributions from different overlapping atomic orbitals. The results are found to be consistent with preferred epitaxial growth directions observed in BaZrO3/MgO and CeO2/LaMnO3 multilayered thin films.

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Figure 1. Side view of the optimized structure of a BaZrO3(001)/MgO(001) interface terminated by MgO and ZrO2 layers. The high coherency and small misfit strain result in a low interface energy of 0.55 Jm−2.
Self-epitaxy is defined as occurring when the distribution of in-plane misalignment angles of grains around a major orientation axis decreases with increasing film thickness. Such a phenomenon occurs during the crystal growth of some buffer materials, such as CeO$_2$ on an IBAD-MgO template, in coated conductors. To obtain high performance coated conductors as well as high throughput speed for lower cost, control of the self-epitaxy needs to be optimized. However, its growth mechanism is not yet fully understood. In this study, competitive growth of neighboring grains of CeO$_2$ is examined as a possible underlying mechanism of self-epitaxial growth. To this end, a cross-section of a CeO$_2$ layer including CeO$_2$/LMO interface was observed using a transmission electron microscope. CeO$_2$ grains with smaller c-axis inclination angles were found to have grown in preference to their neighbors with larger inclination angles. Since there is a positive, almost linear correlation between in-plane and out-of-plane orientations, the distribution of in-plane misalignment angles around a major orientation axis also decreases with increasing thickness. Part of this work includes results from the “Development of Fundamental Technologies for HTS Coils” project supported by the Ministry of Economy, Trade and Industry (METI) and the “Development of Materials & Power Application of Coated Conductors” project supported by the New Energy and Industrial Technology Development Organization (NEDO).
Characterization of TFA-MOD YBCO Thick Films Prepared from Precursor Solution Using Fluorine Free Yttrium and Copper Salts

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TFA-MOD process is expected to be suitable for low-cost large-scale production of YBCO coated conductors with high-performance. In general, the increase in the film thickness of one coating leads to reduction of coating times in the multi-dip coating system, which gives further cost reduction in MOD process. However, it may cause the formation of defects in the films and degradation of superconductive properties. We have previously developed a new precursor solution consisting of Y-propionate, Ba-trifluoroacetate, and Cu-2-ethylhexanoate in order to increase the film thickness of one coating in the dip-coating technique. The critical thickness of a defect-free film in one coating by using the new precursor solution was about 0.8 μm/coat which was significantly improved from that by the conventional one consisted of Y-TFA, Ba-TFA, and Cu-2-ethylhexanoate (0.3 μm/coat).

The $J_c$ value of 2.7 MA/cm$^2$ ($I_c$ value of 791 A/cm-width) at 77 K, under self-field in the film with 2.9 μm thickness (0.48 μm/coat) was obtained by using the new precursor solution. When the film thickness of one coating was increased to 0.77 μm/coat from 0.48 μm/coat, the $J_c$ value was deteriorated to 1.8 MA/cm$^2$ (2.3 μm, 405 A/cm-width). In this study, we have investigated the relationship between film thickness of one coating and $J_c$ property of TFA-MOD YBCO coated conductors prepared from the new precursor solution and optimized calcination and crystallization conditions to fabricate high-performance coated conductors cost-effectively. Furthermore, attempts to introduce artificial pinning centers into TFA-MOD YBCO films prepared from the new precursor solution have been also performed.

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Influence of the grain-boundary angle in TFA-MOD $Y_{0.77}Gd_{0.23}Ba_2Cu_3O_y$ films on in field critical current density

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Trifluoroacetates-metal organic deposition (TFA-MOD) process is one of the most promising methods for producing REBa$_2$Cu$_3$O$_y$ (REBCO) coated conductors (CCs) since it is a low-cost and high material yield process. $Y_{0.77}Gd_{0.23}Ba_2Cu_3O_y$ (YGdBCO) CCs have higher self-field critical current density ($J_{c,s.f.}$) and in-field $J_c$ properties compared with that of YBCO CCs. However, it is necessary to further improve the in-field $J_c$ properties for power application. The low-angle ($\Delta \phi$) of grain boundaries (GBs) is one of key factors for the enhancement of $J_c$ properties in REBCO CCs.

In this work, we fabricated TFA-MOD YGdBCO films on SrTiO$_3$ (STO) single crystal and CeO$_2$ ($\Delta \phi \sim$3.5 deg.) substrates in order to investigate the influence of GBs on the in-field $J_c$ properties. We demonstrated that YGdBCO/STO films show higher in-field $J_c$ compared with YGdBCO/CeO$_2$ films in spite of the similar $T_c$. In addition, $J_c$ in both YGdBCO/STO and YGdBCO/CeO$_2$ films show a power-law dependence with similar $\alpha$, the value of $\alpha$ is a power-law regime ($J_c \propto B^\alpha$) at intermediate fields. We consider that the reason why YGdBCO/STO films show higher in-field $J_c$ is higher $J_{c,s.f.}$ due to low angled GBs. Thus, the low angle of GBs has an important role in the improvement of not only self-field $J_c$ but also in-field $J_c$ in TFA-MOD REBCO films.

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