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Novel Approach for Modeling an Ionic Imprinted Polymer Based SAW Sensor with COMSOL Multiphysics †

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Abstract: Modeling a Surface Acoustic Wave (SAW) sensor response as a chemosensor and not only as just an electronic transducer was performed with COMSOL Multiphysics. For this study, the SAW's sensing area was functionalized with an ionic imprinted polymer (IIP), designed for the selective detection of lead ions. The idea consists in subdividing the IIP into elementary blocks whose physical properties can be modified separately. Three configurations have been envisaged: the IIP before and after lead ions extraction and the non-imprinted polymer (NIP). The generation of shear-horizontal waves on LiTaO3 piezoelectric substrate is confirmed by recording the displacement amplitude versus time, according to the three space directions. The sensors sensitivity is estimated from the delays induced by the incorporation of the lead ions in the IIP layer. To the best of our knowledge, this approach has never been presented in the literature.

Keywords: SAW sensor; chemosensor; Non-imprinted polymer; ionic imprinted polymer (IIP); IIP before extraction; IIP after extraction; lead ions

1. Introduction

SAW sensors are more and more investigated to detect chemical and biological species in liquid media. The principle is based on monitoring either acoustic waves velocity variations, or wave attenuation. Depending on the chosen design, these variations imply changes in frequency or phase and delay times. Considerable attention has been paid to modeling SAW's responses to understand the characteristics of surface acoustic waves generated in SAW devices. Using COMSOL Multiphysics, 2D finite element models of SAW sensors based on piezoelectric thin films of aluminum-nitride (AlN) or zinc-oxide (ZnO) [1] and of YZ Lithium Niobate [2] were developed. Other works were focused on modeling a 3D Love wave based SAW sensor when considering SiO2 [3] and ZnO [4] as guiding layers.

This original study concerns the 3D simulation, using COMSOL Multiphysics, of a SAW sensor functionalized with a Pb(II) imprinted polymer. The ion imprinting technique consists in creating artificial recognition sites in polymeric matrices which are complementary to the ionic template in terms of size, shape and spatial arrangement of the functional groups. Our interest in Pb(II) has been dictated by the fact that this ion has always been linked to ecological and public health problems. Its high toxicity and omnipresence in rivers, wastewaters and even in drinking water, as revealed in Flint crisis, have made it one of the most investigated heavy ions.

Simulation method and results are presented in the following sections.

2. Materials and Methods

A 3D SAW sensor model was built on a 36°rotated Y-cut lithium tantalite piezoelectric substrate (LiTa03) through the COMSOL software. The device is a delay line with a pair of interdigital transducers (IDT) which serve to generate and receive the acoustic waves. Both the IDTs and the sensitive area, the zone separating the IDTs, are made of 100/238 pm Cr/Au thin layers on LiTaO3 substrate.

To simulate an IIP-based SAW, the sensing area was subdivided in elementary blocks whose physical properties can be modified separately and whose dimensions are equal to that of a Pb^{2+} ion. Three configurations have been considered: a non-imprinted polymer (NIP) where all the elementary blocks were filled with a polymeric material, IIP where some of blocks are filled with lead ions (IIP before extraction) or with vacuum (IIP after extraction). Periodic boundary conditions were applied along the z axis in order to simulate the entire device with a reduced geometry. Free tetrahedral mesh was created on the Cr/Au thin layers while, a swept mesh was applied on the sensitive layer (Figure 1).

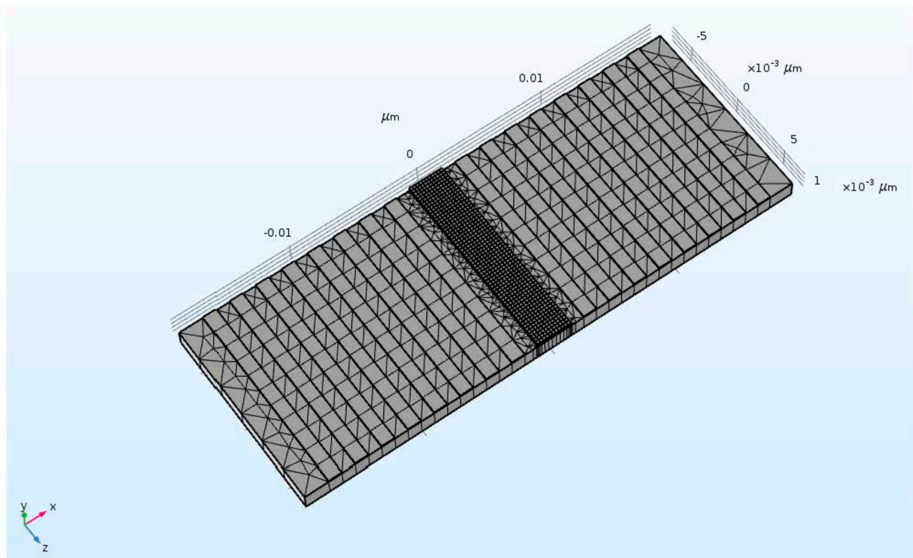


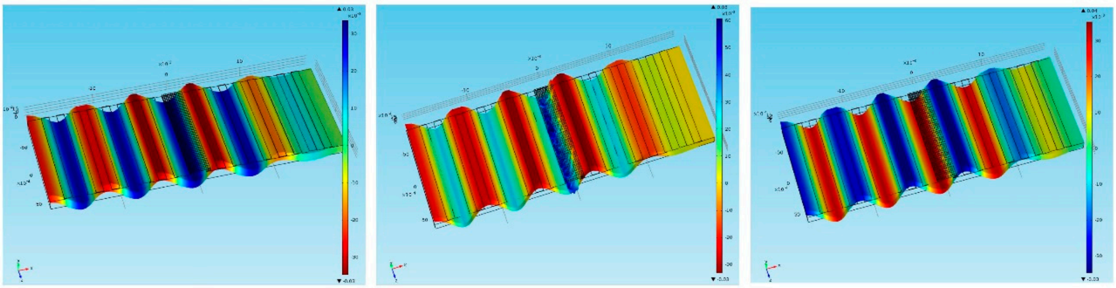
Figure 1. The mesh geometry.

3. Results

A 8MHz SAW sensor was chosen for investigation in this paper. The thickness of the sensitive area is 338 pm. A transient analysis is performed through COMSOL software to obtain the displacements and output voltages versus time.

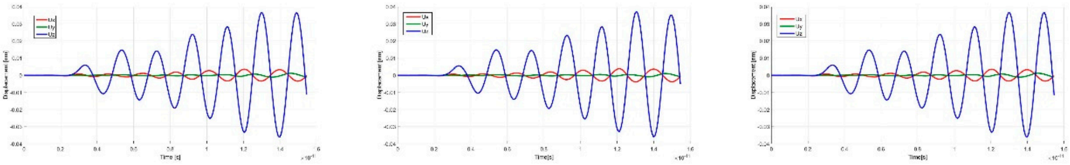
Figure2 reports the 3D field displacements for NIP and IIP before and after extraction (images correspond to 3 snapshots at 9.63 ps).Their further displacement's amplitudes in the three directions, versus time, are presented in Figure 3a–c. The same emplacement has been considered. Results indicate that in all considered cases, the in-plane horizontal displacements are more important than the vertical ones, confirming thus the shear-horizontal nature of the generated waves.

Further calculations have concerned comparison between a NIP/SAW sensor and a non-extracted IIP/SAW one. Results indicate that acoustic waves generated in the first configuration are in advance by about 47 fs, with respect to the second one. This delay corresponds to an equivalent phase shift of about 8.71°. Compared to a non-extracted IIP/SAW senor, the extracted one is in advance by about 49 fs, which corresponds to 9.08°phase shift.



(a) Non-imprinted polymer **(b)** IIP before extraction **(c)** IIP after extraction

Figure 2. Snapshots of the displacement in z direction at 9.63 ps for: (**a**) the non-imprinted polymer. (**b**) the IIP before extraction. (**c**) the IIP after extraction.



(a) Non-imprinted polymer **(b)** IIP before extraction **(c)** IIP after extraction

Figure 3. Displacement's amplitudes in the x, y and z directions with time for: (**a**) the non imprinted polymer (NIP), (**b**) the IIP before extraction and (**c**) the IIP after extraction.

Table 1. Comparison results of NIP/SAW sensor to IIP/SAW device before and after extraction.

	IIP/SAW Device before Extraction	IIP/SAW Device after Extraction
Delay(fs)	47	49
Shift Phase (°)	8.71	9.08

To calculate the mass sensitivity S of the IIP/SAW sensor, the number of the extracted ions was varied. The variation of output voltage compared to IIP after extraction is shown in Figure 4. Sensitivity was computed from the slope of time delay/mass curve and was found of order of 1.5504 s/pg.

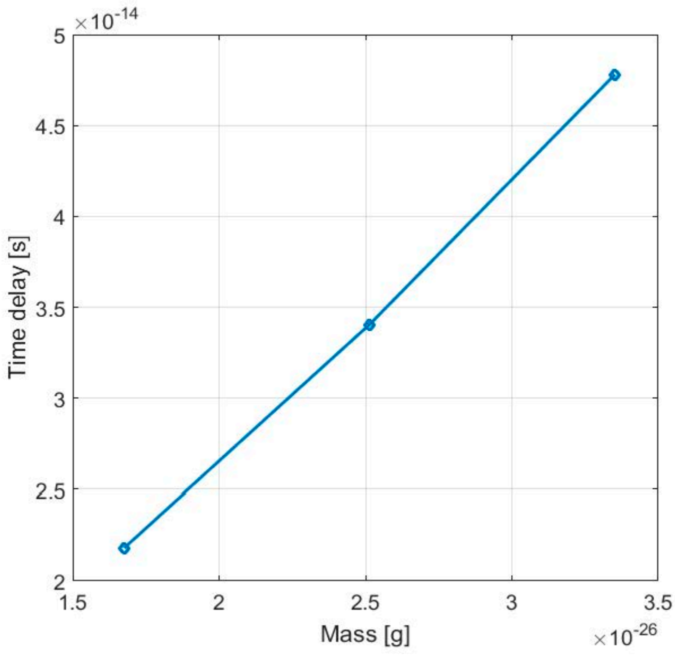


Figure 4. The mass sensitivity of the IIP/SAW device.

Experimental measurements will be conducted in order to confirm these theoretical results.

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Conflicts of Interest: The authors declare no conflict of interest.

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