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Fabrication of (Ba,Sr)TiO$_3$ Epitaxial Thin Films and Characterization of Microwave Waveguiding Structures

Gun Bhakdisongkhram, Youji Yamashita, Takashi Nishida,
Kiyoshi Uchiyama and Tadashi Shiosaki
Graduate School of Materials Science, Nara Institute of Science and Technology (NAIST), 8916-5 Takayama-cho, Ikoma,
Nara 630-0192, Japan. Fax: 0743-72-6069, e-mail: g-bhakdi@ms.naist.jp

$Ba_xSr_{1-x}TiO_3$ (x=0.5) (BST) films were epitaxially deposited on c-cut sapphire substrates by rf sputtering. A coplanar waveguide line was fabricated and both the phase shift and loss tangent of the samples were measured using the on-wafer through-reflect-line (TRL) calibration comparison method. After applying an external bias of 200 V to the coplanar waveguide line fabricated on the BST layer, the phase of the line changes according to the dependence of BST permittivity on bias. The high phase shifts (6.3° per cm) and low loss tangent (0.009) resulted from high crystalline quality of the epitaxial BST film grown on the c-cut sapphire.

Key words: BST, films, microwave, phase shift, substrate

1. Introduction

Dielectric nonlinearity in ferroelectric thin films, which is a result of applying an external electrical bias to the films, will be a crucial characteristic for compact frequency-agile microwave devices [1-2]. $Ba_xSr_{1-x}TiO_3$ (BST) film exhibits high permittivity, considerable loss tangents and high nonlinearity, and therefore is considered a promising material for microwave devices. In order to achieve higher nonlinearity, most efforts have focused on growing the BST films epitaxially on some single-crystal substrates such as MgO and $LaAlO_3$ [3]. These substrates are chosen because their lattice constants and thermal expansion coefficients are close to those of BST films. However, high costs and the deliquescence of the surfaces of these substrates are the practical problems for application in commercial BST microwave devices. As an alternative choice, single-crystal sapphire substrates possess low dielectric losses and are relatively cheap. However, the lattice structure of sapphire is very different from that of the BST film. This raises the question that even if the BST can be epitaxially grown on the sapphire substrates, it is unclear whether or not they will be suitable for microwave devices.

This paper demonstrated the coplanar waveguide structure on BST films. The phase of a microwave signal in the waveguide changes whenever the BST films are under an external electrical bias, corresponding to the change of the permittivity of BST films. The high crystalline quality of the epitaxial BST film was found to be the primary cause of its high tunability and low loss tangent.

2. Experimental

$Ba_xSr_{1-x}TiO_3$ (x=0.5) films were deposited onto 0.5 mm-thick substrates of MgO, c-cut sapphire, and r-cut sapphire at 600°C by rf-magnetron sputtering. The thickness of deposited films after 5 h was approximately 1 μm. The sputtering gas pressure was 2-7 Pa, with an Ar/O$_2$ gas ratio of 9/1. The resultant stoichiometric composition of the Ba$_{0.5}$Sr$_{0.5}$TiO$_3$ films was confirmed by X-ray fluorescence spectroscopy. The crystalline structure of deposited films was confirmed by *X*-ray diffraction (XRD) analysis.

Test patterns are coplanar waveguide lines which were fabricated on the BST film layer using a conventional photolithography technique. As a top electrode, aluminum thin film of 1.0 μm thick was deposited onto the BST by vacuum evaporation, and then was patterned by wet etching. The widths of both the signal line and slot were designed to be 25 μm to obtain the characteristic impedance of 50 ohm. The signal path was 1 cm long.

Microwave measurements were carried out with a network analyzer (R3767CH, Advantest) over the frequency range from 0.1 to 7 GHz. The propagation constant was calculated from *S*-parameters of the coplanar waveguide lines through the TRL calibration method. Details of the coplanar waveguide structures and the measuring method are given in [4]. The phase of a signal on the coplanar line and the loss tangent of the BST thin film were calculated from the propagation constant of the microwave signal in the waveguide.

3. Results and Discussion

3.1 Crystalline structure of deposited films

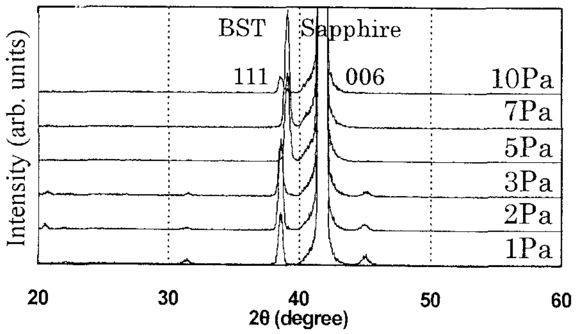

Fig. 1. XRD θ-2θ scans for BST deposited on c-cut sapphire under various gas pressures.

Figure 1 shows the results of XRD θ-2θ scans for BST deposited on c-cut sapphire under various sputtering gas pressures. These results indicate that BST on the c-cut sapphire substrates tended toward preferential (111) orientations.

Rocking-curve scans were recorded to determine whether the films were fully coherent. From the XRD rocking-curve results, the BST film deposited on the c-cut sapphire substrate at sputtering gas pressure of 7 Pa had a (111) rocking-curve full width at half maximum (FWHM) of 0.6°. This indicates that the film was fully coherent.

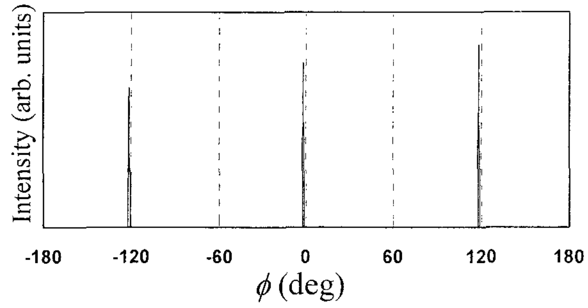

Fig. 2(a). ϕ-scans of the c-cut substrate.

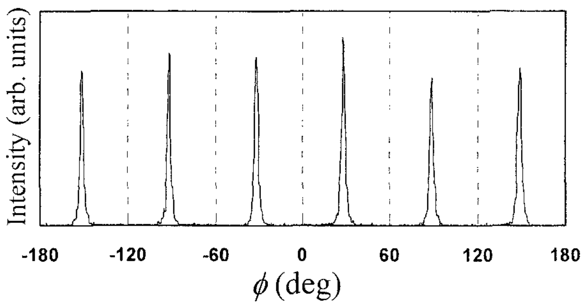

Fig. 2(b). ϕ-scans of the BST film deposited c-cut substrate at 7 Pa.

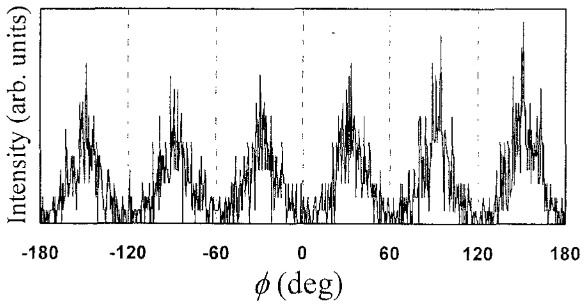

Fig. 2(c). ϕ-scans of the BST film deposited c-cut substrate at 2 Pa.

Table I: Phase shift of $Ba_xSr_{1-x}TiO_3$ thin films

case	Substrate	Ba ratio (x)	Film thickness	Applied bias: slot width	Phase shift	Loss tangent
1 (7 Pa)	c-cut sapphire	0.5	1 μm	80 kV/cm: 25 μm	6.3°/cm @3 GHz	0.009 @7 GHz
2 (2 Pa)	c-cut sapphire	0.5	1 μm	80 kV/cm: 25 μm	1.5°/cm @3 GHz	0.026 @7 GHz
3 (2 Pa)	MgO	0.5	1 μm	80 kV/cm: 25 μm	4.4°/cm @3 GHz	0.008 @7 GHz
(*ref.*[5])	r-cut sapphire	0.5	1 μm	80 kV/cm: 25 μm	0.7°/cm @3 GHz	0.016 @7 GHz
(*ref.*[6])	r-cut sapphire	0.5	0.2 μm	20 kV/cm: 20 μm	11.6°/cm @20 GHz	0.05~0.07 @7-20 GHz
(*ref.*[7])	alumina	0.6	5 μm	25 kV/cm: 16 μm	1.26°/cm @24 GHz	0.09 @24 GHz

To determine whether the films were epitaxially grown, ϕ-scans were recorded. Figures 2(a)-(c) show the results of ϕ-scans of the c-cut substrate and the BST films sputtered under the gas pressure of 7 Pa and 2 Pa, respectively. From this, we observe good BST [011] || c-cut sapphire [012] epitaxy. We concluded that the film deposited on the c-cut substrate was epitaxially grown. In addition, the works on MgO, r-cut sapphire substrate and Si substrates were investigated in our previous work, which showed that epitaxial BST film grown on MgO was the most suitable for microwave devices application [5].

3.2 Phase shift and loss tangent in coplanar line structure

After a DC bias was applied, the signal phase shifted as the permittivity of the BST film changed. Because the permittivity of the substrate under an applied bias is very small in comparison to that of the BST film, the phase shift under the influence of the DC bias occurs because of the film. The phase shift per unit line length is defined as the difference between the signal phase at zero bias and that under a DC bias across a slot of 25 μm. The results of the phase shift at 3 GHz and a bias of 200 V are shown for comparison (Table I). Details of calculation for phase shifts and loss tangents can be found in reference [5]. As illustrated in Table I, in comparison with the resultant phase shifts, the BST grown on c-cut sapphire showed the largest phase shift in the coplanar waveguide lines, followed by the MgO and r-cut sapphire substrates. From this result and the results in § 3.1, the high crystalline quality in BST film was observed to strongly influence the phase shift, which is highly correlated with the tunability (i.e., the dependence of permittivity on DC bias) of the deposited film. Others have investigated similar microwave properties of thin [6] and thick [7] BST films (Table I). Note that phase shift increases almost linearly with increasing frequency and nonlinearly with the applied bias, and the larger slot (25 μm) in our experiment should, in comparison, result in a smaller phase shift. The highest loss tangent was found in the BST films deposited on r-cut sapphire, followed by those deposited on c-cut sapphire and MgO substrate. Accordingly, the loss of BST on MgO and c-cut sapphire is low because the films deposited were epitaxially grown.

Less-oriented films have a different stoichiometry at different regions and especially at grain boundaries; this is considered the primary cause of the high loss in a less-oriented film. Thus, the loss is low when the BST film is highly oriented.

4. Conclusions

BST film was epitaxially grown on a c-cut sapphire substrate and was found to be suitable for microwave devices. The BST film was epitaxially grown on the c-cut sapphire substrate and preferred a (111) orientation. The crystalline quality of the BST film resulted in high phase shifts (6.3° per cm) and low loss tangents (0.009). These results imply that high-quality BST films deposited on c-cut substrate are suitable for microwave device applications.

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