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Numerical Analysis and new formulas of the response stage, on recovery step, of a new SAW Structure with disappeared layer RR-P3HT in detection DMMP

Tomasz Hejczyk[1], Jarosław Wrotniak[2], Paulina Powroźnik[3], Wiesław Jakubik[3]
[1] The Academy of Creative Development – the Foundation Marklowice, Poland,
[2] Institute of Electronics, Silesian University of Technology, Gliwice, Poland
[3] Institute of Physics CSE, Silesian University of Technology, Gliwice, Poland
Corresponding t.hejczyk@ente.com.pl

Summary:
This document presents the results of numerical analyses of the SAW gas sensor in the non-steady state. The effect of SAW velocity changes depending on how the surface electrical conductivity of the sensing layer is predicted. The conductivity of roughness sensing layer above the piezoelectric waveguide or quartz depends on the profile of the diffused gas molecule concentration inside the layer. Numerical results for the profile concentration gas DMMP (CAS Number 756-79-6) for layer (RR)-P3HT in the non-steady state in recovery step are shown. The main aim of the investigations was to study the thin film interaction with target gases in the SAW sensor configuration based on diffusion equation for polymers. The numerical results based on the code written in Python, are described and analyzed.

Keywords: gas sensor, numerical modeling, SAW gas sensor, Ingebrigtsen's formula, DMMP, (RR)-P3HT, numerical acoustoelectric analysis (NAA)

Introduction

The main aim of the investigations was to study thin film interaction with target gases in the SAW sensor configuration based on simple reaction-diffusion equation [1]. Diffusion equations provide theoretical bases for analyses of physical phenomena like heat transport or mass transport in porous or roughness substrate. The paper summarizes the acoustoelectric theory, i.e. Ingebrigtsen's formula, dynamics gas diffusion concentration profiles, and predicts in recovery steps the influence of a thin layer RR-P3HT [2] on the SAW wave velocity in a acoustic waveguide.
Diffusion of gas molecules into the sensor layer will change its physical properties, especially the electrical conductivity. This effect causes a change in boundary conditions for wave propagation. There is a change in wave attenuation, and a change in the velocity of propagation. In SAW sensors there may occur two effects: electrical (acoustoelectrical) and mass effect. In this paper we considered only the electrical effect, important in a sensor with a conducting sensor layer. The behavior of the gas concentration profile DMMP under non-steady-state conditions during recovery steps (see Fig. 1) was presented. The paper presents only final equation describing time – dependent concentration profiles in the recovery step – DMMP profiles.

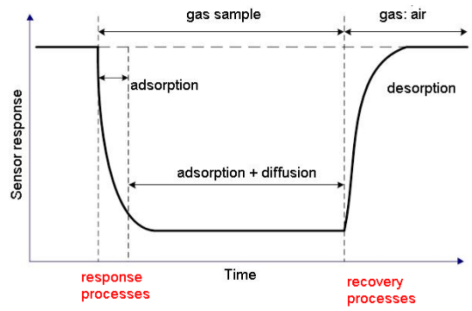

Fig. 1. Gas diffusion dynamics in the response on recovery step processes of a thin layer RR-P3HT gas sensor of DMMP

Model of a gas sensor and influence of the diffusion gas on the acoustoelectric effect

The diffusion of gas particles into the sensor layer causes the formation of a certain profile of the distribution of concentration of these particles deep into the layer. The phenomenon of the diffusion of gas into the sensor layer is of essential importance in the case of porous or rouhgness layer with a developed surface. Such layers are built up in expressly performed technological processes.

In order to optimize the structure of the sensor it is important to get an analytical model of the SAW sensor. A stationary model will be supplemented by time dependences permitting investigations concerning the dynamic characteristics of SAW gas sensor.

In a sensor with an acoustic surface wave (SAW) the optically sensitive active sensor layer is deposited on a quartz [2]. In sensors which operate basing on the acoustoelectric phenomenon the electric conductivity of the sensor layer is affected by the ambient gas. This process becomes essential when the layer is porous or roughness. Of special importance is in the case of Knudsen's diffusion, when the diameter of the pores amount to 1–100 nm. Practically, Knudsen's diffusion is most essential in the application of sensors. The profile of the concentration of the gas molecules in the layer conditioned by value of the ratio of the constant reaction rate *k*, polymer parameters like: *B, s,* and the coefficient of diffusion D_K but numerical analysis and it's accuracy depend from number of iterations *n* *(see Fig 3).*

The diffusion is a kinetic phenomenon, depending on time. The profile of the distribution of gas molecules in the layer changes, therefore, with the lapse of time as well as in transient and recovery step. Time analysis of this phenomenon permits to test regeneration of the sensor as a function of time.

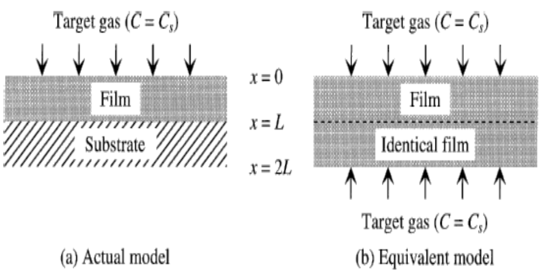

Fig. 2. Actual a) and equivalent model b) on recovery step [1]

The distribution of the concentration of gas molecules in the layer is the function of time *t* and the depth *x* in a resistance sensor (see Fig. 2), making use of Fourier's transformat, has been dealt with N. Matsunaga [1]. In this paper was expressing the concentration *C(x,t)*, in recovery step [1] basis on polymer layer, using general diffusion patterns adapted to the phenomenon: eg. (1,2).

$$\frac{\partial C(x,t)}{\partial t} = D\frac{\partial C^{2}(x,t)}{\partial x^{2}}_{\square} - kC(x,t)_{\square} - Bs\frac{\partial C^{\square}(x,t)}{\partial x^{\square}} \qquad (1)$$

where the general solution is as follows

$$C(x,t) = v(x,t) + w(x,t) + z(x,t) \qquad (2)$$

Numerical analysis of the acoustoelectric interaction in the sensing layer in recovery step

This problem was analyzed numerically, assuming a constant concentration of the gas molecules at the surface of the sensor layer and in its surroundings. Changes of the relative velocity of the wave were determining numerically, viz. the concentration of the gas molecules on the surface C_s. The analysis was performed in the unsteady state, changing the time within the range from *t*=10^{-15} sec to *t*= 10^{-6} sec in recovery step (see Fig.3).

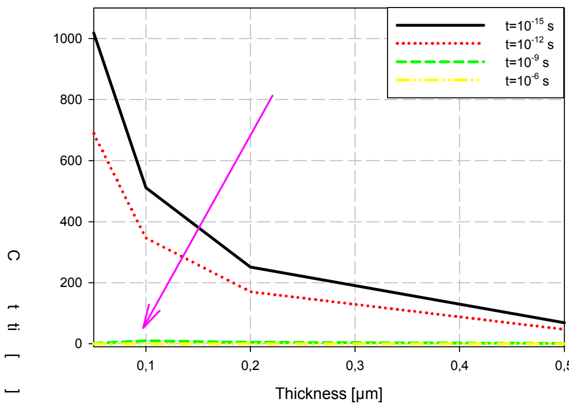

Fig. 3. Numerical results - profiles of the concentration of gas depending on time, thickness 50-500 nm, *B*= 10^5, *D*= 10^6 μm^2 /s, *n*=100, basis on numerical solution eq (1)

Summary

Recovery states are distinctly visible in the range of time from 10^{-9} to 10^{-6} sec.

References

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