# Epitaxial Growth of Single-Domain (110) BiFeO3 Thin Films

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# Abstract

BiFeO<sub>3</sub> has been the subject of investigation for applications in spintronics due to its unique multiferroic room-temperature properties and spin cycloid magnetic texture. However, ferroelectric domain walls create discontinuities in spin cycloids, so a single-domain structure is desired to maximize the feasibility of BiFeO<sub>3</sub> for spintronics. Previous work has demonstrated successful growth of single-domain BiFeO<sub>3</sub> along orientations other than (110). This project demonstrates epitaxial growth of (110) BiFeO<sub>3</sub> that is single-domain based on analysis of the characteristic 221 RSM peak, but further testing is needed to verify these conclusions.

#### Introduction

Improvements beyond traditional electronic devices have been guiding research in this new age of technology. Namely, spintronics, quantum-mechanical devices that utilize magnetism to store information, have become an area of interest due to its predicted low-power computing capabilities [1].

Simultaneously, interest in pseudocubic perovskite BiFeO<sub>3</sub> (BFO) has been on the rise because this material demonstrates multiferroic properties at room temperature, including ferroelectricity and antiferromagnetism [2]. These multiferroic properties, respectively, are supported by the high Curie temperature of  $T_c = ~1100$  K [3] and the high Néel temperature of  $T_N = ~640$  K of BFO [2]. Furthermore, BFO has high polarization at ~90 µC/cm<sup>2</sup> that can be oriented along any of the <111> directions [4].



Figure 1. The general 3-dimensionsal view of the pseudocubic perovskite structure of BFO demonstrating the [111] polarization vector [4].

In addition, the spin and polarization are coupled via the Dzyaloshinskii-Moriya interaction, creating a canting of the magnetic moments, which results in a spin cycloid [5]. This magnetic texture becomes ordered within ferroelectric domains and acts as highways for spin travel, but domain walls create discontinuities that interrupt spin travel [5]. If we create a material with only one ferroelectric polarization direction and no domain walls we will have no disruption to the spin cycloids. Single-domain BFO thin films have been grown successfully on orientations other than the (110) [3], and they demonstrate applicability to spintronics due to the room temperature multiferroic properties of BFO.

This paper gives an overview of the epitaxial growth methods used, details the characterization methods of BFO (110), and discusses the results from these experiments.

#### Methods

A growth series of varying thicknesses of the BFO thin film was developed on SrTiO<sub>3</sub> (STO) (110) substrates. Three samples at ~10nm, ~60nm, and ~100nm of BFO were grown directly on STO (110) substrates. Two samples at ~30nm and ~60nm BFO had ~30nm of an SrRuO<sub>3</sub> (SRO) bottom electrode between the BFO film and the STO substrate. The SRO bottom electrode favors single-domain growth of subsequent BFO [6] and grounds the film during experiments that apply an electric field. The film deposition technique used was molecular-beam epitaxy (MBE). MBE is an ultrahigh vacuum technique that uses heated elemental sources to create beams of metal cations that oxidize on the substrate target.

The growth parameters for BFO require elemental bismuth and iron sources and distilled ozone. The substrate temperature is controlled via resistive heating at 675°C ( $\pm$  5°C). The bismuth and iron sources are heated to achieve the optimum 8:1 flux ratio of bismuth to iron for stoichiometric BFO growth. The distilled ozone consists of 80% O<sub>3</sub> and 20% O<sub>2</sub> with a pressure of 5 x 10<sup>-6</sup> Torr.

The film growth was monitored in situ with reflection high-energy electron diffraction (RHEED).

Ex situ, film growth and quality were characterized using x-ray reflection (XRR), x-ray diffraction (XRD), and atomic force microscopy (AFM). Reciprocal space mapping (RSM) was used to interpret the domain structure.

#### **Results and Discussion**

The XRR data (Figure 2a) confirms the thicknesses of the BFO and SRO films in each sample. The XRD spectra (Figure 2b) capture the 110 and 220 peaks and demonstrate correct stoichiometry and orientation of all materials present. Thus, the XRD implies phase purity of the BFO films and the SRO films.



Figure 2. a) XRR scans of the samples and b) XRD peaks of the BFO, SRO, and STO (110) families as expected.

AFM results allow qualitative and quantitative measurement of sample surface topography. The qualitative aspect permits observation of surface type, growth mechanism, and topographical impurities. BFO (110) films typically form striped domains on the surface [4, 6], which was observed in most samples (Table 1). The root-mean-square (RMS) roughness value for the AFM scans quantitatively represents the roughness of the surface (Table 1). These data points reveal that all samples besides the ~10nm BFO sample were of target quality.

 
 Table 1. AFM results of surface RMS roughness and topographical type for each sample.

Sample	RMS Roughness	Surface Type
10nm BFO	1.903nm	Spotted
60nm BFO	1.955nm	Striped
100nm BFO	1.433nm	Striped
30nm BFO/SRO	2.391nm	Striped
60nm BFO/SRO	4.218nm	Striped

RSMs at specific reciprocal lattice reflections are typically used to show film strain but may also be used to indicate structural variations. The 221 peak positions fingerprint ferroelectric domain variations for the material used [3]. If peak-splitting of the 221 BFO peak is observed, this means there are two or more structural polarization variants; therefore, the sample is not single-domain (Figure 3a). Likewise, if no split 221 BFO peaks are observed, this indicates that there is only one polarization variant present, making the sample single-domain (Figure 3b).



**Figure 3.** RSMs of the 221 peak demonstrating **a**) peak-splitting and multiple domains in the ~60nm BFO sample and **b**) a single 221 BFO peak and a single-domain structure in the ~100nm BFO sample.

### **Conclusion and Future Work**

Analysis of the 221 RSMs of each sample reveal that the ~100nm BFO (Figure 3b), ~30nm BFO/SRO, and ~60nm BFO/SRO samples are single-domain. The reciprocal lattice reflection for ~10nm BFO was indeterminate of a single or double peak, requiring further testing. The ~60nm BFO sample demonstrated peak-splitting, so it is not single-domain (Figure 3a).

Overall, most MBE growths of BFO (110) were single-domain based on analysis of RSM at the 221 reciprocal lattice reflection. Further testing to confirm this analysis will utilize piezoforce microcopy to observe the ferroelectric domains and nitrogen vacancy magnetometry to observe magnetic domains and spin cycloids.

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