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Novel millimeter-wave gas sensor using dielectric resonator with sensitive layer on TiO_2

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***Abstract*— A new generation of gas sensors that operates at millimeter-wave frequency range is presented. The sensor uses a dielectric resonator operating with whispering-gallery modes. Here the dielectric resonator is covered by TiO_2 thin film as sensitive layer. A gas or humidity adsorption makes the TiO_2 dielectric permittivity changing and such changing modifies the resonant frequencies of high-Q whispering-gallery modes within the dielectric resonator. From the measurement of these resonant frequencies the humidity concentration can be derived. Here, the proof of concept is demonstrated through full wave electromagnetic simulations. This humidity (gas) sensor can be remotely interrogated and has great potential for wireless sensing network applications.**

I. INTRODUCTION

The explosion of the market telecommunications allowed the emergence of new wireless gas sensors operating at microwave and millimeter frequencies [1]. The existing semiconductors sensors generally composed by sensitive layer such as TiO_2, SnO_2, WO_3, etc, are well-known due to their high sensitivity for gases and low cost production. In presence of gas, the electrical properties of these materials change and lead a modification in their conductivity. This kind of sensor operates at high temperatures which increases their power consumption. Their operating mode at low frequencies requires techniques of modulation to insure the wireless connection and consequently, the system becomes cumbersome and requires batteries and power supplies [2, 3].

In microwave domain, the dielectric resonator is a good candidate for gas detection due to its large surface area and sensitivity for external environments. These main issues raised potential to be used a very high efficient structure in this context [4]. The excitations of the dielectric resonator (DR) with Whispering-Gallery Modes (WGM) have many advantages over the conventional excitation Transverse Electrical (TE) or Transverse Magnetic (TM) modes. DR operating with WGM has relatively large dimensions and a higher quality factor Q. Moreover, it can be excited differently, and can run in the azimuthally direction, that gives it potentialities to detect gas perturbation in every directions. In this study, we design and simulate a DR structure coupled with microwave waveguides in coplanar technology. This coupling allows very high selective performances [5].

The TiO_2 is used here as the sensitive layer, as it is very sensitive to gas adsorption. Moreover, this metal oxide presents permittivity relaxation at very high frequencies due to the presence of gases, which could be exploited to build a new detector in the microwave and millimeter-wave regimes [6, 7].

II. DESIGN OF THE GAS DETECTOR BASED ON WHISPERING-GALLERY MODES

In this study, we design and simulate a dielectric resonator structure that incorporates a TiO_2 sensitive layer coupled with microwave waveguides in coplanar topology for high performance in term of gas sensitivity.

The proposed resonator-based sensor is shown in Fig.1 (a). It consists of two main blocks: the coplanar waveguides (CPW) (see fig.1 (b)) used for electromagnetic propagation and the DR with TiO_2 layer used for gas detection (see fig.1 (c)). These two parallel CPW are deposited over a SiO_2/SiN_x membrane with Ti/Au metallization with ε_r=1.09, L=13mm, W=300µm, S=30 µm and H_{metal} =1µm. The CPW impedance characteristic is 75Ω. We choose the DR material composition with BaSmTiOxide from TEMEX CERAMICS because it presents high Q-factor, and high temperature stability [8]. The DR characteristics are the following: dielectric constant equals to 78, typical Q-factor around 1600 at 5GHz, diameter D_{DR} =6.5 mm and thickness H_{DR} = 350µm. The DR is mounted above the coplanar lines by using Al_2O_3 dielectric spacer (ε_r=9.8) [8] with diameter D_{spacer}=2.7mm and height H_{spacer}=260µm. From full wave electromagnetic simulations, the dimensions of the spacer leads to the desired electromagnetic coupling between the WGM modes in the DR and the fundamental quasi-TEM mode in the two CPW (H_{spacer} =230 µm and H_{spacer} =280µm).

We choose TiO_2 material as film layer with relative dielectric permittivity of 80 [9] and with thickness of H_{TiO2}=10µm. The whole sensor is laid out on a high resistive silicon substrate with ε_r=11.6 and thickness of H_{Si}=350µm. In order to work with the band-pass filter between port 1 and port 3, the ports 2 and 4 are shunted by standard 50Ω-impedances.

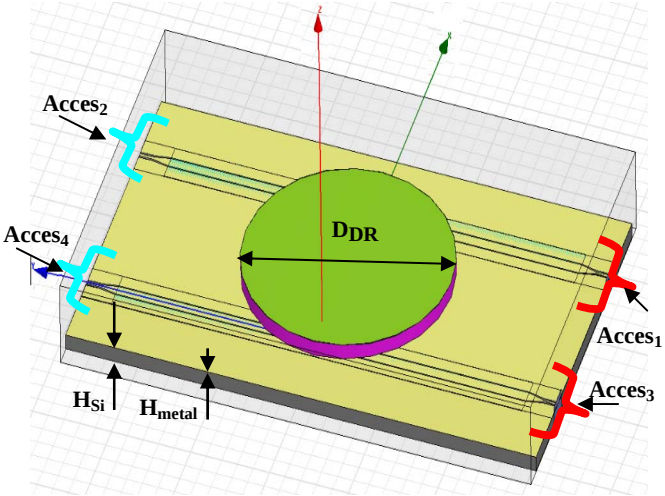

Figure 1. (a) Sensor schematic concept: Cell used to measure the gas concentration.

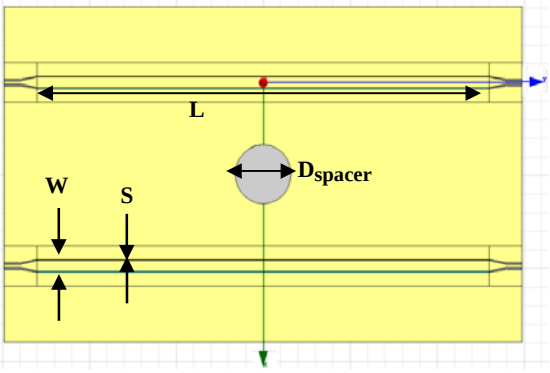

Figure 1. (b) Two coplanar lines micro-machined;

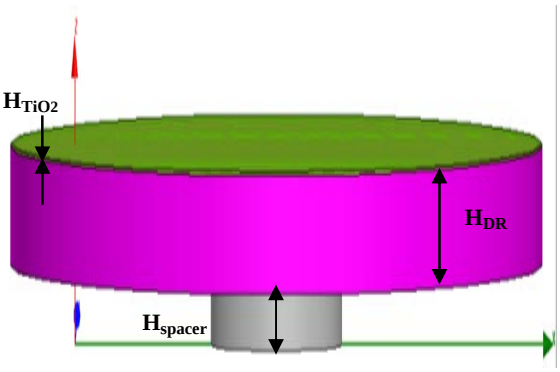

Figure 1. (c) Dielectric resonator with sensitive layer TiO_2 and spacer.

III. Description of the Detection Principle and Simulation Results

Figure 2 shows the functionality of the structure in large operating millimeter-wave frequency band. The DR operating with $WGH_{6.2.0}$ shows a resonant frequency at 33.24GHz with a quality factor of 370. We chose this frequency because there is low insertion losses (-5.70dB) and provides a good coupling between CPW quasi-TEM mode and the WGM in the DR. The magnitude of this coupling is depicted versus frequency in Figure 2. There is a significant coupling magnetic field between the coplanar waveguides and the dielectric resonator.

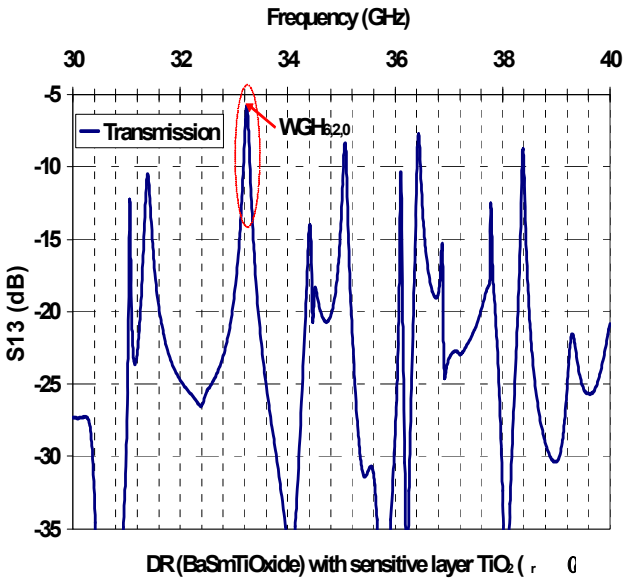

Figure 2. Simulation results of the structure coupling coefficient (magnitude of S_{13}) using full-wave electromagnetic simulation (HFSS™).

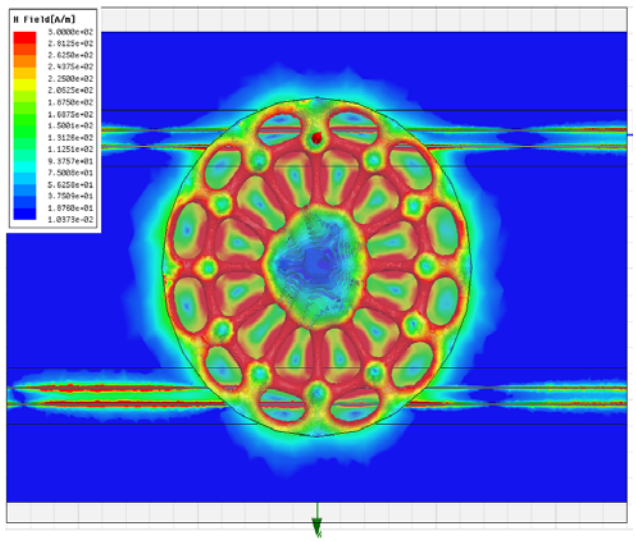

Figure 3. Amplitude of the $WGH_{6,2,0}$ mode magnetic field at resonant frequency 33.24 GHz.

The magnitude of the $WGH_{6.2.0}$ magnetic field at this resonant frequency (33.24GHZ) is depicted in Figure 3 and shows a characteristic distribution of Whispering-Gallery Modes.

IV. Influence of Humidity on the Sensor

Thanks to results reported in literature, the permittivity of TiO_2 material depends on the humidity (H_2O) [10]. For example, in presence of H_2O the dielectric permittivity of TiO_2 tends to decrease by 18%. To analyze the impact of this change in permittivity on the resonant frequency of the WGM, we perform full-wave electromagnetic simulations based on the Finite-Element Method (HFSS™) [11] by adopting relative dielectric permittivity taken between 70 and 90. This variation is found to be 10% on the permittivity of TiO_2. As shown in Figure 4, the resulting resonant frequency of WGM-based resonator takes values that can reach almost 7% on the resonant frequency of the $WGH_{6,2.0}$ mode.

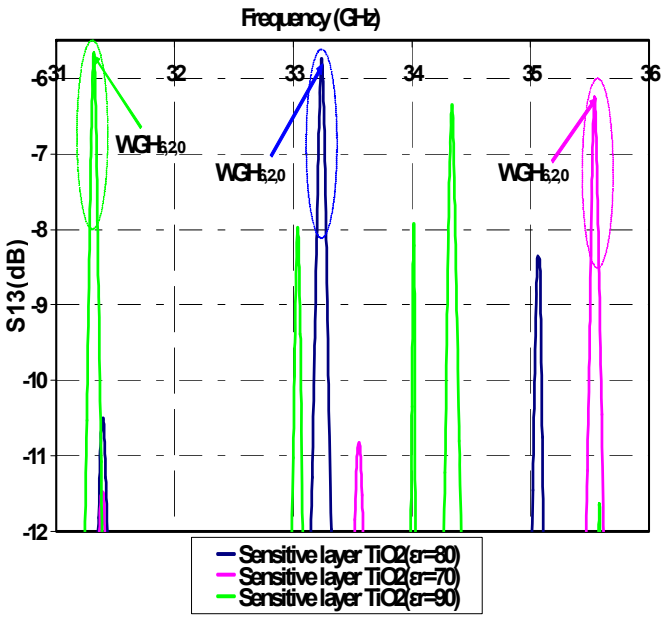

Figure 4. Transmission coefficient at the $WGH_{6.2.0}$ mode in presence of H_2O.

The absorption of another gaseous molecule can generate the same effects, thus we can conjecture that we can design an excellent sensor of gas in the broad sense. Experimental validations are under way.

Moreover we have recently shown an example of detection of ethylene gas with a sensitive layer SnO_2 and keeping the same design of the presented detector [12].

V. Conclusion

The potentialities of a novel gas sensor using Whispering-Gallery Modes have been proved thanks to full wave electromagnetic simulations. The high sensitivity in the frequency response of the proposed gas (humidity) detector device based on high-Q Whispering-Gallery Modes is very interesting for developing unique gas detection with ease of integration of the radio-frequency function. These Gas sensors are now under fabrication and experimental validation will be available soon.

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