Anisotropic defect structure and transport properties of YBa 2 Cu 3 O 7−δ films on vicinal SrTiO 3 (001)

J. Brötz, H. Fuess, T. Haage, J. Zegenhagen, Ch. Jooss, A. Forkl, and R. Warthmann

Citation: Journal of Applied Physics **85**, 635 (1999); doi: 10.1063/1.369421
View online: http://dx.doi.org/10.1063/1.369421
View Table of Contents: http://scitation.aip.org/content/aip/journal/jap/85/1?ver=pdfcov
Published by the AIP Publishing

Anisotropic defect structure and transport properties of $YBa_2Cu_3O_{7-\delta}$ films on vicinal $SrTiO_3(001)$

J. Brötz[a] and H. Fuess
FG Strukturforschung, FB Materialwissenschaft, TU-Darmstadt, Petersenstrasse 23, D-64287 Darmstadt, Germany

T. Haage and J. Zegenhagen
Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

Ch. Jooss, A. Forkl, and R. Warthmann
Max-Planck-Institut für Metallforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

(Received 14 July 1998; accepted for publication 6 October 1998)

The microstructure of $YBa_2Cu_3O_{7-\delta}$ thin films grown on vicinal $SrTiO_3(001)$ has been studied as a function of the vicinal angle by x-ray diffraction using the two-dimensional *q*-scan technique. Our results reveal a strong correlation between the miscut of a $SrTiO_3(001)$ substrate and the anisotropic defect structure of the film. Furthermore, we observed an anisotropy of the corresponding critical current density up to 4.6 depending on the angle of miscut. © *1999 American Institute of Physics.* [S0021-8979(99)09401-3]

Epitaxial, superconducting thin films of $YBa_2Cu_3O_{7-\delta}$ (YBCO) grown on $SrTiO_3(001)$ exhibit superb crystalline quality and excellent electronic characteristics. We have shown previously how to modify and optimize the transport properties of these epitaxial layers by employing the process of self-organization via deposition on annealed, $SrTiO_3(001)$ surfaces.[1,2] With a precisely chosen crystallographic miscut and proper annealing, the structure of $SrTiO_3(001)$ surfaces can be defined down to the atomic level.[3]

With the surface normal slightly oriented towards [010], vicinal $SrTiO_3(001)$ surfaces exhibit a regular sequence of steps in the [010] (*T*) direction and kink-free, straight step edges along the [100] (*L*) direction. Step heights correspond practically exclusively to the unit cell height of $SrTiO_3$(0.39 nm). The width in the *T* direction of the long, smooth, and straight terraces is determined by the angle of miscut. This extraordinary regular step structure is also observed on surfaces with an almost 10° miscut in the [010] direction.[2,4] The microstructure of epitaxial YBCO films grown on these substrates by pulsed laser deposition, exhibits a high density of defects, such as antiphase boundaries (APB's) and stacking faults (SF's).[4] These defects with a width of 2–3 nm cause strong correlated flux pinning, resulting in a critical current density up to $j_c = 8 \times 10^{11}$ A/m^2.[1]

Crystals and thin films of the $RBa_2Cu_3O_{7-\delta}$, R=Y or rare earth (RBCO) family typically exhibit twinning and due to the fact that the twin boundaries are aligned along the diagonal of the *a*/*b* basal plane of the orthorhombic unit cell, i.e., along $[110]_{YBCO}$ or $[\bar{1}10]_{YBCO}$, the microstructure of the crystalline material consists of an assembly of four domains corresponding to the two twin couples aligned along the [110]- and [110]-direction of the $SrTiO_3$ substrate.[5,6] This fourfold domain structure can be observed in *q* space via x-ray diffraction and results in a fourfold splitting of reflections with sufficient in-plane momentum transfer.

In a recent paper we have analyzed the microscopic structure of YBCO thin films on $SrTiO_3$ (001) in detail as a function of the substrate miscut angles, employing x-ray diffraction and the two-dimensional *q*-scan technique. We observed that with proper chosen miscut angles the microscopic domain structure of the thin films can be dramatically influenced. With a substrate miscut towards [100]/[010], about 80% untwinned films can be produced at a miscut angle of 10°. Already rather small miscut angles of about 1° in the [110]/[$\bar{1}$10] direction lead to the disappearance of one of the twin couples.[7] Here we employ the *q*-scan technique to provide details about the anisotropic defect microstructure of the thin films.

Figure 1(a) illustrates the split $(202)_{YBCO}/(022)_{YBCO}$ reflections of a 60-nm-thick YBCO film grown on a $SrTiO_3(001)$ surface with 10° miscut towards [010]. The data are obtained by a STOE four-circle diffractometer with graphite monochromatized Co K_α radiation ($\bar{\lambda} = 1.7902$ Å). The peak positions of the four different suborientations in this figure which are described by the subscripts $S_1^- \ldots S_2^+$ according to Wadhawan,[8] reveal that the *c* axis of the YBCO film is aligned to the [001] direction of the $SrTiO_3$ and not to the optical surface of the vicinal $SrTiO_3(001)$, whereas YBCO films on vicinal substrates with a larger misfit like vicinal MgO (001) with $a = 4211$ Å are predominantly aligned to the surface normal.[9] The structure of twinning and the relative peak intensities within the two twinning systems deviate from films grown on well oriented $SrTiO_3$ substrates. This is due to an anisotropic strain at the interface which is described in detail by Brötz *et al.*[7] The reflections in Fig. 1(a) are measured with the momentum transfer, i.e., the *Q* vector, towards the *L* direction ([100]) whereas the corresponding reflections in

[a]Electronic mail: broetz@hrzpub.tu-darmstadt.de

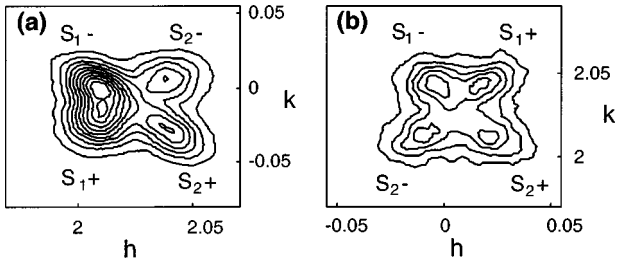

FIG. 1. q scan of the splitted YBCO $(202)_{\mathrm{YBCO}}/(022)_{\mathrm{YBCO}}$ reflections of a 60-nm-thick YBCO film grown on $SrTiO_3(001)$ with a miscut of 10° towards [010], measured towards [100] (L)-direction (a) and towards [010] (T)-direction (b). The indices h and k are given in terms of the cubic $SrTiO_3$ cell.

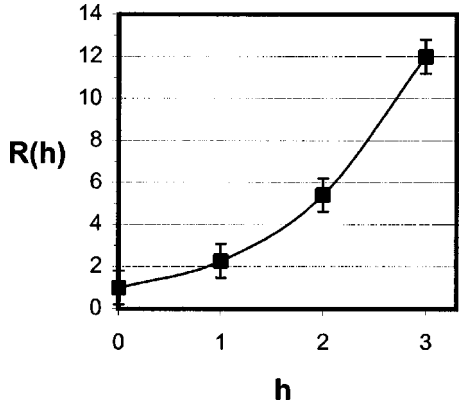

FIG. 2. Anisotropic defect structure of 60-nm-thick YBCO grown on 10° miscut $SrTiO_3$, given by the ratio $R(h)$, which represents the sum of the determined peak intensities of YBCO $(h02)_{\mathrm{YBCO}}/(0h2)_{\mathrm{YBCO}}$ reflections towards L direction, normalized to the corresponding peak intensities towards T direction (see also Fig. 1).

Fig. 1(b) are recorded with the momentum transfer along the T direction ([010]). Thus, we are probing the correlation of the YBCO film structure along and normal to the terraces, respectively. In contrast to YBCO grown on well oriented substrates where the corresponding peak intensities of the film are equal in both directions, we find here a significant difference between the peak intensities. The intensities of the four reflections in L direction are 5.4 times larger than in T direction. This finding suggests an anisotropic distribution of defects within the film. While Lowndes *et al.*[10] found columnar defects in YBCO films grown on vicinal $LaAlO_3$, we assume a planar alignment of defects along the step edges in YBCO films grown on vicinal $SrTiO_3$. The lattice of the film is in the T direction (perpendicular to the step edges) discontinued by antiphase boundaries and stacking faults, whereas defect-free growth can be achieved in the L direction (along the step edges).

To investigate the two-dimensional peak shape of each orientation measured towards the L and the T direction [see Figs. 1(a) and 1(b)] we unfolded the measured intensities by the two-dimensional resolution function of our four-circle diffractometer.[11]

Although the intensity and consequently the crystallinity is significantly lower towards the T direction, we could only find a slight increase in the width of the rocking curves. However, we found by this method that the peaks of the S_1^- and S_2^+ orientations are broadened towards [110], while the peaks of the S_1^+ and S_2^- orientations are broadened towards [110]. This suggests that the twin system $[S_1^-, S_2^+]$ ($[S_1^+, S_2^-]$) is strained towards [110] ([110]), respectively. The coupling between the YBCO film and the $SrTiO_3$ substrate is therefore significantly stronger towards [110] ([110]) than towards [100] or [010].

Figure 2 displays the ratio $R(h) = \mathrm{Int.}(h02)_{\mathrm{YBCO},L}/\mathrm{Int.}(h02)_{\mathrm{YBCO},T}$ for different h values. It is obvious that $R(h)$, which represents the anisotropy of the crystallinity, increases with h. This is due to the enhanced projection of the Q vector on the plane spanned by the L and T direction.

The influence of the vicinal angle θ on the anisotropy of the defect structure, given by $R(3)$ is shown in Fig. 3. The anisotropy is significantly increased by larger angles of miscut and reaches values of $R(3) = 12$ for $\theta = 10°$. Since the terrace width w_S at the $SrTiO_3$ surface decreases with increasing vicinal angle θ according to the relation $w_S = 0.39\ \mathrm{nm}/\tan(\theta)$,[4,12] our result implies that the anisotropy of the defect structure of the film is more or less linearly correlated with the density of steps at the substrate surface. The intensities of the reflections in the L direction do not decrease noticeably with θ (in contrast to the reflections in the T direction) which means that the defect structure is strongly anisotropic with a high, miscut dependent density along the T and a low miscut independent density along the L direction. This is just the description for a planar defect structure, with the planes aligned along the L and normal to the T direction.

While the transition temperature T_c of YBCO films grown on vicinal $SrTiO_3(001)$ substrates is only slightly reduced compared to films grown on well-oriented $SrTiO_3(001)$ substrates,[1] we found a strong influence of the vicinal angle θ on the critical current density j_c which is shown in Fig. 4. The critical current density is measured towards the L and T direction by means of the magneto-optical Faraday effect in an external field $B_{\mathrm{ext}} = 40$ mT, at 4.2 K and the inversion of Biot–Savart's law (for experimental

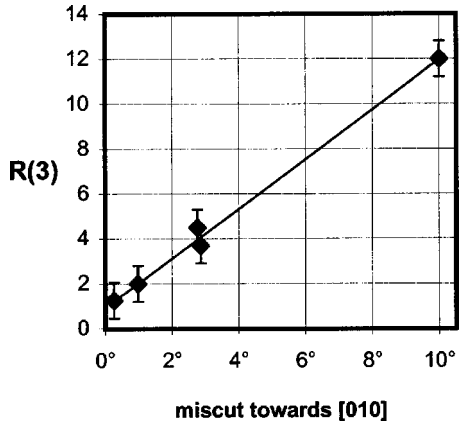

FIG. 3. Enhanced anisotropy of the defect structure in 60-nm-thick YBCO films by the miscut of vicinal $SrTiO_3$ substrates. $R(3)$ represents the sum of the determined peak intensities of YBCO $(302)_{\mathrm{YBCO}}/(032)_{\mathrm{YBCO}}$ reflections towards L direction, normalized to the corresponding peak intensities towards T direction.

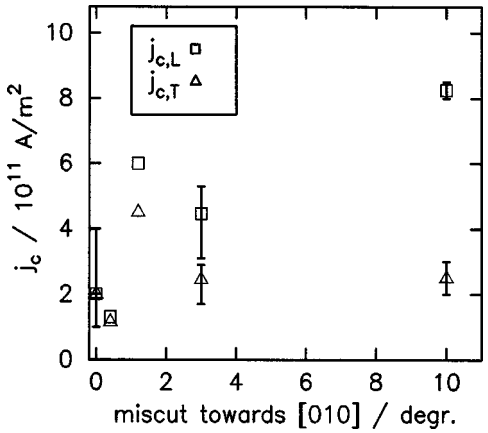

FIG. 4. Critical current densities $J_{c,L}$ and $J_{c,T}$ vs the angle of miscut for YBCO films on vicinal $SrTiO_3(001)$ substrates. $J_{c,L}$ and $J_{c,T}$ are measured in *L* and *T* direction, respectively, at a temperature of 4.2 K and an external field of 40 mT.

details see Refs. 13 and 14). While $j_{c,T}$ (perpendicular to the step edges) is only slightly increased by the miscut, we found a significant increase of $j_{c,L}$ although our films exhibit no screw dislocations and hardly any columnar growth features due to the prevailing step flow growth modus on vicinal substrates.[1,12] The increase of the critical current density in *L* direction up to $j_{c,L}=8\times10^{11}$ A/m^2 is therefore due to a strong correlated pinning perpendicular to the defect planes (normal to the *T* direction), which are generated by the step edges at the $SrTiO_3$ surface.

In summary, we observed an anisotropic defect structure in YBCO films in direct correlation with the miscut of vicinal $SrTiO_3(001)$ substrates by means of x-ray diffraction and the two-dimensional *q*-scan technique. The resulting anisotropic critical current density is directly correlated to the observed anisotropic defect structure.

Support of this work by the Fonds der Chemischen Industrie and the Bundesminister für Bildung und Forschung is gratefully acknowledged.

[1] T. Haage, J. Zegenhagen, J. Q. Li, H.-U. Habermeier, M. Cardona, C. Jooss, R. Warthmann, A. Forkl, and H. Kronmueller, Phys. Rev. B **56**, 8404 (1997).
[2] T. Haage, J. Q. Li, B. Leibold, M. Cardona, J. Zegenhagen, and H.-U. Habermeier, Solid State Commun. **99**, 535 (1996).
[3] See, e.g., Q. D. Jiang and J. Zegenhagen, Mater. Res. Soc. Symp. Proc. **474**, 373 (1997), and references therein.
[4] T. Haage, H.-U. Habermeier, and J. Zegenhagen, Surf. Sci. Lett. **370**, 158 (1997).
[5] J. D. Budai, M. F. Chrisholm, R. Reenstra, D. H. Lowndes, D. P. Norton, L. A. Boatner, and D. K. Christen, Appl. Phys. Lett. **58**, 2174 (1991).
[6] T. Steinborn, G. Miehe, J. Wiesner, E. Brecht, H. Fuess, G. Wirth, B. Schulte, M. Speckmann, H. Adrian, M. Maul, K. Petersen, W. Blau, and M. McConnel, Physica C **220**, 219 (1994).
[7] J. Brötz, T. Haage, J. Zegenhagen, and H. Fuess, Phys. Rev. B **57**, 3679 (1998).
[8] V. K. Wadhawan, Phys. Rev. B **38**, 8936 (1988).
[9] S. K. Streiffer, B. M. Lairson, and J. C. Bravman, Appl. Phys. Lett. **57**, 2501 (1990).
[10] D. H. Lowndes, D. K. Christen, C. E. Klabunde, Z. L. Wang, D. M. Kroeger, J. D. Budai, S. Zhu, and D. P. Norton, Phys. Rev. Lett. **74**, 2355 (1995).
[11] J. Brötz, T. Wieder, and H. Fuess (unpublished).
[12] L. Méchin, P. Berghuis, and J. E. Evetts, Physica C **302**, 102 (1998).
[13] C. Jooss, R. Warthmann, A. Forkl, and H. Kronmueller, Physica C **299**, 215 (1998).
[14] C. Jooss, R. Warthmann, A. Forkl, T. Haage, J. Zegenhagen, H.-U. Habermeier, and H. Kronmueller, Physica C **282–287**, 2311 (1997).