Extracting the Electromechanical Coupling Constant of Piezoelectric Thin Film by the High-Tone Bulk Acoustic Resonator Technique

Chong Zhou, Wei Pang, Qiang Li, Hongyu Yu, Xiaotang Hu, and Hao Zhang

***Abstract*—In this paper, a new approach is proposed to rapidly and accurately measure the electromechanical coupling constant K_t^2 of thin film piezoelectric material, which is critically important for real-time quality control of the piezoelectric film growth in mass production. An ideal lossy bulk acoustic resonator (LBAR) model is introduced and the theory behind the method is presented. A high-tone bulk acoustic resonator (HBAR) was fabricated on a silicon wafer. The impedance response of the resonator was measured, from which the K_t^2 of the piezoelectric material was extracted. To illustrate the potential of the proposed technique to extract material properties, two HBAR devices employing AlN as the piezoelectric material were fabricated using an RF sputter system with known good and bad deposition conditions; the extracted K_t^2 values of the piezoelectric material are compared.**

I. Introduction

The advancement of modern wireless communication systems requires high-performance filters and frequency reference elements with high operation frequency, miniature size, and low cost. Bulk acoustic wave (BAW) resonators are well suited for mobile telecommunication systems operating at high frequencies from 0.5 to 10 GHz and have been intensively developed for the past 20 years [1]. A BAW resonator typically consists of a layer of piezoelectric thin film sandwiched between two thin metal electrodes. When an alternating electrical voltage is applied between the two electrodes, the consequent electric field between the electrodes interacts with piezoelectric material to generate acoustic waves within the piezoelectric material. Electromechanical coupling constant K_t^2 of the piezoelectric material is a parameter of exceptional importance for BAW filters [2]. A greater K_t^2 usually indicates a larger separation of the series and parallel resonances, which is crucial for producing RF BAW filters with wide bandwidth [3].

Manuscript received November 1, 2011; accepted January 18, 2012. This material is based upon work supported by the Ph.D. Program Foundation of the Ministry of Education of China # 20100032120056 and the National Nature Science Foundation of China # 61006074.

C. Zhou, W. Pang, X. Hu, and H. Zhang are with the State Key Laboratory of Precision Measuring Technology and Instruments, Tianjin University, Tianjin, China (e-mail: haozhang@tju.edu.cn).

Q. Li is with the School of Electronic Information Engineering, Tianjin University, Tianjin, China.

H. Yu is with the School of Earth and Space Exploration, Arizona State University, Tempe, AZ.

DOI http://dx.doi.org/10.1109/TUFFC.2012.2280

AlN is a desirable BAW material with relatively high K_t^2. It is frequently prepared by sputtering. The quality of the deposited AlN film is often examined by X-ray diffraction (XRD) and presented in terms of XRD peak-width rocking-curve full-width at half-maximum (FWHM) angle [4]. It is important to note that a small FWHM angle is a necessary condition to achieve high K_t^2, but it is by no means a sufficient condition. Even if XRD shows perfect crystal orientation and satisfactory FWHM angle, an amorphous AlN starting layer could be placed during the deposition process, which would greatly undermine the K_t^2 of the film [5].

The most obvious way to extract the K_t^2 of the piezoelectric material is to fabricate a thin film bulk acoustic wave resonator (FBAR) or a solidly mounted resonator (SMR) and then measure the resonant frequency and antiresonant frequency, from which the effective electromechanical coupling coefficient $K_{t,\text{eff}}^2$ of the resonator is calculated. However, the resonator structure is complicated and there are many factors influencing the $K_{t,\text{eff}}^2$ of the resonator in the fabrication process; ultimately, the extracted K_t^2 of the piezoelectric material may be inaccurate [6].

In this paper, a very intuitive and simple approach based on a single-mask process high-tone bulk acoustic resonator (HBAR) structure to extract K_t^2 of thin film piezoelectric material was developed. As shown in Fig. 1, an HBAR consists of a piezoelectric layer sandwiched by two metal electrodes, and a support substrate underneath the sandwich structure. The bottom electrode serves as an electrical ground plane, and the top electrode is patterned in a ground-signal-ground configuration for probe measurements. K_t^2 of the piezoelectric material can be directly extracted by measuring input impedance of the HBAR. One can get an intuitive impression of the K_t^2 characterization from the Smith circle measured and displayed on a network analyzer.

II. Theory

To get a high quality (Q) factor, the HBAR should have a substrate that has a small acoustic attenuation, such as sapphire, crystal quartz, etc. [7]. Because the thickness of the substrate is large compared with the acoustic wavelength, the device operates at a very high harmonic of its

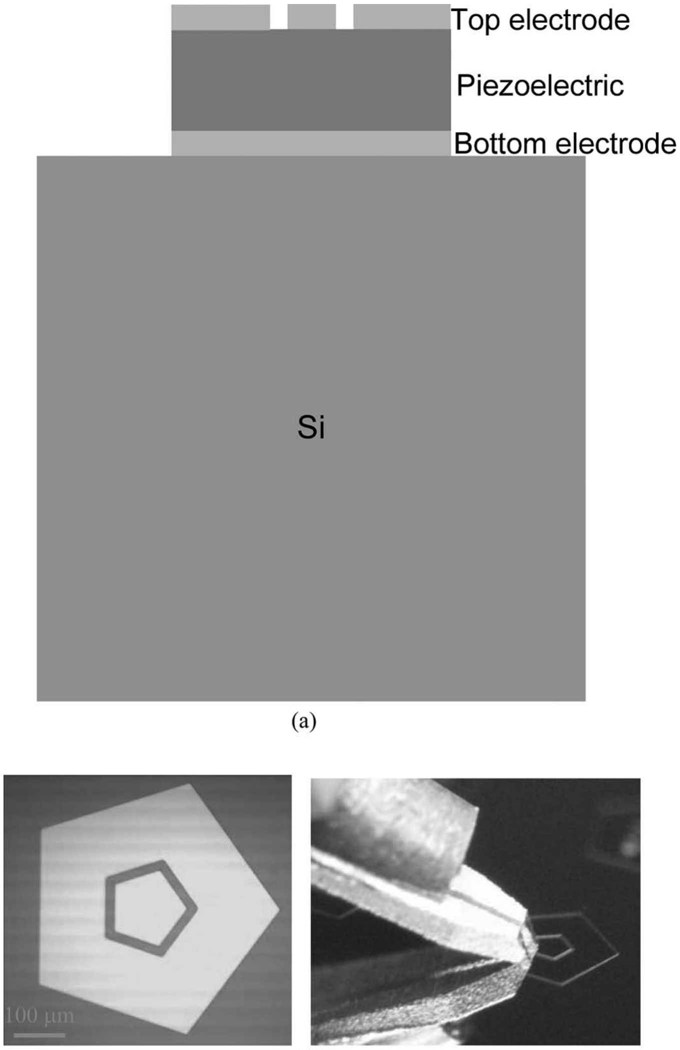


Fig. 1. (a) Cross-sectional schematic of a high-tone bulk acoustic resonator (HBAR). (b) Photographs of a fabricated HBAR device.

fundamental. The electrical response consists of a series of resonances and anti-resonances with frequency separation that is approximately inversely proportional to the thickness of the substrate [8]. In general, it is very difficult to obtain a closed-form solution for the electrical impedance of the HBAR because of the presence of a large number of resonances. To simplify the theoretical analysis, a critical assumption is made. The substrate is assumed to be infinitely long or very lossy, which means that the wave incident to the substrate will never be reflected back. In other words, no standing wave is supported in the substrate. We define this type of device as a lossy bulk acoustic resonator (LBAR).

The active area of the LBAR is determined by the overlap area of the top signal and bottom electrodes. The lateral dimension of the device is significantly larger than the thickness of the composite structure, to justify the one-dimensional acoustic wave propagation assumption. A one-dimensional Mason model [9] was applied to analytically calculate the electrical response of the device. The piezoelectric layer was modeled as an electrical port and

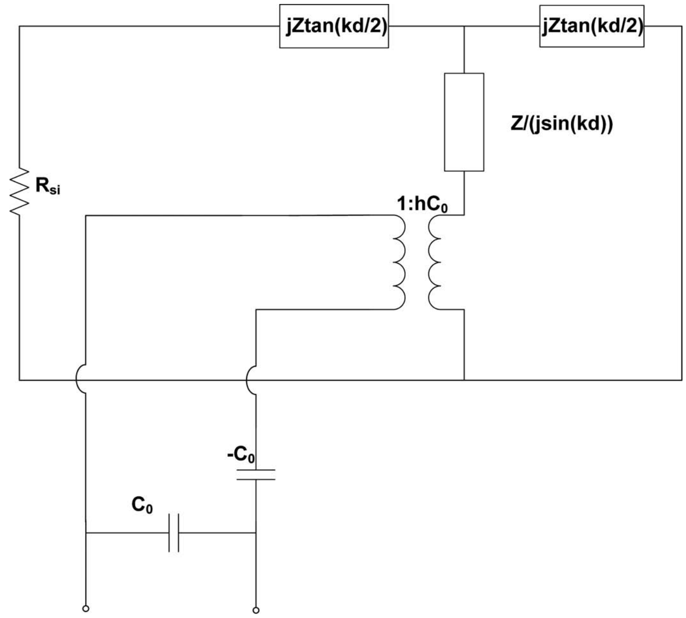


Fig. 2. Equivalent circuit of a lossy bulk acoustic resonator with thin metallic electrodes.

two mechanical ports through the use of an ideal electromechanical transformer, as shown in Fig. 2. With the exception of the piezoelectric layer, any layer in the acoustic structure can be modeled as an ideal electrical transmission line with characteristic impedance equal to the acoustic impedance of the material. From the microwave theory, the infinitely long transmission line can be replaced by a resistance which is equal to the characteristic impedance of the transmission line Z_0. The equivalent circuit of an LBAR with metallic electrodes thin enough to be negligible is shown in Fig. 2.

The electrical input impedance of the LBAR is expressed as

$$\begin{aligned} Z_{\mathrm{in}} &= \frac{1}{j\omega C_0} + \frac{(Z_{\mathrm{S}}/Z_{\mathrm{T}})\sin(kd) + 2j(1-\cos(kd))}{\sin(kd) - j(Z_{\mathrm{S}}/Z_{\mathrm{T}})\cos(kd)} \frac{K_t^2 v_{\mathrm{a}}}{d\omega^2 C_0} \\ &= \frac{1}{j\omega C_0} + Z', \end{aligned} \tag{1}$$

where Z_{S}, Z_{T}, d, v_{a}, and k are the acoustic impedance of the substrate, acoustic impedance of the piezoelectric material, thickness of the piezoelectric layer, acoustic velocity, and wave number in the piezoelectric layer, respectively. C_0 is the capacitance of the piezoelectric layer sandwiched by the top and bottom electrodes. ω is the angular frequency of the applied signal. K_t^2 is the electromechanical coupling constant of the piezoelectric material.

Because Z' is a complex number, it can be rewritten as a sum of the real and imaginary parts:

$$Z_{\mathrm{in}} = \frac{1}{j\omega C_0} + [Z_{\mathrm{r}}(\omega) + jZ_{\mathrm{i}}(\omega)] \frac{K_t^2 v_{\mathrm{a}}}{d\omega^2 C_0}, \tag{2}$$

where Z_{r} and Z_{i} are the real part and imaginary part, respectively, and are given by

$$Z_{\mathrm{r}}(\omega) = \frac{Z_{\mathrm{S}} Z_{\mathrm{T}} (1 - \cos(kd))^2}{Z_{\mathrm{T}}^2 \sin^2(kd) + Z_{\mathrm{S}}^2 \cos^2(kd)} \tag{3}$$

$$Z_{\mathrm{i}}(\omega) = \frac{\sin(kd)[1 + \cos(kd)](Z_{\mathrm{S}}^2 - 2Z_{\mathrm{T}}^2)}{Z_{\mathrm{T}}^2 \sin^2(kd) + Z_{\mathrm{S}}^2 \cos^2(kd)}. \tag{4}$$

Resonance is defined as the frequencies at which $Z_{\mathrm{i}}(\omega) = 0$; therefore, the fundamental resonant frequency is given by

$$\omega_{\mathrm{r}} = \frac{\pi v_{\mathrm{a}}}{d}. \tag{5}$$

In the case of $\omega_{\mathrm{r}} = \pi v_{\mathrm{a}}/d$, $\cos(kd) = -1$, $Z_{\mathrm{r}}(\omega_{\mathrm{r}})$ is very close to the maximum:

$$Z_{\mathrm{r}}(\omega_{\mathrm{r}}) = \frac{4Z_{\mathrm{S}}/Z_{\mathrm{T}}}{D} = \frac{4}{Z_{\mathrm{S}}/Z_{\mathrm{T}}}. \tag{6}$$

The corresponding electrical impedance Z_{in} is

$$Z_{\mathrm{in}} = \frac{1}{j\omega_n C_0} + \frac{4}{Z_{\mathrm{S}}/Z_{\mathrm{T}}} \frac{K_t^2 v_{\mathrm{a}}}{d\omega_n^2 C_0}. \tag{7}$$

R_{r} is defined as the real part of Z_{in} at the resonant frequency:

$$R_{\mathrm{r}} = \frac{4}{Z_{\mathrm{S}}/Z_{\mathrm{T}}} \frac{K_t^2 v_{\mathrm{a}}}{d{\omega_0}^2 C_0} = \frac{4}{\pi} \frac{Z_{\mathrm{T}}}{Z_{\mathrm{S}}} \frac{K_t^2}{\omega_0 C_0} = \frac{4}{\pi^2} \frac{Z_{\mathrm{T}}}{Z_{\mathrm{S}}} \frac{K_t^2 d^2}{v_{\mathrm{a}} \varepsilon_{\mathrm{r}} \varepsilon_0 A}. \tag{8}$$

From (8), we can get

$$\frac{R_{\mathrm{r}}}{K_t^2} = \frac{4}{\pi^2} \frac{Z_{\mathrm{T}}}{Z_{\mathrm{S}}} \frac{d^2}{v_{\mathrm{a}} \varepsilon_{\mathrm{r}} \varepsilon_0 A}. \tag{9}$$

where ε_{r}, ε_0, and A are the relative permittivity, vacuum permittivity, and the active area of the device, respectively. According to (9), with fixed values of piezoelectric layer thickness d and active area A of the LBAR, R_{r}/K_t^2 is a constant.

For the LBAR structure with negligible electrodes, e.g., a simple two-layer structure, the ratio of R_{r} to K_t^2 is a constant value. However, in a practical piezoelectric device, the electrodes cannot be too thin for a low series resistance. To verify whether these conclusions are applicable to the multilayer structure, a program based on the Mason model has been developed to simulate the multilayer LBAR structure. Similarly, the substrate is assumed to be infinitely long, and is replaced by a resistor in the model. To verify the validity of the model, a high-loss silicon wafer was used as the substrate to form the multilayer device shown in Fig. 1. The simulation and experimental results are in very good agreement over a very wide frequency range, as shown in Fig. 3. Unlike conventional high-Q HBARs, the series of resonances and anti-resonances are nearly undetectable in the electrical frequency response of the multilayer HBAR employing the high loss substrate, which indicates that almost all the acoustic energy incident into the substrate is absorbed.

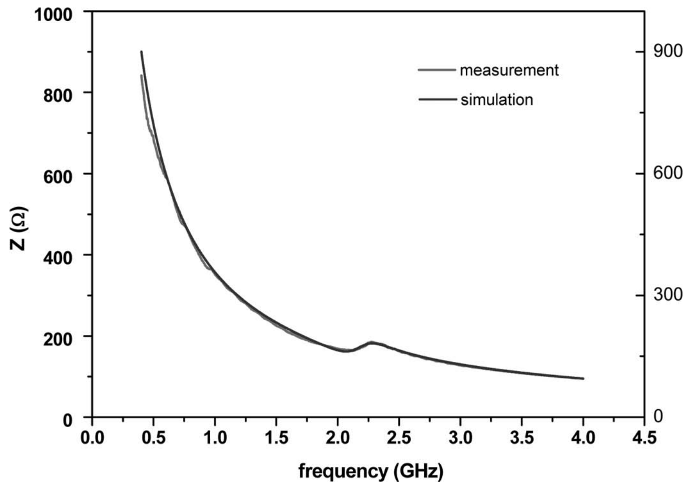


Fig. 3. Simulated and measured frequency responses of a lossy bulk acoustic resonator.

To study the relationship between the K_t^2 and R_r of a multilayer LBAR structure, the value of R_{r} is simulated with the K_t^2 variation, and the result is plotted in Fig. 4. The maximum of the real part of the input impedance R_{m} is plotted in the same figure. Both R_{r} and R_{m} are linear functions with respect to K_t^2 ranging from 1% up to 30%, except the slopes of the two lines are slightly different, which validates the conclusion that the ratio of R_{r} to K_t^2 or R_{m} to K_t^2 is approximately a constant value for a multilayered LBAR structure. Therefore, the value of K_t^2 could be extracted from either the real part of Z_{in} at the resonant frequency or the maximal value of the real part of the measured input impedance of the resonator.

The simulated S_{11} parameters of LBARs with different K_t^2 values are plotted in the Smith chart, as shown in Fig. 5. The S_{11} of an LBAR plotted in the Smith chart is a resonant circular curve. If the piezoelectric layer thickness

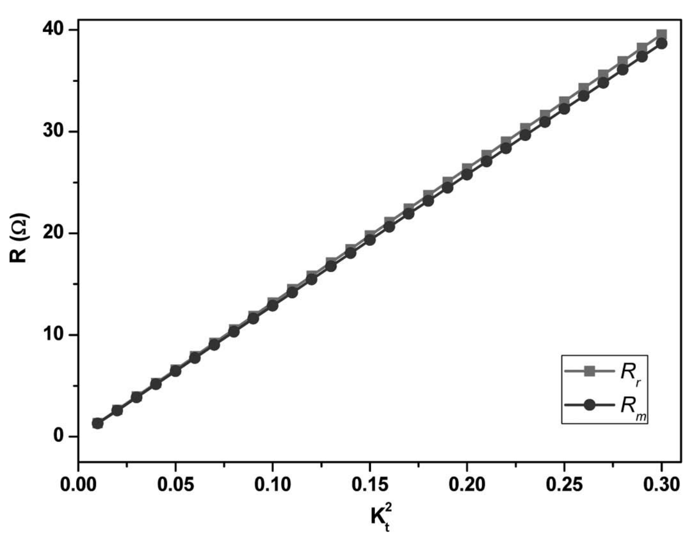


Fig. 4. Relationship between R and K_t^2 of a multilayer lossy bulk acoustic resonator structure.

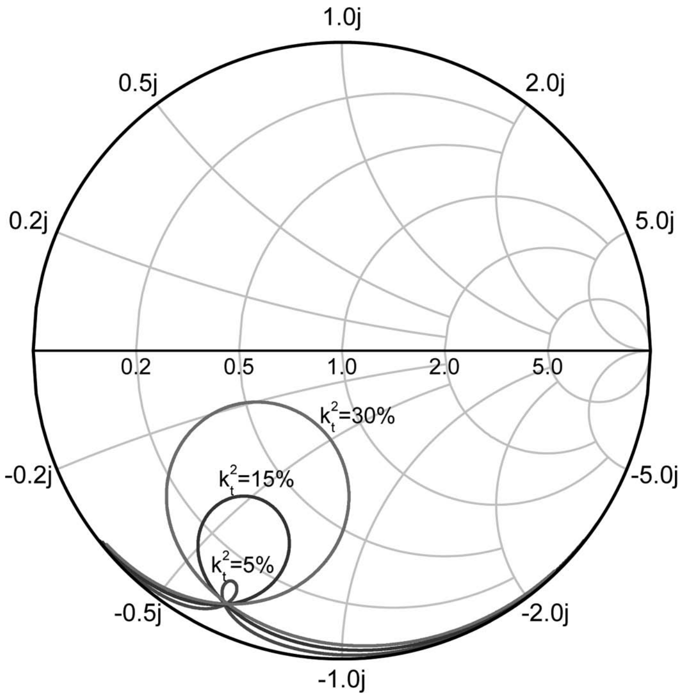


Fig. 5. Smith chart showing simulated S_{11} parameters of lossy bulk acoustic resonators with different values of K_t^2.

d and active area A of the LBAR are fixed, the size of the resonant circle is determined by K_t^2 of the piezoelectric material. The bigger the resonant circle is, the larger is the K_t^2. Therefore, one would get an intuitive impression about the value of K_t^2 by reading the measured impedance of the resonator plotted in the Smith chart.

In the Mason model and the preceding simulations, a resistance representing the complete absorption of acoustic waves in the substrate, equivalent to the acoustic impedance of the substrate material, was adopted. However, the commonly used substrates such as silicon have a finite thickness, and also many of them do not present significant attenuation to the acoustic wave. Therefore, in a more realistic model, the thickness of the substrate should be finite, and the loss factor of a propagating acoustic wave in the substrate is introduced. The simulation results are displayed in Fig. 6, which are the real part of the input impedance Z of an HBAR formed on low-loss substrate and an ideal LBAR. The dark gray curve is the result of the LBAR using the ideal model in which the substrate is replaced by a resistance, and the light gray curve is that of the HBAR using the realistic model. The lighter curve is fatter than the dark curve because a large number of harmonic resonances are excited which are densely spaced in the frequency spectrum of the low-loss HBAR. With the increasing substrate loss, the harmonic resonances become weak, and the fat, lighter curve becomes slimmer, ultimately matching the darker curve. The darker curve is approximately the mean of the lighter curve.

An LBAR is an ideal device and is not convenient to fabricate. A low-loss HBAR is a more realistic device for practical use. After a low-loss HBAR is fabricated and measured, the noisy raw impedance data are then averaged using a moving square or Gaussian average window to get a smooth data curve, from which the K_t^2 of the piezoelectric material is extracted. Taking into account that the frequency interval of the resonances and antiresonances superimposed on the electrical response are approximately inversely proportional to the thickness of the substrate, an alternative approach is to design a low-pass filter to filter out the high-tone components of the signal produced by the substrate resonance. A clean spectral curve is obtained at the output of the filter, which is then used to calculate K_t^2 using the same procedure.

III. Experiments

To illustrate the potential of the proposed technique to extract material properties, two HBAR devices were fabricated, using AlN as the piezoelectric material. The AlN thin films in the two devices were prepared in an RF magnetron sputtering system. One AlN film was deposited using known good deposition conditions, and the AlN film in the other device was deposited using known bad deposition conditions. The deposition conditions include substrate temperature, RF power, process pressure, surface roughness, etc. The substrates used to fabricate the two devices were 500-μm-thick silicon wafers, polished on one side. A 0.3-μm molybdenum thin film is deposited on the substrate as the bottom electrode. Following the deposition of the bottom electrode, an 0.8-μm AlN layer is deposited in the RF sputtering system. A 0.3-μm molybdenum thin film is then deposited and patterned as the top electrode. The active area of the device is an irregular polygon of about 3×10^4 μm^2.

In Fig. 7, the measured real part of the input impedance of the two HBAR devices are plotted in light gray. The data after performing the averaging function are shown in darker gray in the same figures. From the maximum

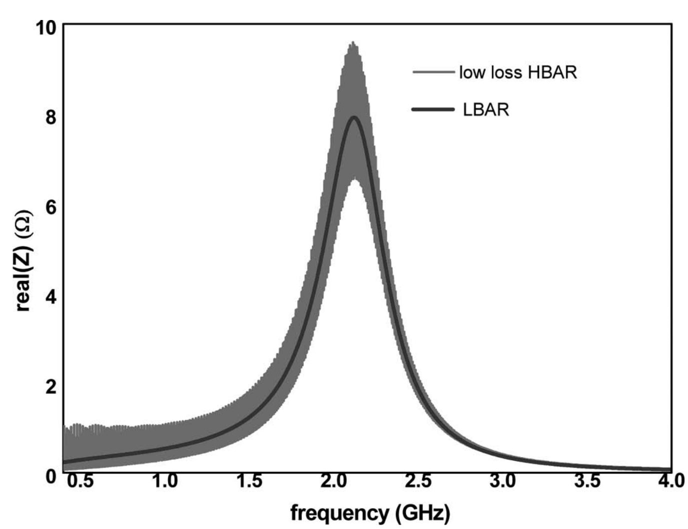


Fig. 6. Real part of the input impedance of the low-loss high-tone bulk acoustic resonator (HBAR) and the lossy bulk acoustic resonator (LBAR).

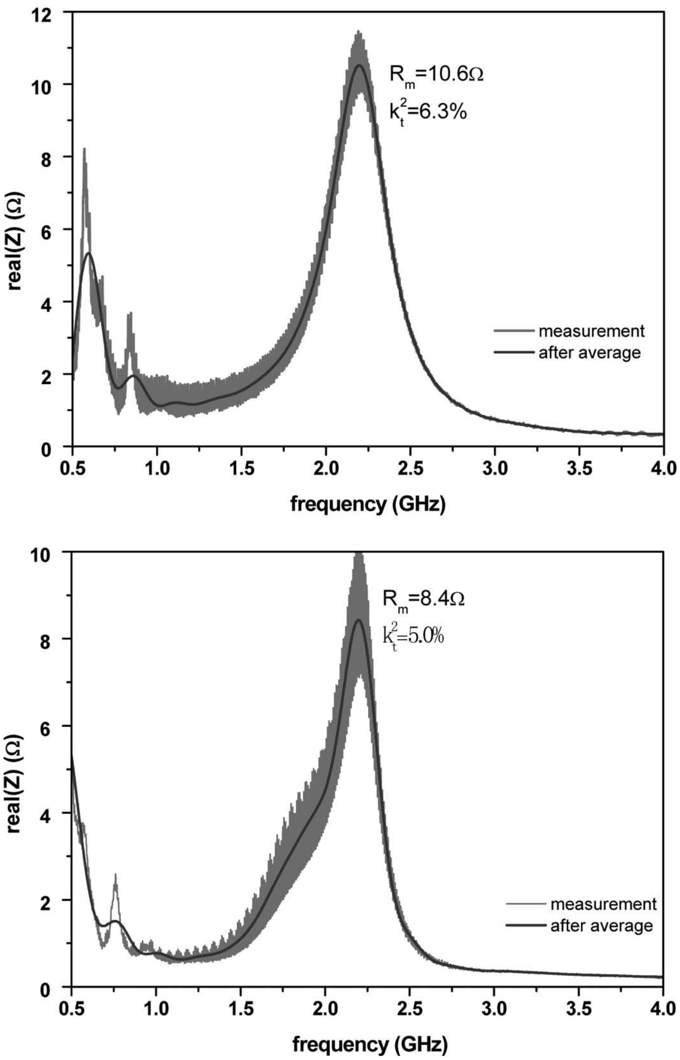


Fig. 7. The measured real part of the input impedance of the two high-tone bulk acoustic resonator (HBAR) devices employing the AlN piezoelectric films prepared in a sputter system with known (top) good and (bottom) bad deposition conditions.

resistance R_{m} and the relation between R_{m} and K_t^2 as described in Fig. 4, the electromechanical coupling constants K_t^2 of the two AlN films are extracted as 6.3% and 5.0%.

IV. Conclusion

A very simple method to extract K_t^2 of thin-film piezoelectric material was developed in this paper. In the new method, K_t^2 can be directly extracted by measuring the input impedance of an HBAR. The theory behind the method was presented and experiments were performed to validate the theory. This study provides a new tool to evaluate the quality of a grown piezoelectric film.

References

[1] K. M. Lakin, K. T. McCarron, J. Belsick, and J. F. McDonald, “Thin film bulk acoustic wave filters technology,” in *Proc. IEEE Radio and Wireless Conf.*, 2001, pp. 89–92.

[2] R. Ruby, “Review and comparison of bulk acoustic wave FBAR, SMR technology,” in *Proc. IEEE Ultrasonics Symp.*, 2007, pp. 1029–1039.

[3] K. M. Lakin, J. Belsick, J. F. McDonald, and K. T. McCarron, “Improved bulk wave resonator coupling coefficient for wide bandwidth filters,” in *Proc. IEEE Ultrasonics Symp.*, 2001, pp. 827–831.

[4] R. Aigner, “Bringing BAW technology into volume production: The ten commandments and the seven deadly sins,” in *Proc. 3rd Int. Symp. Acoustic Wave Devices for Future Mobile Communication Systems*, 2007, pp. 85–91.

[5] T. Kamohara, M. Akiyama, N. Ueno, K. Nonaka, and H. Tateyama, “Growth of highly c-axis-oriented aluminum nitride thin films on molybdenum electrodes using aluminum nitride interlayers,” *J. Cryst. Growth*, vol. 275, no. 3–4, pp. 383–388, 2005.

[6] R. S. Naik, J. J. Lutsky, R. Reif, and C. G. Sodini, “Electromechanical coupling constant extraction of thin-film piezoelectric materials using a bulk acoustic wave resonator,” *IEEE Trans. Ultrason. Ferroelectr. Freq. Control*, vol. 45, no. 1, pp. 257–263, 1998.

[7] H. Zhang, W. Pang, H. Yu, and E.S. Kim, “High-tone bulk acoustic resonators on sapphire, crystal quartz, fused silica and silicon substrates,” *J. Appl. Phys.*, vol. 99, no. 12, art. no. 124911, 2006.

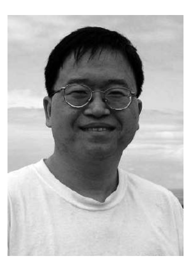
[8] Y. Zhang, Z. Wang, and J. D. N. Cheeke, “Resonant spectrum method to characterize piezoelectric films in composite resonators,” *IEEE Trans. Ultrason. Ferroelectr. Freq. Control*, vol. 50, no. 3, pp. 321–333, 2003.

[9] J. F. Rosenbaum, *Bulk Acoustic Wave Theory and Devices.* Boston, MA: Artech House, 1988.

Chong Zhou was born in Hubei, China, on August 15, 1988. He obtained the B.S. degree from Tianjin University, Tianjin, China, in 2010. He is now a graduate student there, pursuing his M.S. degree in electrical engineering. His research interests include bulk acoustic wave device modeling and characterization, FBAR duplexer and oscillator design, and RF and microwave circuit design, calibration, and measurement.

Wei Pang received the B.S. degree from Tsinghua University, Beijing, China in 2001, and the Ph.D. degree in electrical engineering from the University of Southern California, Los Angeles, CA, in 2006. He worked in the wireless semiconductor division of Avago Technologies, Fort Collins, CO. He is currently a Professor in the College of Precision Instrument and Optoelectronics Engineering, Tianjin University, China. He has published 50 refereed papers in the areas of MEMS for RF wireless communications, biological detection, wireless sensor platforms, and medical ultrasound. He is an author of two issued and 10 pending U.S. patents.

Photographs and biographies were not available for **Qiang Li**, **Hongyu Yu**, and **Xiaotang Hu** at time of publication.



Hao Zhang received the M.S. degree in physics and Ph.D. degree in electrical engineering from the University of Southern California, Los Angeles, in 2002 and 2006, respectively. He is currently a Professor in the College of Precision Instrument and Optoelectronics Engineering, Tianjin University, China. His research interests are in the fields of RF/microwave MEMS, MEMS sensors, microfluidics, and biochips.