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Role of SiO_2 Layers in Third-Order Nonlinear Effects of Temperature Compensated BAW Resonators

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***Abstract*—This work applies a comprehensive nonlinear characterization process of two Temperature Compensated Bulk Acoustic Wave (TC-BAW) resonators. In both resonators, the SiO_2 layers have a remarkable impact on the generation of third-order intermodulation products (IMD3), confirming the impact of the SiO_2 on the generation of passive intermodulation. A unified model considering the electro-thermo-mechanical constitutive relations of the piezoelectricity is used, that allows to discern on the origin of the IMD3, either it comes from intrinsic nonlinearities of the materials, or from self-heating mechanisms.**

Keywords— Nonlinear, BAW, SMR, Silicon Dioxide, Aluminum Nitride, nonlinearities, IMD3, third order intermodulation products

I. Introduction

It is well known that passive intermodulation in the antenna, connectors and filters of the RF front-ends is becoming a potential drawback in the future implementation of new radio communication standards. In particular, IMD3 generation is receiving special attention in the recent carrier aggregation schemes, in which transmitters and receivers share the antenna and their operating bands are very close located. In such scenarios, the IMD3 generated in the N-Plexer might fall in a receiver band producing desensitization.

Continuous demands on further size reduction of the RF front-end receiver comes along with the need of high linear and temperature stable performances which turns out into very stringent requirements, hard to achieve. As it is well known, Solidly Mounted Resonators (SMR) topology allows to design TC-BAW resonators and filters using, in the acoustic reflector, a stacked configuration of different materials with positive and negative temperature derivatives of the stiffness constant. Silicon Dioxide (SiO_2) is the most common choice whose layer thicknesses are designed to compensate the temperature derivatives of the other materials. However, SiO_2 has a potential impact on the generation of harmonics and intermodulation products (IMD) [1].

This work describes the role of the SiO_2 in the generation of IMD3 due to its nonlinear stiffness constant, and also the impact that it has on the IMD3 arising from self-heating mechanisms.

The paper starts in Section II by recalling the electro-thermo-mechanical model described in [2]. All the intrinsic nonlinear sources coming from the piezoelectric layer [2]-[4], and from the other electrodes and acoustic reflector [1] are considered. Section III briefly introduces the IMD3 generation by intrinsic and by thermal effects, and how they can be discerned. It also recalls about the materials in charge of generate intrinsic IMD3. Section IV describes the two resonators measured and simulated and their linear responses. Section V analyzes the IMD3 in both resonators due to thermal and intrinsic properties of the materials used in the stack. It also demonstrates how the IMD3 generated by some materials of the stack, cancel each other resulting in a lower observable IMD3.

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II. Electro-Thermo-Mechanical Mason Model

The electro-thermo-mechanical model [2] is able to analyze most of the nonlinear manifestations occurring in SMR BAW resonators. The model is based on the nonlinear distributed Mason model described in [3], [4] to which [2] coupled the thermal domain to account for self-heating IMD3 in a similar way as it was previously done in [5]. Being this model completely reported in [2], here we outline the constitutive equations that the field magnitudes must fulfill at each unit-cell of the discretized model, either in the piezoelectric layer or any layer comprising the resonator.

The electro-thermo-mechanical constitutive equations of the piezoelectric layer relate the field magnitudes stress T, strain S, electric field E, electric displacement D and temperature θ to each other using the constants $c^{E\theta}$, e^{θ}, $\varepsilon^{S\theta}$, τ^E, ρ^S, which are the stiffness, piezoelectric, dielectric, thermal pressure and pyroelectric constants respectively, and can be read as:

$$\begin{aligned} T &= c^{E\theta}S - e^{\theta}E - \tau^{E}\theta + \Delta T_{NL}, \\ D &= e^{\theta}S + \varepsilon^{S\theta}E + \rho^{S}\theta + \Delta D_{NL}, \end{aligned} \tag{1}$$

where the nonlinear terms ΔT_{NL} and ΔD_{NL}, considering only the dominant nonlinear coefficients detailed in [2], are

$$\begin{aligned} \Delta T_{NL} &= c_2^{E\theta}\frac{S^2}{2} + \varphi_6 S\theta + \varphi_5 SE + c_3^{E\theta}\frac{S^3}{6} + \chi_7\frac{SE^2}{2} - \chi_9\frac{S^2E}{2} \\ &\quad - \varphi_7 E\theta, \\ \Delta D_{NL} &= \varepsilon_2^{S\theta}\frac{E^2}{2} - \varphi_5\frac{S^2}{2} + \varphi_2 E\theta + \varphi_3 SE - \chi_7\frac{S^2E}{2} + \chi_9\frac{S^3}{6} \\ &\quad + \varphi_7 S\theta, \end{aligned} \tag{2}$$

All the constants appearing in (2) are nonlinear coefficients of the piezoelectric material, Aluminum Nitride (AlN) in our case, which provoke specific frequency patterns of harmonics or intermodulation products. These specific patterns are very useful to establish the characterization processes [1]-[4], which foresee to discern which parameters are dominant in the generation of a given Harmonic or IMD product in a certain range of frequencies.

For the non-piezoelectric layers, the nonlinear equations relating S, T and θ can be written as

$$T = c_{NP}S + T_C, \qquad (3)$$
$$T_C = \frac{1}{2}c_{2,NP}S^2 + \frac{1}{6}c_{3,NP}S^3 + \varphi_{6,NP}S\theta,$$

where the subscript *NP* indicates a given material from which the resonator is formed.

Equations (2) and (3) are the basis of the nonlinear distributed Mason model [1]-[4]. Figure 1 shows a unit-cell of the piezoelectric material. The nonlinear sources T_C and V_C appearing in the acoustic and electric branch respectively come from arranging (1) to get S and D as the independent variables instead of S and E, as the Mason model requires [3].

The BAW resonator is emulated by cascading many of these unit-cells and those corresponding to the other layers [1].

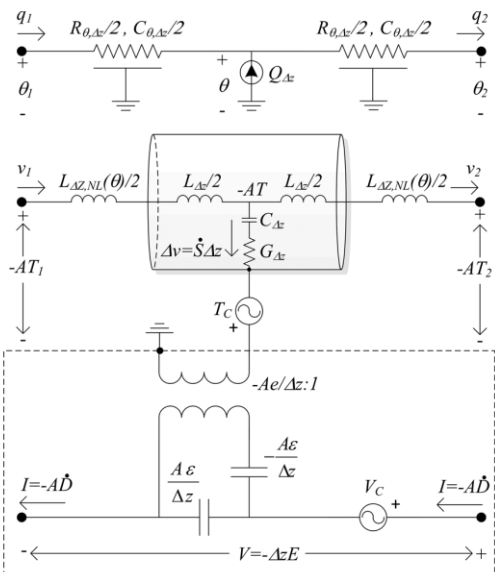

Fig. 1. Nonlinear unit cell of the piezoelectric layer [2].

III. IMD3 Generation

As stated in the introduction, this work focuses on the IMD3 generation by intrinsic nonlinearities, that is the nonlinear terms of (2) and (3) that do not depend on θ, or by self-heating mechanisms in the device [2].

A. *Intrinsic IMD3 generation*

References [1]-[4] reported the most important materials and their corresponding nonlinear coefficients generating intrinsic H2 and IMD3. In [3] was established that the responsible of the high peak of H2 around the resonance frequency was the AlN through the parameter φ_5 in (2), and the IMD3 generation was due to its third-order stiffness constant $c_3^{E\theta}$. Later, [1] reported that the SiO_2 layers forming the acoustic reflector of SMR resonators might also contribute to the H2 and IMD3, especially in TC resonators. In particular, the second-order stiffness constant $c_{2,SiO}$ plays a significant role not only in the generation of H2, but also in the IMD3 generated by remixing effects, in which the second harmonics and IMD2 product in a two-tone experiment are remixed again with the fundamental signals to produce IMD3.

B. *IMD3 generated by self-heating effects*

It is well known that self-heating effects can also produce IMD3. The heat generated by the instantaneous dissipated power of a signal formed by two tones spaced Δf will follow time fluctuations at this frequency Δf [5]. If the separation between tones is small (few tenths of kHz or less), those fluctuations are very slow, being the material able to follow the dynamic variations of the temperature, changing the material properties that are temperature dependent. The Δf-varying material properties will modulate the fundamental signals producing IMD3 distortion. The slower the variation, the higher the IMD3 because of the specific heat of the material that determines the capability of the material to change its temperature under a dynamic heat flux.

Heat propagation is modeled as a lattice RC (thermal resistance and heat capacity) circuit in which current and voltage are equivalent to heat and temperature [5]. The distributed RC network acts as a low-pass filter eliminating the higher frequency components and therefore the IMD3 has a clear dependence with Δf. This dependence allows to discern between intrinsic nonlinearities or self-heating mechanisms if proper experiments are conducted as it is shown in Section V.

IV. BAW Resonators and Linear Measurements

This section briefly describes the two one-port resonators measured in this work and their linear characterization through broadband measurements of the input impedance. Both resonators are TC SMR-BAW resonators designed to operate at the LTE-B30 band. These resonators are referred as RSER and RSHU through the paper, and they were respectively designed as series and shunt resonators in a ladder filter topology. Both resonators are AlN resonators with the same layer configuration. The acoustic reflector alternates Tungsten (W) and Silicon Dioxide (SiO_2) layers and the electrodes are based in Aluminum Copper (AlCu) and W. The difference between both resonators is the layer thicknesses, which cannot be disclosed for confidential reasons.

At this point, it is important to recall that the only material that has a positive temperature-dependent coefficient, φ_6 in (3), is the SiO_2. In TC resonators, SiO_2 thicknesses are designed in order to compensate the temperature derivatives of the other layers. For this reason, SiO_2 layers are thicker than in other resonators.

In any nonlinear characterization process, the first step is to accurately model the broadband linear response of the device. In particular, in this case the viscosity of the materials must be also adjusted because it defines the losses in each layer and therefore the generated heat. The material losses are adjusted in the model to emulate the Q factors of the spurious resonances appearing in the broadband measurement. The frequency pattern of the IMD3 generated in the resonator, depend on those spurious resonances, so a proper modeling of them is required [1]. To illustrate this, Fig. 2 depicts the agreement between measurements and simulations of the linear response of the RSHU resonator.

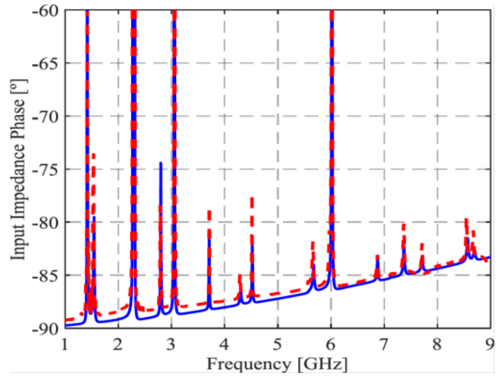

Fig. 2. Measured (dashed-red) and simulated (blue) input impedance phase of the RSHU resonator.

V. Nonlinear Measurements

This section provides a characterization of the nonlinear response to discern the origin of the IMD3, either it comes from intrinsic nonlinearities of the materials, or from self-heating mechanisms. The procedure consists on 2-tone (f_1 and f_2) experiments, sweeping the separation, $\Delta f = f_2\text{-}f_1$, between them, and measuring the IMD3. The distributed nonlinear model consists in discretizing the resonator in 60 unit-cells for the piezoelectric layer, and 100 unit-cells for the other layers forming the stack, in order to follow properly the field magnitude distribution along the stack at any frequency of interest. Two different experiments have been analyzed.

A. *First experiment (fixed f_1 and swept f_2)*

The first experiment, consists on feeding the one-port resonators with two fundamental tones, f_1 and f_2, in which f_1 remains fixed at 2.33 GHz and f_2 is swept around f_1. The input power to the device of the fundamental signals is 21 dBm. The reflected signal is measured, capturing the IMD3 generated inside the resonators. This experiment allows to identify the intrinsic nonlinear material constants that are the main contributors to the IMD3. In this experiment, the thermal effects do not have a significant impact due to the large separation between tones, which is 2 MHz.

Figure 3(a) and Fig. 3(b) depict the measured and modeled IMD3 responses for RSER and RSHU resonators, respectively. The nonlinear parameters used in the model are the same than those reported in [1] providing a good agreement with the measurements. Figure 3 also plots the isolated contribution of the AlN and SiO_2 layers. As it can be observed, the IMD3 is due to the contribution of both materials, producing some cancellation between them at some frequencies. At the same time, it can be observed how the SiO_2 layers are the main responsible of the spurious peak appearing at 2.24 GHz and 2.26 GHz, for RSER and RSHU respectively. As detailed in [1], the IMD3 produced by the SiO_2 layers, seems to be generated by second order nonlinear terms, producing H2 at higher frequencies. At the H2 frequencies a spurious resonance (see Fig.2) exits that enhance the H2 level. This H2 is remixed with the other fundamental signal causing IMD3.

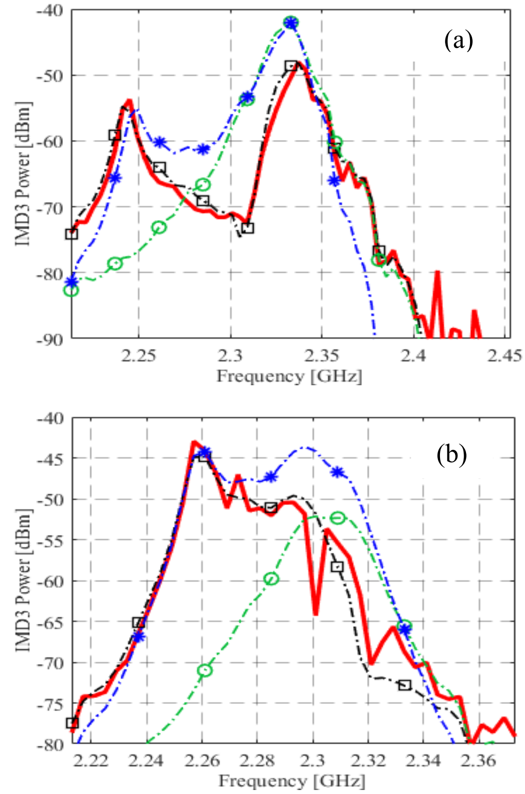

Fig. 3. IMD3 ($2\cdot f_1\text{-}f_2$) measurement and simulations sweeping f_2 and f_1 remaining fixed at the central frequency of 2.33 GHz for resonator RSER (a) and RSHU (b). Measurement (thick red), simulation (black squares), only AlN coefficients (green circles) and SiO2 coefficients (blue asterisks).

B. *Second experiment (Δf-sweep)*

In the second experiment, the central frequency of the two tones remains fixed at a given frequency, and the separation Δf between tones is swept, going from a few hertz up to 40 MHz. This experiment allows us to evaluate the IMD3 due to thermal effects.

First of all, we have measured the IMD3 of the resonator RSER. The central frequency remains fixed at 2.33 GHz, the frequency in which the intrinsic IMD3 is maximum accordingly with the previous experiment.

Figure 4 depicts the measured and simulated IMD3 (only the IMD3 at $2\cdot f_1\text{-}f_2$ is shown for simplicity). The profile of the thermal RC network and its low-pass behavior can be clearly seen from few hertz's up to 1 MHz. This indicates that the IMD3 comes from self-heating mechanisms. For tone spacing larger than 1 MHz, the IMD3 level generated by thermal effects is lower, and the intrinsic IMD3 dominates. The temperature derivatives considered for the AlN are φ_2=195$\cdot 10^{-6}\cdot \varepsilon^{S\theta}$, φ_7=$10^{-6}\cdot e^{\theta}$ and φ_6 = -119.4$\cdot 10^{-6}\cdot c^{E\theta}$. The used values for the other materials are $\varphi_{6,SIO2}$=291.9$\cdot 10^{-6}\cdot c^{E\theta}$, $\varphi_{6,W}$=-136.5$\cdot 10^{-6}\cdot c^{E\theta}$ and $\varphi_{6,\mathrm{AlCu}}$ =-727.5$\cdot 10^{-6}\cdot c^{E\theta}$.

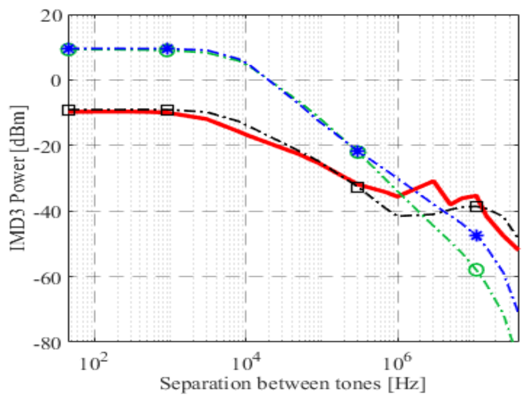

Fig. 4. IMD3 ($2{\cdot}f_1$-f_2) measurement and simulations sweeping the separation between tones at the central frequency of 2.33 GHz for resonator RSER. Measurement (thick red), intrinsic and thermal effects (black squares), thermal effects produced by positive temperature-dependent coefficients (blue asterisks) and thermal effects produced by negative temperature-dependent coefficients (green circles).

Analyzing separately the IMD3 generated by thermal effects, this is, the IMD3 due to only the temperature- coefficient of the SiO_2 on one hand, and the one generated by all the other temperature derivatives on the other hand, it is observed that the simulated IMD3 levels are higher than the measured IMD3. It is clear then that the IMD3 due to thermal effects is cancelled in the TC resonators. Note that designing the TC stack to compensate changes of the ambient temperature, does not necessarily implies that the IMD3 was cancelled. The temperature profile trough the stack of materials might be different for variations of the steady ambient temperature than for heating sources (losses) distributed through the stack.

The same experiment has been carried out for the RSHU resonator. The central frequency was fixed at 2.29 GHz. Figure 5 (a) shows that the nonlinear temperature coefficients found in this work fits quite well the measurements also for this resonator. As in the RSER resonator, the isolated contribution of the SiO_2 and the other materials overestimates the measured IMD3. The cancellation in this case is even higher than in the previous case, being more than 30 dB.

One last experiment has been done. Figure 5 (b) shows the IMD3 response for the RSHU resonator when the central frequency is set up at 2.33 GHz (close to its shunt resonance). In that case, the measured IMD3 is 20 dB lower than in the previous case but still the cancellation effect is significant.

VI. Conclusions

This work demonstrates that a good characterization of the nonlinear response on BAW resonators helps to identify the contribution to the IMD3 of the materials forming the stack, discerning between thermal and intrinsic IMD3 generation. Finally, it demonstrates how SiO_2 layers, besides help to avoid frequency shift in the linear response due to temperature changes, also cancel the IMD3 signals generated in the AlN layer, improving the performance of the resonators.

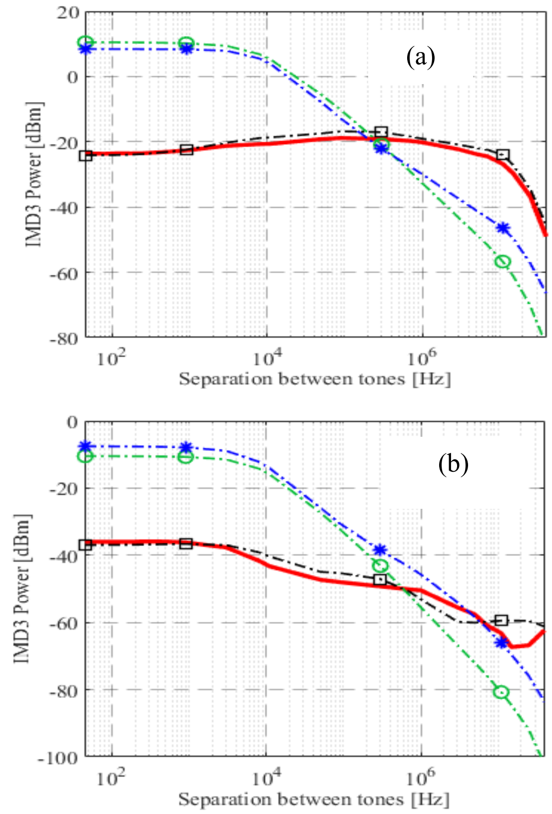

Fig. 5. IMD3 ($2{\cdot}f_1$-f_2) measurement and simulations sweeping the separation between tones at the central frequency of 2.29 GHz (a) and 2.33 GHz (b) for resonator RSHU. Measurement (thick red), intrinsic and thermal effects (black squares), thermal effects produced by positive temperature-dependent coefficients (blue asterisks) and thermal effects produced by negative temperature-dependent coefficients (green circles).

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