SYNTHESIS AND CHARACTERIZATION OF $(Ba_xSr_{1-x})Ti_{1+y}O_{3+z}$ THIN FILMS AND INTEGRATION INTO MICROWAVE VARACTORS AND PHASE SHIFTERS*

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Precise control of composition and microstructure is critical for the production of $(Ba_xSr_{1-x})Ti_{1+y}O_{3+z}$ (BST) dielectric thin films with the large dependence of permittivity on electric field, low losses, and high electrical breakdown fields that are required for successful integration of BST into tunable high frequency devices. Here we review recent results on composition-microstructure-electrical property relationships of polycrystalline BST films produced by magnetron sputter deposition, that are appropriate for microwave devices such as phase shifters. Films with controlled compositions were grown from a stoichiometric $Ba_{0.5}Sr_{0.5}TiO_3$ target by control of the background processing gas pressure. It was determined that the (Ba+Sr)/Ti ratios of these BST films could be adjusted from 0.73 to 0.98 by changing the total $(Ar+O_2)$ process pressure, while the O_2/Ar ratio did not strongly affect the metal ion composition. Film crystalline structure and dielectric properties as a function of the (Ba+Sr)/Ti ratio are discussed. Optimized BST layers yielded capacitors with low dielectric losses (0.0047), among the best reported for sputtered BST, while still maintaining tunabilities suitable for device applications. These BST films were used to produce distributed-circuit phase-shifters, using a discrete periodic loading of a coplanar waveguide with integrated BST varactors on high-resistivity silicon. Phase shifters yielding 30 degrees of phase shift per dB of insertion loss were demonstrated at 20GHz.

Keywords: magnetron sputter-deposition, BST films, film stoichiometry, tunability, loss, leakage, phase shifters

INTRODUCTION

The charge storage capacity, low leakage, high dielectric nonlinearity, high breakdown field, and low microwave losses of $(Ba_xSr_{1-x})Ti_{1+y}O_{3+z}$ (BST), given appropriate BST/electrode/substrate processing and integration strategies, make it suitable for application to Gbit DRAMs [1,2] and high frequency devices [3-7], even when using polycrystalline BST films exhibiting epitaxial film-like properties [8].

BST films with controlled composition and properties can be produced by RF magnetron sputter-deposition, using a single BST oxide target. However, it is critical to understand the effect of processing parameters to achieve optimum composition, microstructure and properties of the BST layer and capacitors. Specifically, the electrical properties of BST films are sensitive to Ti non-stoichiometry measured by the (Ba+Sr)/Ti ratio [8-11]. It is found that sputtering from single stoichiometric oxide targets produce non-stoichiometric oxide thin films (e.g., $SrTiO_3$, $Ca_{1-x}Sr_xCuO_2$, and $YBa_2Cu_3O_x$ [12-14]), which can be avoided by growing films under high gas pressure using target-substrate off-axis geometry [15] or compositionally-adjusted targets [12,14] BST targets with various (Ba+Sr)/Ti [9] and Ba/Sr ratios [16] were utilized to produce compositionally adjusted BST films by physical vapor deposition. Our magnetron sputter-synthesis work demonstrated that: (a) (Ba+Sr) / Ti ratios of BST films can be adjusted simply by using a single stoichiometric BST target coupled with accurate control of the total $Ar+O_2$ process pressure [6], (b) BST capacitors involving layered BST films with high tunability-low loss or intermediate tunability-very low loss individual layers result in capacitors with simultaneous low loss and high tunability [17] and (c) high performance phase shifters can be fabricated [18,19] using our sputter-deposited BST films [7, 17] integrated with high resistivity Si substrates.

SYNTHESIS AND PROPERTIES OF SPUTTER-DEPOSITED BST FILMS USING A SINGLE BST TARGET

BST thin films (70-80 nm thick) were produced and extensively characterized at Argonne National Laboratory (ANL), using RF magnetron sputtering in Ar-O_2 gas mixtures. The substrate and target (a sintered stoichiometric $Ba_{0.5}Sr_{0.5}TiO_3$ disc) were positioned parallel to each other in an on-axis configuration with 10 cm separation. BST films were deposited at 650°C on Pt(120nm) / TiO_2(40nm) / SiO_2(300nm) / Si or Pt(120nm)/SiO_2(300nm)/Si substrates. High resistivity silicon (>10 kΩ-cm) substrates were used in anticipation of microwave circuit applications. Test capacitors were produced by depositing 100 µm diameter Pt top electrodes at 350°C through a shadow mask, followed by annealing the whole capacitor at 550°C for 30 minutes in air, in order to minimize contamination at the top Pt electrode/BST interface and improve its structure.

RBS, XRD, field emission SEM, and SPM were used to investigate the thickness, composition, crystallographic orientation, microstructure, and roughness of the BST films, respectively. Dielectric properties (relative permittivity, ε, and dielectric loss, $\tan \delta$) were measured as a function of applied electric field at 10 kHz and 0.1 Vrms oscillation level, using a HP 4192A impedance analyzer. Capacitance and loss were also characterized at 1MHz using a Keithley C-V meter.

Figure 1 (a) shows the variation of the (Ba+Sr)/Ti and Ba/Sr ratios in BST films as a function of the total (Ar+O_2) deposition pressure with the O_2/Ar ratio fixed at 1/5. The ratio of (Ba+Sr)/Ti changed from 0.73 to 0.98 for films grown with total gas pressure from 22 to 58 mTorr. The growth rate of the BST films depends on the total process pressure (Figure 1 (b)). Variation of the O_2/Ar ratio in the 1:1-1:5 range did not affect the metals composition of the BST films.

BST films with (Ba+Sr)/Ti ratios ≥ 0.9 exhibited a polycrystalline structure characterized by (100), (110), and (111) peaks in the XRD spectra [7], which disappeared for (Ba+Sr)/Ti ratios below 0.85. This, coupled with the relatively high permittivities still found for these samples, suggests that high-Ti BST films are nanocrystalline, although TEM work is necessary for confirmation.

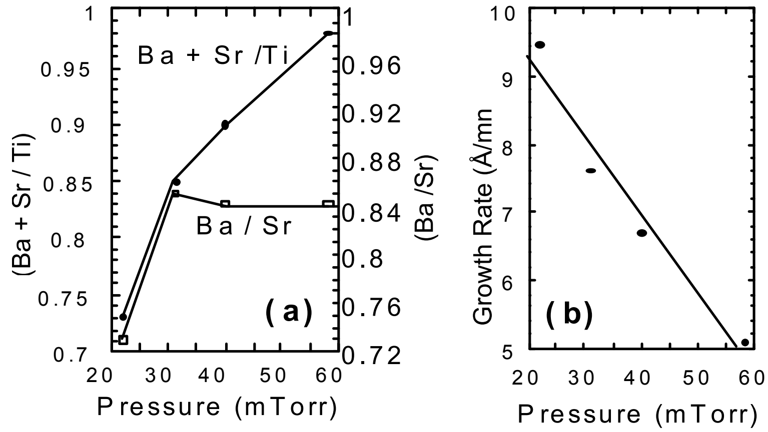


FIGURE 1. (a) Variation of (Ba+Sr)/Ti and Ba/Sr ratios for BST films deposited at 650°C from a stoichiometric target with a Ba/Sr ratio of 50/50, and (b) growth rate as a function of the total pressure ($Ar+O_2$) [7].

The rms roughness measured by SPM was approximately 3 nm for BST films with (Ba + Sr) / Ti ≥ 0.9 and 2 nm for BST films with (Ba+Sr)/Ti ≤ 0.85, correlating with the structural changes indicated by XRD spectra. BST films with (Ba+Sr)/Ti ratios > 0.9 exhibited a dense and granular microstructure, while BST films with (Ba+Sr)/Ti ratios < 0.85 exhibited a featureless microstructure.

Figure 2 shows the field-dependent dielectric properties of BST capacitors measured at 10 kHz. The BST film with (Ba+Sr)/Ti = 0.95 [Figure 2(a)], displayed the largest tunability [~ 74% (ε_{max}- ε_{min}/ ε_{max})], while the lowest dielectric loss of 0.0047 at zero bias was found for the sample with (Ba+Sr)/Ti = 0.73 [Figure 2 (b)]. The relationships governing permittivity and loss for these films remain to be fully explored. The BST capacitor with the highest figure of merit K= tunability/tan δ corresponds to a (Ba+Sr)/Ti ratio of 0.73.

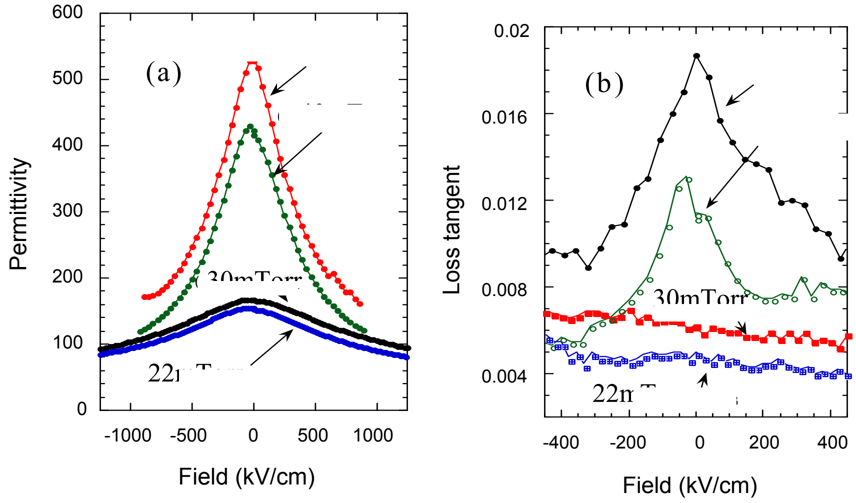


FIGURE 2. (a) Permittivity and (b) loss tangent measured at 10 kHz and 0.1V oscillation, for BST deposited at various ($Ar+O_2$) pressures. The permittivity was measured until capacitor breakdown occurs [7]

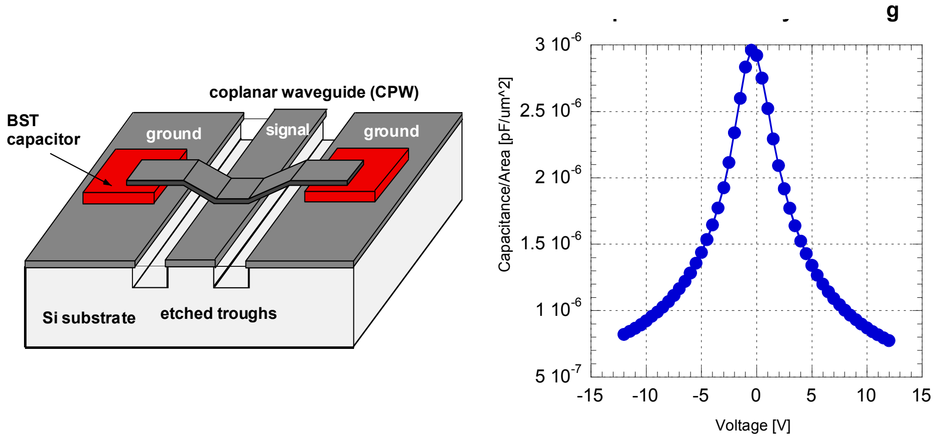
Capacitors with BST near stoichiometric films [(Ba+Sr)/Ti = 0.95] displayed high tunability (74 %) and high dielectric loss (tan δ= 0.0187), while capacitors with Ti-rich BST layers [(Ba+Sr)/Ti = 0.73] exhibited low dielectric loss (tan δ = 0.0047) and less tunability (47.6 %) [see Figures 2 (a) and (b)]. Based on this result, we recently produced capacitors with layered BST films with each layer optimized for maximum tunability or minimum loss [17]. The optimized capacitors involved (Ba+Sr)/Ti = 0.73 layers at the Pt electrodes / BST interface, and a central layer with (Ba+Sr)/Ti = 0.95 ratio. This layered structure yielded BST capacitors with simultaneous high tunability and low loss. While single layer stoichiometric [(Ba+Sr)/Ti = 0.95] BST capacitors exhibited ~1 MV/cm breakdown field, layered BST capacitors [(Ba+Sr)/Ti = 0.73 / 0.95 / 0.73] with bottom and top interface layers exhibited breakdown at 2.8 MV/cm, since for this field the leakage is still below the irreversible resistance degradation. In addition, the layered BST capacitors exhibit low leakage (~ 6 x10^{-9} A/cm^2). Typical tunabilities and loss for these films are 3:1 and 1% (@ 1MHz), respectively.

PHASE SHIFTERS BASED ON OPTIMIZED MAGNETRON SPUTTER-DEPOSITED BST FILMS

The BST thin films described above have been incorporated into monolithic microwave integrated capacitors in thin-film phase-shifters circuits. The approach taken in this work was to fabricate monolithic parallel-plate capacitors using standard IC processes, and integrate these with microwave coplanar-waveguide transmission-line structures. Figure 4 (a) illustrates a simple parallel-plate capacitor structure integrated in shunt along a coplanar transmission-line (CPW). For lowest possible loss, the silicon substrates can be micromachined in the CPW gap region as shown. This also has the advantage of reducing the capacitance per unit length on the unloaded-line, allowing for larger capacitive loading in a circuit. Figure 3 (b) shows a typical capacitance versus voltage curve for the parallel plate devices fabricated at University of California-Santa Barbara (UCSB) on a 100nm film with a zero-bias dielectric constant of ~300, using BST films from Argonne National Laboratory (ANL) and UCSB.

Monolithic delay lines were then implemented using this technology. The delay lines are distributed circuits using a coplanar waveguide periodically loaded with thin-film BST varactors, as shown in Figure 4. When designed correctly, this structure is a synthetic transmission line with a phase velocity that can be controlled by changing the value of the external loading capacitors. The parallel plate capacitor topology utilizes the tunability of the BST film effectively and requires lower control voltages than interdigitated electrode designs. Conductor losses are low in this topology.

UCSB has recently [6] used this topology to demonstrate analog phase shifter circuits using monolithic GaAs varactors loading a coplanar waveguide (CPW) transmission line in K-band, resulting in < 4 dB insertion loss at 20 GHz and a continuously programmable delay of 0-360 degrees at this frequency.



(a) (b)

FIGURE 3: a) Integrated thin-film capacitor structure on a coplanar waveguide. b) Low-frequency (1 MHz) C-V curve of a typical UCSB/ANL device showing 4:1 capacitance variation.

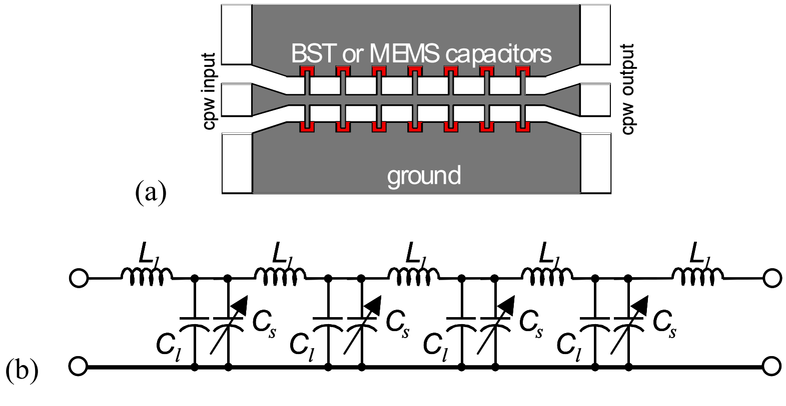
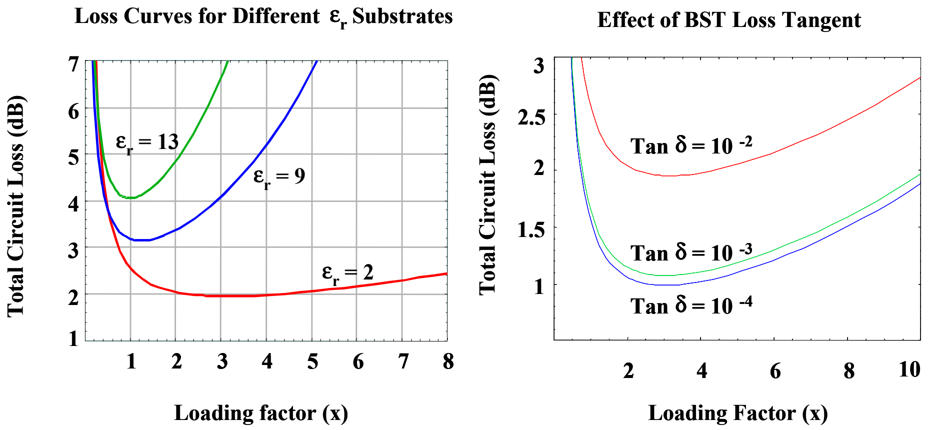


FIGURE 4: (a) Distributed circuit phase shifter using a periodically-loaded coplanar waveguide. (b) Equivalent circuit of the distributed phase shifter.

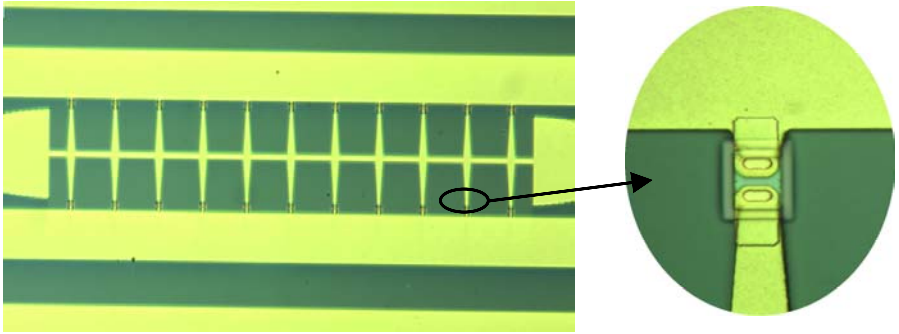
Excellent performance of the phase shifters was the result of careful modeling of the circuit, especially with respect to RF losses, which allowed us to optimize the structure for low insertion loss and high performance. An especially important parameter is the loading factor ‘x’, which is the ratio of the variable capacitor per unit length to the unloaded line capacitance per unit length. For a given variable capacitor technology and substrate dielectric constant there exists an optimum loading factor which results in a circuit with the lowest possible insertion loss. This has been experimentally verified by measuring the losses on GaAs varactor loaded transmission lines, and it was found that losses for the optimally loaded transmission line are dominated by the losses in the variable capacitor. Thus, further efforts to reduce the losses of the circuit must concentrate on reducing losses in the variable capacitor, which favors the use of thin-film BST technology.



(a) (b)

FIGURE 5 – Predicted losses for BST-based circuits like that of fig.3. (a) Influence of substrate dielectric constant ($\tan\delta=0.02$, or $Q=50$); (b) Influence of loss tangent ($\varepsilon_r=2$).

To demonstrate the potential of BST thin film varactors for distributed phase-shifters, a loss analysis was carried out for different substrate dielectric constants and for different values of loss tangent of the BST film. The results are displayed in Figure 5, which shows that there is a certain optimum loading factor for minimization of the total circuit loss. The total circuit loss decreases with a decrease in the substrate dielectric constant, due to a subtle interplay between conductor loss and characteristic impedance. Since the BST technology allows a range of substrates to choose from, it should be possible to achieve substantially lower loss than with GaAs-based circuits. Another set of calculations we performed was to investigate the effect of the BST thin film loss tangents on the total phase shifter losses and the results are shown in Figure 5(b). At loss tangents of 10^{-3} or lower (specified at 10 GHz) the performance is limited by conductor loss only, indicating that significant improvements over diode-based circuits can be obtained with material improvements.



(a) (b

FIGURE 6: a) Photograph showing a periodically loaded line phase shifter fabricated at UCSB. b) Details of parallel plate BST capacitor used in the circuit.

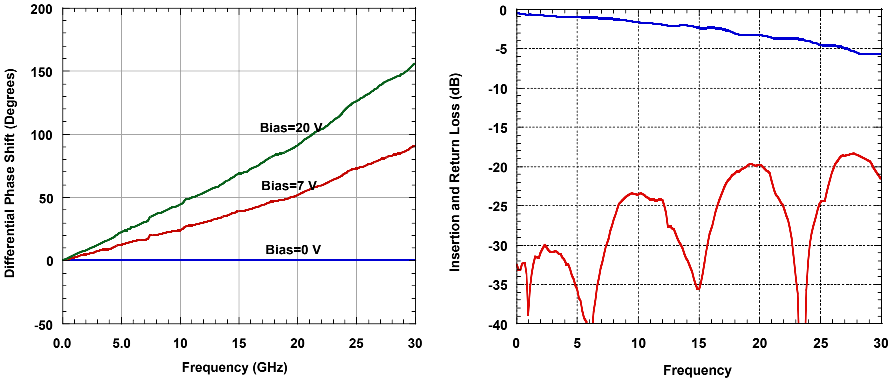


FIGURE 7: Measured performance of a periodically loaded line phase shifter fabricated at UCSB.

UCSB has recently [19] demonstrated a BST-based periodically loaded line phase shifter as shown in Figure 6. The phase shifter was capable of producing up to 160° of phase shift at 30 GHz. The phase shift increases linearly with frequency as expected for a variable time delay element. The preliminary results of this phase shifter are shown in Figure 7. Note that this phase shifter has not yet been fully optimized, however the result seems to confirm the potential of thin film BST technology. Advances in the materials are required to further improve on this result.

CONCLUSIONS

In conclusion, we have shown that BST films with high tunabilities, low losses, and high dielectric breakdown fields can be grown using magnetron sputter deposition with judiciously chosen process parameters. Specifically, control is demonstrated of the composition (i.e., the (Ba+Sr)/Ti ratio) of BST films grown from a single stoichiometric target by use of tailored target-substrate geometry and deposition pressure. These results are consistent with a mechanism based on the pressure dependencies of the individual fluxes of Ba, Sr, and Ti impinging on the substrate (i.e., the different constituents have different, pressure dependent angular scattering distributions in the gas phase, due to their different masses). Figures of merit, defined as the ratio of tunability to dielectric loss, of approximately 100 have been obtained under optimized deposition conditions, with among the lowest losses at zero bias (0.0047) reported for physical vapor deposited BST films. In addition, we demonstrated that BST capacitors with magnetron-sputter-deposited layered BST films exhibit enhanced tunability, minimized dielectric loss and leakage current, and increased dielectric breakdown, which make them suitable for high frequency devices.

Periodically loaded line phase shifters with up to 160° of phase shift at 30 GHz were fabricated using BST capacitors involving the magnetron sputter-deposited BST films produced in our program. The phase shift increased linearly with frequency as expected for a variable time delay element. The phase shifters produced in our program are not fully optimized yet, however the result presented in this paper indicate the potential of thin film BST technology for high frequency devices. Advances in the materials are required to further improve on this result.

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