EXPERIMENTAL STUDY OF ALUMINIUM NITRIDE THIN FILM MICROWAVE BULK ACOUSTIC WAVE RESONATORS, ACOUSTICALLY ISOLATED FROM SUBSTRATE

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1. ABSTRACT

The interest to the thin film microwave bulk acoustic wave resonators acoustically isolated from substrate is stimulated by modern trends in the development of communication systems such as the handling the more high frequencies achievement of higher reliability, improving of electrical parameters and miniaturization. Thin film resonators (TFR) well fit to these requirements.

This report is devoted to the systematic study of TFR's made of AlN piezoelectric films with metal electrodes acoustically isolated from the substrate by a set of quarter wavelength layers made of SiO_2 and W having a big contrast in their acoustic impedances. Such sets of layers deposited onto rather thick well polished silicon substrate are working like a Bragg mirror effectively reflecting acoustic waves.

Various resonator configurations were studied. Half-wavelength and quarter wavelength in thickness TFR's were investigated with the Bragg structures designed as the reflectors providing zero and pi phase shift correspondingly. The dependence of the resonator properties on the number of layers in the mirror (5, 6, 7, 9) was investigated near the resonant frequencies 1.7, 2.3, and 5.4, 5.5 GHz. A good agreement between experimental and calculated data was obtained when experimentally found values of K^2 and directly measured thickness of the layers (by SEM) composing the structure had been used. It was found that the best agreement between data was regularly achieved for smaller (than table data) values of sound velocity in AlN films and higher values of the attenuation coefficients for layers. It means that in the case of a small thickness of the AlN and other films their mechanical properties may differ from the data for bulk material.

2. SAMPLES AND EXPERIMENTAL PROCEDURE

Polycrystalline aluminum nitride thin films were deposited with reactive radio frequency magnetron sputtering. The target was a 508 mm diameter 99.9999% Al disk. The system was pumped down to a base pressure smaller than 2×10^{-7} Torr before admitting the gas in. The films were grown at in 1 mTorr N2 and with a power of 300 W applied to the target. Well *c*-axis oriented films with a columnar microstructure were obtained. The vertically cut side surface observed under a scanning electron microscope exhibits a high density of crystallite in regular columnar structure.

We used the x-ray diffraction method to study the structure of the AlN films. There existed only one diffraction peak corresponding to the crystal plane (002) occurring at 2θ=36.09°. The peaks and their sharpness indicate that the *c*-axis of the AlN crystallites is perpendicular to the AlN–Al_2O_3 interface and that the (002) plane is parallel to it. The FWHM of 2.53° in the rocking curve represent the well-aligned columnar structure normal to the substrate. The estimated average size of the crystallites was 470Å.

Resonator structures were composed by AlN thin film with top and bottom metal thin film electrodes being deposited over Bragg-type multylayer structure fabricated on the polished sides (100)-silicon wafer substrates. Thin films of W were chosen as a high acoustic impedance material and that of SiO_2 - as a low acoustic impedance material for the Bragg reflector, respectively.

To make Bragg reflector layers, W and SiO_2 of quarter wavelength thickness were in situ deposited on the Si substrate by rf magnetron sputtering. AlN and Al were deposited on the Bragg reflector layers by rf magnetron sputtering. We fabricated nine layers Bragg reflector of W-SiO_2 pairs using r.f. sputtering method and fabricated AlN piezoelectric and Al electrodes using pulsed dc sputtering. SiO_2 and W or ZnO layers were *in-situ* deposited on Si(100) substrate by rf sputtering. Al electrodes and AlN piezoelectric layer were *in-situ* deposited at room temperature by asymmetric bipolar pulsed dc reactive sputtering. The film thickness and microstructure were observed using a field emission scanning electron microscope.

For the measurement of the electromagnetic wave reflection coefficient S_{11}, the HP8753D network analyzer was used. The connection between the network analyzer and the samples under investigation was performed using special microwave probes that could operate up to 40 GHz in matched regime. Using the obtained S_{11} data, all other parameters of the structure such as the magnitude of electric impedance and the phase of electric impedance were calculated. These data was used for acoustic characterization of thin films and the resonators.

3. EXPERIMENTAL RESULTS

Initially two series of results were analysed. The first one was experimental data of the study of a thin-film resonator made of Al-AlN-Al with 5 and 6-layer Bragg reflector composed of SiO_2 and W layers. The composition of the resonators with 6 layers was:

Al – AlN – Al / SiO_2 – W – SiO_2 – W- SiO_2 – W / Si

The results of experiment with one of the resonators are presented in Fig.1. In this example the Bragg structure was designed for the frequency 2.4 GHz. So, the thicknesses of all the layers composing the structure were equal to quarter wavelength. For perfect resonator operation the thickness of the AlN film must also correspond to 2.4 GHz. But the thickness of the resonator AlN film was equal to 2.95 μm corresponding

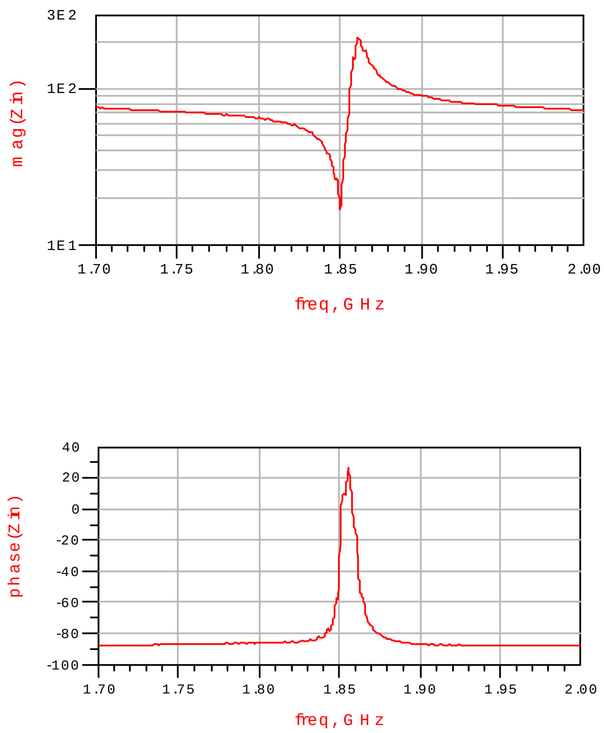

Fig.1 Example of the magnitude and phase frequency dependences of the structure with Bragg reflector, the area of the upper electrode is 200X200 μm^2.

to a half-wave length on the frequency 1.95 GHz. Nevertheless a rather strong resonance peaks have been observed. This fact is confirming experimentally the fact that the Bragg reflector is a wideband structure.

In order to understand and evaluate the observed results the numerical modeling was made using the expressions from [1] for input electric impedance of a piezoelectric layer loaded by upper and lower electrodes. The expression for transformation of acoustic impedance was repeatedly used in order to take into account Bragg mirror placed between lower electrode and the substrate. The attenuation in the layers and in substrate was taken into account using complex wave vectors for acoustic wave propagation. In simulations almost exact coincidence in resonant frequencies of the experimental and calculated data was obtained. But for best fit in these and subsequent data a slight decrease in the value of sound velocity (some few percents) required. It means that the elastic properties of the thin AlN film are not perfect and probably non uniform along the thickness. It was found for the resonators with different size of the upper electrode (150X150 μm^2, 200X200 μm^2, 400X400 μm^2) the decrease in the magnitude of impedance with the increase of the electrode area and it was in agreement with the numerical calculations.

The comparison of the data for the resonators of different types showed that there was no great difference in the results because of improper operation of the Bragg reflector.

The next two series of the results were obtained for the Al-AlN TFR structures with Bragg reflector layers with reversed order of the sequence. The structures under study were: Al – AlN /W– SiO_2 – W – SiO_2 – W – SiO_2 / Si and Al – AlN / W – SiO_2 – W – SiO_2 – W / Si

These structures were the λ/4 resonators. New point is that last tungsten layer simultaneously plays the role of the bottom electrode. The resonant frequency of the AlN layer almost correspond to the resonant frequency of the Bragg reflector. The structures worked much better than the structure discussed before. The rather smooth curves in all the cases are seen. The possible reason for it is the substitution of Al as bottom electrode by W. This material, and it is well known, provides a much better and perfect adhesion.

The measurements of the difference Δf between the frequencies of the resonance and anti resonance let us to evaluate electromechanical constants. In accordance with BVD model iet can be found as:

$$K_t^2 = \frac{\pi}{2} \cdot \frac{f_s}{f_p} \cdot \tan\left(\frac{\pi}{2} \cdot \frac{f_p - f_s}{f_p}\right) \qquad (1)$$

The estimations show that the measured value of k^2 is significantly smaller (sometimes more than 2 times) than table values for crystalls (6.4%). The possible explanation of this fact is the penetration of the metal from the electrodes (more probably upper Al) to AlN film.

Another set of experimental data is presented below for more carefully designed resonators. These resonators and Bragg reflector structures were formed correspondingly by the next sequence of layers:

Al(0.05)-AlN(1.12)/W(0.43)-SiO_2(0.67)-W(0.43)-SiO_2(0.67)-W(0.43)/Si(500);

Al(0.05)-AlN(1.12)/W(0.43)-SiO_2(0.67)-W(0.43)-SiO_2(0.67)-W(0.43)- SiO_2(0.67)/Si(500);

The thickness of the layers is shown in brackets in μm. In these resonators the tungsten layer under AlN film also played the role of the bottom electrode.

It was possible to achieve such a very good fitting of the data between experimental data and the results of calculation if the parameters of AlN and other layers parameters were slightly changed with respect to the table values. It seems to be reasonable – thin film material parameters may differ from the table bulk material data. In the process of the fitting the values of K^2 were found directly from the difference in the positions of resonance and anti-resonance peaks in frequency domain. To fit the value of the measured frequency of the resonance the velocity of sound in AlN was taken less (equal to 10.375 km/sec instead of table value 11.007km/sec).

The width of resonance peaks and the quality factor depend on the attenuation constants in the layers composing the structure and energy escaped into the substrate. To find the role of the attenuation in different layers the calculated values of the quality factor when the losses in various layers and various groups of layers were taken into account are listed in the Table 1 (lines 1-3 for five-layer structure, 4,5 for six-layer structure).

The first line corresponds to resonator in which all the losses in the structure except the substrate are neglected. All the energy losses are connected with the dissipation in the substrate. It means that five-layer Bragg reflector structure provides rather good acoustic isolation and high value of the quality factor can be

Table 1.

Si	SiO_2	Al	AlN	W	Q
7.2	0	0	0	0	6.2 10^4
7.2	0	0	27	0	780

7.2	44	13.65	27	5.14	303
7.2	44	13.65	27	5.14	290
7.2	0	0	0	0	>10^5

reached. In the second line the losses in AlN are involved in the consideration. Due to high losses in this film almost ten time decrease in quality factor is expected. The further decrease in quality factor is observed when acoustic losses in SiO_2 and W layers that are forming Bragg reflector structure are taken into account. The measured value of the quality factor for 6 layers in the Bragg structure appeared to be even slightly less than in case of five-layer Bragg reflector. It seems to be unexpected because the additional SiO_2 layer may provide mach better acoustic isolation of the resonator from the substrate (The calculated value of the quality factor exceeds 10^5 when only energy escape to the substrate is a source of the losses as it is shown in last line of the table. This value is higher than in ideal case for 5 layers when Q=6.2 10^4). The explanation of this fact can again be found if to take into account big additional losses in SiO_2 layer.

From the consideration of the data shown in the table one can conclude that for the achievement of high values of quality factor it is necessary to select low loss materials both for resonator layers themselves and for the materials used in Bragg reflector structures.

The data shown in line 1 in the table illustrates that even in case of the ideal resonator with the absence of the attenuation in its layers the quality factor due to relatively small numbers of layers in Bragg reflector is not high. They are explained by energy escape into substrate. The accounting of the losses in piezoelectric film strongly decreases Q, as it is shown in line 2 of the Table 1.

The next set of resonators with 7 layers Bragg reflector structures were formed correspondingly by the next sequence of layers:

Mo(0.21)-AlN(1.67)-Mo(0.21)/SiO_2 (0. 69)-W(0.56)-SiO_2 0.69) -W(0.56) -SiO_2 (0. 69)-W(0.56)-SiO_2(0.69)/Si(500);
Al(0.026)-AlN(2.76)-Al(0.026)/SiO_2 (0. 80)-W(0.50)-SiO_2 (0.80)-W(0.50) -SiO_2 (0. 80)-W(0.50)-SiO_2(0.80)/Si(500);

Both types of resonators were designed as λ/2 TFR structures and show a very prominent result. The TFR in first case was formed by relatively thin AlN film (its proper resonant frequency was 3.1GHz) and very thick electrodes made of molybdenum. The whole three layer system was resonating on 1.757GHz in a very good agreement with the classical dispersion equation for multilayer composite resonator structure:

$$qd + \frac{Z_{Mo}}{Z_{AlN}} \cdot \arctan \delta_1 t_1 + \frac{Z_{Mo}}{Z_{AlN}} \cdot \arctan \delta_2 t_2 = \pi \qquad (2)$$

Here q and d –are the wave vector and the thickness of the piezoelectric layer, δ_1, δ_2 t_1, t_2 –are correspondingly the wave vectors and thickness of electrode layers.

In spite of some discrepancy between necessary and real thickness of Bragg reflector layers (resonant frequency for SiO_2 is 1.6 GHz and for W is 2.32 GHz) all resonators has demonstrated very nice characteristics The best values of Q were: for the first structure Q_s= 463, Q_p= 383; for second structure Q_s= 488, Q_p=322. The variation of the aperture of the upper electrode results in the impedance change which in order of magnitude agrees with the theory. The whole set of experimenal dependences was fitted point to point if to increase the losses in AlN and in SiO_2.

In our experiments a big discrepancy between the frequencies in the Bragg reflector and TFR took place in the case of TFR structure Al-AlN-Al with 7 layers in the Bragg reflector. The frequency at which W layers provided λ/4 thickness was 2.58 GHz, for SiO_2 this frequency was 1.36 GHz. The resonator frequency 1.81 GHz, corresponded to λ/2 thickness of Al-AlN-Al structure (taking into account in calculations the thickness and sound velocities in Al electrodes). Nevertheless rather high values of Q_s= 488 has been achieved.

It is interesting to compare the results of direct measurements of K^2 for Mo-AlN-Mo and Al-AlN-Al resonators. The evaluation, using the previous standard formula, gave for Mo-AlN-Mo resonator the value 4.5%, and for Al-AlN-Al only 2.58%. But in fact for the thick Mo layers this expression is not valid. Rigorous taking into account of the real wave properties of thick electrode layers results in the expression:

$$K_t^2 = \frac{f_s}{f_p} \cdot \left(\frac{\pi - 2\psi_p}{2} \right) \cdot \frac{\cos\left[\frac{f_s}{f_p} \cdot \left(\frac{\pi - 2\psi_p}{2} + \psi_s \right) \right]}{\sin\left[\frac{f_s}{f_p} \cdot \left(\frac{\pi - 2\psi_p}{2} \right) \right] \cdot \cos\psi_s} \qquad (3)$$

here: $\psi_{p,s} = \arctan \frac{Z_1^0}{Z_t} \tan w_1^{p,s}$,

Z_1^0, Z_t , $w_1^{p,s}$ -are correspondingly acoustic impedances of electrode (both electrodes are similar), piezoelectric film, phase gain in electrode layer on the resonance frequencies. The evaluation using these expressions gives the value of K^2 for Mo-AlN-Mo 3.2%. From comparison of these figures an important conclusion can be done. The acoustic quality of AlN film grown on Mo is better than on Al. Composite resonator structure composed of the thick Mo electrodes and AlN film increase gap between series and parallel resonances with respect to this value calculated from material coupling constant.

It was interesting to compare these data with the results of study of the TFR made on the same substrate on the same resonance frequency but with relatively thin Mo electrodes (0.05μm) and thick AlN (2.5μm). It was found that due relatively thick and relatively perfect AlN film the measured value of K^2= 4.76% became higher, but the quality factor of the resonator decreased (Q_s= 251) because of higher value of acoustic wave attenuation in AlN than in Mo.

The role and the influence of the attenuation in the layers of the Bragg-reflector layers was clearly clarified in the experiments with two types 9 layer of Bragg reflector designed for more high frequency operation. Their structures were:

Al(0.05)-AlN(0.885) -Al(0.05)/ SiO_2 (0.19)- W(0.215)-SiO_2 (0.19)-W(0.215)-SiO_2 (0.19)-W(0.215)-SiO_2(0.19)-W(0.215)- SiO_2(0.19)/Si(500);
Al(0.05)-AlN(0.847) -Al(0.05)/ SiO_2 (0.21)- ZnO(0.31)-SiO_2 (0.21)-ZnO(0.31)-SiO_2 (0.21)-ZnO(0.31)-SiO_2(0.21)-ZnO(0.31)- SiO_2(0.21)/Si(500);

The Bragg reflectors were composed of W-SiO_2 pairs and ZnO-SiO_2 pairs. Tungsten has much high value of the material impedance (101.02 kg/m s) than ZnO (35.95 kg/m s). So it is expected that the quality factor in the case of W-SiO_2 pairs must be higher than for ZnO-SiO_2 pairs due to much more effective acoustic isolation.

The results of numerical analysis and the fitting for the Bragg structure made of ZnO-SiO_2 pairs are shown in Table 2.

In the first line the expected value of Q factor for lossless ZnO-SiO_2 pairs is given. Due to high number of layers the value is very high. The taking into account of the losses only in AlN film results in almost two order of

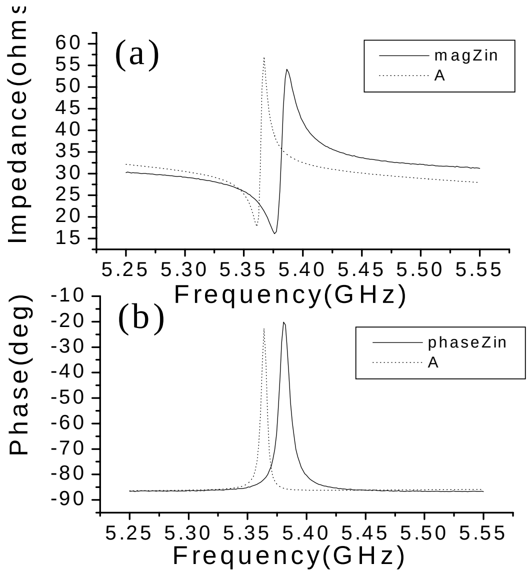

Fig.2 The measured and calculated data of modulus a) and phase b) of AlN film λ/2 thickness resonators with 9 layers of W-SiO2. Solid line - experiment, dashed line - the result of numerical calculation.

Table 2

Si	AlN	Al	ZnO	Q
7.2	0	0	0	$2.9\ 10^5$
7.2	10	0	0	334
7.2	10	13.65	0	267
7.2	10	13.65	28.5	38.7

magnitude decrease in the Q factor. Subsequent taking into account of the losses in Al and ZnO layers results in the decrease of Q up to the value 38.7.

The example of measured and calculated data of modulus a) and phase b) of AlN film λ/2 thickness resonators with 9 layers of W-SiO2. Solid line-experiment, dashed line-the result of numerical calculation (resonant frequencies were not fitted) are shown on Fig.2.

In Table 3 the results of numerical analysis and the fitting for the Bragg structure made of W-SiO_2 pairs are shown.

Table 3

Si	AlNi	Al	W	Q
7.2	0	0	0	$>10^8$
7.2	10	0	0	345
7.2	0	0	7.14	498
7.2	10	13.65	7.14	105

In the first line the data for the lossless resonator and Bragg reflector structure is given. This value is higher than in the previous case. The reason is the better isolating properties of the lossless Bragg reflector in case of W-SiO_2 pair than in case of ZnO-SiO_2 due to higher acoustic impedance contrast. Account of the losses in the piezoelectric film immediately results in drastic drop in quality factor. For the comparison the data given in row 3 illustrates the influence of the losses only in Bragg reflector on the quality factor. In the last row the results of fitting and calculating losses in all layers composing the structure are presented. The value Q=105 case of W-SiO_2 Bragg reflector is greater than 38.7 in case of ZnO-SiO_2 Bragg reflector as a result of better acoustic isolation. In both cases the ultimate value of quality factor is a relatively low. It is a sequence of the losses both in Bragg layer and ZnO film.

The last investigated structure was TFR with 9 layers in the Bragg reflector with the electrodes made of Mo:

Mo(0.105)-AlN(0.347) -Mo(0.105)/ SiO_2 (0.158)-W(0.175)-SiO_2 (0.158)-W(0.175)-SiO_2 (0.158)-W(0.175)-SiO_2(0.158)-W(0.175)- SiO_2(0.158)/Si(500);

The resonators were designed as λ/2 TFR structures and their experimental study showed a very good results. These TFR's were formed by relatively thin AlN film (its proper resonant frequency was 14.9 GHz) and very thick electrodes made of molybdenum. The three layer system was resonating near 5.4GHz in a satisfactory agreement with the dispersion equation for multilayer composite resonator structure (2). Again Bragg reflector layers had resonant frequencies far from necessary for λ/4 on the desired frequencies 5.4GHz (for SiO_2 it was 6.96 GHz and for W is 7.4 GHz). But again a very good impedance magnitude and phase characteristics were obtained for two values of the size of the aperture 100 and 150µm. Just like the previous case the quantitative agreement with the results of numerical simulations could be achieved if the BAW attenuation coefficient was increased a few times in SiO_2 slightly in other layers and the value of K^2 taking less than 2%. The best values of Q were Qs= 607(aperture size 100µm), Q_p= 849 (aperture size 150µm);

6. CONCLUSIONS

Study of thin AlN films in resonators showed that the acoustic losses are the same or slightly higher, sound velocity and electromechanical coupling coefficient are less than in bulk material. Half wavelength and quarter wavelength in thickness TFRs were investigated with the Bragg structures designed as the reflectors providing zero and pi phase shift correspondingly. A good agreement between experimental and calculated data was obtained when experimentally found values of K^2 and directly measured thickness of the layers (by SEM) composing the structure has been used. It was experimentally confirmed that Bragg reflectors are extremely wide band structures not very critical to the individual layer thickness.

New important results were obtained when the Al electrodes were substituted by relatively thick W and Mo films. It was found due to very perfect adhesion and low estimated acoustic losses these materials not only can effectively serve as the electrodes but also can provide better conditions for AlN growing than Al film interface.

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7. REFERENCES

[1] G.S.Kino, Acoustic waves: devices, imaging, and analog signal processing. Prentice-Hall Inc., Englewood Cliffs, NJ.