Design of Rayleigh SAW Resonators for Applications as Gas Sensors in Highly Reactive Chemical Environments

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Abstract **- This work presents the performance and important design considerations of the first successful highly efficient Rayleigh surface acoustic wave (RSAW) resonator filters using gold (Au) electrode structure. Au metallisation provides corrosion immunity when the devices are operated as polymer coated gas sensors in chemically reactive environments. It is shown that Au, due to its 7 times higher density than Al, provides about 13 times higher frequency sensitivity and a stronger velocity perturbation in resonant devices compared to their RSAW counterparts with aluminium (Al) electrodes. This results in strong excitation of unwanted surface skimming bulk wave (SSBW) modes and transverse wave guide modes (TWGMs) in such resonant Au devices. Practical guidelines for the choice of correct device geometry, Au thickness and spacer variations to maximize coupling to the desired RSAW mode, increase resonator efficiency and loaded Q, as well as minimize interference with parasitic TWGMs are given. Experimental 433 MHz two-port resonators and dual mode inline coupled filters with insertion loss in the -8 to -12 dB range and loaded Q values in the 4500 to 6000 range are presented with emphasis on their polymer coating and gas probing behavior.**

Keywords-Rayleigh SAW resonators, sensors, gold electrodes, film thickness, SSBW modes, transverse waveguide modes.

I. INTRODUCTION

Rayleigh surface acoustic wave (RSAW) resonators coated with chemosensitive polymer films are widely used in a variety of sensor systems for chemical and biological gas detection [1,2]. In most cases, the sensor devices in modern commercialized SAW based gas detection systems and electronic noses are RSAW resonators on temperature stable ST-cut quartz. These acoustic devices are operated in oscillator circuits and, due to their high electrical quality factor (Q) and low insertion loss, they provide excellent noise immunity and high measurement resolution and accuracy [3]. A major problem in such systems is that, if the sensors are operated in chemically reactive gas-phase environments, the aluminium (Al) electrode structure of the sensor device is often attacked by the detected gas or gas mixture which forms corrosive acids or bases with the humidity of the ambient air. The problem is further aggravated by the sensing polymer film at the device surface greatly increasing the amount of adsorbed agent and moisture coming in contact with the electrode structure. As a result of that, the sensor performance degrades and the device electrode structure is destroyed after a limited number of measurement cycles. The solution to that problem is the implementation of RSAW resonant devices using corrosion proof electrode metallisation such as gold (Au). Au-RSAW devices of this type, operating at 433 MHz with a typical loaded Q as high as 5000 and insertion loss in the -8 to -10dB range in the uncoated state have been recently reported [4]. To confirm the corrosion immunity of the Au devices and compare it with Al resonators, fully functional samples were submerged in water based alkaline and acid solutions of NaOH (0.1 mol, pH 13) and HCl (1 mol, pH 0) [4]. These analytes were found to completely remove the electrode structure of the SAW devices with Al metallisation within an hour. No evidence of structure degradation was found in the Au devices after 96 hours of test.

The design of RSAW resonators on ST-cut quartz for use as polymer coated gas sensors may be quite different from resonator designs intended for use in low-noise oscillators for communications. Such oscillators aim at achieving ultimate phase noise performance [5], therefore, the resonators stabilizing them, are typically designed for unloaded Q-factors close to the material limit for the acoustic wave mode used, often referred to as Q×F product or material Q. The material limit is a constant in which Q is the resonator's unloaded quality factor and F is its frequency. For the RSAW mode, the Q×F product has the value of 1.05×10^{13} Hz and RSAW resonators featuring unloaded Q values as high as 80 to 90% of the material Q for RSAW can readily be designed [5]. Our experience has shown, however, that such high-Q devices are not appropriate for sensor applications since, in order to maintain high loaded Q in the oscillator loop, they use a fairly weak coupling to the electrical load which is typically 50Ω. Normally, this is achieved with a small number of active fingers in the interdigital transducers (IDTs) and an aperture tailored to a compromise between loaded Q and insertion loss such that the resonator operates at about 50% of the material Q when terminated with 50Ω impedance [5]. When a sensing film is applied to the surface of such a high-Q device, the Q degrades and loss increases rapidly with film thickness [6]. This makes the device unusable at thick sensing films as used for sufficient gas sensitivity. Earlier investigations on the polymer coating and gas sensing behavior of SAW resonators have shown that resonator devices with strong coupling to the load can stand substantially higher mass loading and, therefore, thicker sensing films on their surface for the same amount of loss increase and Q degradation compared to weak coupling devices, featuring very high Q in the uncoated state [6-9]. In order to obtain high coupling to the electrical load without additional electrical matching networks which can affect the stability of the sensor oscillators, we have increased the number of active IDT fingers and the acoustic aperture to values allowing a well behaved resonance and reasonably low insertion loss even when the devices are coated with thick polymer films. As a result of that, their loaded and unloaded Q in the uncoated state are generally lower than in devices designed for operation close to the material limit [4], however, their polymer coating and gas sensing performance is substantially better. The design geometries for the strong coupling Au RSAW devices used in this work are given in Ref. [4] and will not be discussed here in more detail.

This paper treats peculiarities and important design considerations that need to be taken into account when designing RSAW resonators with Au metallisation and strong coupling to the load for sensor applications. The influence of metallisation parameters and spacers on the device performance is experimentally investigated and discussed in detail. Successful designs and their performance are presented.

II. Peculiarities of RSAW Resonators with Gold Electrode Structure

The RSAW devices with Au electrode structure, subject of this work, use the classical two-port resonator configuration shown in Fig. 1 a) [10]. They consist of two interdigital transducers surrounded by two reflector gratings to launch and detect a standing RSAW pattern within the resonant cavity. A coupling grating of the length *L* between the two IDTs sets the

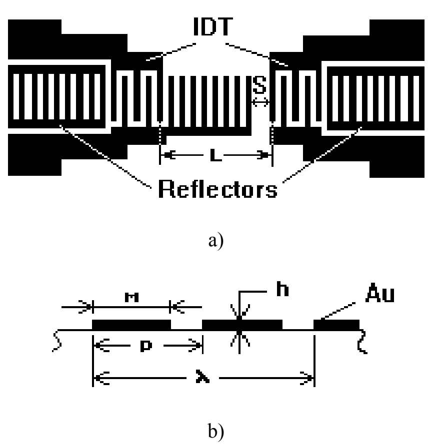


Fig. 1. Geometry (a) and metallisation parameters (b) of a RSAW based two-port resonator with Au electrode structure.

number of longitudinal modes inside the cavity and the spacer *S* adjusts the location of the standing wave maxima in such manner w.r.t. the IDT fingers that one of the longitudinal modes that we call main resonance, is excited and detected by the IDTs at maximum efficiency and lowest loss while the other longitudinal modes are sufficiently well suppressed [11]. Thus, the structure in Fig. 1 a) can support single-mode operation which is important for stable operation of the sensor oscillator stabilized with this device. In all sensor devices we used the synchronous IDT configuration [12] in which the IDTs, being synchronously placed with the reflectors, are part of them and contribute to the overall reflection inside the cavity. This type of geometry places the resonance close to the lower stopband edge and is less sensitive to fabrication tolerances compared to peak positioned designs [12]. As mentioned in the Introduction, the number of finger pairs in the IDTs and the acoustic apperture have been maximized in such manner that the resonators provide strong coupling to 50Ω load [4].

The second important set of design parameters is the Au metallisation which is critical for proper device operation. As shown in Fig. 1 b), the metallisation parameters are the *m/p* ratio and the Au thickness *h*. In this work we found that small variations of the *m/p* ratio around the optimum number of 0.5 at which reflection is maximum, did not have a serious effect on the device performance. These variations were found to shift the resonance frequency and to slightly affect the magnitudes of the adjacent longitudinal modes w.r.t. each other. The Au thickness *h*, however, was found to have a critical effect on the resonator performance and this is the reason why we will give it a more detailed consideration in this paper.

The RSAW Au devices were fabricated in a standard photolithographic process using lift-off technology. The Au film was deposited on the ST-cut quartz wafers in an e-beam evaporator on top of a thin titanium (Ti) layer which was found to provide excellent adhesion of the gold to the quartz substrate.

A. *The influence of the Au thickness on the frequency sensitivity of RSAW resonators*

Although the properties of Au stripes for designing efficient RSAW reflectors on piezoelectric quartz were investigated three decades years ago [13-15], we are not aware of successful RSAW resonators with Au-stripe electrode structure published so far, although very impressive results have been reported with the leaky SAW (LSAW) mode recently [16]. The LSAW mode may be quite useful for liquid sensors, but it does not provide sufficient sensitivity in gas sensors, that is why, our efforts were directed towards the RSAW mode. The reason why Au-RSAW resonators on quartz are more difficult to design than their Al counterparts is that:

1. *Au is about 7 times heavier than Al and*
2. *Au is substantially softer than Al.*

By having 7 times higher density than Al, Au metallisation introduces a very strong mass loading effect for RSAW propagation on the quartz substrate. Therefore, the effective

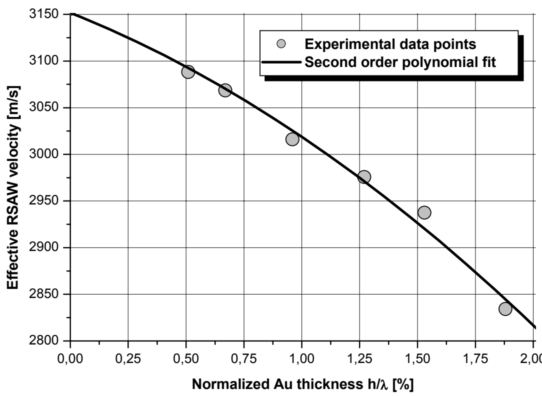


Fig. 2. Effective RSAW propagation velocity in a two-port resonator with Au electrode structure versus normalized Au film thickness.

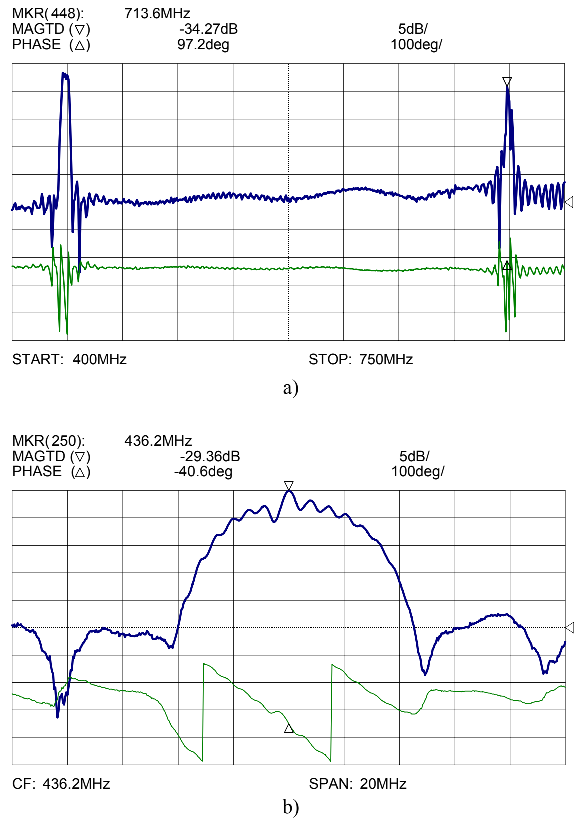


Fig. 3. Frequency (upper plots) and phase (lower plots) responses of a two-port RSAW resonator with Au metallisation and strong excitation of a parasitic SSBW mode. The broadband responses (a) indicate the lower-frequency RSAW mode at about 436 MHz and the SSBW mode at about 70% higher frequency. The narrowband RSAW responses (b) indicate very weak resonance behavior (ripples) on top of the sin(x)/x response of the IDTs.

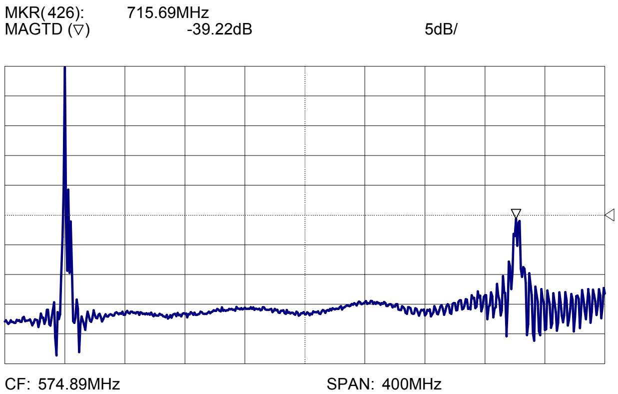
wave velocity $v_{eff} = f_o.\lambda$ within the resonator structure, where f_o is the main resonance frequency, will be much more sensitive to Au thickness variations compared to RSAW resonators with Al metallisation. This is evident from Fig. 2 which represents an experimental data plot of v_{eff} versus Au thickness, normalized by the acoustiv wavelength λ in a 433 MHz two-port resonator which was fabricated with the same photomask but different Au thicknesses. The experimental points in Fig. 2 were derived from measurements on the resonant frequency at each Au thickness. The value of v_{eff} at $h/\lambda = 2\%$ is by 10.6% lower than the free-surface propagation velocity of 3156m/s for ST-cut quartz. It is interesting to note that the reduction of v_{eff} in a similar 433 MHz RSAW device with Al metallisation was found to be 13 times smaller at the same 2% Al thickness compared to the device from Fig. 2, although the density of Al is only 7 times lower than Au.

In another experiment, we left the Au thickness constant at about 100nm and varied the Ti film thickness underneath the Au film which we used as adhesion layer. Despite the fact that Ti is also a very light metal, the sensitivity of the resonant frequency w.r.t. small variations in the Ti film thickness was measured as 2680ppm/nm versus 12570ppm/nm for Au. Thus the sensitivity of the resonant frequency to Au variations is only 4.7 times higher for Au and in no relation to the density ratio between the two metals. This high frequency sensitivity to small mass variations on the device surface implies that RSAW resonators with Au metallisation will also make very good gas sensors with substantially higher gas sensitivity compared to their Al counterparts.

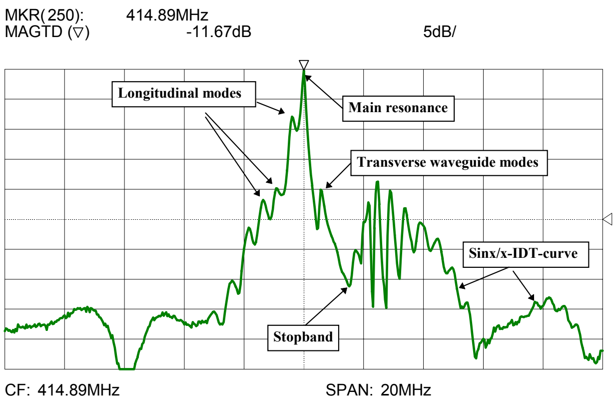
B. The influence of the Au thickness on the excitation of parasitic SSBW modes in Au RSAW resonators

Another critical effect caused by the high density of Au which is not observed in RSAW resonators with Al metallisation is that the mass loading of the surface causes a strong excitation of a parasitic surface skimming bulk wave (SSBW) mode with about 70% higher effective propagation velocity. Its response is seen on the right-hand side of the broadband frequency and phase response data plot in Fig. 3 a) where its magnitude is about as high as the magnitude of the RSAW mode on the left-hand side of the plot. This means that in this case, the IDTs couple equally strong to both, the RSAW and the SSBW mode instead of providing maximum coupling to the desired RSAW mode. The effect of the insufficient IDT coupling to the RSAW mode on the resonance behavior of the device from Fig. 3 a) is shown in Fig. 3 b). Only a few weak resonance ripples are seen on top of the sin(x)/x IDT response. The insertion loss of this resonator is in excess of -29dB.

In a systematic effort to maximize IDT coupling and obtain a strong and well behaved resonance at the RSAW mode of interest, we found that in a structure as the one from Fig. 1 a) it is impossible to completely eliminate the SSBW mode. However, by carefully optimizing the Au film thickness, it is possible to maximize coupling to the RSAW mode and simultaneously minimize it at the SSBW one, despite the fact that both modes operate at different frequencies. The results for the Au-thickness optimized device from Fig. 3 is shown in Fig. 4. As evident from Fig. 4 a), the SSBW response at 716 MHz is now suppressed by 27 dB w.r.t. the RSAW response which has a strong single-mode resonance response and an insertion loss of -11.7 dB. The main RSAW resonance in Fig. 4 b) is well behaved and by about 8 dB higher than the adjacent



a)



b)

Fig. 4. Broadband (a) and narrowband (b) frequency response of the device from Fig. 3 with an Au thickness optimized for maximum coupling at the RSAW mode and highest suppression at the undesired SSBW mode.

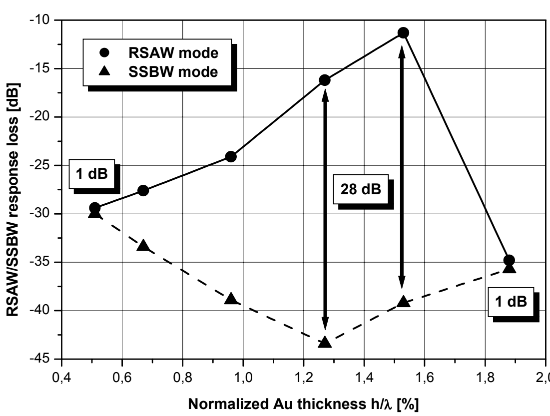


Fig. 5. Insertion loss behavior of the RSAW and SSBW modes versus Au thickness for the device from Fig. 3 and 4.

longitudinal modes on its left. The higher stopband edge, as well as a transverse waveguide mode (TWGM) on the right-hand slope of that resonance are also clearly visible.

The experimental data plots in Fig. 5 show the insertion loss behavior for both modes as a function of Au film thickness. It is clearly evident that at h/λ = 0.5 and 1.9% Au thickness, both modes have the about the same (within 1 dB) insertion loss which is about -30 and -35dB, respectively. In the thickness range from 1.25 to 1.55% the loss difference between both modes is 28 dB which means that in this case, the IDT coupling to the SSBW mode is very low. At h/λ=1.55% which is optimum for this device, RSAW insertion loss is minimum and most of the devices, fabricated at that thickness, were found to have an insertion loss in the -10 to -12dB range and a loaded Q of about 5500.

C. *Excitation of transverse wave guide modes*

In an attempt to minimize unmatched device loss and maximize coupling to the load, as necessary for RSAW sensor devices intended for operation with thick soft polymer films, we tried to maximize the acoustic aperture of Au devices that have been thickness optimized for maximum coupling to the RSAW mode (see Section II B). The result for a device with 85λ aperture is shown in Fig. 6. The -7.7 dB insertion loss and loaded and unloaded Q values of 5000 and 8540, respectively, indicate that this device operates at about 35% of the material Q for RSAW on quartz and show that it is indeed possible to design a highly efficient RSAW single-mode resonator with Au metallisation. The efficiency of a RSAW device with Al metallisation which can be designed to operate at 80 to 90% of the material Q at this frequency [5], cannot quite be reached mainly due to viscous loss caused by the fairly poor stiffness of Au. Our current investigations, however, show that the strong coupling device from Fig. 6 provides excellent low-loss performance and very high gas sensitivity when coated with thick soft polymer films. Therefore, operation at higher unloaded Q in the uncoated state is not really necessary. A major issue of concern for this device, however, is the excitation of strong TWGMs which appear as closely spaced spikes on the right-hand slope of the main resonance in Fig. 6.

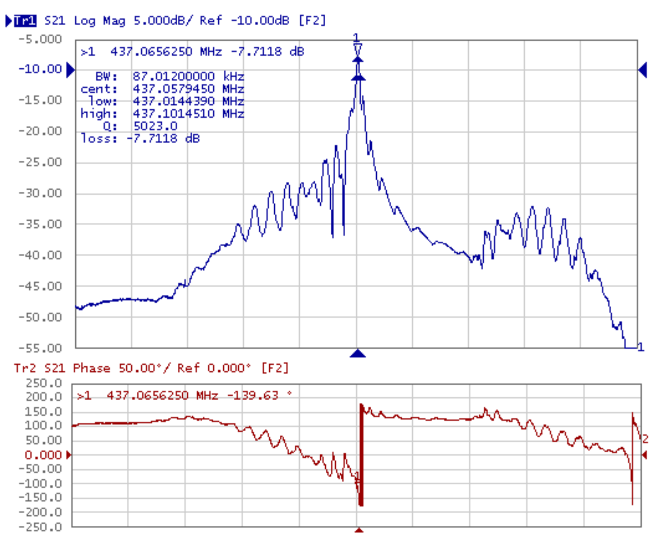


Fig. 6. Frequency (upper plot) and phase (lower plot) responses of a low-loss thickness optimized Au RSAW two-port resonator with 85λ aperture for strong load coupling. Horizontal scale: 1.5MHz/div.

We found that these TWGMs are very sensitive to small variations in Au thickness from device to device on the quartz wafer and sometimes interfere with the main resonance causing increased device loss and distortion. This, in turn, reduces the yield of good devices on the wafer and increases fabrication cost. Also, TWGMs propagate in a zig-zag way along the resonant cavity departing from the temperature compensated X-direction of RSAW propagation for ST-cut quartz and are, therefore, very temperature sensitive. We found that strong TWGM interference with the main resonance may occur if the sensor devices are operated over a wide temperature range.

A common method for TWGM suppression in RSAW resonators is reflector weighting. This method can reduce TWGM influence to acceptable levels, however, it also reduces resonator efficiency. In one of our designs we implemented random interruption of the reflector strips as shown in Fig. 7. As expected and evident from Fig. 8 a), finger interruption reduced the distortion on the frequency and phase responses caused by the TWGMs. The explanation of that effect is that TWGMs, due to their zig-zag way of propagation, get scattered by the discontinuities in the reflector while the main standing wave suffers less from these discontinuities since it propagates in a direction normal to the reflector strips. Nevertheless, the comparison of identical devices with and without finger interruptions (see Fig. 8 a) and b)), shows that the device with the weighted reflector suffers by 4 to 5 dB higher insertion loss than its unweighted counterpart. In both cases, the aperture was 70λ. The 15λ apperture reduction in the unweighted device from Fig. 8 b) results in about 1 dB loss increase compared to the 85λ device from Fig. 6, however, the resonance in that device did not suffer from TWGM interference any longer. The TWGMs were suppressed by at least 7 to 8 dB in that device (see Fig. 8 b)) and this suppression was found sufficient for stable device operation over a wide temperature range and for good reproducibility of the devices on the wafer. The strong coupling device from Fig. 8 b) also provides excellent polymer coating and gas probing behavior and was the final choice for the multichannel gas analysis sensor system which the Au devices were intended for.

D. *Spacer variation in RSAW two-port resonators with Au metallisation*

An attempt to roughly predict the mode behavior of the devices described in this work and in [4] was made by using a standard coupling-of-modes (COM) algorithm similar to the one described in [17, 18]. The COM algorithm provides very

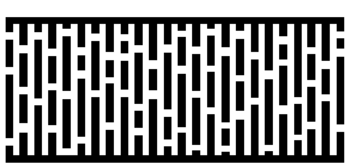
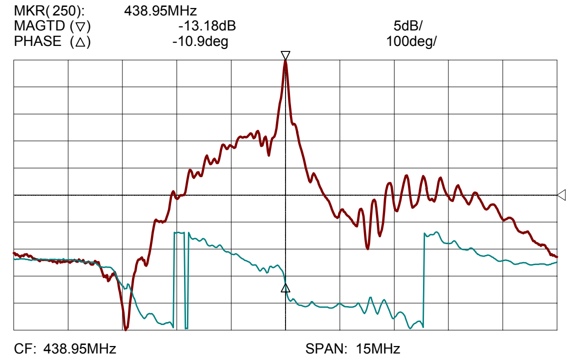
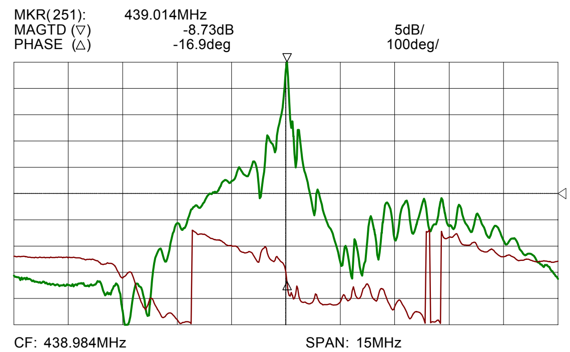


Fig. 7. Reflector with randomly broken fingers for TWGM suppression.



a)



b)

Fig. 8. Comparison of two identical Au devices (a) with and (b) without random interruption of the reflector fingers according to Fig. 7. Upper and lower data traces are the device frequency and phase responses, respectively.

reliable results when applied to RSAW resonators with Al metallisation since all COM parameters for Al stripes are well known. Unfortunately, there is very little data in literature about Au stripes and because of that, we did not succeed in obtaining satisfactory COM analysis data for Au RSAW devices. That is why, the final performance adjustment in the devices from this work was performed experimentally by altering the spacer *S* in Fig. 1 a) in small λ/16 steps within half of a wavelength in order to adjust the cavity length *L* in such manner that the standing wave maxima coincide with the centers of transduction for one longitudinal mode as necessary for single-mode operation of the resonator device [11]. The results of this spacer variation is shown in Fig. 9 for the Au-thickness optimized device from Fig. 6. The data show that lowest device loss, highest Q and best single-mode operation are achieved at a cavity length $L \approx n\lambda/2$ which, surprisingly, is different from the behavior of RSAW two-port resonators with Al-stripe structure where optimum single-mode performance is achieved at $L \approx n\lambda/2 - \lambda/8$ [19]. We attribute this different behavior to the high density of gold and to some degree of dispersion, accordingly, as observed in surface transverse wave (STW) based resonators [11]. It should of course be noted that the optimum cavity length may differ from design to design, therefore, a spacer variation is highly recommended as a final optimization step in each Au RSAW design, as suggested for STW devices [11].

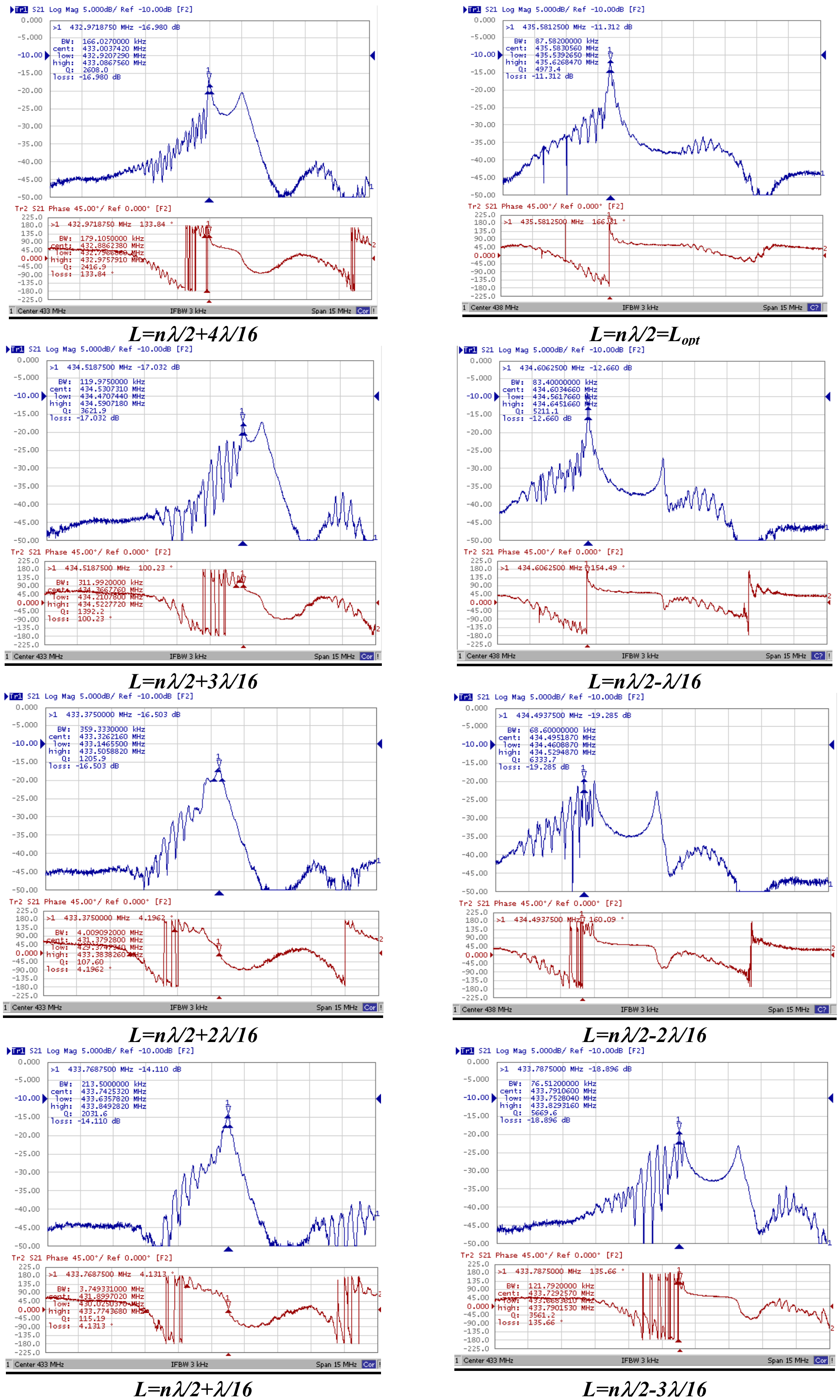


Fig. 9. Spacer variation in the device from Fig. 6. The upper and lower data plots are the frequency and phase responses, respectively.

III. Workflow for the Design of RSAW Resonators with Gold Electrode Structure

Based on our experience with the design and evaluation of RSAW resonators with Au metallisation for sensor applications, we would like to suggest the following workflow for practical device design.

1. *If you have reliable simulation algorithms for COM and TWGM analysis and reliable experimental data for Au metallisation to work with in the simulation process, use them. Try to work as close as possible to the goal frequency of your final design.*
2. *Choose an initial device geometry with sufficient active IDT finger pairs (at least 30 [15]) to provide strong load coupling and perform TWGM analysis to see what maximum apperture you can afford in your device without TWGM interference with the main resonance. Avoid IDT and reflector weighting since this reduces resonator efficiency but make sure that the selected apperture provides at least 7 to 8 dB TWGM suppression w.r.t. the main resonance without weighting.*
3. *Perform COM analysis on that device and see if the device geometry that you have selected can be optimized for single-mode operation. Every time you change the number of IDT finger pairs and/or cavity length, observe the longitudinal mode behavior at different spacers untill you get the resonant loss, Q and single-mode behavior that you want.*
4. *Before fabricating your device, design the photomask in such manner that a spacer variation is possible.*
5. *Fabricate the device and perform a careful Au thickness optimization providing maximum coupling at the RSAW mode and highest SSBW suppression.*
6. *Perform a spacer variation on the Au thickness optimumized device to adjust minimum resonant loss and single-mode operation.*
7. *Check if the loss and Q are acceptable, perform polymer film deposition and make sure, the device retains reasonably low loss and a well behaved resonance under polymer load [6-9]. If not, start the design all over again with increased values for IDT fingers and aperture.*
8. *Once the device works satisfatory in the uncoated and polymer coated state, rescale the photomask and Au thickness to the desired frequency.*

IV. Further Successful RSAW Resonant Sensors with Gold Metallisation

Except for the successful single-mode device in Fig. 8 b) that we discussed already, we would like to present performance data from two more RSAW Au designs that were found to provide excellent gas sensitivity, a well behaved resonance and reasonably low loss when coated with thick soft polymer sensing films. The strong coupling device, characterized in Fig. 10, is a highly efficient single-mode two-port resonator with an extended resonant cavity. On one hand, the extended cavity increases sensor area and, therefore, gas sensitivity, on the other hand it helps the device retain a high phase slope at thick polymer coatings which improves stability and noise of the sensor oscillator in the system. Note that there is no evidence of TWGMs on the resonant slopes. This was achieved by using the correct aperture in an unweighted IDT/reflector geometry and by maximizing the cavity length which also helps reducing the TWGMs. As a result of that, the -11.3 dB device insertion loss is somewhat higher than in the short-cavity device from Fig. 8 b) but the loaded Q of 5740 is a respectable number.

In practical RSAW based sensor systems [3], dual-mode inline coupled resonator filters (ICRFs) are often the preferred choice for the sensor device due to the fact that such filters have twice as high phase variation range within their pass band compared to single-mode devices. This is evident from the phase response of the ICRF device in Fig. 11 which also provides excellent gas sensor performance.

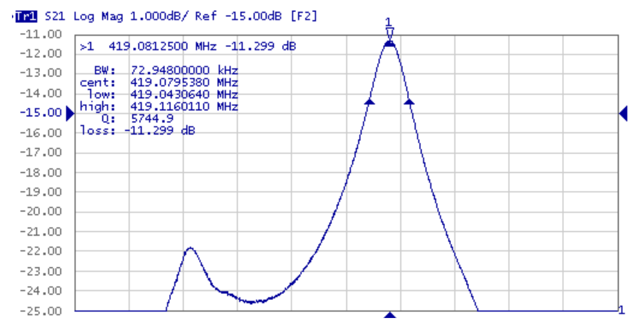


Fig. 10. Frequency response of an extended cavity Au RSAW sensor device with improved TWGM suppression. Horizontal scale: 100 kHz/div.

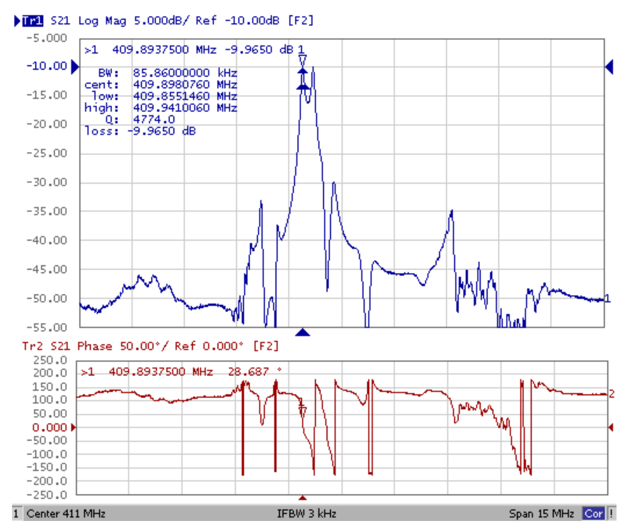


Fig. 11. Frequency (upper plot) and phase (lower plot) responses of an Au RSAW inline coupled dual mode resonator filter with increased phase slope within its pass band.

When coated with a polymer film, the left longitudinal mode vanishes but the right one still retains a high phase slope over a wide phase variation range. This greatly reduces the stability of the sensor oscillator when the RSAW device is operated at thick soft polymer films in environments of high gas concentrations. As evident from Fig. 11, in the uncoated state, this ICRF device provides -10dB of insertion loss and has a respectable loaded Q of 4770. There is no evidence of TWGMs which is attributed to the suitably selected aperture and the long coupling grating between the two IDTs in the device geometry.

The polymer and gas probing behavior of the Au RSAW devices from this work is subject of a different study the results of which will be published soon.

V. Summary and Conclusions

We have presented design considerations, experimental data and performance of the first successful RSAW resonators using gold electrode structure. The devices use strong coupling to the electrical load as appropriate for operation as polymer coated gas phase sensors. The Au metallisation protects the sensors from corrosion and makes them suitable for operation in highly reactive chemical environments. It was shown experimentally that Au, due its 7 times higher density and lower stiffness compared to Al, causes 13 times higher frequency sensitivity and a strong parasitic excitation of parasitic SSBW and TWGM modes in practical sensor devices, and this complicates their design. However, by carefully selecting the device geometry and Au thickness, it is possible to suppress unwanted modes and maximize IDT coupling and resonator efficiency at the desired RSAW mode. Guidelines for practical device design with emphasis on operation under heavy polymer film coating were also presented. The performance of practical single- and dual-mode devices in the 430 MHz range, featuring insertion loss in the -8 to -12 dB range and loaded Q values in the 4500 to 6000 range, was presented and discussed. All Au devices were found to provide superior polymer coating and gas probing performance compared to their earlier Al counterparts and feature excellent corrosion immunity when operated in chemically reactive gas phase environments.

Acknowledgment

The author wishes to gratefully acknowledge Forschungszentrum Karlsruhe in Germany for supporting this work and SAW Components Dresden GmbH, Germany for fabricating the Au RSAW resonators used in this study.

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