Original Paper

phys. stat. sol. (a) **203**, No. 2, 379–385 (2006) / **DOI** 10.1002/pssa.200521385

Ferroelectric thin-film characterization using a coplanar waveguide bandstop filter

Qingduan Meng[*, 1], **Xueqiang Zhang**[1], **Fei Li**[1], **Jiandong Huang**[1], **Xiaohong Zhu**[1], **Dongning Zheng**[1], **Bolin Cheng**[2], **Qiang Luo**[3], **Changzhi Gu**[3], and **Yusheng He**[1]

[1] National Lab for Superconductivity, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, P.R. China
[2] Key Laboratory of Optical Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, P.R. China
[3] Laboratory of Microfabrication, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, P.R. China

Received 30 March 2005, revised 5 September 2005, accepted 3 October 2005
Published online 25 November 2005

PACS 77.22.Ch, 77.22.Gm, 77.55.+f, 84.40.Az

A new structure for the characterization of the permittivity of ferroelectric thin films at microwave frequencies is proposed. This new structure involves a coplanar waveguide (CPW) bandstop filter based on a ferroelectric thin film. Using the resonant frequency and Q value of the CPW bandstop filter, the dielectric constant (ε_r) and the loss tangent (tan δ) of the ferroelectric thin film were determined by comparing the measured responses with simulated results. To demonstrate this new structure, a CPW bandstop filter was fabricated on MgO substrate coated with $Ba_{0.5}Sr_{0.5}TiO_3$ (BST-0.5). The dielectric parameters determined as a function of temperature and external bias are reported.

1 Introduction

Barium strontium titanate is considered to be an important material for tunable microwave devices, such as phase shifters, tunable filters, and high-Q resonators for radar and communication applications [1–3], because of its large electric field tunability and low dielectric loss. For optimal performance of these tunable devices, it is important to study the temperature- and electric field-dependent behaviors of ferroelectric thin films. In the past few years, capacitive coupled microstrip resonators [4–7] and coplanar waveguide (CPW) transmission line structures [8, 9] have been developed for ferroelectric thin-film characterization at microwave frequencies. In the capacitive coupled microstrip resonator structure, two microstrip half-wavelength resonators are employed, and an additional lumped planar capacitor is mounted above the coupling gap, which locates between the two half-wavelength resonators. The resonant frequency and Q value are altered by the lumped planar capacitor. In this structure, it is difficult to assemble devices for a smaller lumped planar capacitor and narrower gaps, and this method is mainly based on the lumped ferroelectric capacitor. At higher frequency, it is limited because the model for the lumped capacitor is invalid. Also, in order to characterize the electric field dependence of the permittivity for ferroelectric thin films, bias circuits are unavoidable, which provide a strong decoupling between dc circuits and the microwave ones. This is unfavorable in the miniaturization of practical devices.

In the CPW transmission line structure, a dc voltage can be directly applied to the ferroelectric film through the ports of the device, so the dc bias circuit is no longer necessary, which is beneficial for mini-

[*] Corresponding author: e-mail: qdmeng@ssc.iphy.ac.cn

aturization of devices and also avoids the problem of frequency range limit from the bias circuits. However, this structure is not suitable for finding the loss tangent of the ferroelectric thin film because of the difficulty of excluding the conductor loss. Combining the advantages of the CPW transmission line structure and the resonant method, a new structure is proposed for studying the permittivity of ferroelectric thin films at microwave frequencies. Here the new structure is named a CPW bandstop filter.

2 Principle of measurement

The CPW bandstop filter structure proposed in this paper is shown in Fig. 1, which mainly consists of a CPW quarter-wavelength open-circuit stub connected perpendicularly to the main CPW transmission line. Usually the substrate is a certain well-known material, such as MgO, $LaAlO_3$, etc., coated with a ferroelectric thin film. The pattern layer is usually a conventional metal or high-temperature superconductor thin film. When the quarter-wavelength open-circuit stub is employed, the signal at the resonant frequency will not be transmitted to port 2 from port 1, thus an attenuation is formed in the transmission response curve of the CPW bandstop filter, and the resonant frequency of the quarter-wavelength open-circuit stub is given by

$$f_{(\mathrm{GHz})} = \frac{300}{\frac{\lambda_{(\mathrm{mm})}}{4}\sqrt{\varepsilon_{\mathrm{eff}}}}\,, \tag{1}$$

where $\varepsilon_{\mathrm{eff}}$ is the effective dielectric constant of the open-circuit stub [10]. It is apparent that as $\varepsilon_{\mathrm{eff}}$ increases, the resonant frequency of the open-circuit stub decreases and vice versa. Therefore from the measured resonant frequency the effective dielectric constant of the open-circuit stub can be deduced, which is determined by the dimensions of the center strip (including the gaps) of the stub, the thickness, and the permittivity of any layer under the conducting layer.

In order to obtain the dielectric constant of the ferroelectric thin film from the measured response curves of the filter, a commercially available computer-aided design program, Sonnet suites, was employed to simulate the frequency response of the filter. The dielectric constant of the ferroelectric thin film can be derived via a comparison between the simulated and measured resonant frequencies. The loss tangent of the ferroelectric thin film can be also be determined by comparing the measured Q value of the filter with the simulated one, which is defined by the formula $Q = f_0/\Delta f_{3\mathrm{dB}}$.

In the proposed structure, the CPW is utilized, so the dc bias voltage is easily applied to the ferroelectric thin film through the ports of the CPW structure. To study the electric field dependence of the ferroelectric thin film, the gaps of the open-circuit stub are designed to be much narrower than the gaps of the main CPW transmission line, as shown in Fig. 1. When a dc bias voltage is applied, the electric field

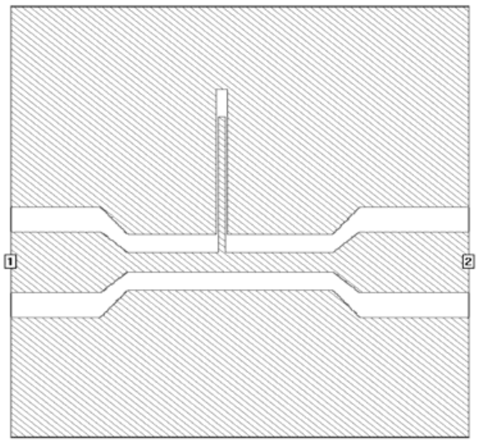

Fig. 1 Schematic of the CPW bandstop filter. A coplanar waveguide transmission line is connected perpendicularly to a quarter-wavelength open-circuit stub.

intensity located at the open-circuit stub is much stronger than that at the main CPW transmission line. Hence the dielectric properties of the ferroelectric thin film near the open-circuit stub will change dramatically with the external dc bias voltage, whereas only very small variations can occur elsewhere. The advantage of using very narrow gaps in the open-circuit stub design is that the maximum output bias voltage (40 V) supplied by a vector network analyzer (e.g. Agilent 8510 C) could be high enough to produce the required field intensity for the electric field dependence measurements, and therefore an additional bias circuit is no longer necessary in the proposed filter structure.

3 Results and discussion

3.1 Accuracy of the software and the validity of the proposed structure

In order to verify the accuracy of the Sonnet suites software used in the simulation and the validity of the proposed structure, both computer simulations and microwave measurements were carried out for the filter made from MgO substrate coated with a 2.5 μm gold thin film. The dimensions of the filter were as follows. The length, width and gaps of the quarter-wavelength open-circuit stub were 2780, 75, and 15 μm, respectively, and the width and gaps of the main transmission line were 215 and 105 μm, respectively. The length, width, and thickness of the MgO substrate were 10 mm, 5 mm, and 500 μm, respectively.

In the simulation, when the dielectric constant and the loss tangent of the MgO substrate were chosen as 9.75 and 1.6×10^{-5}, respectively, the simulated and measured responses show good agreement in the frequency range of interest, as shown in Fig. 2. Firstly, the measured resonant frequency of the filter (12.0825 GHz) has almost the same value as the simulated one (12.0828 GHz). The difference between the simulated and the measured resonant frequencies (0.003%) is small and negligible. Secondly, the measured response curve is almost superposed on the simulated one below the resonant frequency; only at frequencies above 12.165 GHz does deviation occur. This kind of deviation maybe attributed to the processing or assembling techniques of the actual device. Comparing the deduced dielectric constant of the MgO substrate (9.75) with the reported values (9.8) in Refs. [11, 12], a small difference of 0.05 is obtained; the relative deviation is about 0.5%, which is very small and negligible. This result indicates that the proposed structure is applicable and the Sonnet suites software is accurate in the characterization of the dielectric constant of the MgO substrate. Because a gold thin film was used to form the pattern layer, its contribution to the loss of the filter is so large that this structure cannot be utilized to characterize the loss tangent of the MgO substrate. However, when the loss tangent value of the substrate is greater than 0.01, this structure is applicable. Furthermore, the Sonnet suites software supports the precise simulation for multilayer structures [13, 14], so it is applicable to simulate the MgO substrate coated with the ferroelectric thin film.

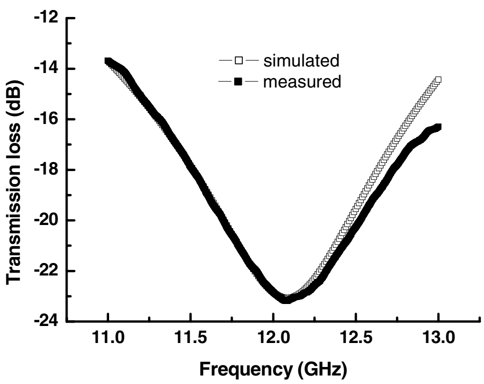

Fig. 2 Measured and simulated responses of the filter based on MgO substrate coated with a gold film at room temperature.

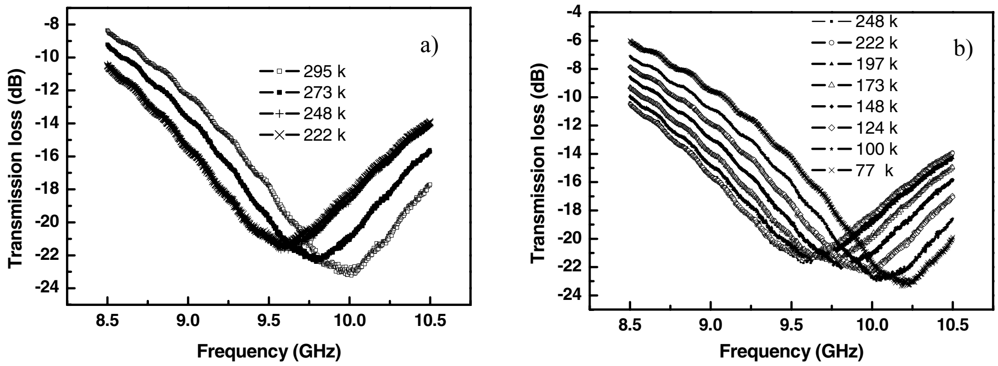

Fig. 3 Measured responses of the bandstop filter with a BST-0.5 thin film at various temperatures, as indicated.

3.2 Determination of the dielectric constant of $Ba_{0.5}Sr_{0.5}TiO_3$ thin film

A filter based on MgO substrate coated with a 300 nm thick $Ba_{0.5}Sr_{0.5}TiO_3$ (BST-0.5) thin film was fabricated and measured. The measured transmission responses with temperatures are shown in Fig. 3. The temperature-dependent responses show two opposite trends and thus can be divided into two groups. In the first group (see Fig. 3a), the resonant frequency of the filter is shifted to lower values from 9.9650 to 9.5700 GHz with decreasing temperature. The two curves for 248 and 222 K are too close to be distinguishable, indicating that the temperature for the frequency shifted to the lowest value must be somewhere between. In the second group (see Fig. 3b) the resonant frequency moves back and towards higher frequency from 9.5700 to 10.2050 GHz when the temperature drops further from 222 to 77 K.

When an electric field is applied to the BST-0.5 thin film, its dielectric constant is expected to become smaller, resulting in the resonant frequency shifting towards higher frequency. The measured frequency responses of the filter with the BST-0.5 thin film did reveal such a change under different externally applied voltages. As an example, Fig. 4 shows the responses of the filter measured at 248 K under 0 and 30 V. It can be seen that a frequency shift of 190.0 MHz occurs which is actually the largest among all the results examined at different temperatures.

To determine the dielectric constant of the BST-0.5 thin film from the above experimental results, computer simulations were then carried out. Most of the parameters needed in the simulation were either validated from previous tests (e.g. the parameters of MgO substrate, see Fig. 2), or measured from experimental samples (e.g. the thickness of the BST-0.5 thin film and conductivity of the gold layer), and

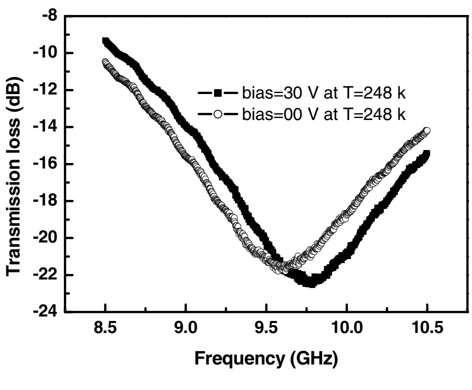

Fig. 4 Measured responses for the filter with the BST-0.5 thin film under bias of 0 and 30 V at 248 K.

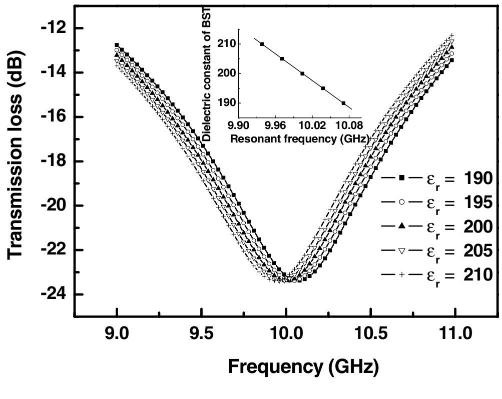

Fig. 5 Simulated responses of the filter with the BST-0.5 thin film for different dielectric constants at room temperature.

the only unknown parameters were the dielectric constant and loss tangent of the BST-0.5 thin film. Here, we could assign the loss tangent a reasonable value (i.e. tan $\delta = 0.01$), and leave the dielectric constant as the only arbitrarily chosen parameter. Figure 5 shows the simulated results with the dielectric constant of the BST-0.5 thin film being selected as 190, 195, 200, 205, and 210, with the loss tangent being fixed at 0.01. The measured conductivity of the gold layer was 2.26×10^7 S/m at 295 K. It is apparent that when the dielectric constant of the BST-0.5 thin film increases from 190 to 210 in steps of 5, the simulated resonant frequency of the filter decreases from 10.0709 to 9.9387 GHz in steps of about 33.0 MHz. Furthermore, the derived relationship between the dielectric constant of the BST-0.5 thin film and the resonant frequency of the filter, shown in the inset of Fig. 5, follows a simple linear relation:

$$\varepsilon_{\mathrm{BST}} = 1713.9 - 151.3 \times f_0 \tag{2}$$

which is applicable for determining the dielectric constant of the BST-0.5 thin film from the measured resonant frequencies. As an example, let us substitute the measured resonant frequency at 295 K into Eq. (2) and the dielectric constant of the BST-0.5 thin film at 295 K can be easily derived: $\varepsilon_r = 206.0$ at zero bias and $\varepsilon_r = 196.5$ at 30 V dc bias. Following this process, the dielectric constant of the BST-0.5 thin film at all the other tested temperatures can be obtained, as shown in Fig. 6. It was observed that the Curie temperature for the BST-0.5 thin film measured in this study is about 230 K, which is consistent with previously reported values [15, 16]. Furthermore, compared with the dielectric constant value (450) for a thickness of 800 nm [15, 16] and the dielectric constant value (240) for a thickness of 290 nm [17], it is apparent that the dielectric constant value (200) determined in the present study for the BST-0.5 thin film with a thickness of 300 nm is reasonable.

3.3 Determination of loss tangent of the BST-0.5 thin film

In order to determine the loss tangent for the BST-0.5 thin film at 295 K, different simulations were conducted. In these simulations, the dielectric constant was fixed as a constant ($\varepsilon_r = 200$) and a set of loss tangent values were selected, keeping all the other parameters as before. Typical simulation results are shown in Fig. 7. When the loss tangent of the BST-0.5 thin film is selected from 0.0001 to 0.1 in steps of factors of 10, the resulting Q values of the filter are 16.67, 16.64, 16.02, and 11.56, respectively. An additional selected value (0.05) was also used and the resulting curve is also plotted in Fig. 7. Figure 7 shows that the Q value of the filter is most sensitive when the loss tangent value for the BST-0.5 thin film is selected from 0.1 to 0.01. In this loss tangent value range, detailed simulations were then carried out and the results can be well fitted by a quadratic polynomial (see Fig. 8):

$$\tan \delta = 0.5946 - 0.0592\, Q + 0.0014\, Q^2 \,. \tag{3}$$

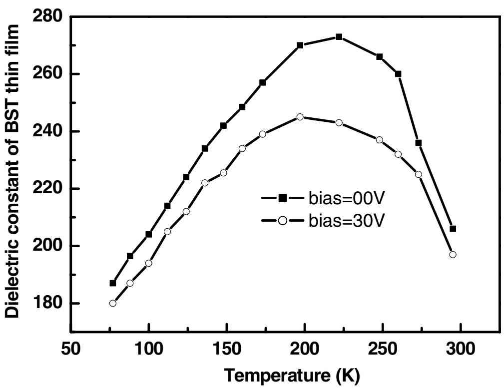

Fig. 6 Measured relative dielectric constant of the BST-0.5 thin film as a function of temperature at 0 and 30 V external bias.

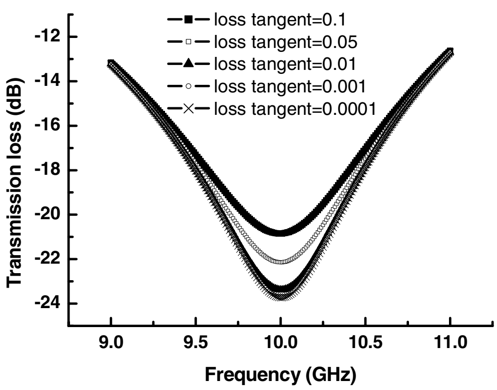

Fig. 7 Simulated responses of the filter with the BST-0.5 thin film for different loss tangent values at room temperature.

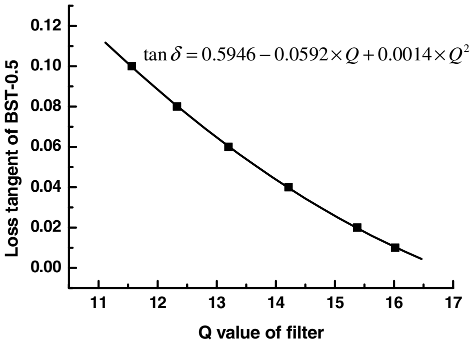

Fig. 8 Loss tangent of the BST-0.5 thin film versus simulated Q values of the filter.

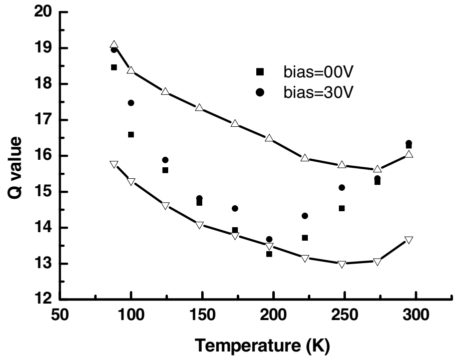

Fig. 9 Temperature dependence of the measured Q value of the filter with the BST-0.5 thin film at 0 and 30 V bias. Simulated Q values with loss tangents of 0.05 (∇) and 0.01 (Δ) for the BST-0.5 thin film are also plotted (the lines are guides for the eye).

By substituting the measured Q value at 295 K into Eq. (3), the loss tangent for the BST-0.5 thin film at 295 K can be easily determined: $\tan\delta = 0.007$ at zero bias and $\tan\delta = 0.006$ at 30 V dc bias. Following the above process, relations similar to Eq. (3) for the loss tangent and the Q value at different temperatures can be derived and the loss tangent of the BST-0.5 thin film at all other tested temperatures can then be obtained. The whole process, however, requires many sets of simulations and is indeed a very time-consuming work. For a quick and simple estimation, we only simulated two sets of temperature-dependent Q values with tangent losses of 0.05 and 0.01, respectively, and plotted them together with all the experimental data at 0 and 30 V dc bias voltages, as shown in Fig. 9. It can be seen that the loss tangent of the BST-0.5 thin film is a maximum around 200 K. This temperature is a little lower than the Curie point of the BST-0.5 thin film. As the tested temperatures move away from the Curie temperature range, the loss tangent change becomes smaller, especially at room temperature and liquid nitrogen temperature (the lowest tested temperature), where the loss tangent reaches a minimum. Furthermore, the Q value of the filter under 30 V bias is larger than that under zero bias voltage at the same temperature, indicating that the loss tangent of the BST-0.5 thin film under 30 V bias is less than that at zero bias. All these results are in accord with other reports [15, 18].

4 Summary

The dielectric properties of BST-0.5 thin films have been studied using a new CPW bandstop filter structure. The temperature and voltage dependences of the permittivity for the BST-0.5 thin films have been reported. The results obtained are consistent with reported values. This implies that the proposed structure is accurate and applicable for characterizing the permittivity of ferroelectric thin films.

Acknowledgement This project was partly supported by the National Center for Nanoscience and Technology, China.

References

[1] G. Subruamanyam, F. Keuls, and F. Miranda, IEEE Microw. Guid. Wave Lett. **8**, 78 (1998).
[2] E. G. Erker, A. S. Nagre, Y. Liu, P. Periaswamy, T. R. Taylor, J. Speck, and R. A. York, IEEE Microw. Guid. Wave Lett. **10**, 10 (2000).
[3] M. J. Lancaster, J. Powell, and A. Porch, Supercond. Sci. Technol. **11**, 1323 (1998).
[4] D. Galt, J. Price, J. Beall, and T. Harvey, IEEE Trans. Appl. Supercond. **5**, 2575 (1995).
[5] A. B. Kozyrev, V. N. Keis, G. Koepf, R. Yandrofski, O. I. Soldatenkov, K. A. Dudin, and D. P. Dovgan, Microelectron. Eng. **29**, 257 (1995).
[6] J. Sok, J. S. Lee, and E. H. Lee, Supercond. Sci. Technol. **11**, 8759 (1998).

[7] C. Y. Tan, Linfeng Chen, K. B. Chong, and C. K. Ong, Rev. Sci. Instrum. **75**, 136 (2004).
[8] C. Krowne, S. Kirchoefer, and J. Pond, IEEE Digest **MIT-S**, 1193 (2000).
[9] P. Suherman, T. Jackson, Y. Koutsonas, R. Chakalov, and M. Lancaster, IEEE Digest **MTT-S**, 265 (2004).
[10] J. S. Hong and M. J. Lancaster, Microstrip Filters for RF/Microwave Application (Wiley, New York, 2001).
[11] MgO magnesium oxide single crystal substrates, SPI supplies, http://www.2spi.com/.
[12] J. Krupka, R. G. Geyer, M. Kuhn, and J. Heyen Hinken, IEEE Trans. Microw. Theory Tech. **42**, 1886 (1994).
[13] Q. J. Zhang, M. Yagoub, X. Ding et al., Electric Components and Technology Conf. (2002), p. 701.
[14] S. Gevorgian, H. Berg, H. Jacobsson, and T. Lewin, IEEE Microw. Mag. **4**, 60 (2003).
[15] S. D. Harkness IV, R. K. Singh, C. Mueller et al., Mater. Sci. Eng. B **41**, 379 (1996).
[16] F. Miranda, C. Mueller, C. Cubbage et al., IEEE Trans. Appl. Supercond. **5**, 3191 (1995).
[17] Hang-Ting Lue and Tseung-Yuen Tseng, IEEE Trans. Ultrason. Ferroelectr. Freq. Control **48**, 1640 (2001).
[18] K. Bethe, Philips Res. Rep. **2**, 1 (1970).

