Characteristics of Dual Mode AlN Thin Film Bulk Acoustic Wave Resonators

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***Abstract*—Thin film bulk acoustic wave resonators (FBAR) using piezoelectric AlN thin films have attracted extensive research activities in the past few years. Highly c-axis oriented AlN thin films are particularly investigated for resonators operating at the fundamental thickness longitudinal mode. Depending on the processing conditions, tilted polarization (c-axis off the normal direction to the substrate surface) is often found for the as-deposited AlN thin films, which may leads to the coexistence of thickness longitudinal mode and shear mode for the thin film resonators. Knowing that the material properties are strongly crystalline orientation dependent for AlN thin films, a theoretical study is conducted to reveal the effect of tilted polarization on the frequency characteristics of thin film resonators. The input electric impedance of a thin film resonator is derived that includes both thickness longitudinal and thickness shear modes in a uniform equation. Based on the theoretical model, the effective material properties corresponding to the longitudinal and shear modes are calculated through the properties transformation between the original and new coordinate systems. The electric impedance spectra of dual mode AlN thin film resonators are calculated using appropriate materials properties and compared with experimental results. The results indicate that the frequency characteristics of thin film resonators vary with the tilted polarization angles. The coexistence of thickness longitudinal and shear modes in the thin film resonators may provide some flexibility in the design and fabrication of the FBAR devices.**

Keywords - AlN thin film, FBAR, dual mode resonator

INTRODUCTION

The need for better filters and signal conditioning is continuously changing to address a wide range of applications including controls, signal processing, RF and microwave communications, navigation and many others. It has been known for quite some time that bulk acoustic wave (BAW) and surface acoustic wave (SAW) devices, which couple the mechanical resonances to the electrical signals being conditioned by electromechanical transduction mechanism through the use of piezoelectric materials, have very desirable characteristics for filtering applications. The currently used surface acoustic wave (SAW) and bulk acoustic wave (BAW) resonators or filters are in general off-chip devices with considerably large sizes. For mobile communication applications in the GHz range, small sized bandpass filters with low insertion loss and good out of band rejection are required. More recently, with the strong progress in thin film technologies for complex materials systems such as PZT, ZnO and AlN, thin film bulk acoustic wave (FBAR) resonator and filter concepts are gaining more and more importance for microwave frequency control applications [1-17]. In bulk acoustic wave (BAW) resonator, an acoustic wave is excited electrically in a piezoelectric layer. Hereby the fundamental thickness vibration mode is employed. For resonators operating in the GHz range, thin film piezoelectric layer on the order of one micron in thickness with desirable electromechanical properties (high Q and desirable bandwidth) are required. Among these materials, AlN is very attractive due to its interesting properties such as high thermal conductivity, high electrical insulation, and chemical stability. In addition, it has a large band gap of 6.2 eV and high acoustic velocity, 10400 m/s; and it is piezoelectric in its crystalline form. These characteristics make it possible to design and fabricate high frequency resonators and bandpass filters for signal processing and communication devices. On the other hand, ZnO and PZT thin films, with large electromechanical coupling coefficients, are attractive for filters with wider bandwidth. If thin film bulk acoustic resonator devices of sufficient performance can be fabricated, they will be the best choice to replace the current crystal, ceramic or SAW devices due to their compactness and good compatibility with the high frequency Si or GaAs integrated circuit processing. In fact, Agilent International Inc. has commercialized AlN FBAR duplexers for applications in some telecommunication systems [18].

The BAW devices are also be used in many other fields such as used as sensors for physical, chemical and biological applications. However, the performance capability of the BAW resonator using thickness longitudinal wave mode will be adversely affected when the resonator is used in the liquid environment such as in biosensing or viscosity measurement application, because the liquid will absorb most of the acoustic

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energy at the resonator/liquid interface. For this reason, thickness shear mode (TSM) resonators are gaining more and more research interest due to their highly efficient performance in the liquid environment. Conventionally, thickness shear mode BAW devices have been made of AT- or BT-cut quartz crystal plates that are with relatively low fundamental resonant frequency, typically of 5, 10 or 25MHz. If thickness shear mode piezoelectric thin films could be deposited or grown, high frequency thin film shear mode BAW resonators and transducers would be fabricated, expectedly provides higher sensitivity in sensory applications in liquid phases.

Recently, high frequency shear mode BAW resonators using ZnO and AlN piezoelectric thin films have been investigated by several research groups [19-21]. Piezoelectric ZnO thin films with c-axis parallel to the substrate plane have been successfully deposited on the glass substrate [19, 20]. The ZnO film/glass composite shear mode resonators can be excited and high resonance frequencies have been achieved. Also, the ZnO solidly mounted bulk acoustic wave resonators operating in the shear mode was fabricated by Link et al. [21]. The operating ZnO thin film has a tilt angle which enables the resonator can be excited in the shear mode. Wittstruck et al. [22] reported the fabrication of the $Mg_xZn_{1-x}O$ thin film bulk acoustic wave (BAW) resonator with c-axis of the $Mg_xZn_{1-x}O$ film long the plane surface in the BAW structure, which can, thus an acoustic shear wave mode can be excited, providing potential application for the thickness shear mode sensing. The resonance frequency and coupling coefficient can be varied by controlling the mole percentage of the Mg composition in the $Mg_xZn_{1-x}O$ thin film. In the case of AlN thin films, tilted polarization has been realized by using a modified sputtering method [23, 24]. Both thickness longitudinal and thickness shear modes are obtained in a single SMR BAW resonator. Bjurström et al. [25-28] studied the variation of the electromechanical coupling and the quality factor of the AlN BAW resonators, for both the longitudinal and shear modes, as a function of the tilt degree of film texture. A dual mode device with a micro-fluidic transport system was fabricated to investigate the device performance in the water medium.

In this paper, we present the theoretical simulation results for the longitudinal-shear dual mode BAW resonator. The input electric impedance spectrum of the device will be obtained by extending the Mason model considering the coexistence of the two modes [29]. In the simulation, the tilt angle of the piezoelectric AlN thin film varies from 0 to 90 degree with respect to the normal direction of the substrate. The material properties crystalline orientation dependence of the AlN thin film is considered in the simulation.

THEORY

A. Transformation of the material properties

For the characterization of bulk acoustic wave resonator, it is important to identify the piezoelectric, dielectric and mechanical properties of the piezoelectric layer. Considering a piezoelectric thin film BAW resonator, the material properties tensors related to longitudinal and shear wave mode are crystalline orientation dependent. We consider the material properties directly related to the longitudinal and shear modes as the effective material properties while the thin film have a tilted polarization. The effective material properties can be obtained by transferring the materials properties in the c-axis crystalline direction to the normal or in-plane direction of the substrate, which corresponds to a rotation of the coordinate system. Here we need to derive the relations of dielectric constant ε, piezoelectric coefficient d, and elastic stiffness c between two different orientations.

The transformation of dielectric, piezoelectric, and elastic constants to a new coordinate system can be derived by applying the transformation rules of the second, third, and forth tenors respectively. Assuming $\{e_i\}$ and $\{e_i'\}$ are the original and new coordinate systems, respectively. We can have

$$\varepsilon' = A\varepsilon A^t \quad (1)$$

$$d' = AdN^t \quad (2)$$

$$c' = McM^t \quad (3)$$

where ε', d', c' are the properties in new axis system, and the transformation matrix is

$$\boldsymbol{A} = \begin{bmatrix} \boldsymbol{a}_{11} & \boldsymbol{a}_{12} & \boldsymbol{a}_{13} \\ \boldsymbol{a}_{21} & \boldsymbol{a}_{22} & \boldsymbol{a}_{23} \\ \boldsymbol{a}_{31} & \boldsymbol{a}_{32} & \boldsymbol{a}_{33} \end{bmatrix} \quad (4)$$

and

$$M = \begin{bmatrix} a_{11}^2 & a_{12}^2 & a_{13}^2 & 2a_{12}a_{13} & 2a_{11}a_{13} & 2a_{11}a_{12} \\ a_{21}^2 & a_{22}^2 & a_{23}^2 & 2a_{22}a_{23} & 2a_{21}a_{23} & 2a_{21}a_{22} \\ a_{31}^2 & a_{32}^2 & a_{33}^2 & 2a_{32}a_{33} & 2a_{31}a_{33} & 2a_{31}a_{32} \\ a_{21}a_{31} & a_{22}a_{32} & a_{23}a_{33} & a_{22}a_{33}+a_{23}a_{32} & a_{21}a_{33}+a_{23}a_{31} & a_{21}a_{32}+a_{22}a_{31} \\ a_{11}a_{31} & a_{12}a_{32} & a_{13}a_{33} & a_{12}a_{33}+a_{13}a_{32} & a_{11}a_{33}+a_{13}a_{31} & a_{11}a_{32}+a_{12}a_{31} \\ a_{11}a_{21} & a_{12}a_{22} & a_{13}a_{23} & a_{12}a_{23}+a_{13}a_{22} & a_{11}a_{23}+a_{13}a_{21} & a_{11}a_{22}+a_{12}a_{21} \end{bmatrix} \quad (5)$$

In equations (4) and (5), $a_{ij} = e_j . e_i$. And the matrix N in the equation (2) can be determined by

$$\boldsymbol{N}^t = \boldsymbol{M}^{-1} \quad (6)$$

From equations (1) to (3), we can get the effective material properties related to the longitudinal and shear wave mode. In the calculation, we need to use the elastic compliance which is the inverse of elastic stiffness.

$$[\boldsymbol{s}_{ij}] = [\boldsymbol{c}_{ij}]^{-1} \quad (7)$$

B. Electric impedance

Fig. 1 shows the schematic structure for the single layer piezoelectric resonator. For the single layer bulk acoustic wave resonator, the electric field is applied along the thickness direction; and for simplicity, the thicknesses of the top and bottom electrodes are ignored. The polarization direction or the crystalline c-axis direction has a tilted angle θ with respect to normal direction of the top or bottom electrode plane. For the longitudinal mode, the constitutive equations were derived with coordinate system $\{x_i\}$ where the axis x_3 is normal to the electrode plane. On the other hand, coordinate system $\{x_i'\}$ is

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used in the shear wave mode where axis x_3' is parallel to the electrode plane.

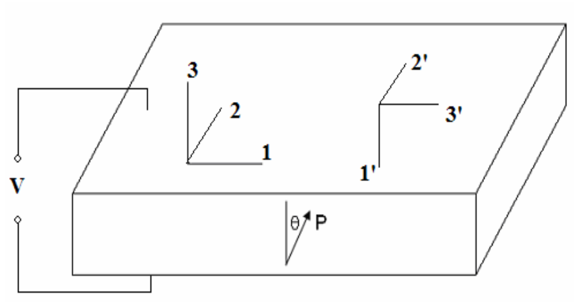

Figure 1. Structure of single layer bulk acoustic wave resonator

For the thickness longitudinal vibration mode, we have

$$\boldsymbol{T_3} = \boldsymbol{c_{33}^D} \cdot \boldsymbol{S_3} - \boldsymbol{h_{33}} \cdot \boldsymbol{D_3} \tag{8}$$

$$\boldsymbol{E_3} = -\boldsymbol{h_{33}} \cdot \boldsymbol{S_3} + \beta_{33}^S \cdot \boldsymbol{D_3} \tag{9}$$

where T is the mechanical stress, S is the mechanical strain, E is the electric filed, D is the electric displacement, c is the elastic stiffness constant, h is the piezoelectric constant, $\beta = \mathbf{1}/\varepsilon$ is the inverse of dielectric constant.

Similarly, for thickness shear vibration mode,

$$T_5' = c_{55}^{D'} \cdot S_5' - h_{15}' \cdot D_1' \tag{10}$$

$$E_1' = -h_{15}' \cdot S_5' + \beta_{11}^{S'} \cdot D_1' \tag{11}$$

For the resonator shown in Fig. 1, the electric voltage can be obtain by the equations (8) to (11)

$$\begin{aligned} V &= \int_0^t E \cdot dz \\ &= \int_0^t (-h_{33} \cdot S_3 - h_{15}' \cdot S_5' + D_3 / \varepsilon_{33}^S) \cdot dz \\ &= \frac{I}{j\omega C_0} + \frac{v_1 + v_2}{j\omega} \cdot h_{33} + \frac{v_1' + v_2'}{j\omega} \cdot h_{15}' \end{aligned} \tag{12}$$

where v_1 and v_2 are the "acoustic" currents or acoustic velocities of the top and bottom surface plane of the resonator corresponding to the longitudinal mode respectively, $\omega = 2\pi f$ is the angular frequency, I is the electric current. $\boldsymbol{C_0} = \varepsilon^s \boldsymbol{S}/\boldsymbol{t}$ is the clamped capacitor of the resonator with effective area S and piezoelectric film thickness t, where ε^s is the dielectric constant of piezoelectric materials under constant strain condition. Also from Mason model, we have

$$F_1 = jZ_0 v_1 \tan(\frac{kt}{2}) - \frac{jZ_0}{\sin(kt)}(v_1 + v_2) + \frac{h_{33}}{j\omega} \cdot I \tag{13}$$

$$F_2 = jZ_0 v_2 \tan(\frac{kt}{2}) - \frac{jZ_0}{\sin(kt)}(v_1 + v_2) + \frac{h_{33}}{j\omega} \cdot I \tag{14}$$

where F_1 and F_2 are the forces on the top and bottom surface of the resonator respectively, I is the electric current, $k = \omega / v$ is the wave number. $Z_0 = S\rho v$ is the acoustic impedance of the piezoelectric layer with mass density ρ. Piezoelectric constant h can be derived by $h = e/\varepsilon^S$ where e is the piezoelectric stress constant. Similarly, for the shear mode, we have

$$F_1' = jZ_0' v_1' \tan(\frac{k't}{2}) - \frac{jZ_0'}{\sin(k't)}(v_1' + v_2') + \frac{h_{15}}{j\omega} \cdot I \tag{15}$$

$$F_2' = jZ_0' v_2' \tan(\frac{k't}{2}) - \frac{jZ_0'}{\sin(k't)}(v_1' + v_2') + \frac{h_{15}}{j\omega} \cdot I \tag{16}$$

Assume that the top and bottom surfaces are exposed to air, thus they can be treated under a mechanical free boundary condition; i.e., $F_1 = F_2 = F_1' = F_2' = 0$. From equations (12)-(16), the input electric impedance of the piezoelectric resonator can be obtained as

$$Z_{in} = \frac{V}{I} = \frac{1}{j\omega C_0}(1 - k_{33}^2 \frac{\tan(kt/2)}{kt/2} - k_{15}^2 \frac{\tan(k't/2)}{k't/2}) \tag{17}$$

where $k_{15}^2 = \frac{h_{15}'^2}{\beta_{11}^{S'} c_{55}^{D'}}$ and $k_{33}^2 = \frac{d_{33}^2}{\varepsilon_{33}^S s_{33}^D}$ are the electromechanical coupling coefficient for the shear mode and longitudinal mode respectively. It should be point out that the acoustic velocities for the longitudinal mode and shear mode are $v_{33} = \sqrt{\frac{c_{33}^D}{\rho}}$ and $v_{15}' = \sqrt{\frac{c_{55}^{D'}}{\rho}}$ respectively. From equation (17), we can calculate the input electric impedance spectrum as the function of the frequency and therefore the resonance frequencies, quality factors and electromechanical coupling coefficients can be obtained with the spectrum.

In this paper, the electric impedance spectrum of piezoelectric AlN thin film resonator is calculated to demonstrate the resonance frequency crystalline orientation dependence. Tables 1 and 2 list the material properties of AlN thin film used in the calculation [30, 31]. The thickness of the piezoelectric thin films is assumed to be 5 microns. It should be noted that in the calculation, a small imaginary part is added to the acoustic velocity to avoid singularity. Also, the mechanical Q factor of the AlN thin film can be approximately given by [32]

$$Q \approx \frac{1}{2} \cdot \frac{v'}{v''} \tag{18}$$

where $\boldsymbol{v}'$ and $\boldsymbol{v}''$ are the real and imaginary parts of the acoustic velocity of the thin film. The piezoelectric strain coefficient d can be derived by

$$[\boldsymbol{d}] = [\boldsymbol{e}][\boldsymbol{S}] \tag{19}$$

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Table 1. Material properties of AlN thin film used for calculating the coupling coefficients

Elastic stiffness constants (GPa)						Dielectric constant (10^{-11}F/m)		Density (kg/m^3)
c_{11}	c_{12}	c_{13}	c_{33}	c_{44}	c_{66}	ε_{11}	ε_{13}	ρ
410	140	100	390	120	135	8.0	9.0	330

Table 2. Piezoelectric properties of AlN thin film and device parameters used in the simulation

Piezoelectric constants (C/m^2)			Thickness	Area
e_{31}	e_{33}	e_{15}	(μm)	(m^2)
-0.58	1.55	-0.48	5	9×10^{-8}

RESULTS AND DISCUSSIONS

For a single layer BAW resonator, the resonance frequencies of the longitudinal and shear wave modes are dependent on the elastic stiffness properties and the film thickness. Since the effective elastic stiffness constants are different for the films with different crystalline tilted angle θ, the resonance frequencies of the resonators for a specific thin film thickness are different.

Fig. 2 shows the effective elastic stiffness constants c_{33} and c'_{55} as the functions of the tilted angle θ. Here the angle θ can also be treated as the rotation angle between the original and the new coordinate systems in the simulation. It can be seen that the values of the effective c_{33} and c'_{55} change with rotation angle, which makes the resonance frequencies of the longitudinal and shear modes dependent on the polarization orientation of the piezoelectric film. Besides the elastic constants, the dielectric constants and the piezoelectric coefficient are also crystalline orientation dependent.

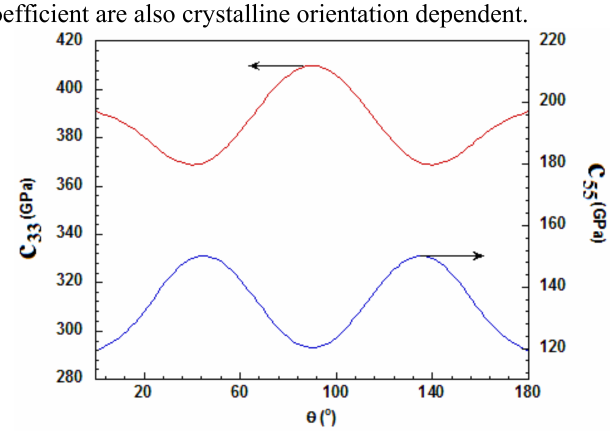

Figure 2. The elastic stiffness constants crystalline orientation dependence

From equation (17), we can calculate the input electric impedance spectra of BAW resonators with different tilted polarization angles. To our knowledge, no mechanical quality factor data have been reported in the literature for AlN shear mode FBARs. Thus the mechanical Q, which are assumed to have the value 200, are used in the simulation for the impedance spectra in this study. The mechanical quality factor data for the longitudinal mode have been reported in many AlN FBAR studies, usually in the range of 60 to 400, depending on the AlN thin film deposition processing and FBAR fabrication processing steps. Here longitudinal mode Q factor is also assumed to be 200 in the simulation. Fig. 3. to Fig. 9. are the electric impedance spectra of the single layer AlN BAW resonators with different tilted polarization angles, which vary from 0 degree to 90 degree with the increment of 15 degree. The figures show that the resonance frequencies of the longitudinal mode and shear mode are around 1.1 GHz and 0.6 GHz respectively. When the tilted angle is 0 degree, which means the *c*-axis of the AlN thin film is normal to the electrode plane, only the thickness longitudinal exists. On the other hand, when the angle is 90 degree, the thickness shear mode dominates the operation of the resonator. Interestingly, for the thickness longitudinal mode, the resonance peak decreases with the titled polarization angle from 0 degree to 45 degree. At 45 degree the peak becomes almost invisible, while the thickness shear mode dominates the resonance spectrum. The resonance frequencies for a specific mode vary with the change of the tilted polarization angles, which induces the variation of the material elastic properties as we discussed before. Since the piezoelectric coefficients, elastic constants and the dielectric constants are all crystalline orientation dependent, the electromechanical coupling coefficients k_{33} and k_{15} will also be dependent on the crystalline orientation. Thus, resonance peaks of the impedance spectra will also be different with the change of the tilted polarization angle.

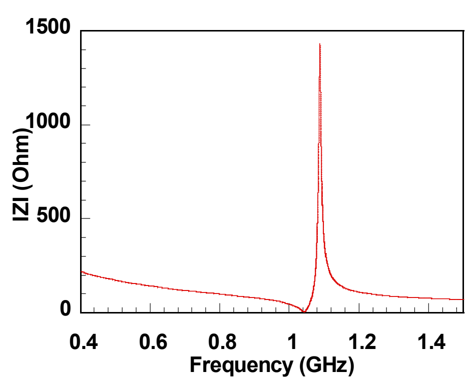

Figure 3. Input electric impedance of the dual mode resonator; θ=0

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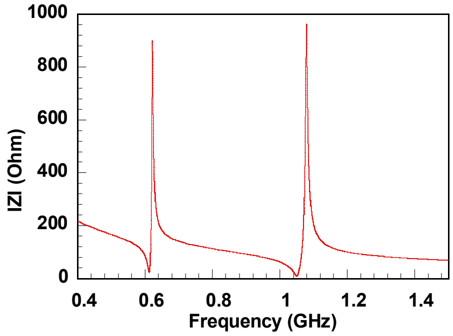

Figure 4. Input electric impedance of the dual mode resonator; θ=15°

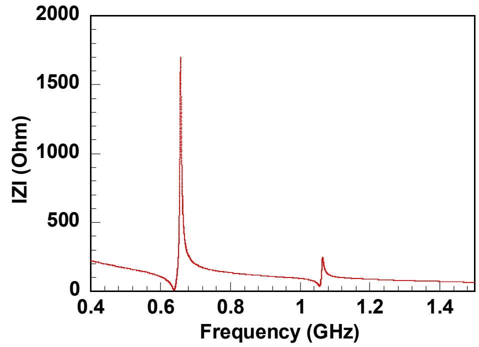

Figure 5. Input electric impedance of the dual mode resonator; θ=30°

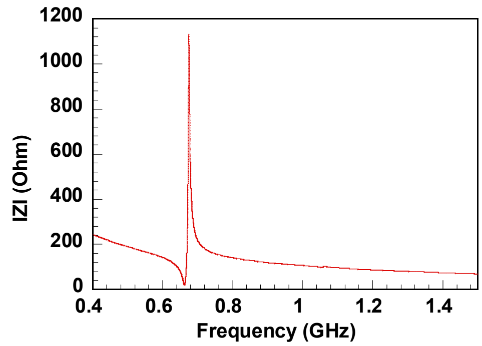

Figure 6. Input electric impedance of the dual mode resonator; θ=45°

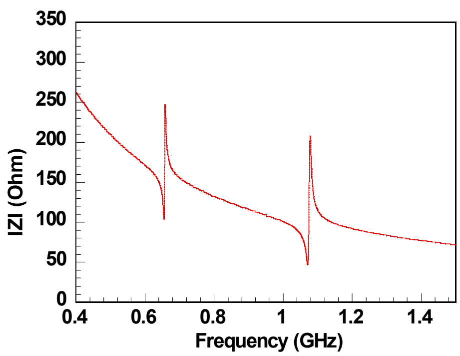

Figure 7. Input electric impedance of the dual mode resonator; θ=60°

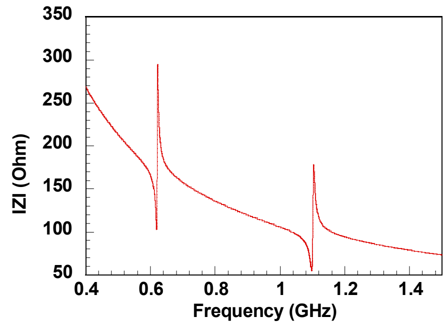

Figure 8. Input electric impedance of the dual mode resonator; θ=75°

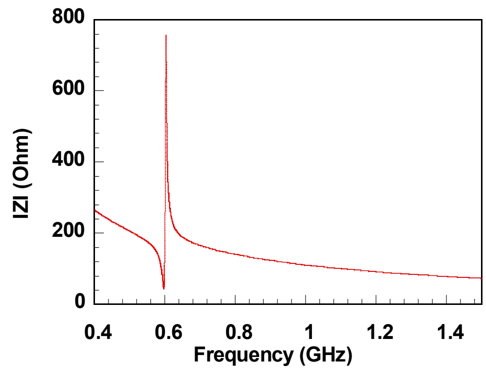

Figure 9. Input electric impedance of the dual mode resonator; θ=90°

The simulation results show that the shear and longitudinal wave modes can coexist in the resonator operation for certain frequency ranges. It provides more flexibility in choosing a specific mode for different applications for the BAW resonators. For instance, one can pick a thickness shear mode with specific resonance frequency for sensing applications in the liquid medium.

CONCLUSIONS

The AlN piezoelectric thin film deposited by DC reactive sputtering is often found to have a tilted polarization angle with respect to the substrate normal direction, which lead to the coexistence of the thickness longitudinal and thickness shear modes for the AlN FBARs. The AlN material properties including the piezoelectric coefficients, elastic constants and dielectric constants used in the simulation of the electric impedance are all crystalline orientation dependence. The effective material properties used in the dual-mode resonator simulation can be obtained by transferring the properties in the c-axis orientation to the normal or in-plane direction of the substrate, which corresponds to a rotation of the coordinate system. The crystalline orientation dependence of material properties makes the resonance frequencies and other characteristics of the BAW resonator dependent on tilted polarization angles. By extending the Mason model, the input electric impedance of the single layer dual-mode BAW resonator is derived. The impedance spectra of the AlN piezoelectric thin film resonators with tilted polarization angles have been simulated. The simulation results clearly

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reveal the crystalline orientation and materials property dependence of the thickness longitudinal and thickness shear resonance modes of the AlN FBARs. The coexistence of the dual modes may provide more flexibility in resonator design, fabrication and device applications.

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