

Microwave dielectric characteristics and finite element analysis of MgTiO₃–CaTiO₃ layered dielectric resonators

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Abstract

MgTiO₃ and CaTiO₃ ceramics were stacked in different schemes to yield the layered dielectric resonators, and the microwave dielectric characteristics were evaluated with TE₀₁₁ resonant mode. With increasing the thickness fraction of CaTiO₃, the measured resonant frequency and Q_f value decreased, while the effective dielectric constant and temperature coefficient of resonant frequency increased. The stacking scheme also had significant effect on the microwave dielectric properties. Finite element method was used to predict the microwave dielectric characteristics of the layered dielectric resonators, and the predicted results indicated good agreements with the experimental ones. The temperature-stable resonators could be attained by adjusting the thickness fractions of CaTiO₃ since MgTiO₃ and CaTiO₃ had reverse temperature coefficients of resonant frequency.

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1. Introduction

Dielectric ceramics have been widely used for microwave applications as resonators in the microwave circuits.¹ To attain temperature-stable resonators with small size and high Q value, the dielectric ceramics should have high dielectric constant ($\epsilon_{r,\text{eff}}$), high Q_f value and near-zero temperature coefficient of resonant frequency (τ_f).^{1,2} However, the temperature stability for many ceramics is poor in spite of the possible high dielectric constant and high Q_f value, and it should be improved. The most frequently used method to tune τ_f is to form solid solution using two materials with opposite temperature coefficients.^{3–6} However, not all ceramics can be improved by this method since the possible incompatibility of ionic radius, ionic charge or crystal structure will bring undesired secondary phase and damage the Q_f value much.

Layered dielectric resonator is introduced to improve the temperature stability of the dielectric resonator as a new approach.^{7–12} By stacking one dielectric ceramic with positive temperature coefficient of resonant frequency with another

ceramic with a negative one, near-zero temperature coefficient can be obtained without damaging the high Q_f value much.^{7–12} Though much work on layered resonator has been carried out, many problems have not been understood deeply yet, such as the effects of the thickness ratio and stacking scheme on the microwave dielectric properties. Also, accurate prediction is needed for further understanding the layered resonators, especially for designing the temperature-stable resonators.

In the previous work, we have discussed the effects of the composition ratio and stacking scheme on the microwave dielectric properties of the co-fired layered ceramic resonators and found some interesting and special characteristics.¹³ However, residual stresses in the ceramics due to the different thermal expansion coefficients of the components should have effects on the properties of the layered resonators, and the effects are difficult to be analyzed quantitatively. Even worse, the stresses may cause cracks in the samples. The effects of the residual stresses should be excluded for further understanding the layered resonators. In the present work, the component ceramics of the layered resonators are prepared separately and then stacked directly. The air gap between the different layers is very thin and its effect can be neglected. MgTiO₃ and CaTiO₃ ceramics are selected as the components of the layered resonators, whose microwave

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dielectric properties vary much from each other¹⁴ so that the variations of the properties can be easily observed. The TE_{011} mode with which the layered resonators work is investigated for its simplicity and typicality. The effects of the thickness fraction of $CaTiO_3$ and stacking scheme on the microwave dielectric properties are discussed. Also, the microwave dielectric properties of the layered resonators are predicted by finite element method according to the corresponding properties of $MgTiO_3$ and $CaTiO_3$ ($\epsilon_r = 17.17$, $Q_f = 92,000$ GHz, $\tau_f = -50$ ppm/ $^\circ$ C for $MgTiO_3$ and $\epsilon_r = 174.3$, $Q_f = 11,260$ GHz, $\tau_f = 804.1$ ppm/ $^\circ$ C for $CaTiO_3$ in the present work), and the predicted properties are compared with the experimental results. Finite element method pays attention to the temperature-stable resonators in particular, and the corresponding predicted microwave dielectric properties are given.

2. Experimental

$MgTiO_3$ and $CaTiO_3$ powders were synthesized by a solid-state reaction process. MgO (97%), $CaCO_3$ (99%) and TiO_2 (99.5%) raw powders with proper ratio were mixed by ball milling in distilled water with zirconia media for 24 h and then calcined at 1100°C in air for 3 h to synthesize $MgTiO_3$ and $CaTiO_3$, respectively. $MgTiO_3$ and $CaTiO_3$ powders with organic binder of PVA water solution were pressed into cylindrical compacts and sintered at 1350°C in air for 3 h. The as-sintered pellets with near the same diameter of 10.60 mm were thinned to desired thicknesses, and then were polished well with paralleling and smooth surfaces. The pellets were stacked axis-symmetrically with different schemes and thickness ratios. The stack was then sandwiched by the two gold-coated copper plates of the Hakki-Coleman setup¹⁵ and it could work as a dielectric resonator. The total thickness for all these layered resonators was 5 mm. Three stacking schemes in the present experiment are shown in Fig. 1, and they are denoted by $MgTiO_3/CaTiO_3$, $MgTiO_3/CaTiO_3/MgTiO_3$ and $CaTiO_3/MgTiO_3/CaTiO_3$, respectively. (Stacking scheme of $CaTiO_3/MgTiO_3$ should also be considered. But in fact, both experiments and theory indicated that the microwave dielectric properties for stacking schemes of $CaTiO_3/MgTiO_3$ and

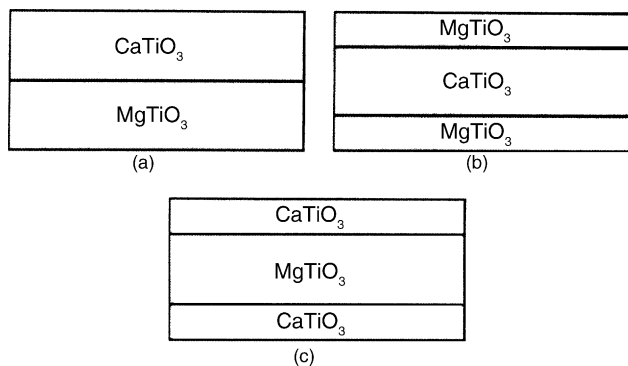


Fig. 1. Stacking schemes for the $MgTiO_3$ – $CaTiO_3$ layered resonator: (a) $MgTiO_3/CaTiO_3$; (b) $MgTiO_3/CaTiO_3/MgTiO_3$; and (c) $CaTiO_3/MgTiO_3/CaTiO_3$.

Table 1

Experimental parameters for the $MgTiO_3$ – $CaTiO_3$ stacks

Stacking sequence	Thickness ratio				
	3:1	2:1	1:1	1:2	1:3
$MgTiO_3/CaTiO_3$	3:2:3	1:1:1	1:2:1	1:4:1	1:6:1
$MgTiO_3/CaTiO_3/MgTiO_3$	1:6:1	1:4:1	1:2:1	1:1:1	3:2:3
Thickness fraction of $CaTiO_3$	0.25	0.333	0.5	0.667	0.75

$MgTiO_3/CaTiO_3$ were the same for TE_{011} mode since the top and bottom metal plates were equivalent.) The thickness ratios and corresponding thickness fractions of $CaTiO_3$ for the layered resonators with different stacking were shown in Table 1.

The resonant frequency, temperature coefficient of resonant frequency between 20 and 80°C and Q_f value were determined with TE_{011} mode by an Agilent 8720ES network analyzer using the Hakki-Coleman method.¹⁵ Assuming the stack as a homogeneous dielectric, the effective dielectric constant ($\epsilon_{r,eff}$) of the layered resonator could be evaluated from the resonant frequency and dimensions of the stack by an accurate formula.^{15,16}

3. Finite element analysis

The axis symmetry exists for TE_{011} mode and the electric field only has a rotational component E_θ that is also axis symmetrical, so two-dimensional finite element method can be used to analyze the layered dielectric resonators and only half of the cross section needs to be analyzed. The resonator with such dimensions is in trapped state for TE_{011} mode,¹⁷ where the electromagnetic energy is confined in and near the sample. Finite element analysis for the layered resonators also shows that the electric field far away from the sample is very weak, so the space far away from the sample can be neglected. Only the space within 25.3 mm from the symmetry axis is considered for finite element analysis as shown in Fig. 2, and the triangular first-order element is employed. Many resonant frequencies corresponding to TE_{0np} modes can be attained after resolving the overall matrix equation, and the lowest one is the resonant frequency for TE_{011} mode. Also, the electric field intensity of each node can be given. The detailed analyzing process has been reported by Kooi et al.¹⁸ and Zeng et al.¹⁹ and it will be not discussed in this paper.

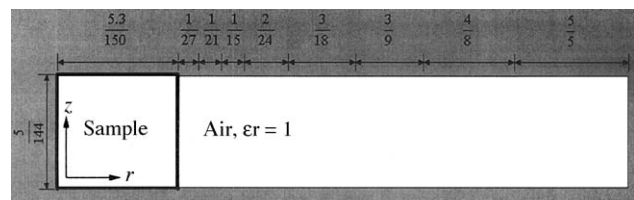


Fig. 2. Half of the cross-section of the layered resonator for finite element analysis, where the fractional number n/m denotes that the length is n millimeter and divided into m segments averagely.

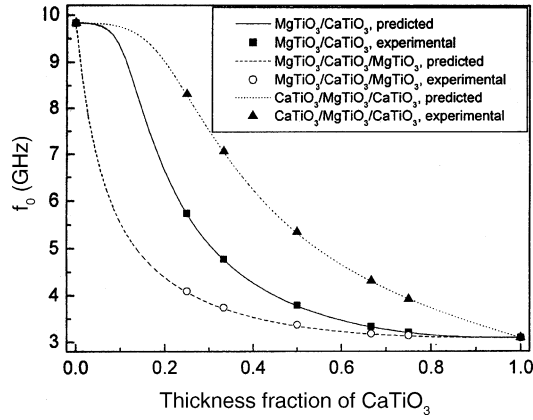


Fig. 3. Resonant frequency of the MgTiO₃–CaTiO₃ layered resonator as function of thickness fraction of CaTiO₃.

From the electric field distribution, the electric filling factor of each layer can be calculated by

$$P_{e,i} = \frac{(1/2) \int_V \epsilon_{r,i} \vec{E} \times \vec{E}^* dV}{\sum_i ((1/2) \int_V \epsilon_{r,i} \vec{E} \times \vec{E}^* dV)} = \frac{\int_S \epsilon_{r,i} E_\theta^2 \times r dS}{\sum_i (\int_S \epsilon_{r,i} E_\theta^2 \times r dS)} \quad (1)$$

For the layered resonators working with TE_{01δ} mode, Alford and his associates have shown that the temperature coefficient of resonant frequency obeys

$$\tau_f = G + \sum_i (\tau_{f,i} P_{e,i}) \quad (2)$$

where G is the effect of the shield due to the thermal expansion of the cavity wall and $\tau_{f,i}$ is the temperature coefficient of resonant frequency for each component with the electric energy filling factor of unity.^{11,12} It also acts for TE₀₁₁ mode where $G=0$, so

$$\tau_f = \sum_i (\tau_{f,i} P_{e,i}) \quad (3)$$

For layered and monomorph dielectric resonator, there is

$$\tan \delta = \frac{f_0}{Q_f}, \quad (\tan \delta)_i = \frac{f_0}{(Q_f)_i} \quad (4)$$

and

$$\tan \delta = \frac{\sum_i ((\tan \delta)_i P_{e,i})}{\sum_i P_{e,i}} \quad (5)$$

so the Q_f value of the layered resonator can be calculated by

$$Q_f = \left(\sum_i \frac{P_{e,i}}{(Q_f)_i} \right)^{-1} \times \sum_i P_{e,i} \quad (6)$$

4. Results and discussion

Figs. 3–5 show the experimental and predicted resonant frequency, effective dielectric constant and temperature coefficient of resonant frequency of the layered resonators with TE₀₁₁

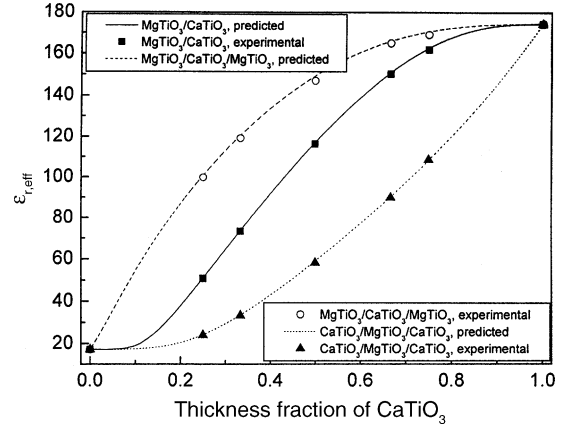


Fig. 4. Effective dielectric constant of the MgTiO₃–CaTiO₃ layered resonator as function of thickness fraction of CaTiO₃.

mode as function of the thickness fraction of CaTiO₃. The dots and lines correspond to the experimental and predicted values, respectively. To judge the accuracy of finite element analysis, the relative error is given as the difference between the predicted and experimental results divided by the experimental result. The relative errors for the resonant frequency, effective dielectric constant and temperature coefficient of resonant frequency are within -0.78 – 0.14% , -0.28 – 1.58% , and -1.1 – 1.4% , respectively. It is indicated that the finite element analysis can give accurate prediction for the resonant frequency, effective dielectric constant and temperature coefficient of resonant frequency of the layered dielectric resonators.

With increasing the thickness fraction of CaTiO₃, the resonant frequency decreases, while the effective dielectric constant and temperature coefficient of resonant frequency increase for the same stacking scheme. The variations do not fit any known model for dielectric composites, such as series model, parallel model or logarithmic model.²⁰

The stacking scheme also has significant effect on the microwave characteristics of the layered resonators. For the same thickness fraction of CaTiO₃, the highest resonant frequency of the layered resonator is for the stacking scheme of CaTiO₃/MgTiO₃/CaTiO₃. It is followed by MgTiO₃/CaTiO₃, and the lowest resonant frequency is obtained

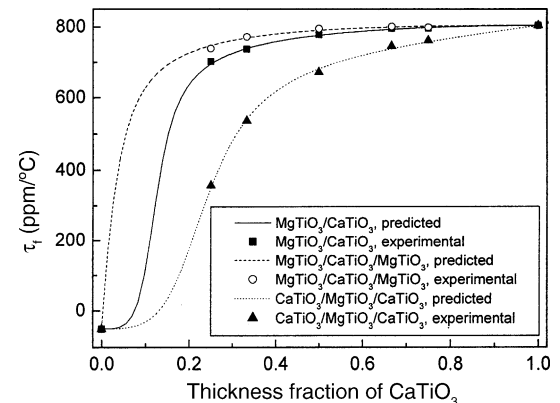


Fig. 5. Temperature coefficient of resonant frequency of the MgTiO₃–CaTiO₃ layered resonator as function of thickness fraction of CaTiO₃.

Table 2

Electric filling factors of MgTiO₃ and CaTiO₃ of the MgTiO₃/CaTiO₃ layered resonators with the thickness fraction of CaTiO₃ of 0.5, predicted by finite element method

Stacking scheme	Thickness ratio	P_e (CaTiO ₃)	P_e (MgTiO ₃)
MgTiO ₃ /CaTiO ₃	1:1	0.967	0.032
MgTiO ₃ /CaTiO ₃ /MgTiO ₃	1:2:1	0.983	0.016
CaTiO ₃ /MgTiO ₃ /CaTiO ₃	1:2:1	0.959	0.040

for MgTiO₃/CaTiO₃/MgTiO₃, while reverse comparative results are given for the effective dielectric constant and temperature coefficient of resonant frequency. A brief explanation is given through analyzing the layered resonators with the same CaTiO₃ thickness fraction of 0.5 but with different stacking schemes. The contours of the electric field intensity simulated by finite element method are shown in Fig. 6(a–c), with the relative electric field intensity marked. The densest electric field distribution in CaTiO₃ is observed for MgTiO₃/CaTiO₃/MgTiO₃, and it is followed by MgTiO₃/CaTiO₃ and finally CaTiO₃/MgTiO₃/CaTiO₃. Also, electric filling factor for CaTiO₃ gives the same comparative results, as shown in Table 2. Denser electric field and larger electric filling factor for CaTiO₃ mean that CaTiO₃ contributes more to the final microwave dielectric properties of the layered resonators. Also, CaTiO₃ has much higher dielectric constant and temperature coefficient of resonant frequency than MgTiO₃, so the properties of the layered resonators with different stacking schemes are quite different as mentioned above, though they have the same thickness fraction of CaTiO₃.

Figs. 6(a–c) and 7(a and h) also indicate the difference of the electric field distribution between the layered and monomorph dielectric resonators. The shape of the contour of the electric field intensity for MgTiO₃/CaTiO₃/MgTiO₃ resonator is almost the same to that for the monomorph resonator, except for the slight difference of the relative electric field intensity. MgTiO₃/CaTiO₃ resonator has unsymmetrical electric field distribution for its unsymmetrical stacking schemes and it is the most significant difference from the monomorph resonator. The above two kinds of layered resonators only have slightly different contour shape from the monomorph resonator, while the CaTiO₃/MgTiO₃/CaTiO₃ resonator is quite different and of special interest. Unlike the monomorph dielectric resonator for which the electric field concentrate in only one area, two concentrating areas may exist for CaTiO₃/MgTiO₃/CaTiO₃ layered resonators, as shown in Fig. 6(c). To further understand the change of the electric field distribution, more contours are shown in Fig. 7(a–h) for CaTiO₃/MgTiO₃/CaTiO₃ layered resonators with different thickness fraction of CaTiO₃. With increasing the thickness fraction of CaTiO₃, the top and bottom CaTiO₃ layers seem to ‘pull’ the contour from the middle MgTiO₃ layer (Fig. 7(b–d)), and then split it (Fig. 7(e and f)). We can attribute the interesting electric field distribution to the much larger dielectric constant of CaTiO₃ than that of MgTiO₃. As known for all, the electric field tends to concentrate in the area with large dielectric constant for dielectric resonator.¹⁶ For CaTiO₃/MgTiO₃/CaTiO₃ layered res-

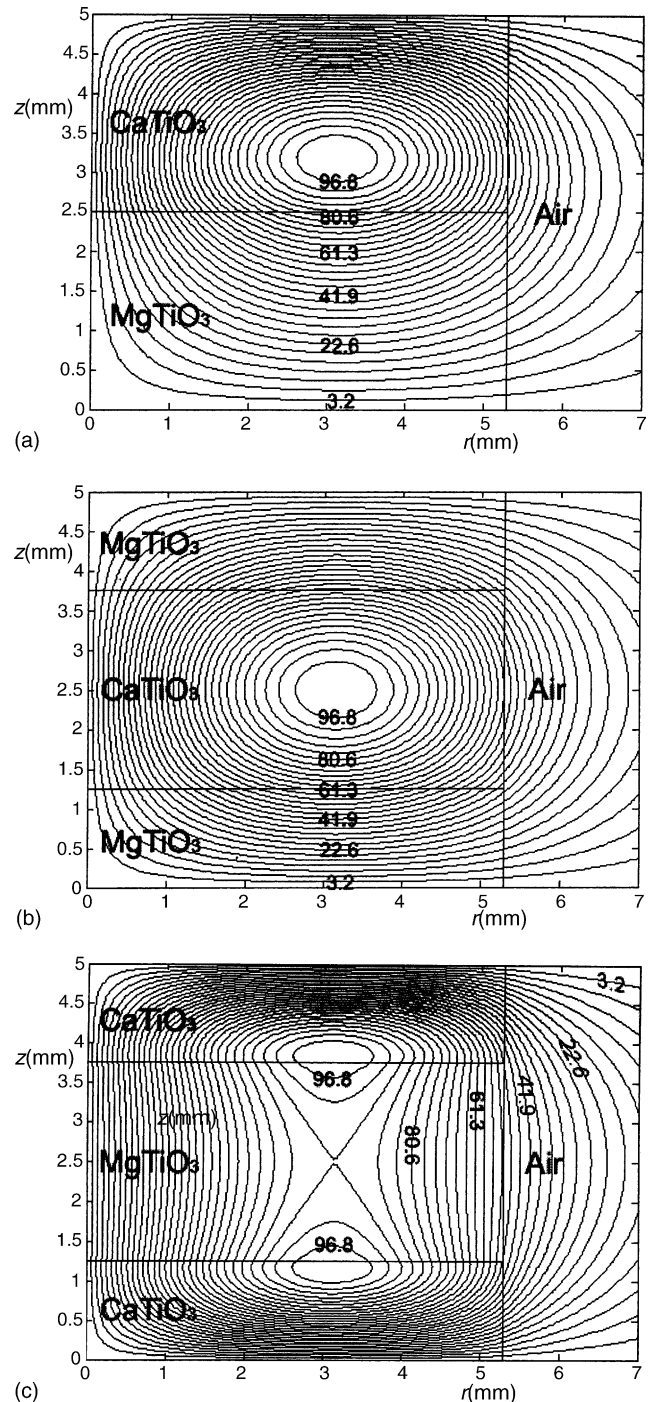


Fig. 6. Simulated contours of the electric field intensity for the differently stacking layered resonators with the same CaTiO₃ thickness fraction of 0.5 with TE₀₁₁ mode: (a) MgTiO₃/CaTiO₃; (b) MgTiO₃/CaTiO₃/MgTiO₃; and (c) CaTiO₃/MgTiO₃/CaTiO₃.

onator, the electric field tends to concentrate in the top and bottom CaTiO₃ layers which are equivalent. So the contour may be split when the thickness fraction of CaTiO₃ is in a given range for CaTiO₃/MgTiO₃/CaTiO₃ layered resonator, while only a little change occurs for MgTiO₃/CaTiO₃/MgTiO₃ and MgTiO₃/CaTiO₃.

The measured Q_f value for the MgTiO₃–CaTiO₃ resonator as function of the thickness fraction of CaTiO₃ is shown in Fig. 8(a),

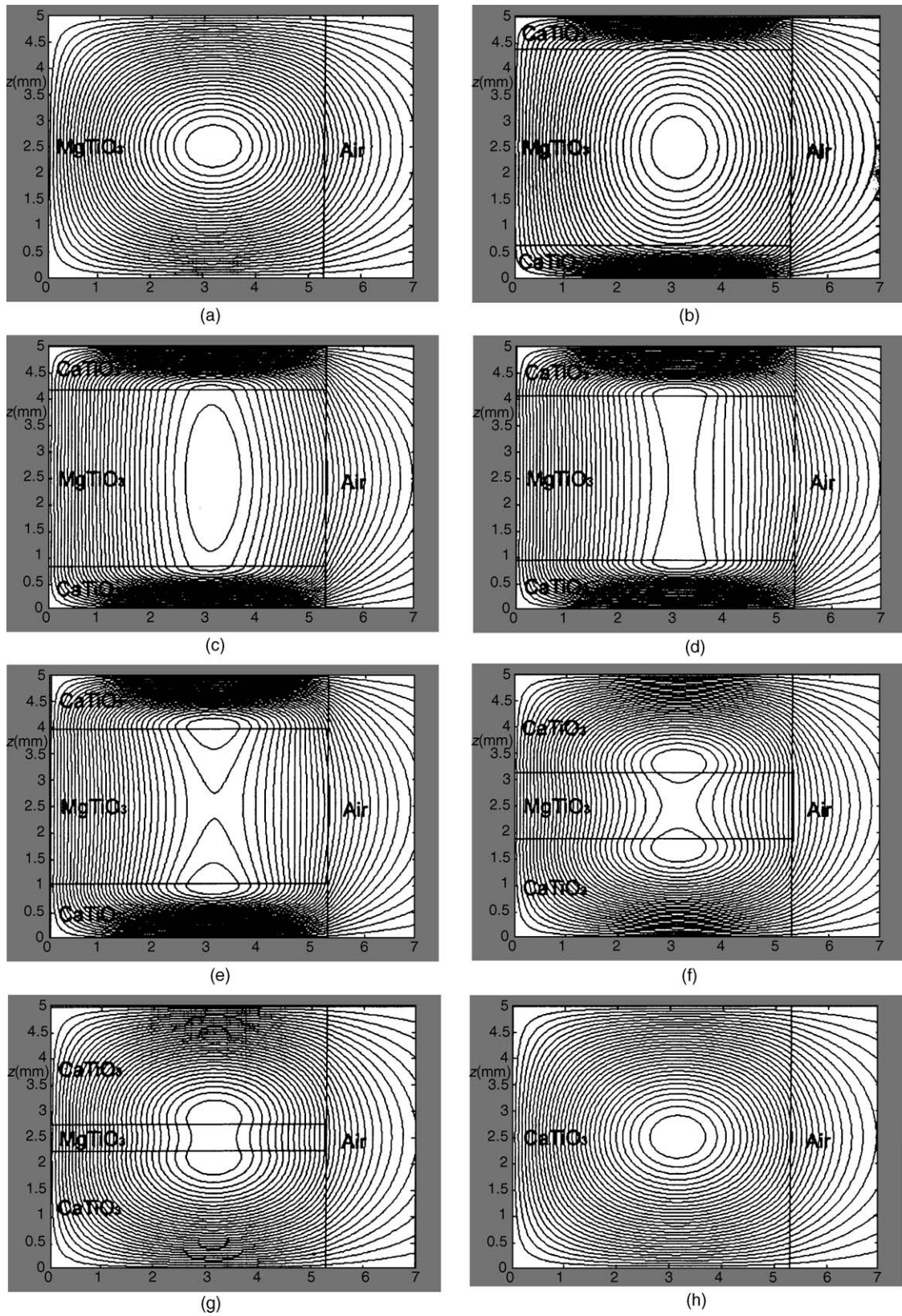


Fig. 7. Change of the electric field distribution of $\text{CaTiO}_3/\text{MgTiO}_3/\text{CaTiO}_3$ resonators with TE_{011} mode, where the corresponding thickness fraction of CaTiO_3 is (a) 0; (b) 0.25; (c) 0.33; (d) 0.38; (e) 0.42; (f) 0.75; (g) 0.90; and (h) 1.

Table 3
Predicted temperature-stable layered MgTiO₃–CaTiO₃ resonators with different stacking schemes

Stacking scheme	Thickness fraction of CaTiO ₃	f_0 (GHz)	$\epsilon_{r,\text{eff}}$	Q_f (GHz)	τ_f (ppm/°C)
MgTiO ₃ /CaTiO ₃	0.0759	9.6433	17.85	61,370	0
MgTiO ₃ /CaTiO ₃ /MgTiO ₃	0.0029	9.5686	18.14	61,370	0
CaTiO ₃ /MgTiO ₃ /CaTiO ₃	0.1314	9.6189	17.94	61,370	0

as the dots indicate. For the same stacking scheme, the Q_f value decreases with increasing the thickness fraction of CaTiO₃. The stacking scheme also has effect on the Q_f value. For the same thickness fraction of CaTiO₃, the highest Q_f value is obtained for the stacking scheme of CaTiO₃/MgTiO₃/CaTiO₃. It is followed by MgTiO₃/CaTiO₃, and the resonator with stacking scheme of MgTiO₃/CaTiO₃/MgTiO₃ indicate the lowest Q_f value. The experimental results do not fit the prediction very well, as shown in Fig. 8(a), and the error is attributed to the difference between the samples¹⁰ and the uncertainties of the Q measurement.²¹ Even this, the predicted trends are consistent with the experiments. Fig. 8(b) gives the overall variations of the predicted Q_f values. For each stacking scheme, sudden rise of Q_f value can be found when the thickness fraction of CaTiO₃ decrease to a certain value.

It should be noted that the temperature-stable layered resonators can be attained since MgTiO₃ and CaTiO₃ have reverse temperature coefficients of resonant frequency. Finite element method gives the predicted thickness fractions of

CaTiO₃ and corresponding microwave dielectric characteristics for the temperature-stable layered dielectric resonators, as shown in Table 3, and high Q_f values can be attained. To obtain temperature-stable layered resonators, the thickness fractions of CaTiO₃ for different stacking schemes differ much from each other, while the corresponding microwave dielectric characteristics only differ a little.

5. Conclusion

The microwave dielectric characteristics for the layered MgTiO₃–CaTiO₃ resonators with TE₀₁₁ resonant mode have been discussed in detail. The stacking scheme, as well as the thickness fraction of CaTiO₃, has significant effect on the resonant frequency, effective dielectric constant, temperature coefficient of resonant frequency and Q_f value. Layered dielectric resonator proves to be an effective method to tune the temperature coefficient of resonant frequency, and the temperature-stable dielectric resonators can be attained by this method. The predicted microwave dielectric properties by finite element method fit the experimental results well and finite element method is a useful tool to analyze the layered dielectric resonators.

Acknowledgements

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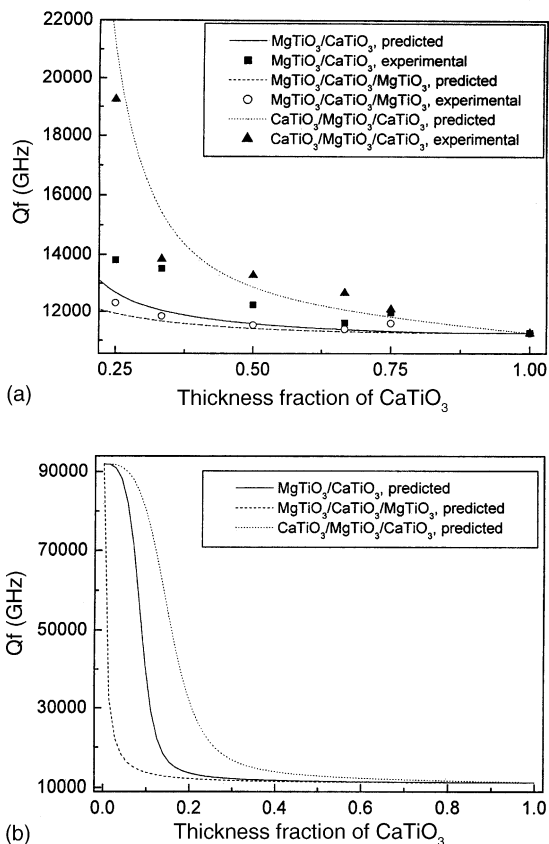


Fig. 8. Q_f value of the MgTiO₃–CaTiO₃ layered resonator as function of thickness fraction of CaTiO₃.

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