STRESS CONTROLLED PIEZOELECTRIC ALN-MEMS-RESONATORS WITH MOLYBDENUM ELECTRODES FOR GHZ APPLICATIONS

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Abstract — We present design, fabrication and characterisation of piezoelectric AlN MEMS resonators with usage of molybdenum as material for the bottom electrode. The stress control during the sputter process and influence on the film quality of molybdenum by adding a thin (50nm) aluminium nitride nucleation layer beneath are shown. Two design variants with and without a structural silicon layer underneath the bottom electrode are presented. Equal layers in both design variants result in the possibility of comparing their performance RF properties like piezoelectric coupling factor and quality factor.

Keywords: piezoelectric MEMS resonator, aluminium nitride (AlN), molybdenum (Mo), Lamb wave resonator, stress control, nucleation layer

I - Introduction

Acoustic Lamb wave MEMS resonators on silicon (Si) substrates with the piezoelectric material aluminium nitride (AlN) gain more and more attention as they show a great potential for electronically reconfigurable RF applications as filters and oscillators [1-3]. Furthermore, molybdenum is an excellent start material for RF applications as filters and oscillators [1-3]. Further, molybdenum is an excellent start material for RF applications as filters and oscillators [1-3].

The scope of this article lies on Lamb wave MEMS resonators including a structural silicon layer beneath. The fabrication process is the stress control of the different layers with respect to the resulting functional reliability. By adding a thin (50nm) AlN nucleation layer underneath, we achieved a considerable increase of the film quality of the bottom electrode. We show the realisation of two different variants of resonators either with or without a structural silicon layer underneath the piezoelectric stack.

Equal layers in both let us systematically compare the two designs for the first time. The design including a Si layer is expected to reveal a higher quality factor than the other design should show a higher electromechanical coupling coefficient. Depending on the application an optimal configuration can be chosen.
where $d_{31}$ is the transverse piezoelectric modulus, $\varepsilon_r$ the relative permittivity, $E_p$ the Young’s modulus and $t_{fe}$ the thickness of the AlN layer, and $\varepsilon_0$ the dielectric permittivity of vacuum.

The quality factor $Q$ is determined by $f_n$ the effective mass $m_{eff}$ of the resonator body and the effective damping coefficient $d_{eff}$ comprising all loss mechanisms including material damping, substrate and viscous losses:

$$Q = 2\pi f_n \frac{m_{eff}}{d_{eff}}$$  (3)

It can be concluded from Eqs. (2) and (3) that increasing the resonator thickness $t$ provides higher $Q$ without diminishing the $Q \times \kappa^2$ product.

C. Finite element simulations

A three step finite element (FE) analysis was done to identify the longitudinal modes of the resonators. The longitudinal modes of interest were extracted from the modal solution by the Modal Assurance Criterion (MAC). In the region of the longitudinal frequencies a broadband harmonic analysis was performed for determination of the electrical and mechanical behaviour of the resonator with a piezoelectric excitation. As a result, the admittance and the mean value of the deformation can be obtained, as illustrated by Fig. 2.

The simulated deformation indicates that due to a number of local frequency maxima a unique identification of the longitudinal mode is only possible in conjunction of the admittance measurement.

$$\begin{array}{c}
\text{Material} \\
\text{Unit} \\
\text{Mo} \\
\text{Pt} \\
\text{Al}
\end{array}
\begin{array}{c}
\text{Bulk Resistance} \\
\mu\Omega\text{cm} \\
5.7 \\
10.7 \\
2.8
\end{array}
\begin{array}{c}
\text{Density} \\
g/cm^3 \\
10.2 \\
21.5 \\
2.7
\end{array}
\begin{array}{c}
\text{Thermal Expansion} \\
10^{-6} 1/K \\
5.1 \\
8.9 \\
22.9
\end{array}
\begin{array}{c}
\text{Acoustic Velocity} \\
10^3 m/s \\
6.2 \\
2.7 \\
6.3
\end{array}$$

B. Stress control and film quality

The Mo bottom electrode as well as the AlN layer above is deposited in different chambers of one single sputter cluster. With prevention of the interception of vacuum conditions, no native oxide film on the Mo surface is formed and the contamination with water or dust molecules is minimised, which results in an ideal nucleation surface for AlN [7, 10, 13].

Stress control of the Mo layer is achieved by an appropriate choice of sputtering parameters. The increase of power and decrease of pressure result in reduced tensile stress. Furthermore by increasing the target-substrate distance only sputtered atoms with high kinetic energy reach the substrate. As a consequence, more energy is transferred to the growing film and the intrinsic stress becomes more compressive. The same criteria work well for adjusting the intrinsic stress of the piezoelectric AlN layer.

It was found that a thin (50nm) AlN nucleation layer leads to a strong improvement of the molybdenum film quality and hence to an improvement of the quality of the AlN layer above.

C. Fabrication of the resonators

For the resonators without an additional Si layer (left-hand side Fig. 4) the fabrication process starts with single side polished silicon wafers (100). The second resonator design (right-hand side Fig 4) is produced out of silicon-on-insulator (SOI) wafer (100). The important fabrication steps are shown in Fig. 3. The Mo (100 nm) and AlN (600nm) layers are processed in the cluster system CS400 of von Ardenne (Fig. 3a). The resonator body is patterned in a chloride dry etch process using a ICP CVD silicon dioxide (SiO2) mask (Fig. 3b) [14]. The Mo bottom electrode around the resonator is etched using a solution of H2O2 and H2O. The patterned top electrode (Al) and the metal bond pads (Al) are realised via lift-off processes (Fig. 3c). The resonators without a Si layer are released in an isotropic dry etch process utilizing the gases SF6 and O2 (Fig. 3d). Here the AlN nucleation layer shows a second benefit as a protection layer for Mo. The Si layer of the second resonator
design is patterned by an anisotropic silicon dry etch process (Fig. 3d). For releasing the resonators the box layer (SiO₂) is etched in a hydrogen fluoride vapour process (Fig. 3e).

IV – Characterization

The resonant properties of the structures were tested at room temperature under normal ambient conditions.

A. RF Measurements

We performed a two-port wafer network analysis using a SUSS PM4 prober and Agilent PNA-X analyser. An open-short-load-trough calibration was carried out using a standard calibration substrate. The resonator properties were extracted from the admittance matrix \( Y \) as calculated from the measured scattering matrix \( S \).

The curves of the transconductance \( y_{21} \) for two selected resonators with the same dimensions except for the structural Si layer are shown in Figs. 5 and 6.

B. Laser Doppler Vibrometry

Laser Doppler vibrometry (LDV) measurements were executed with UHF-120 from Polytec. Beside the frequency response, mode shapes were measured by scanning over a user defined grid along the surface of the resonator [15].

Figs. 5 and 6 show the measured response where the vibration maximum is in accordance with the electrical admittance measurement. The quality factor derived from LDV data for the longitudinal mode agrees with RF results.

As expected, further mechanical frequency peaks beside the longitudinal mode are not reflected by the electrical measurements (cf. Sec. II.C).

Table 2: Summary of measurement results under normal ambient conditions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Unit</th>
<th>AlN</th>
<th>AlN-Si</th>
</tr>
</thead>
<tbody>
<tr>
<td>Length ( l )</td>
<td>µm</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>Thickness ( t )</td>
<td>µm</td>
<td>0.85</td>
<td>2.85</td>
</tr>
<tr>
<td>Mode Number ( n )</td>
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<td>5</td>
</tr>
<tr>
<td>Resonant Frequency ( f_5 )</td>
<td>MHz</td>
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<td>217.00</td>
</tr>
<tr>
<td>Coupling Factor ( \kappa )</td>
<td>%</td>
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<td>0.23</td>
</tr>
<tr>
<td>Quality Factor ( Q )</td>
<td></td>
<td>425</td>
<td>1670</td>
</tr>
</tbody>
</table>

V – Results and Discussion

A. Stress control and film quality

The stress of the Mo bottom electrode can be adjusted in a wide range between compressive and tensile area. (see Figs. 7 and 8).

![Figure 7: Intrinsic stress (left) and XRD Mo(110) reflection (right) upon varying power and pressure in DC sputtering process.](image)

When adapting the sputtering parameters it is important to sustain the required crystalline orientation of the film. As the X-ray diffraction (XRD) results show, for Mo both criteria correlate with each other (see Figs. 7 and 8).
Fig. 9 indicates the influence of the target to substrate distance on the intrinsic stress of the AlN layer. The stress can be adjusted easily between +300 MPa and -400 MPa.

Figure 8: Variation of XRD Mo(110) reflection (left) and of intrinsic stress (right) upon changing target-substrate distance in sputtering process – at 600W; 1·10⁻³ mbar.

Figure 9: Variation of intrinsic stress in the AlN layer upon increasing the substrate to target distance.

By adding a thin (50 nm) AlN nucleation layer for the Mo bottom electrode, the crystalline quality of the AlN layer above is enhanced significantly, as it can be seen in Fig. 10 clearly. A full-width, half-maximum of the rocking curve (FWHM) of about 2 degrees was achieved.

Figure 10: Left-hand side: XRD reflections of Mo(110) and AlN(002) including AlN nucleation layer (green and black curve) – red curve without AlN nucleation layer; Right-hand side: SEM picture of the layer composition

B. Characterization

The measured resonant frequencies from both, LDV and RF measurements, coincide with the results obtained from analytical modeling (Eq. 1) and FE simulations (cf. Figs. 5, 6). As expected, the resonant frequencies of AlN-Si resonators fall below those of the pure AlN resonators. This is attributed to the lower $v_{ph}$ of the AlN-Si resonator which is mainly caused by the smaller Young’s modulus of Si compared to AlN. Close to the desired resonant modes, the FE simulations reveal additional local maxima of the out-of-plane displacement which are also present in the LDV measurements (compare Figs. 2a, b with Figs. 5, 6). Consequently, unambiguous mode identification by LDV is only possible in combination with RF measurements.

The $Q$ factors derived from RF measurements could be confirmed by LDV and are comparable to the results obtained by other researchers for similar structures (cf. Table 2) [8]. According to theory, the measured $Q$ factors approximately scales linearly with the additional Si layer thickness without compromising the signal amplitudes at resonance.

VI – Conclusions

We show the adjustment of stress in the Mo film over a wide range between +1000 MPa and -100 MPa. A FWHM of the AlN Layer of about 2 degrees by increasing the Mo film quality was achieved. As a consequence the suitability of Mo as material for piezoelectric AlN Lamb wave MEMS resonators was shown.

Due to the higher $Q$ factors, the resonators with additional Si layer are favoured for RF applications as oscillators and filters. At wavelengths of about 10 µm, GHz range can be addressed with these structures by accordingly downscaled electrode dimensions.

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References