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# Characterization of $(Ba_{0.5}Sr_{0.5})$ TiO<sub>3</sub> Thin Films for Ku-Band Phase Shifters

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> This report is a formal draft or working paper, intended to solicit comments and ideas from a technical peer group.

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# CHARACTERIZATION OF (Ba<sub>0.5</sub>Sr<sub>0.5</sub>)TiO<sub>3</sub> THIN FILMS FOR Ku-BAND PHASE SHIFTERS

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The microstructural properties of  $(Ba_{0.5}Sr_{0.5})TiO_3$  (BSTO) thin films (300, 700, and 1400 nm thick) deposited on LaAlO<sub>3</sub> (LAO) substrates were characterized using high-resolution x-ray diffractometery. Film crystallinity was the parameter that most directly influenced tunability, and we observed that a) the crystalline quality was highest in the thinnest film and progressively degraded with increasing film thickness; and b) strain at the film/substrate interface was completely relieved via dislocation formation. Paraelectric films such as BSTO offer an attractive means of incorporating low-cost phase shifter circuitry into beam-steerable reflectarray antennas.

Keywords: ferroelectric; paraelectric; thin film; microstructure; phase shifter

## INTRODUCTION

Next-generation wireless communication systems will require communication channels with much higher data transfer rates than current systems. For example, the Iridium system has recently been deployed and allows for uplink (user-to-satellite) data transfer rates of 2.4 kilobits per second<sup>[1]</sup>. By contrast, Teledesic, which is planning to become operational in 2002, will allow for uplink data transfer rates of up to 2.04 megabits per second<sup>[2,3]</sup>. To support such high data transfer rates, broadband channels at Ku-band (12-18 GHz), K-band (18-26 GHz) and higher frequencies must be used. Furthermore, since the satellite moves relative to the user in low earth orbiting (LEO) systems, steerable-beam antennas are required to maintain the user-to-satellite link. The need to process signals at such high frequencies while simultaneously tracking the satellites presents a challenging problem; beam steering and signal processing require electronically tunable devices, yet the nonlinearities inherent in tunable devices cause signal degradation and higher bit error rates<sup>[4,5]</sup>. For low frequency, low bandwidth systems tunable

devices based on silicon varactors and diodes work well. However, because of intractable materials limitations<sup>[6,7]</sup>, it is doubtful that silicon-based devices can meet the performance requirements or cost constraints for beam-steerable antennas, tunable oscillators, and tunable filters in next-generation broadband satellite systems.

Our interest in (Ba, Sr)TiO<sub>3</sub> (BSTO) thin films arises from the fact that the properties of these materials appear highly suited for broadband, tunable devices. The paraelectric films have dielectric constant ( $\varepsilon_r$ ) values of typically 2000-3000, and  $\varepsilon_r$  is tuned via a dc voltage. Ideally, we would like the films to display high tunability, low losses, and no hysteresis (either as a function of voltage or temperature). Prior work has established that the capacitance and tunability of the films is independent of frequency up to 30 GHz, and dielectric losses at frequencies above 10 GHz are comparable or lower than in Si-based tunable devices which perform similar functions<sup>[8,9]</sup>. Furthermore, the planar configuration of the thin film devices make them highly attractive for monolithic patterning of phase shifter arrays, which is a key step in the development of low-cost beam-steerable antennas such as the reflectarray antenna shown in Figure 1. Other applications currently under development are tunable local oscillators and tunable filters<sup>[10]</sup>.



FIGURE 1 Schematic diagram of beam-steerable reflectarry antenna. RF power is supplied to the radiating elements by a single solid-state amplifier, and beam steering is accomplished by electronically controlling the phase between radiating elements (diagram reprinted by permission of C.A. Racquet). The tunability and dielectric loss of paraelectric films at GHz frequencies is highly dependent on film microstructure. Prior work has established that tunability is maximized in highly epitaxial films with minimal strain<sup>[11,12]</sup>. Furthermore, substantially higher tuning/loss ratios are observed in films with planar (both electrodes on top of the film) rather than with parallel plate configurations<sup>[13]</sup>. However, a detailed understanding of how film strain impacts tunability and loss is lacking. The objectives of this paper are to differentiate in-plane from out-of-plane strain in BSTO films of varying thickness and correlate film microstructure with tunability and loss.

### EXPERIMENTAL PROCEDURE

The BSTO films were deposited on single-crystal LaAlO<sub>3</sub> (LAO) substrates using pulsed laser deposition. The substrate temperatures and oxygen pressures during deposition were 750 °C and 100 millitorr, respectively. The BSTO films reported in this study were 300, 700, and 1400 nm thick. The films were patterned into phase shifters using a conventional lift-off technique, and the metallization consisted of a 10 nm Cr adhesion layer deposited directly on the BSTO film, followed by a 2  $\mu$ m thick Au layer. The BSTO films were not selectively etched. Ground planes comprised of 10 nm Cr/2  $\mu$ m Au layers were also deposited on the backside of the substrate. A detailed descriptions of the 8-element phase shifter design and microwave performance at cryogenic as well as room temperatures have been reported<sup>[14,15]</sup>. Phase shift and insertion loss were measured at room temperature, in an evacuated chamber, using an HP 8510 network analyzer.

The microstructure of the films was characterized using high-resolution x-ray diffractometry. The out-of-plane lattice parameters and full-width half-maximum (FWHM) values were obtained via  $\omega$ -scans of the BSTO and LAO (002) peaks. The in-plane lattice parameters were obtained via asymmetric  $\omega$ -scans across the BSTO and LAO (103) and ( $\bar{1}$ 03). Since the x-ray incidence and exit angles differ for the asymmetric scans, the in-plane and out-of-plane contributions to the Bragg diffraction vector also differ, thus enabling us to generate two equations to solve for the in-plane ( $a_{\parallel}$ ) and out-of-plane ( $a_{\perp}$ ) lattice parameters. In addition, the extent to which strain caused by lattice mismatch at the film/substrate interface is relieved by dislocations at the interface can also be measured. This technique is widely used to characterize semiconductor heterostructures<sup>[16]</sup>, and is applicable to paraelectric films when the films are of sufficiently high crystalline quality so as to yield observable diffraction peaks using the high-resolution x-ray diffractometer.

#### RESULTS

Asymmetric  $\omega$ -2 $\theta$  scans about the (103) BSTO and LAO peaks for the 300 nm film are shown in Figure 2. The film-to-substrate peak distances and shapes of the peaks were virtually identical for the ( $\overline{1}03$ ) peaks, except the  $\omega$  values range from 56-60°. The  $\omega$  angles were chosen so as to fulfill the diffraction conditions for glancing incidence or glancing exit configurations. These data provide several insights into the film microstructure. First, the film crystallinity is much poorer than that of the substrate; the FWHM of the BSTO peak is 0.23°, whereas the substrate FWHM is 0.015°. Next, the substrate-to-film distance between the glancing incidence and glancing exit peaks are identical, indicating that interfacial strain is completely relieved by dislocations. We observed complete relaxation at the film/substrate interface for all of the BSTO/LAO films.



FIGURE 2  $\omega$ -2 $\theta$  scan about the (103) BSTO and LAO diffraction peaks. Data taken under glancing incidence conditions.

A reciprocal space map of the BSTO and LAO (103) diffraction peaks is shown in Figure 3. The axes are drawn so that the y-axis extrapolates to the (0, 0) reciprocal lattice point. The fact that a line drawn from the LAO peak to the BSTO peak also extrapolates to the reciprocal lattice origin indicates the film is completely relaxed relative to the substrate. Furthermore, the graph shows the BSTO peak is substantially broader in the x-direction than in the y-direction, indicating poorer crystallinity in the direction parallel to the film surface than perpendicular to it.



FIGURE 3 Reciprocal lattice map of LAO and BSTO (103) peaks. The position of the BSTO peak relative to LAO indicates relaxation at the BSTO/LAO interface, and the broadness of the BSTO peak indicates degradation of the film crystallinity.

We observed a decrease in film crystallinity with increasing thickness. The full-width, halfmaximum values for the BSTO (002) and (103) peaks are shown in Figure 4. Also shown is the maximum x-ray intensity from the (002) peaks. The lowest FWHM values for both the (002) and (103) peaks were observed in the 300 nm thick film. Both the (002) and (103) FWHM values increased with increasing film thickness, indicating that the crystalline quality of thicker films was inferior to that of thinner films. However, the rate at which the film quality degrades is different; with increasing film thickness, the (002) FWHM increases more rapidly than the (103) peaks, indicating that increasing film thickness is more detrimental to the out-of-plane than the in-plane. The degradation in film crystallinity is further verified by examining the (002) peak intensities. There was a slight increase in peak intensity as the film thickness was increased from 300 to 700 nm, however, the sharp drop in intensity for the 1400 nm thick film attests to the fact that the film crystallinity degraded with increasing film thickness.



FIGURE 4 X-ray diffraction full-width, half-maximum (FWHM) values of the (002) and (103) peaks, and (002) peak intensity as a function of BSTO film thickness.

There was no clear correlation between lattice parameter and film thickness or tunability. Figure 5 shows  $a_{\parallel}$  and  $a_{\perp}$  for BSTO films with varying film thicknesses. In all three cases,  $a_{\parallel}$  and  $a_{\perp}$  were slightly higher than the ideal lattice parameter, and the expansion was more pronounced in the  $a_{\parallel}$  direction. However, for the films reported in this study, the variations in lattice parameters at different film thicknesses were modest. We note that for films not reported in this study, which were deposited under different conditions (i.e. temperature and  $O_2$  pressure) and using other techniques such as sputtering, film strain can be much more pronounced and thus have a direct impact on tunability.



FIGURE 5 In-plane  $(a_{\parallel})$  and out-of-plane  $(a_{\perp})$  lattice parameters of BSTO/LAO films as a function of film thickness. Both  $a_{\parallel}$  and  $a_{\perp}$  are slightly expanded relative to the ideal lattice parameter.

The ultimate objective of our film characterization studies is to optimize phase shifter performance. Figure 6 plots phase shift and K factor, which is a figure of merit used to rate phase shifter performance (=phase shift (degrees)/insertion loss (dB)), at  $\approx 15$  GHz. The phase shift is relatively constant for varying film thicknesses, which is counterintuitive. We expect the phase shift to increase with increasing film thickness<sup>[14]</sup>, and the fact that phase shift does not substantially increase with increasing BSTO thickness, coupled with the degradation in film crystallinity for thicker BSTO films, indicates that the drop in film crystallinity is extremely deleterious to tuning. Furthermore, the K factors are substantially higher for the thinner films, indicating that phase shifters with the best figures of merit require highly crystalline BSTO thin films.



FIGURE 6 Phase shift (degrees) and K-factor (phase shift/insertion loss (dB)) as a function of film thickness for BSTO 8-element phase shifters.

#### DISCUSSION

The goal of this work is to quantify the microstructural properties of BSTO films so as to understand how phase shifter tuning and loss are impacted by film. For crystalline BSTO thin films, a number of film parameters can be determined using high-resolution x-ray diffractometry. For the BSTO/LAO films, the crystalline quality was highest in the thinnest film (300 nm). This was also the film that yielded the best phase shifter figure of merit. Increasing the film thickness provided little or no enhancement in phase shift, which was correlated with a drop in film crystallinity for the thicker films.

We did not observe any correlation between film strain and phase shifter performance. This was surprising because there is a large lattice mismatch (4%) between the BSTO films and LAO. The lack of strain dependence was attributed partly to the fact that the deposition process was optimized so as to minimize film strain, and partly to complete strain relaxation at the film/substrate interface.

The microstructural feature that most significantly influenced tunability was film crystallinity. The thin crystallinity both perpendicular and parallel to the film surface was best in the 300 nm film, and degraded with increasing film thickness. For the 300 nm film, the film crystallinity was better in the  $a_{\perp}$  than  $a_{\parallel}$  directions, as evidenced by the FWHM of the (002) and (103) peaks (0.056 vs. 0.097 degrees, respectively). Because the reflectarray antenna design is configured with the RF and DC electric fields parallel to  $a_{\parallel}$ , this data suggests that improving the in-plane crystallinity of the thin films will lead to higher tunability and perhaps higher K-factors in the phase shifters.

#### CONCLUSIONS

Beam-steerable reflectarray antennas that use tunable paraelectric films in the phase shifter circuitry offer an attractive means of maintaining low-cost communication links for broadband communication systems at Ku-band and higher frequencies. However, optimization of the film microstructure and phase shifter design requires a detailed understanding of how film microstructure impacts microwave tuning and loss. We observed that the tunability of BSTO films deposited on LAO substrates was most heavily influenced by the film crystallinity, and the thinnest films (300 nm) displayed the best crystallinity and phase shifter figure of merit. Film strain was completely relaxed at the BSTO/LAO interface, and did not have a discernable impact on tunability.

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