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Numerical Analysis and new formulas on steady step of a new SAW Structure with disappeared layer RR-P3HT in detection DMMP

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Summary:
This document presents the results of numerical analyses of the SAW gas sensor in the 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 steady state 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), steady state

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 steady step the influence of a thin layer RR-P3HT [2] on the SAW wave velocity in a acoustic waveguide.
The behavior of the gas concentration profile DMMP under steady-state conditions (see Fig. 1) was presented. The paper presents only final equation describing time – dependent concentration profiles in the steady step – DMMP profiles in exposition on light [2]. Basis on diffusion equations and application convolution on signals we can proving theses to practise Laplace mathematical transformation to solve this problem.

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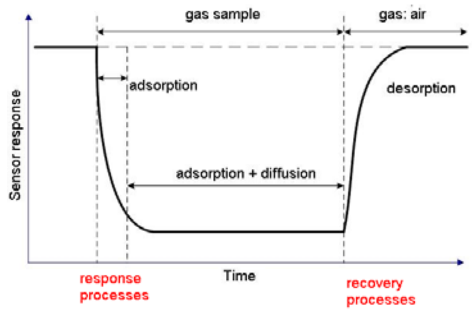

Fig. 1. Gas diffusion dynamics on steady step processes of a thin layer RR-P3HT gas sensor of DMMP – constants part of characteristics between response and recovery stage

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

In the steady state, the system can be considered linear $C(x,t)=C_s$, like an automation system with linear, proportional characteristics, e.g. k_p. This is indicated by the solution presented in the literature [2]. In a sensor with

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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.

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 and steady state. Time analysis of this phenomenon permits to test steady state of the sensor as a function of time in conditions of disappearing pol

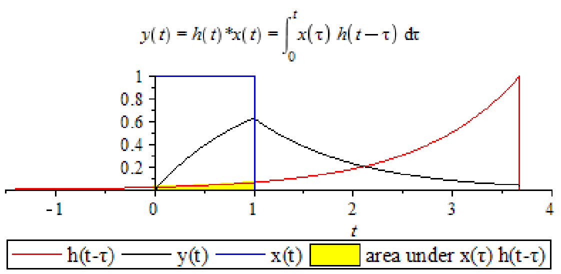

Fig. 2. Convolution of signals

In this paper was expressing the concentration *C(x,t)*, in steady step [1] basis on polymer layer, using general diffusion patterns adapted to the phenomenon: eg. (1,2).

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

where the general solution is as follows

$$C_A = C_1\, exp\left(\frac{\sqrt{4k_1+b_1^2}}{2}x + \frac{b_1}{2}x\right) + C_2\, exp\left(\frac{b_1}{2}x - \frac{\sqrt{4k_1+b_1^2}}{2}x\right)$$

where C_1 C_2 are integral constans

(2)

Numerical analysis of the acoustoelectric interaction in the sensing layer in steady 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. vs. number of kwants, basis on following formula:

$$v(x,t) * g(t) = C_S\frac{\lambda\alpha}{nhc}\left[1 - \exp\left(\frac{-\lambda\alpha}{nhc}\right)t\right]\ v(x,t) \qquad (3)$$

where number of kwants are constant (see Fig. 3), and number of kwants are variable (see Fig. 4).

The analysis was performed in the steady state, changing the time within the range from t=10^{-9} sec to t= 10^2 sec in steady step (see Fig.3).

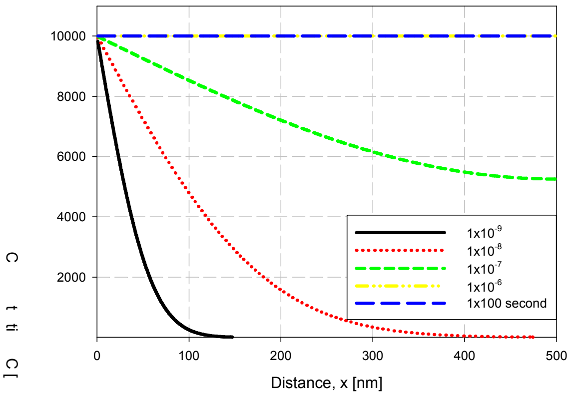

Fig. 3. Numerical results in time – concentration depends charge of light, number of kwants = constans

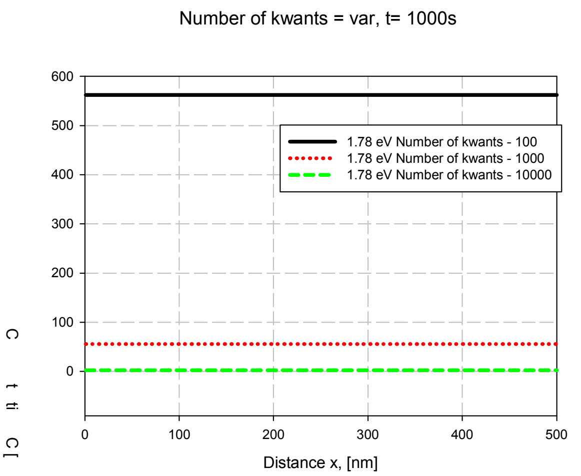

Fig. 4. Numerical results depends from number of kwants – concentration depends charge of light

Summary

Steady states are distinctly visible in the range of time from 10^2 sec.

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