Structural Characterization of Superconducting $YBa_2Cu_3O_{7-\delta}$ Thin Films: An X-ray Diffraction Study

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Abstract:

Among discovered superconductors, cuprate superconductors are notable for their high critical temperature, which makes them ideal for modern applications. In this study, we focus on one of these cuprate superconductors, $YBa_2Cu_3O_{7-\delta}$ (YBCO). With the goal of creating high-quality *a*- and *c*-axis YBCO films, YBCO films were grown utilizing oxide molecular beam epitaxy (MBE) and analyzed via reflection high energy electron diffraction (RHEED), X-ray diffraction (XRD), and X-ray reflection (XRR). RHEED allowed for *in-situ* monitoring of the film growth, and XRD was used to analyze structural quality, to assess the changes need to make better films, and to find the lattice constants. Finally, XRR allowed for the surface roughness and the film thickness to be assessed. Overall, these methods allowed for the growth of high-quality *a*- and *c*-axis YBCO thin films.

Summary of Research

In 1986, the first cuprate superconductor, Ba-La-Cu-O, was discovered [1]. Its discovery started off what is now decades long research into "high-temperature" cuprate superconductors [2]. This research focused on making higher-temperature superconductors and discovering the best methods available to create these materials. From this, thin film superconductors emerged as a way to precisely engineer superconductors.

Our research project is focused on one of those high-temperature superconductors: $YBa_2Cu_3O_{7-\delta}$ (YBCO). YBCO is of interest because it is a superconductor with a critical temperature around 90K, giving it the advantage that it can be supercooled to its superconducting state using liquid nitrogen for engineering applications. YBCO is a structurally versatile member of the cuprate family that can be synthesized either in *a*-axis or *c*-axis, where superconductivity takes place in the Cu-O planes for both cases [2]. One important application of YBCO *a*-axis thin films is their role in fabricating Josephson Junctions [3, 4].

The aim of this project was to achieve high-quality *a*- and *c*-axis YBCO thin films by utilizing *in-situ* and *ex-situ* diffraction techniques, *i.e.* RHEED and XRD. For high-quality oxide thin film synthesis, oxide molecular beam epitaxy (MBE) is of great significance, as it possesses atomic-layer precision capabilities. Accordingly, the YBCO thin films were grown via oxide MBE. The growth process began with selecting the proper substrate to promote high-quality YBCO growth. For this project, magnesium oxide (100) MgO was the chosen substrate for *c*-axis YBCO growth, and lanthanum aluminum oxide (100) LAO was the chosen substrate for *a*-axis YBCO growth.

On growth days, the MBE effusion cells were heated from idle temperatures to the required growth temperatures and were preferably allowed to stabilize upon reaching the desired growth temperature. Afterwards, a quartz crystal microbalance (QCM) was used to calibrate individual elemental fluxes. QCM calibrations were followed by specific calibration growths. Once these calibrations were complete, MBE growth of the YBCO thin films began.

Results and Discussion

During growth, the quality of the films was monitored *in-situ* via reflection high energy electron diffraction (RHEED) patterns, which provided information about the surface film quality and crystallinity [5]. Fig. 1 shows an example RHEED image acquired during an *a*-axis YBCO film growth. Within the RHEED pattern, the presence of clear specular spots (streaks) and the faint in-between streaks, as well as the absence of any additional diffraction spots (due to, for example, the formation of secondary phases), indicate that the film is an example of high-quality *a*-axis YBCO, where the red arrows indicate the signatures of *c*-axis in-plane reflections.

Once growth was complete, the films were analyzed in the PARADIM four-circle x-ray diffractometer. The X-ray diffraction (XRD) analyses were used to determine the phase purity and quality of the MBE grown YBCO thin films. By using XRD in conjunction with MBE, the effects of different growth parameters could be identified. Using this combination, the ideal temperatures for *a*-axis growth were determined. The temperature dependence of *a*-axis YBCO growth is presented through three different samples in Fig. 2. Additionally, X-ray reflection (XRR) was used to characterize the YBCO films, particularly in the determination of thin film thicknesses. Reflectivity oscillations characteristic of thin film XRR measurements, including Kiessig fringes, were used to determine the thickness of the MBE-grown thin films quantitatively.

Conclusion

In conclusion, the goal to improve the quality both of *a*- and *c*-axis YBCO thin films was achieved. Our work shows that it is possible to create high quality thin films of both *a*- and *c*- axis YBCO through specific growth temperatures and precise stoichiometry control. Fig. 3 exhibits achieved examples of high-quality *a*- and *c*- axis YBCO grown via MBE. Furthermore, the oxygen content is crucial for preliminary characterization and is interrelated with the *c*-lattice parameter [6]. We were able to determine the *c*-axis and *a*-axis lattice parameters, with special focus being given to *c*-axis lattice parameter, using the Nelson-Riley extrapolation function to calculate the lattice constants. For one of the selected samples, the *c*-lattice parameter is found to be ~11.74 Å (inset, Fig. 3).

Future Work

In future work, we plan to observe the electrical properties of the *a*- and *c*- axis YBCO thin films and to investigate the YBCO thin films via scanning transmission electron microscopy (STEM). One can also aim to integrate the *a*-axis YBCO into Josephson Junctions, devices in which two superconducting layers sandwich an insulating layer. Josephson Junction devices have a wide range of applications, making them a worthwhile pursuit for future work.

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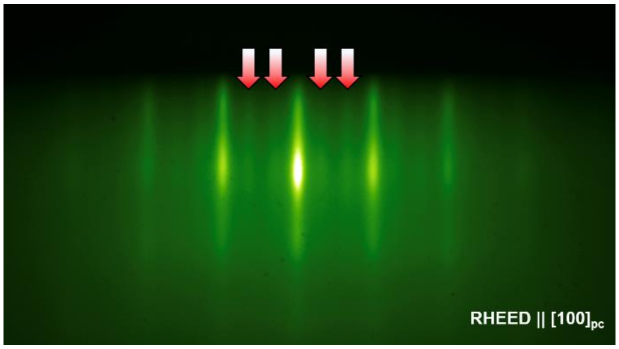

Figure 1. Image of *a*-axis YBCO during MBE growth.

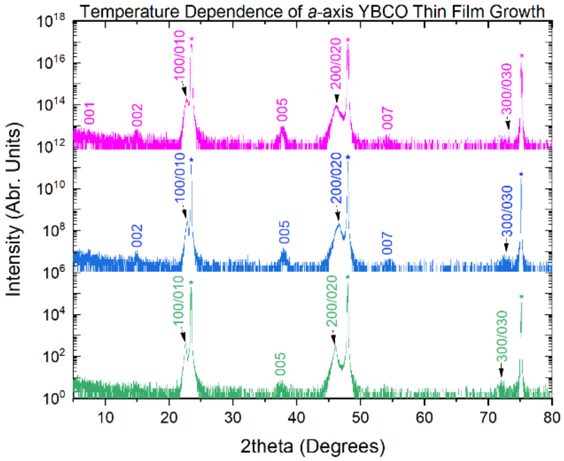

Figure 2. XRD patterns for three different *a*-axis YBCO films on LAO (100) grown at three different temperatures. From top to bottom, the temperatures (measured by a thermocouple) are 445°C (magenta), 435°C (blue), and 425°C (green). The stars indicate the substrate peaks.

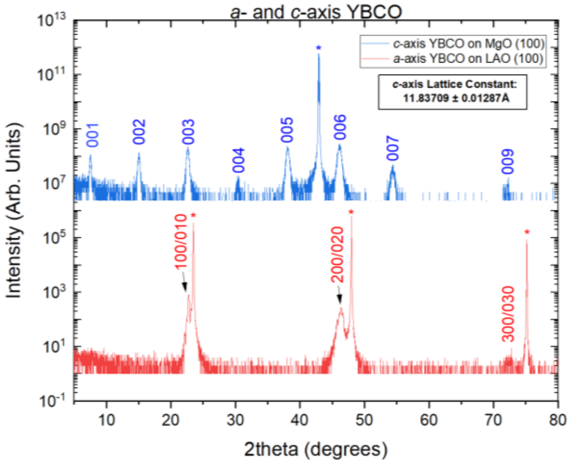

Figure 3. XRD plots of high-quality *a*-axis YBCO (red) and *c*-axis YBCO (blue). The *c*-axis lattice parameter is calculated to be 11.73919 ± 0.00824Å. The stars indicate the substrate peaks.

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