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Numerical Analysis and Modeling of Nonlinear Dielectric Properties of $(Ba_x, Sr_{1-x})TiO_3$ Films

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$(Ba_x, Sr_{1-x})TiO_3$ (BST) films have been widely investigated because of expectations of their applications in microwave devices. In particular, there has been intense interest in new devices that use their nonlinear properties such as tunable devices and frequency mixers. In order to realize such devices, detailed evaluation of their nonlinear properties and numerical modeling are important. In this paper, capacitance-voltage (*C-V*) characteristics of BST films prepared by sputtering were measured, and numerical fitting of a polynomial to the voltage-charge (*V-Q*) characteristics calculated from the *C-V* data was carried out. The results show that the measured data can be expressed with precision by a simple equation containing only linear and third order components, revealing that a practical experimental equation for the design of electrical circuits was obtained. Furthermore, a new equivalent circuit of the nonlinear dielectric film was proposed, and calculation of generation of third order frequency from a BST film capacitor was also performed. The measured third order component agreed exactly with the calculated results, revealing that our equivalent circuit is useful as an analysis method for circuits using nonlinear capacitors.

Key words: BST, nonlinear dielectric properties, equivalent circuit, thin films

1. INTRODUCTION

BST films have been interesting chiefly as a material for microwave devices, because of their good dielectric properties such as high permittivity at high frequencies. [1,2] In order to fabricate microwave integrated circuits using this material, the preparation of BST films has been extensively investigated. [2-4] Since nonlinear dielectric characteristics can be obtained for the film capacitors at low voltages, new devices utilizing nonlinearity have also been anticipated. A frequency tunable device is one such device. Since the operational frequency of the device can be varied by an external bias voltage, a multi-band communication system can be simplified by using such a tunable device. It has been reported that frequency conversion devices such as a frequency mixer and multiplier can also be realized using a nonlinear capacitor. [5] The preparation of BST films and evaluation of device properties have been investigated widely, as mentioned above; however, there have been few reports on detailed analysis of their nonlinear properties, and discussions on circuit design and optimization. Since the impedance of devices using high permittivity materials such as BST decreases, their pattern size needs to be increased due to impedance matching. However, nonlinearity is also suppressed by increasing the size. Thus, optimization of device design is difficult but important.

In this paper, we have evaluated the nonlinear dielectric properties of BST films in detail, and have attempted to analyze the properties numerically in order to obtain an experimental equation for the nonlinear films. From the results, we propose an equivalent electrical circuit for the nonlinear capacitor.

2. EXPERIMENTAL

The $(Ba_{0.5}, Sr_{0.5})TiO_3$ thin films were deposited on $Pt/\alpha\text{-}Al_2O_3(0001)$ substrates by rf magnetron sputtering

(SPF-210H, ANELVA). The sputtering conditions used are summarized in Table I. We have reported that high quality epitaxial films can be obtained not only on conventional MgO substrates but also on sapphire. [3] Lower cost and higher chemical stability can be achieved for devices using sapphire substrates. The compositions and crystalline orientations of the BST films were measured by XRF and XRD, respectively. (111)-oriented BST epitaxial films (Ba/Sr=50/50) were used in the experiments. The Pt top electrodes were also prepared by sputtering, and electrode patterns with about 0.2 mm diameter were formed using a metal mask method.

The electrical properties in the form of *C-V* characteristics of the Pt/BST/Pt capacitors were measured using a low frequency impedance analyzer (4192A, Agilent Co.). An oscillator (FC300, Yokogawa Co.) and digital phosphor oscilloscope (TDS3052, Tektronix Co.) were also used for observations of the dynamic response of electrical circuits using a BST film capacitor.

Table I. Sputtering conditions

Temperature	650°C
rf Power	100 W
Gas Ar:O_2	9:1
Gas Pressure	2 Pa
Deposition Time	60 min
Thickness	200 nm
Target	($Ba_{0.5}Sr_{0.5}$)TiO_3 powder

3. RESULTS AND DISCUSSION

Figure 1(a) shows a schematic of the *C-V* properties of BST films. The nonlinear dielectric property is generally expressed with nonlinear dielectric constants such as ε_1 (linear component), ε_3 (third order component), ε_5 (fifth order component) and so on. Thus, the electric flux density, *D*, is given by

$$D=\varepsilon_1 E+\ \varepsilon_3 E^3+\varepsilon_5 E^5+\cdot\cdot \quad , \qquad (1)$$

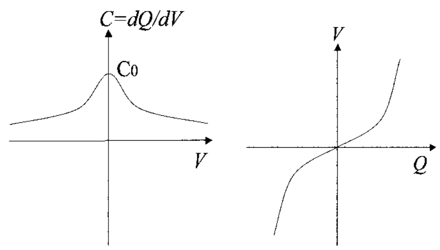
where *E* is the electric field. From this equation, the charge on the capacitor, *Q*, and the capacitance, *C*, are

$$Q=C_0 V+k_3 V^3+k_5 V^5+\cdot\cdot \quad , \qquad (2)$$

and,

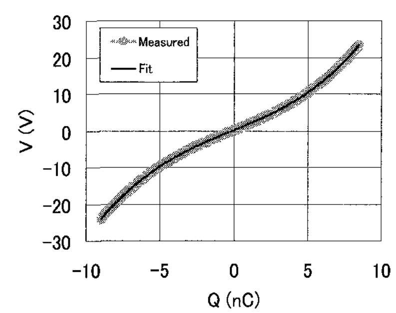
$$C=dQ/dV=C_0+3k_3 V^2+3k_5 V^4+\cdot\cdot \quad , \quad (3)$$

where *V* is the applied voltage, C_0 is the linear component of the capacitance, and k_3 and k_5 are the coefficients for nonlinear properties. In the case of equation (3), the *C-V* curve, as shown in Fig. 1(a), cannot be expressed without higher order coefficients, and the discussion becomes difficult.

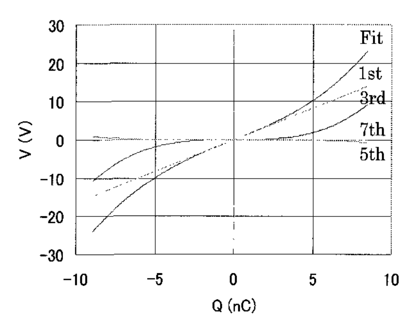


(a) *C-V* properties (b) *V-Q* properties

Fig. 1 Schematic of nonlinear dielectric properties of BST capacitors.



(a) Fitting results



(b) 1st, 3rd, 5th and 7th components

Fig. 2 Fitting of nonlinear dielectric properties using a polynomial function.

From Fig. 1(a), the *V-Q* curve is obtained as shown in Fig. 1(b). In this case, the curve is similar to a simple polynomial curve. Thus, we attempted to write the applied voltage as:

$$V = (Q + \alpha Q^3 + \alpha_5 Q^5 + \cdot\cdot)/C_0 \quad , \quad (4)$$

where α and α_5 are coefficients for nonlinearity, and can be obtained by numerical data fitting. Figure 2 shows the fitting results. The fitting was performed by least squares fitting with a polynomial function of 7th, and good agreement was obtained, as shown in Fig. 2(a). The curves of each component in the polynomial are shown in Fig. 2(b). The *V-Q* characteristics of the BST film prepared could be satisfactorily expressed as a polynomial function of only the first and third degree. The contributions of the 5th and 7th degree were below 4% and 2%, respectively.

The experimental equation can be simplified by eliminating the odd degree and the 5th and higher. Equation (4) can then be written as:

$$V \fallingdotseq (Q + \alpha Q^3)/C_0 \quad . \quad (5)$$

In equation (5), the coefficient of α can be easily obtained from *C-V* measurements without least squares fitting. α is given by:

$$\alpha = \frac{(2+C_0/C_1)^2(C_0/C_1 - 1)}{27(C_0V_1)^2} \quad , \quad (6)$$

where C_1 is the capacitance at a bias voltage of V_1. The *C-V* curves measured and calculated using equation (6) are shown in Fig. 3, revealing that the experimental equation can be utilized fully for the analysis. The parameters C_0, V_1, C_1/C_0 and α in equation (6) were 607pF, 7.6 V, 0.7 and $8.71\times10^{15}C^{-2}$, respectively.

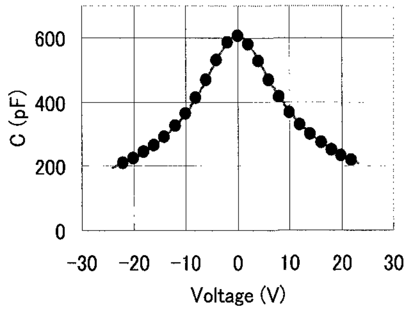
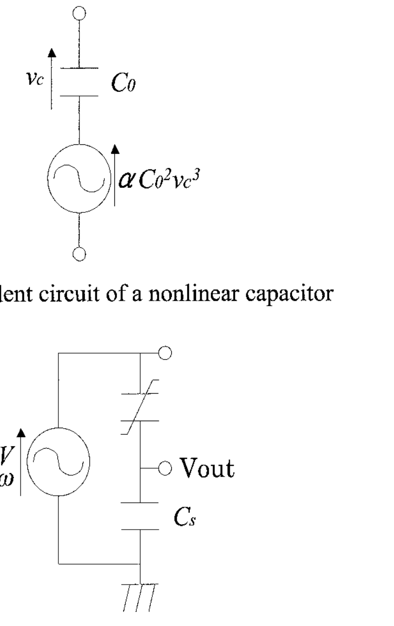


Fig. 3 *C-V* curves measured and calculated using the experimental equation.

In the case of a specimen with high tunability, such as Ba-rich BST, the error of fitting increased. The 5th order should also be used for highly tunable films. However, the equation cannot be applied for a ferroelectric capacitor showing hysteresis properties, such as $BaTiO_3$.

Several researchers have evaluated *C-V* characteristics using the Devonshire and Slater theories in earlier literature. [6,7] Polynomial equations similar to equations (3) and (5) have been expressed. Thus, the mechanism of the *V-Q* properties expressed by a polynomial function such as equation (3) could be explained by these theories.



(b) Test circuit for third harmonic generation

Fig. 4 Analysis of an electrical circuit using a nonlinear capacitor.

From equation (3), an equivalent circuit model of the nonlinear capacitor was obtained, as shown in Fig. 4(a). The simple electrical circuit for third harmonic generation shown in Fig. 4(b) was evaluated. The operation of this circuit is similar to that of the Sawyar-Tower circuit. The capacitance, *Cs*, and applied voltage of the oscillator, *V*, in Fig. 4(b) are 63nF and 9.5 V, respectively. The parameters C_0 and α for the nonlinear capacitor were also 659pF and $1.08\times10^{16}C^{-2}$, respectively. The third harmonic in the measured output voltage was extracted by Fourier transform. The measured voltage of the harmonic and that of the calculation were 5.6 mV and 6.1 mV, respectively. The error of 8% appears to be caused by measurement error, parasitic resistance and stray capacitor. The harmonic signal obtained was very weak, and the conversion efficiency was low. The fabrication of a frequency converter has been previously reported. [8] The converter required very high power as an input source, such as 1 kW, in order to obtain high nonlinearity. Thus, improvement in the circuit is necessary in the future, and the equivalent circuit proposed is useful for such circuit design.

4. CONCLUSIONS

The numerical analysis of a BST nonlinear capacitor was carried out, and a new experimental equation was proposed. The equation is a simple polynomial function of only the first and third degrees, and it agreed closely with measured results. An equivalent circuit model was also obtained using the equation. The circuit could be easily analyzed by the model, revealing that it is useful for optimization of various new nonlinear devices.

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