

Do We Really Need Ferroelectrics in Paraelectric Phase Only in Electrically Controlled Microwave Devices?

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Abstract—Typical paraelectric materials (e.g., SrTiO_3 , KTaO_3 , $\text{Ba}_x\text{Sr}_{1-x}\text{TiO}_3$, $x < 0.5$) and electrically tunable microwave devices based on these materials are briefly reviewed. The analysis shows that in spite of the recent year's extensive efforts, no considerable improvement in the microwave losses in thin paraelectric films has been achieved. Thin films, regardless of fabrication method and substrate type, have much lower dielectric permittivity than bulk single crystals, and the loss tangent at microwave frequencies ($f > 10$ GHz) is of the order of 0.01 (at zero dc-bias field) at room temperature. Nevertheless, quite promising component and subsystem level devices are successfully demonstrated. Use of ceramic (bulk and thick film) ferroelectrics in tunable microwave devices, currently considered for industrial applications, offer cost reduction. In this paper, explicitly for the first time, we consider possibilities and benefits of using ferroelectrics in polar phase in electrically controllable microwave devices. Examples of using ferroelectrics in polar state (e.g., $\text{Na}_{0.5}\text{K}_{0.5}\text{NbO}_3$, SrTiO_3 in antiferroelectric phase) in electrically tunable devices are reported.

Index Terms—Ferroelectrics, paraelectrics, tunable microwave devices.

I. INTRODUCTION

SINCE THE late 1960's and early 1970's, ferroelectrics have been regarded as attractive for applications in electrically tunable microwave devices, and a number of practical devices have been demonstrated over the past several decades [1]–[4]. It is generally assumed (even if not stressed specifically in some publications) that, for applications in electrically tunable microwave devices, ferroelectrics should be in a paraelectric phase. Ferroelectrics in polar phase have not been considered for applications in tunable microwave devices. The reason is that most of the ferroelectrics in polar phase are also piezoelectric, and piezoelectric transformations cause large losses at relatively low microwave frequencies (typically less than 10 GHz). Additional losses in polar phase and at low frequencies are associated with the domain wall movements. Hysteresis, which appears in permittivity–dc field dependence, was another reason hindering the applications of a ferroelectric in a polar phase. Hence, no practical attempts have been undertaken in the past to make electrically tunable microwave devices utilizing the ferroelectric phase. In this

respect, piezoelectric devices [both surface acoustic wave and bulk acoustic wave (including bulk and thin film)] are exceptions, and will not be addressed in this paper. On the other hand, some recent experiments indicate that such "discrimination" is not valid. For example, rather low microwave losses along with substantial tunability [defined as $T_\epsilon(V) = [\epsilon(0) - \epsilon(V)]/\epsilon(0)$] of the dielectric permittivity is observed in ferroelectric (piezoelectric) $\text{Na}_{0.5}\text{K}_{0.5}\text{NbO}_3$ (NKN) films at frequencies up to 50 GHz [5]. This indicates that, at millimeter-wave frequencies, the domain wall movements and piezoelectric transformations do not contribute to the microwave losses, and polar phase ferroelectric may be used in tunable microwave devices if they have substantial tunability. Additionally, theoretical and experimental investigations in the past couple of years show that thin films, typically regarded as paraelectrics, may be in a polar, i.e., strain induced ferroelectric phase [6]–[8]. Consequently, a question arises as to why one should not consider other typical ferroelectrics in polar phase for applications in microwave devices. Applications of ferroelectrics in polar phase may offer additional functionalities and design flexibility. A digital (switchable) filter and compensation of temperature dependences in ferroelectric devices are examples discussed in this paper.

The comparison between ferroelectric and semiconductor varactors show [9] that the frequency range, where the ferroelectric varactors may successfully compete with semiconductor analogs lays above 10–20 GHz, where the quality factor of semiconductor varactors decrease drastically ($Q \sim 1/f$), while the Q factor of ferroelectric varactors may remain rather high and, in some cases, even increase with frequency [5]. However, at low frequencies ($f < 10$ GHz) where the Q factor of semiconductor varactors is rather high, i.e., typically above 50, applications of ferroelectric varactors may be limited since the semiconductor counterparts have the advantage of better integration with monolithic microwave integrated circuits (MMICs).

Tunability and loss tangent are the basic parameters characterizing ferroelectrics for applications in tunable microwave devices. Perhaps the losses are the most critical issue in device applications, and most of the efforts in recent years have been devoted to the optimization of film fabrication processes in terms of microwave loss reduction. However, no substantial reductions of losses have been achieved thus far. For this reason, at least at present, the application of epitaxial ferroelectrics in low-loss narrow-band filters with steep skirts is somehow limited, while they can be successfully used in other tunable microwave devices.

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TABLE I
MICROWAVE LOSSES AND TUNABILITY OF TYPICAL FERROELECTRICS

	Made by	Type	$\tan\delta$	f, GHz	T, K	Tuning %	Ref.
Thin epitaxial films	PLA ¹	Au/STO/LAO	0.0013 ³	16	77	10	[18]
	PLA	Ag/BSTO/MgO	0.2	10	298	30	[26]
	PLA	HTS/STO/LAO	0.0075	6	77	23	[10]
	PLA	Au/Ag/BSTO/MgO	0.006	10	300	56	[27]
	PLA	Ag/BSTO/MgO	0.04	5	300	75	[28]
	PLA	Au/Ti/BSTO/MgO	0.04	8-10	300	50	[29]
		Au/Ti/STO/MgO	0.04			30	
	PLA	STO/LAO	0.04	1.5	100	38	[21]
	PLA	Ag/YBCO/STO/LAO	0.05	11	4	30	[12]
	PLA	Au/Ti/STO/LAO	0.01	1.5-2.5	300	-	[21]
	PLA	Au/YBCO/STO/MgO	0.02	20	20	25	[24]
	PLA	Ag/BSTO/LAO	0.1	10	75		[23]
	PLA	Au/YBCO/STO/LAO	0.006	7.5	79	7	[13]
	Mag ²	Cu/STO/CeO/Sapphire	0.02	3-10	78-100	45	[22]
	Mag	Cu/STO/CeO/Sapphire	0.025	3	78	29	[25]
	PLA	YBCO/STO/LAO	0.0032	4.2	4	-	[19]
	MOCVD ⁴	Pt/BSTO/Pt/SiO ₂ /Si	0.006	20	300	-	[36]
	PLA	BSTO/MgO	0.02	10	300	-	[34]
	PLA	BSTO/MgO	0.06	1-20	300	34	[35]
		BSTO/LAO	0.05			20	
Thick film		Mg doped BSTO	0.0065	10	300	3.66	[33,33]
Bulk	Ceramic	BSTO	0.0056	C-band	300	-	[20]
		STO	0.002	C-band	300	-	
		BSTO:MgO	0.008	10	300	4<	[37]
		BaSrTiO	0.044	18	300	16	[3]
	Single crystal	STO	0.00033	1	77		[10]
		KTO	0.0005	1	77		
		STO	0.0024	22	300	-	[30]
			0.0014	22	170		
		STO	0.00023	2	77		[31]
			0.0005	0.3	300		

¹ Pulsed laser ablation; ² Magnetron sputtering; ³ Estimated from unloaded Q-factor ($Q_0=750$); ⁴ Metal-organic chemical vapor deposition

II. TYPICAL MICROWAVE PARAELECTRICS

Incipient ferroelectrics SrTiO₃ (STO), KTaO₃ (KTO), and Ba_xSr_{1-x}TiO₃ (BSTO, in paraelectric phase, $x < 0.5$) have been traditionally used in electronically controlled microwave devices. These materials are used in the form of single crystals (bulk [10], [11], epitaxial film [11]–[19]), or ceramics (bulk [1]–[3], film [20]) with normal metal or superconductor electrodes. Very little is known about the microwave properties of other ferroelectric materials and microwave devices based on them. Losses and tunability for paraelectrics widely used at microwaves are summarized in Table I. Usually the tunability of

the capacitance $T_c(V) = [C(0) - C(V)]/C(0)$ rather than the tunability of permittivity $T_\epsilon(V)$ is used to estimate parameters of devices and, in some cases, to estimate the effective parameters of the materials. For sandwich-type capacitors (bulk and thin film) $T_c(V)$ is approximately the same as $T_\epsilon(V)$, while it is smaller than $T_\epsilon(V)$ for planar capacitors in the form of a gap between electrodes on the surface of a ferroelectric film. For a planar device, a tradeoff is possible between the tunability and losses. The width of the gap between the planar electrodes relative to the thickness of the ferroelectric film (e.g., in a varactor) may be designed so that the losses are kept low at the expense of reduced tunability. A more complete assessment of

tunable devices for microwave application may be done using a figure-of-merit introduced in [38].

Measurement of the loss tangent in bulk single crystal incipient ferroelectrics have been carried out by using samples without electrodes [30], [31] and with electrodes in a sandwich configuration [10]. In the case where superconductor electrodes are used [10], [11], the losses associated with the electrodes may be ignored. Hence, the loss tangent given for single crystal ferroelectrics in Table I characterize the paraelectric material itself and may be used to estimate the quality of ceramics and epitaxial ferroelectric films.

Microwave measurements of the dielectric properties of epitaxial films represented in Table I are mainly done using planar electrodes applied to one surface of the film only. No contactless microwave ($f < 100$ GHz) measurements of ferroelectric films have been reported thus far, which makes it difficult to distinguish between the losses in the bulk of the film and at the film/ferroelectric interface. Measurement of zero-bias losses tangent at microwave frequencies (up to 20 GHz) in a “sandwich” Pt/BSTO/Pt structure is reported in [36] (see Table I).

Presented in Table I are the experimental results obtained at microwave ($f > 0.3$ GHz) frequencies only. It is neither complete nor perfect since the publications are spread over a large variety of interdisciplinary journals, and often do not specify material parameters explicitly. In contrast to the sandwich-type capacitor structures, in planar capacitors (with the electrodes on one surface of the ferroelectric film), a considerable part of the microwave field is outside the ferroelectric film, i.e., in air or in low dielectric-loss substrate. The field outside the ferroelectric film is larger for larger gaps between the planar electrodes. This means that measured effective dielectric constant, tunability, and loss tangent shown in Table I are lower than the permittivity, tunability, and loss tangent of the film itself. Note that the loss tangent values given in Table I also include the losses in the electrodes (except for a single-crystal STO [30], [31]). In most cases, these losses may be ignored since they are usually smaller in comparison with the losses in the ferroelectric films. The analysis of the previous publications and the results given in Table I show that no substantial improvement in the film quality is achieved despite extensive efforts in the past decade. Although, in some cases, the effective $\tan \delta$ is somehow closer to the $\tan \delta$ of the bulk single crystals, the actual losses in the bulk of the films are still much higher in comparison with the bulk single crystals, especially at room temperature.

Bulk and thick-film ceramic ferroelectrics offer advantages of low cost in mass production. Efforts to apply ceramics in microwave devices had been made in late 1960's [39] and early 1970's [1]. Lower losses, in comparison with the epitaxial films, are observed in ceramic materials, where low-loss nonferroelectric dielectrics are used as additives. Such additives decrease both the losses, dielectric permittivity, and its tunability [32], [33], [37].

In bulk single-crystal paraelectrics (i.e., STO and KTO), the losses increase with the applied dc field [10], which has been theoretically explained by a quasi-Debye relaxation mechanism [40]. On the other hand, in most cases, the losses in the ceramics and epitaxial films go down with the applied dc field. This may lead to a desire to use smaller tuning ranges at higher dc fields.

However, one has to take into account that, at high dc fields, some irreversible changes (electrocoloration due to the ion migration [41], [42]) may take place in the ferroelectric where the dc field is kept high at elevated temperature for a long time.

Recent theoretical predictions [6], [43] and experimental results [7], [8] show that the strain in the films caused by substrate clamping and interfacial charges lead to induced polarization in thin STO films. It then becomes questionable if the epitaxial films regarded as paraelectric are really in paraelectric phase, and if the data shown in Table I should be regarded as related to paraelectric phase. Furthermore, a low-loss polar state is observed even in bulk single crystals of STO at microwave frequencies [10], [11], which traditionally has been regarded as an incipient ferroelectric, i.e., not having polar phase. These observations make it reasonable to study the possibilities of using (in electrically controlled microwave devices) ferroelectrics not only in the paraelectric, but also in the polar phase.

III. FERROELECTRIC DEVICES AND SYSTEMS

In this section, we will very briefly review reported tunable devices and systems based on ferroelectrics. In all published devices, ferroelectrics are regarded as being in a paraelectric phase, although, judging from the above arguments, these statements may not always be true. In most cases, due to the lack of relevant data, it is impossible to distinguish whether the materials used are in paraelectric or polar phase.

A large number of ferroelectric microwave ceramic components, such as varactors, tunable filters [4], and phase shifters [2], [3], [20] have been demonstrated in the past. Some basics of physics and device design are given in [1]. A K -band phase shifter based on thin-film trilayer Pt/BSTO/Pt varactors has been reported recently [14], which seems to be the first publication where sandwich-type varactors are used at these high frequencies. The main advantages of a thin-film trilayer (“sandwich”) design are small dc voltages (< 5 V) and high tunability ($T_c(V) \approx T_e(V)$). The other event worth mentioning is that a startup company is already marketing cost-effective tunable ferroelectric filters and duplexers.

Recently, electronically scanned phased arrays based on ferroelectric phase shifters have been demonstrated. A commercial K -band two-dimensional phased array for one-dimensional (1-D) scanning of the beam has been demonstrated by Paratek.¹

The phase shifters in this array are based on sections of microstrip lines fabricated on bulk ceramic ferroelectric substrate. A K -band eight-element linear phased array based on thick-film ferroelectric varactors (planar electrodes) has been also reported [16]. An experimental K -band 16 element linear phased array using thin BSTO film phase shifters have been demonstrated in [15]. Phase shifters in this system are realized on coupled microstrip lines fabricated on top of 0.3- μm -thick BSTO films epitaxially grown on an MgO substrate by laser ablation.

No tunable microwave devices utilizing polar phase ferroelectrics (at least regarded as such) are reported thus far. In Section IV, we will discuss a couple of examples to demonstrate the possibilities and advantages of using ferroelectrics in polar phase.

¹[Online]. Available: <http://www.paratek.com>

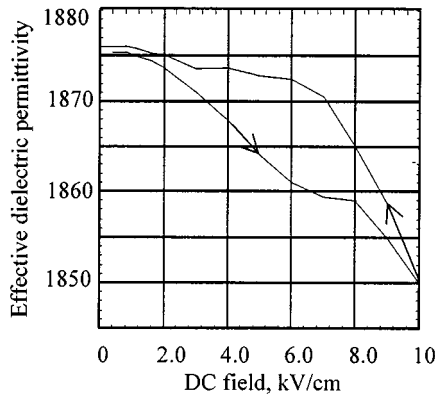


Fig. 1. DC-field dependence of the dielectric permittivity of a bulk single-crystal STO at 77 K.

IV. DEVICES BASED ON POLAR PHASE FERROELECTRICS

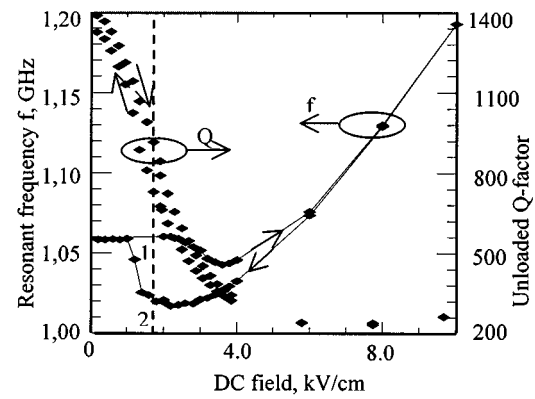
A. Switchable Frequency Resonators

A double hysteresis loop in the dielectric permittivity of single crystal STO at 1.0 kHz and temperatures below 62 K was first reported in [44]. The result was explained theoretically assuming the crystal undergoes an antiferroelectric-to-paraelectric phase transition. The authors observed this phase transition in a specially temperature-treated STO where the cooling was done with short-circuited electrodes. Later similar experimental results have been published at about 1.0 [10] and 1.5 GHz [11]. These experiments show that the paraelectric-to-antiferroelectric phase transition in cooled bulk single-crystal STO may be induced by a dc electric field even at a higher temperature (77 K) regardless of the cooling conditions (i.e., cooling with or without short-circuited electrodes). The dielectric hysteresis at 77 K and 1.5 GHz in an STO single crystal is shown in Fig. 1 [11]. In this experiment, high-temperature superconducting (HTS) electrodes are used to apply the dc field.

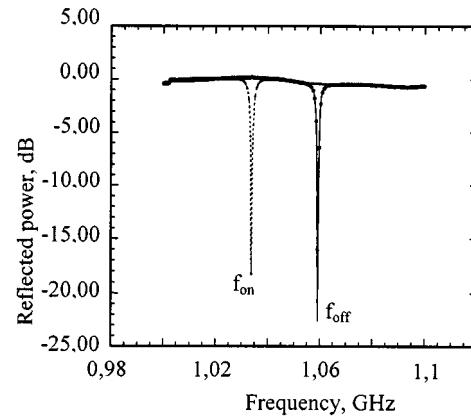
The loop in the dielectric permittivity in Fig. 1 makes an analog dc control of a microwave device problematic. On the other hand, the hysteresis loop in the field-dependent permittivity may be utilized in digitally controlled microwave devices. An example of the dc-bias-dependent resonant frequency and unloaded Q factor for a disk parallel-plate resonator based on a single-crystal STO with superconductor electrodes is shown in Fig. 2(a) [10]. In this experiment, the STO disk was 10 mm in diameter and 0.5-mm thick with HTS electrodes. As follows from Fig. 2(a), there are two distinct resonant frequencies for the same dc field, corresponding to two branches of the $f(V)$ curve. The resonant frequency is less sensitive to the changes of dc bias near points 1 and 2. Fig. 2(b) shows the resonant curve in two states, corresponding to points 1 and 2 in Fig. 2(a). An important feature of such a digitally switched resonator is that the losses (Q factors) are practically the same at the two resonant states. Switchable rather than analog control may be advantageous in many practical applications.

B. Varactors Based on Ferroelectric NKN Films

As was mentioned above, very little is known about the microwave properties of ferroelectrics in polar phase. The dielec-



(a)

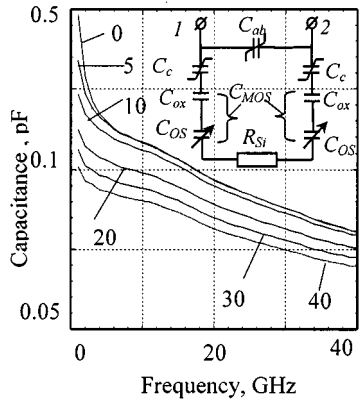


(b)

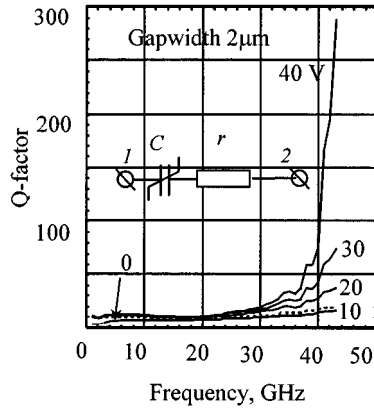
Fig. 2. DC-field dependence of the: (a) resonant frequency and (b) Q factor and resonant curves corresponding to two states (1: off and 2: on). $T = 52$ K and dc field is 1.2 kV/cm.

tric properties of polar NKN films on LaAlO_3 substrates have been studied experimentally [45]. The results were quite encouraging in terms of microwave losses and tunability. Recently, more experiments have been published with NKN films deposited on oxidized silicon substrates [5]. Bulk NKN is characterized by a ferroelectric phase transition at about 600 K, i.e., one should expect that the films at room temperature are in a polar phase. Indeed, thin films on silicon substrate have distinct hysteresis loops with remnant polarization about $10 \mu\text{Coul}/\text{cm}^2$ [46].

Fig. 3 shows the microwave performance of thin NKN film varactor deposited on a high-resistivity silicon substrate [5]. The gapwidth between the planar Au/Ti electrodes [see inset in Fig. 4(b)] is $2 \mu\text{m}$. The details of the NKN film deposition are given in [46]. Fig. 4 shows dc-bias dependences of the capacitance and Q factor of an NKN varactor. As can be seen in Fig. 4(b), a substantial tunability ($>10\%$) is available at frequencies up to 50 GHz, and the Q factor increases with increased frequency and dc bias [see Fig. 3(b)]. The rather high tunability observed at low frequencies ($f < 10$ GHz) is due to the surface barrier at the Si/ SiO_2 interface, i.e., the tunability at low frequencies is mainly due to the metal-insulator-semiconductor (MIS) capacitor [47] with an additional ferroelectric layer [48]. At higher frequencies ($f > 20$ GHz), the MIS structure is practically not tunable, and the observed tunability is due to the ferroelectric film [48]. It is important to note that, in comparison

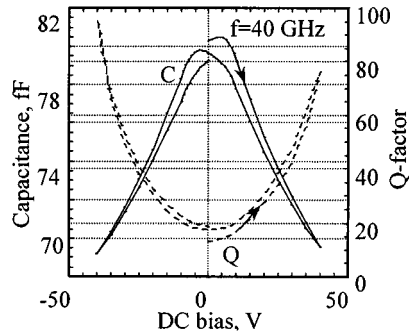


(a)

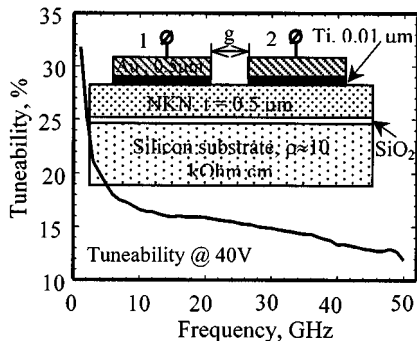


(b)

Fig. 3. (a) Capacitance and (b) Q factor of Au/Ti/NKN/SiO₂/Si planar structure versus frequency $T = 300$ K. NKN film thickness is $0.4 \mu\text{m}$.



(a)



(b)

Fig. 4. (a) Capacitance and Q -factor and (b) tunability of an interdigital capacitor. Finger length is $12 \mu\text{m}$, finger width and spacing are $2 \mu\text{m}$, $T = 300$ K.

with semiconductor analogs, the Q factor of this not yet optimized varactor is rather high at 40 GHz.

The $C(V)$ in Fig. 4(a), measured at 40 GHz, show a typical butterfly shape, which is distorted (reduction of zero-bias capacitance after bias reversals) due to charge accumulation at interfaces and at the grain boundaries in the bulk of the film. In further optimization of the film and devices, this effect has to be reduced. However, the butterfly performance is an inherent property of the polar phase, and it is observed in most epitaxial film ferroelectric varactors, delay lines, and filters. It has been shown theoretically [6], [43] and experimentally [8] that there is only a narrow temperature range where the films are in paraelectric phase, and the butterfly performance does not appear. The substrate/film type, deposition process, and post deposition treatment may be adjusted to have this temperature range in the desired interval. In other cases, the problem can be taken care of electronically if the butterfly type $C - V$ is not distorted and is repeatable.

C. Temperature-Compensated Varactor

The temperature dependence of the dielectric permittivity, which is an inherent property of ferroelectric materials, is a major problem in practical implementations of tunable ferroelectric devices. One can overcome this problem by using ferroelectrics in polar phase if the losses at frequencies of interest are sufficiently low and the tunability of the dielectric permittivity is sufficiently large. Fig. 5(a) shows an example of how this problem can be solved in a planar BSTO capacitor made of two ferroelectric films with different ratios of Ba/Ti. In the experimental results presented in this paper, Ba/Ti = 3 and 1/3 is used [see Fig. 5(a)]. The films are separated by epitaxial MgO to avoid chemical interaction/interdiffusion. The temperatures (T_1 and T_2) [see Fig. 5(a)] where the permittivities peak are different for the two BSTO films with the different Ba/Ti ratios. The losses of the individual films also peak at temperatures T_1 and T_2 . In the temperature interval between the peaks, the film with the larger Ba/Ti ratio is in a polar phase and, with the increased temperature, its permittivity increases. At the same time, the other film is in the paraelectric phase and its permittivity decreases with the increased temperature. The resultant effective permittivity measured between the plates of the varactor (Fig. 5) will depend on the geometry, i.e., thickness and permittivity of the layers, ratio between the total thickness of the films, and the width of the gap between electrodes. The geometry and parameters of the films may be designed to yield a desired temperature coefficient of the capacitance. It may be particularly designed to be independent of temperature in a certain temperature interval. In this case, the device is designed so that the decreased permittivity of the paraelectric film is compensated by the increased permittivity of the film in ferroelectric phase [see Fig. 5(a)]. The results of such experimental temperature compensation are shown in Fig. 5(c). Since the losses of the individual films also peak at temperatures T_1 and T_2 [see Fig. 5(a)], one should expect a maximum Q factor between these two temperatures where the capacitance is not temperature dependent, as can be seen from the experimental results [see Fig. 5(c)]. In the experiments shown in Fig. 5(b) and (c), the total thickness of all epitaxial layers is $0.4 \mu\text{m}$, plates are $125 \times 125 \mu\text{m}^2$, and

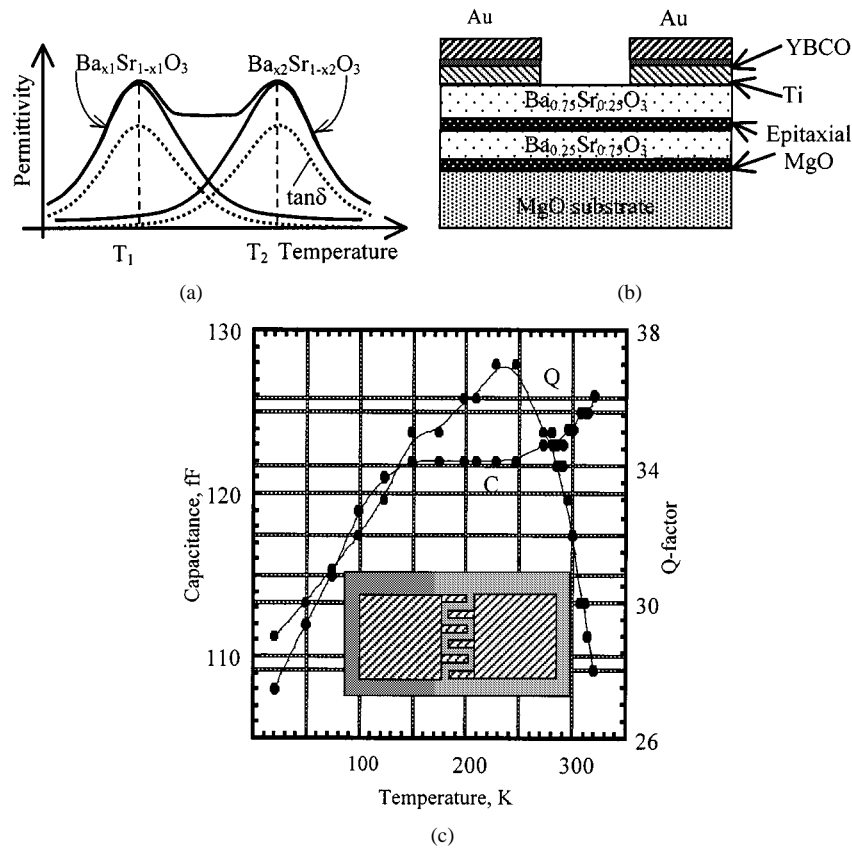


Fig. 5. Concept (a) structure (b) and experimental verification of temperature stabilization.

“fingers” are 12- μm long, 4- μm wide, and 4- μm apart (gap-width).

A similar approach can be used to design temperature-compensated phase shifters and other ferroelectric components. While optimizing the design of temperature-compensated ferroelectric components, one should remember that the temperature where the permittivity peaks depends not only on the composition of the ferroelectric film, but also on the strain interfacial charges [8].

V. CONCLUSIONS

In many cases, the epitaxial ferroelectric films, regarded as paraelectric, may be in strain and/or interface charge-induced ferroelectric phase; nevertheless, they have been successfully used in tunable microwave devices. Given this fact, and referring to the experiments with polar phase ferroelectrics discussed above, ferroelectrics in polar phase should also be considered for microwave applications in tunable microwave devices. Applications of polar ferroelectrics in tunable devices seem to be more practical at frequencies above 10–20 GHz since, at these frequencies, domain wall motions are frozen and there is no piezoelectric transformation of microwave signals, i.e., there are virtually no microwave losses associated with these effects. Moreover, this is a frequency range where ferroelectrics may compete with semiconductors since, above these frequencies, ferroelectrics offer substantially higher Q factors in comparison with semiconductor varactors.

Consideration of the polar phase substantially increases the number of ferroelectrics available for tunable microwave appli-

cations and may lead to the use of new ferroelectrics with lower losses and higher tunabilities. It also offers flexibility in device design, as in the case of a temperature-compensated varactor. Besides standard analog tuning, ferroelectrics in polar phase offer a possibility of digital control. The switchable resonant frequency resonators may particularly be used in switchable filters in modern microwave communication systems filters. In a view of switchable resonator discussed above, it seems interesting to study microwave performance of bulk and thin-film antiferroelectrics.

Hardening of the soft mode in thin epitaxial film [7] is yet another factor speaking in favor of the application of polar phase ferroelectrics at millimeter-wave frequencies. It seems that, due to the hardening of the soft mode, one may expect substantial ferroelectric activity and tunability in polar phase at microwave frequencies.

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