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ALGORITHM FOR PROCESSING GAS SENSOR'S RESPONSE KINETICS DATA USING EXTENDED EXPONENTIAL FUNCTION WITHOUT NUMERICAL DIFFERENTIATION

Abstract. The features of the use of computer technologies for processing experimental data for solving the problems of automation of research of materials for gas sensitive sensors are considered.
An algorithm for processing the kinetic dependence of the response of gas sensors based on the model of an extended exponential function are proposed, which does not use numerical differentiation operations when finding the parameters of this model. This allows to significantly reduce the influence of the presence of data spread in the coordinates of the approximating diagrams that are used in calculating the model parameters, increase the accuracy of their determination and contribute to the implementation of an automated information measuring system for the process of computer processing and analysis of experimental data.
Keywords: gas sensor, response, kinetics, stretched exponential function, algorithm, information-measuring system, software.

Introduction

Computer technologies for processing experimental data have already become widespread in various fields of science and technology. They are used both in studying the well-known problems of high-energy physics and nuclear physics [1], image processing [2], search and creation of new materials [3], and for solving specific scientific and technical problems of studying plasma light sources [4], building intelligent information-measuring systems for monitoring heat-insulating materials [5], etc.

Another specific area where the use of the technologies under consideration seems appropriate is the search and study of materials for gas-sensitive sensors [6].

Studies of this type are associated with the need to process and analyze significant amounts of experimental data. In [7], the prospects for solving such a problem by creating a specialized information-measuring system are shown.

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As is known, one of the key components of the software of such intelligent information-measuring systems is the algorithmization of experimental data processing processes based on the corresponding mathematical models [8-11].

For the primary processing of data obtained in the study of resistive gas sensors in [7,12], a general phenomenological model based on the stretched exponential Kohlrausch-Williams-Wots function $f_{KWW}(t) = exp\left[-\left(\frac{t}{\tau}\right)^{\beta}\right]$, where t – time, β and τ - parameters [13,14]. It was use to describe the kinetics of the relaxation dependences of the response, in particular, at the recovery stage (Fig. 1).

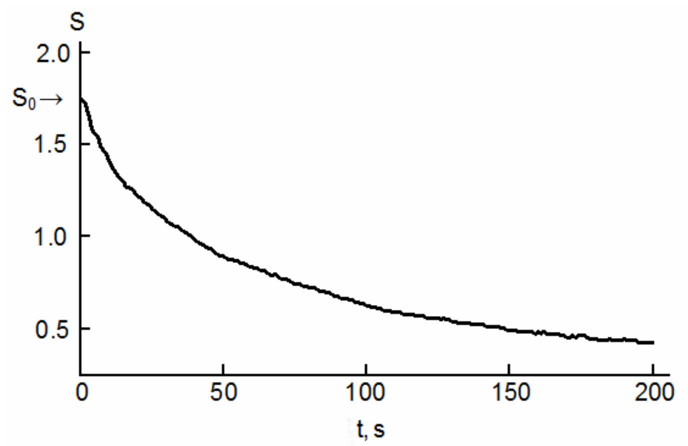

Figure 1 - Typical kinetics of response dependences at the stage of reduction of a sample of a resistive gas sensor (ZnO with the addition of Ag [15])

A distinctive feature of such a model is its suitability for describing relaxation phenomena in disordered systems, in which dynamic processes occur simultaneously in many time ranges [15].

As shown in [6], the use of this approach makes it possible to obtain much more information about the physicochemical phenomena that determine the phenomenon of gas sensitivity of resistive sensor materials. Used in the window application given in [7], it testifies to the reality and efficiency of computer processing of a significant amount of data in the process of carrying out the physical and chemical measurements under consideration. However, the used measurement data processing algorithm does not allow implementing a fully automated specialized IMS in a measuring complex for studying the main characteristics of gas-sensitive sensors. The main reason for this is the need to numerically calculate the derivatives and select the interval in the time dependence of the main parameter, the sensitivity to the active gas, which makes it possible to correctly estimate the parameter β of the KWW function that approximates the sensor recovery kinetics. These functions require participation in the data processing process of the operator [7].

In this paper, we propose and justify an algorithm based on a stretched exponential function, which makes it possible to exclude the participation of the operator in the process of processing and primary analysis of measurement data on the response kinetics of resistive gas sensors.

Description of the algorithm and its features

It should be noted that the data processing algorithm used in [6, 7] does not require any additional assumptions or data. Only the results of measurements of the kinetic dependence S(T) are used in the form of a table (located in a c file of type .txt or .xls). Nevertheless, its disadvantage is the presence of the operation of numerical differentiation when finding one of the resulting data parameters β used in the approximating KWW-function. As a rule, this creates a significant scatter of points in the coordinates of the diagrams of the used approximating dependencies to calculate the specified parameter. As a result, this leads to the fact that it is difficult to implement the automation of the data processing process for the kinetic dependences considered here.

Below it is proposed to use an approach to determining the parameter β, which is based on the assumption of the possibility of correctly fixing the value of the static value of gas sensitivity S_0 by estimating its approximate value in the initial section of its kinetic dependence.

Approximating dependence used as a model for the primary phenomenological analysis of the experimental kinetic dependences of the response of the gas sensitive sensor in the area after the removal of the active gas

$$S(t) = S_0 \cdot exp\left[-\left(\frac{t}{\tau}\right)^{\beta}\right] \tag{1}$$

can be converted to

$$log\left\{-ln\left[\frac{S(t)}{S_0}\right]\right\} = \beta \cdot log(t) - \beta \cdot log(\tau) \tag{2}$$

As follows from (2) in the coordinates $x = log(t)$ and $y = log\left\{-ln\left[\frac{S(t)}{S_0}\right]\right\}$, the considered dependence is a straight line $y - a_0 + a_1 x$, and thus, based on its experimental points in such coordinates, the parameter β of the KWW-model ($\beta = a_1$) can be relatively simply determined without involving the operation of numerical

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differentiation. The coefficients a_1 and a_0 for the considered linear model can be determined by the formulas [16]

$$a_1 = \frac{1}{n} \cdot \left(\sum_{i=1}^{n} y_i - a_0 \sum_{i=1}^{n} x_i \right) \tag{3}$$

$$a_0 = \frac{n \sum_{i=1}^{n} x_i y_i - \sum_{i=1}^{n} x_i \cdot \sum_{i=1}^{n} y_i \cdot}{n \sum_{i=1}^{n} x_i{}^2 - \left(\sum_{i=1}^{n} x_i \right)^2} \tag{4}$$

where i and n are the index for the numbering of readings and their number of experimental kinetic dependence.

However, in the considered approach there is a requirement that the static value of the response S_0 for the studied reduction kinetics be known. In experimental practice, the exact measurement of this parameter is not always possible. On the one hand, this is due to the technically used equipment, that is, the fixation of the considered kinetic dependence begins with a certain time delay, or when the specified static value is not reached within a really reasonable time for a specific experimental study. In connection with this, it is important to study the influence of these factors on the measurement of the value of S_0, in particular, the instrumental error and the time delay of the process of fixing the kinetic dependence considered here.

Influence of inaccuracy of the set parameter S_0

$$log\left\{-ln\left[\frac{S(t)}{S(t_d)}\right]\right\} = \beta \cdot log(t) - \beta \cdot log(\tau) \tag{5}$$

As follows from (5), β can be represented by the coefficient in front of the $log(t)$ argument of the linear dependence of its function $log\left\{-ln\left[\frac{S(t)}{S(t_d)}\right]\right\}$.

On Fig. 2 shows the theoretical dependences of the KWW relaxation model in the proposed coordinates for different β. and the results of the analysis of the influence of the approximate value $S(t_d)$ of the specified parameter S_0 on them.

As can be seen, an underestimated value of S_0 leads to a deviation of the dependence in Fig. 2 from linear only in the range of short times (in this case, less than a few seconds). The results of calculating the value of β in accordance with expression (3) with a different choice of the time range of the data used in Fig. 2 and using the built-in functions of the Mathcad package (slope) are presented in Table. 1.

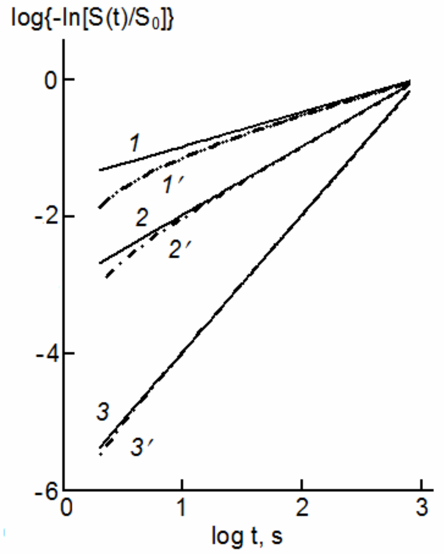

Figure 2 - Theoretical dependences of the KWW relaxation model of the gas sensor recovery response kinetics in the coordinates) (dependencies 1, 2 and 3) and in the coordinates ($log\left\{-ln\left[\frac{S(t)}{S(t_d)}\right]\right\}, log(t)$), where t_d is the delay time for fixing the beginning of kinetics (*1′*, *2′* and *3′*), for parameter values β: 1 and *1′* – 0.5; 2 and 2′ - 1; 3 and 3′ - 2. S_0=100; τ=10 s; t_d =1s

As follows from Table. 1, second column, there is a tendency to some overestimation of the value of the parameter β determined in accordance with the method under consideration at its small values. If the initial part of the kinetic dependence is not used, i.e. to use data for processing starting from a certain time point $t_1 > t_d$ (for example, t_1= 10 s or 1 minute), then the accuracy of determining β can be increased.

Nevertheless, in the range of β from 0.5 to 2, the considered algorithm for processing the kinetic dependence of the response of gas sensors based on the stretched exponential function model allows obtaining adequate results.

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Table 1

Influence on the accuracy of the estimation of the β parameter of the KWW-function selection of the time range for processing the kinetics $S(t)$

Exact value β	Approximate value of β. determined in accordance with (3) by discarding the first points of the initial kinetic dependence $S(t)$ over the time interval		
	t_1=t_d, s	10 s	60 s
0.25	0.374	0.352	0.332
0.5	0.566	0.547	0.533
0.75	0.785	0.771	0.762
1	1.021	1.009	1.004
1.25	1.263	1.254	1.251
1.5	1.508	1.502	1.5
1.75	1.756	1.751	1.75
2	2.004	2	2

Application of the algorithm to the processing of experimental data

On Fig. 3 shows the experimental kinetic dependence of the response at the stage of reduction of a sample of a resistive gas sensor, shown in fig. 1 in coordinates x=$log(t)$ and .

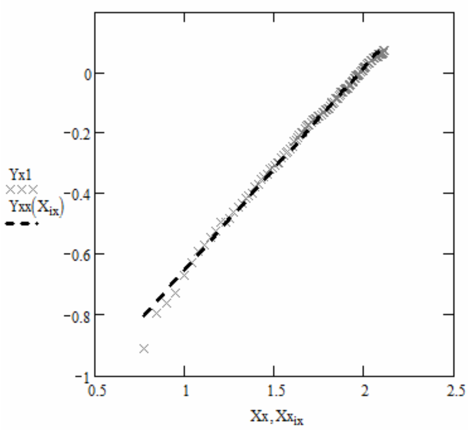

Figure 3 - Dependence of the experimental kinetics of the gas sensor recovery response in the coordinates $log\left\{-ln\left[\frac{S(t)}{S(t_d)}\right]\right\}$ fig. 1 (points - crosses) and its linear approximation used in the considered algorithm for its processing (dotted line)

As can be seen, it satisfies the ideas developed in the previous section. The calculated values of the parameter β^* were 0.643 at t_1 = 10 s and 0.628 at t_1 = 60 s. The estimates coincide with an error of no more than 3%.

Further operations of the algorithm are similar to those given in [12,17,18].

Determination of unknown characteristics τ and S_0 by applying the coordinates $y=ln\ S(t)$ and $x=t^{\beta}$ for experimental data (Fig. 4).

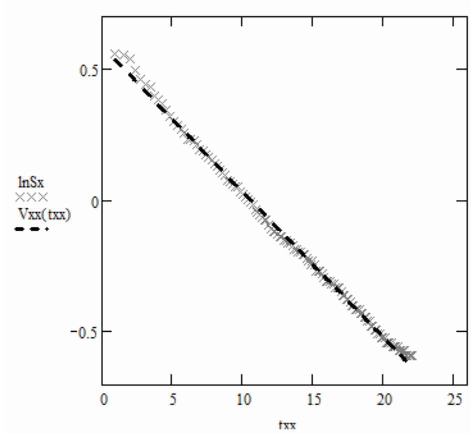

Figure - Dependence of experimental kinetics of gas sensor recovery response in coordinates $\left(lnS(t);t^{\beta}\right)$ fig. 1 (points - crosses) and its linear approximation used in the considered algorithm for its processing (dotted line)

It should be noted that the value of β - is already known. The approximating dependence is represented by a straight line $ln[S(t)] = a_0 + a_1 \cdot t^{\beta}$, where $a_0 = lnS_0$, $a_1 = -\tau^{\beta}$. Thus, $\tau = (-a_1)^{-1/\beta}$ and $S_0 = exp(a_0)$. The coefficients of the above linear regression dependence a_0 and a_1 are determined using formulas (3) and (4) or built-in intercept and slope functions of the Mathcad package. From the data in Fig. 4 you can get τ=88 s and S_0 =1.95. Calculation of the average relaxation time in accordance with [12,16,17]

$$t_{rel} = \int_0^{\infty} f_{KWW}(t)\, dt = \tau/\beta\,((1/\beta)), \tag{6}$$

where is the gamma function.

Comparison of the obtained parameters (β=0.63; t_{rel} = 120 s; τ=90 s; S_0=1.95) with similar ones, which were determined for these data by the method described in [12], showed their satisfactory agreement.

Conclusions

An algorithm for processing the kinetic dependence of the response of gas sensors based on the model of a stretched exponential function is proposed, which does

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not use numerical differentiation operations when finding one of the parameters of this model. and thus allows:

- to eliminate the presence of a scatter of points in the coordinates of the diagrams of the used approximating dependencies for calculating one of the key parameters of the model and its influence on the accuracy of processing;

- refuse the participation of the operator when choosing the optimal time interval from the processed kinetic dependencies for a more accurate assessment of all model parameters;

- allows the implementation of an automated information-measuring system for the considered data processing process.

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Алгоритм обробки даних кинетики відгуку газового сенсора із застосуванням розробленої еспоненційної функції без численного диференціювання

Метою роботи є розробка програмного забеспечння для обробки експериментальних даних кінетики відгуку резистивних газових сенсорів на основі алгоритму моделі розтягнутої експоненційної функції Кольрауша-Вільямса-Уоттса.

У даній статті розглядаються особливості використання комп'ютерних технологій обробки експериментальних даних для вирішення задач автоматизації досліджень матеріалів для газочутливих сенсорів.

У статті запропоновано алгоритм обробки кінетичної залежності відкликання газових сенсорів на основі моделі розтягнутої експоненційної функції, який не використовує операції чисельного диференціювання при знаходженні одного з параметрів цієї моделі. і, таким чином дозволяє: усунути наявність розкиду точок в координатах діаграм апроксимуючих залежностей для розрахунку одного з ключових параметрів моделі і його вплив на точність обробки; відмовитися від участі оператора при виборі оптимального часового інтервалу з кінетичних залежностей для більш точної оцінки всіх параметрів моделі; допускає реалізацію автоматизованої інформаційно-вимірювальної системи для аналізованого процесу обробки даних.

Ключові слова: газовий сенсор, відгук, кінетика, розтягнута експонентна функція, алгоритм, інформаційно-вимірювальна система, програмне забезпечення.

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