

IMPLEMENTATION OF COMPUTER PROCESSING OF RELAXATION PROCESSES INVESTIGATION DATA USING EXTENDED EXPONENTIAL FUNCTION

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Abstract. The object of research is the development of a specialized measuring information system for the study and control of relaxation processes in materials and technical systems. The purpose of the work is the use of computer technologies to eliminate routine operations associated with the processing of experimental data, increase the speed, accuracy and information content of the process of studying the control of gas sensors. A variant of using computer data processing to automate the processing and primary analysis of experimental data of scientific research and control of the physicochemical parameters of gas-sensitive materials is proposed. The developed computer data processing system provides a practical opportunity to use the measurements of the kinetic characteristics of the gas sensitivity of gas sensors for their experimental research and control and, thus, to achieve higher accuracy and information content. The testing of the developed information-measuring system confirmed its operability and compliance with the requirements for improving the accuracy and speed of the processing process.

Keywords: information-measuring system, gas sensor, extended exponential function, hardware, software, data processing

IMPLEMENTACJA KOMPUTEROWEGO PRZETWARZANIA DANYCH BADANIA PROCESÓW RELAKSACYJNYCH Z WYKORZYSTANIEM ROZSZERZONEJ FUNKCJI WYKŁADNICZEJ

Streszczenie. Przedmiotem badań jest opracowanie specjalistycznego systemu informacji pomiarowej do badania i kontroli procesów relaksacyjnych w materiałach i systemach technicznych. Celem pracy jest wykorzystanie technologii komputerowych do wyeliminowania rutynowych operacji związanych z przetwarzaniem danych eksperymentalnych, zwiększenia szybkości, dokładności i zawartości informacyjnej procesu badania kontroli czujników gazu. Zaproponowano wariant wykorzystania komputerowego przetwarzania danych do automatyzacji przetwarzania i podstawowej analizy danych eksperymentalnych badań naukowych i kontroli parametrów fizykochemicznych materiałów wrażliwych na gaz. Opracowany komputerowy system przetwarzania danych zapewnia praktyczną możliwość wykorzystania pomiarów charakterystyk kinetycznych wrażliwości czujników gazu do ich badań eksperymentalnych i kontroli, a tym samym do osiągnięcia wyższej dokładności i zawartości informacyjnej. Testy opracowanego systemu pomiaru informacji potwierdziły jego funkcjonalność i zgodność z wymaganiami dotyczącymi poprawy dokładności i szybkości procesu przetwarzania.

Słowa kluczowe: system informacyjno-pomiarowy, czujnik gazu, rozszerzona funkcja wykładnicza, sprzęt, oprogramowanie, przetwarzanie danych

Introduction

Computer technologies for processing experimental data have already become widespread in various fields of science and technology. They are used both in the study of well-known problems of high-energy physics and nuclear physics [3], image processing [4], search and creation of new materials [2], and for solving specific scientific and technical problems research of plasma light sources [8], construction of intelligent information-measuring systems for monitoring heat-insulating materials [9], etc.

Another specific area where the use of the technologies under consideration seems appropriate is the problem of studying relaxation processes in various materials and technical systems. The analysis of such kinetic dependences allows, as a rule, to obtain the most complete information about the properties of an object [7, 13, 15, 18, 19].

Studies of this type are associated with the need to process and analyze significant amounts of experimental data. The previous paper [12] shows the prospects for solving such a problem by creating a specialized information-measuring system.

The object of research is the implementation of computer processing and primary analysis of data from studies of relaxation processes in materials and systems using the example of resistive gas sensors. This process usually takes a lot of time and requires multiple cycles of processing large arrays of experimental data. First of all this is due to the need to ensure sufficient accuracy and information content of the results obtained. Therefore, to exclude routine operations associated with the processing of experimental data, to increase the speed, accuracy and information content of the research process itself, it seems relevant to automate it using computer technology.

The subject of the study is the methods and methods for constructing hardware and software for a specialized automated information-measuring system, which provided digitization and input of measurement data into memory and data analysis within the framework of the well-known model

of a stretched exponential function [12, 14]. Known methods of computerization of the data processing process, as a rule, reduced to the use of their digitization and input into computer memory [13].

The purpose of the work is the use of computer technologies to eliminate routine operations associated with the processing of experimental data, increase the speed, accuracy and information content of the process of studying the control of gas sensors.

In this paper, the task is to develop a variant of automation of an information system for processing and analyzing measurement data of the response kinetics of resistive gas sensors for research and control of gas sensor parameters.

The most acceptable option for using computer data processing for the described measuring process is the development of an IMS, which should provide a solution to two problems:

- digitization and input of measurement data into the EOM memory in the form of text files;
- processing and analysis of data within the framework of the previously mentioned model of an extended exponential function, in particular, to ensure the determination of its parameters and the construction of their dependences on various factors (temperature, partial pressure of the detected gas, structural features and chemical composition of the sensor used, etc.).

1. Method and technology for measuring gas sensor parameters

The main characteristics of gas sensitive sensors are [1]:

- response kinetics when a certain amount of adsorbent enters/removes into the atmosphere surrounding the sensor (at a constant sensor temperature);
- temperature dependence of the response at a constant concentration of the adsorbent;
- dependence of the response on the concentration of adsorbent at a constant temperature.

The response defined as R_s/R_0 , where R_s is the resistance of the sensor in the medium containing the adsorbent, R_0 – is in air.

Based on the need to measure these characteristics, a measuring device was assembled.

The measuring setup consisted of a sealed chamber with a volume of 20 dm^3 , to which a small expansion tank was attached, a power supply unit, and an electrical circuit. The expansion tank consisted of elastic rubber and was used to equalize the pressure between the volume of the chamber and the surrounding atmosphere. The electrical circuit ensured the reception of a signal from the sensor and its transmission to a personal computer (PC), and the computer itself.

The gas sensor, together with the system for ensuring its heating, was located in the measuring chamber and electrically connected to the rest of the installation. The chamber also housed a thermometer to control the temperature of the gases and a miniature fan to ensure the isotropy of the gaseous medium.

A dosed amount of active gas was injected at the right time into the measuring chamber.

The most well-known implementations of automation of measurements usually reduced to the process of digitizing the input experimental data and loading it in the form of text files into the computer's memory [13]. Their further processing and analysis were carried out manually or using separate computer programs.

The previous papers [12, 14] used a general phenomenological model based on the extended Kohlrausch-Williams-Watts exponential function $f_{kww}(t) = \exp[-(t/\tau)^\beta]$, where t is time, β and τ are parameters [10, 17]. It is used to describe the kinetics of the relaxation dependences of the response, in particular, at the recovery stage.

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 [6]. As shown in the paper [13] the use of such an approach makes it possible to obtain much more information on the physicochemical phenomena that determine the phenomenon of gas sensitivity of resistive sensor materials. Used in the window application given in the paper [12] it indicates the reality and efficiency of computer processing of a significant

amount of data in the process of conducting the physical and chemical measurements under consideration.

2. Software and hardware for digitization and input of measurement data into memory

The hardware for inputting and converting data into digital form is based on the ARM microcontroller STM32F103C8T6 [16], which uses the AMS1117-3.3 chip to provide a stable supply voltage (+3.3 V). The functioning of the microcontroller is carried out using a quartz resonator X1 with a frequency of 8 MHz.

The analog voltage that was digitized came from a voltage divider, to which a constant voltage $U_C = 3.3 \text{ V}$ was applied. The divider was a series connection of a precision current resistor (R_X) and the sensor itself. A part of the voltage taken from the U_{SEN} sensor was impressed to the corresponding output of the microcontroller, which is the input of its 12-bit built-in analog-to-digital converter (ADC). The use of this ADC allows digitization with an accuracy of at least 1 mV.

This connection scheme allows you to define the resistance of the sensor as the ratio of the digitized voltage U_{SEN} and the current I passing through the divider $R_{SEN} = U_{SEN}/I$, where $I = (U_C - U_{SEN})/R_X$.

Communication with a personal computer is carried out via the USB interface. For communication, only two common wires D+ and D- are used, which are connected to the micro-USB connector.

To control the electrical circuit of digitization and enter measurement data into the PC memory, a program created in the Python language and retranslated into the machine code language using the script compiler for Windows – Auto-PY-to-EXE is used. The architectural scheme of the developed program is shown in Fig. 1.

The user interface of the program is shown in Fig. 2. On Fig. 2 area, "1" is used to connect to a PC; in the field "2" – the measured data are displayed. Field "3" is used to set the delay time, the resistance of the current resistor and enable the display of the measured signal in the form of a graph; Field "4" – to set the identifier of the text file, which will be used to write data and comments to the file. Field "5" – chart display area. To start / stop the program, use the "Start / Stop" button.

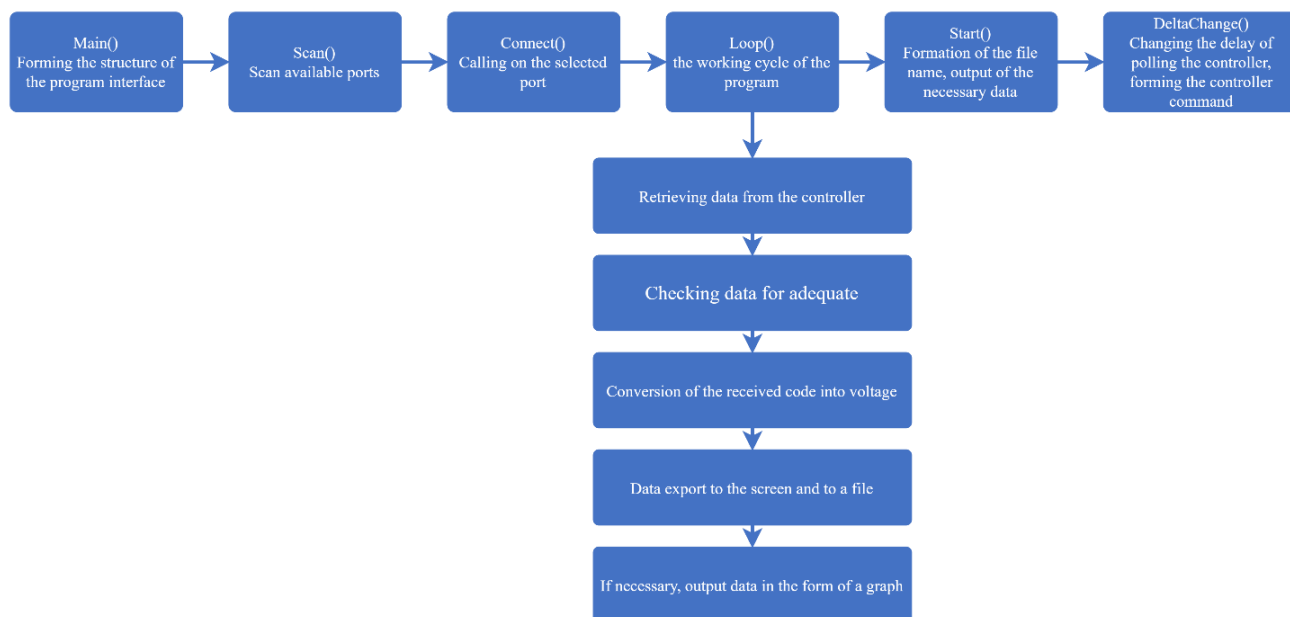


Fig. 1. Architectural scheme of the program for digitization and input of measurement data into memory

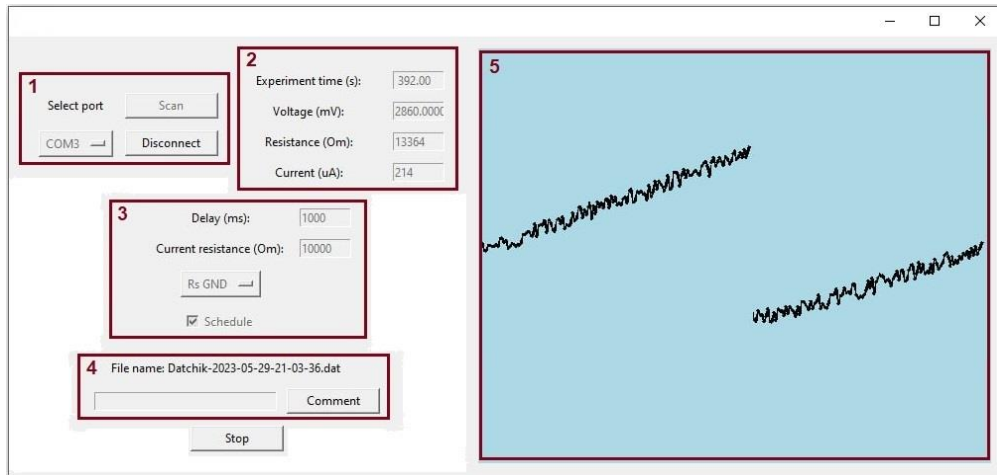


Fig. 2. General view of the interface of the data entry management program

3. Software for data processing and analysis

The presented system of computer technology for processing experimental data provides for the implementation of three modes – test, automated and in the mode with operator’s support. The test mode designed to teach you how to work with the software. Automated mode operates as part of an automated information system for measuring and controlling parameters of gas sensors. In the mode with operator’s support, the processing and analysis of experimental data is carried out step by step, allowing the user to make changes to its algorithm.

The software base on the integrated use of heterogeneous software products and provides the following service functions for processing and analyzing the specified data:

- data entry using Excel text files;
- calculations in the mathematical package "Mathcad" given parameters;
- visualization of the obtained dependencies in the form of graphs;
- providing the necessary textual information about the calculation algorithms used and test examples of their use;
- internet access if needed for more information.

The environment that ensures the operation of the described software product is the Windows operating system. Navigation between sections occurs with the help of buttons and menus of various levels (main, intermediate and working menus) [20].

To control the processing of source data used the Package Monitor, written using the C# language and the Windows Forms Application project type of the Visual Studio platform. The application software modules of the library of computational algorithms are documents of the well-known mathematical package Mathcad (version 15) [5]. In addition, the application uses universal tools for working with files with extensions like .xlsx, .dat(txt), docx and .pdf.

The main elements of the main window are buttons with labels, the names of which correspond to the purpose of the activated software modules (Fig. 3).

Pressing the "Entering the Experiment Date Argument" button calls up the intermediate menus "Task" (Fig. 4a), where the layout of the input and output information is indicated, and it is possible to select one of the proposed operating modes (Fig. 4b): test ("Test Program"), step-by-step with the participation and control of the operator ("My program") or automatic ("Auto Program"). After selecting and pressing the corresponding field, an Excel spreadsheet document file window will be loaded, where you should enter the values of the variable parameter-argument, the effect on the change in the KWW function of which is supposed to be investigated (Fig. 4c).

Its value is entered in the first column of the electronic table, zeros are entered in the remaining three fields, after which the file must be closed.

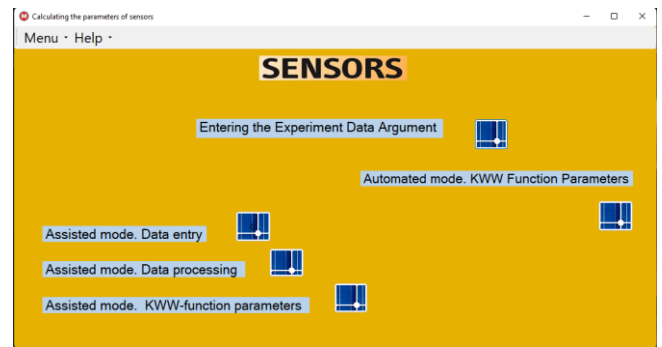


Fig. 3. Main window of the data processing and analysis interface

"Automated mode. KWW Function Parameters" run software in automated mode. It is assumed that the experimental data of measurements of the kinetic relaxation dependence of the sensor response in the form of a text file (.dat) have already been placed in the corresponding software folder. The program of the mathematical package Mathcad in accordance with the algorithm described in the previous paper [11] will perform their processing. After that, the results will be transferred to a file with an .xlsx type extension, where the values of the variable parameter-argument were entered (instead of zeros, Fig. 4), as well as them – a graphical visualization of the values of the parameters of the KWW-function with the given values of the parameter-argument in the program itself processing.

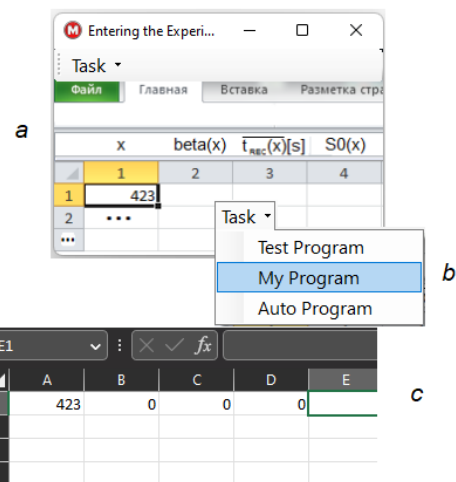


Fig. 4. Intermediate windows for choosing a mode (a and b) and switching to an Excel file (c) to set the value of the argument (the measurement identification factor, in this example, temperature)

Activation of the button "Assisted mode. Data entry" provides input of experimental data of measurements of the kinetic relaxation dependence of the sensor response into an Excel spreadsheet type file (or text file) for the test mode and the mode with operator support. In this case, the structure of intermediate windows is used, similar to that shown in Fig. 4.

The remaining buttons "Assisted mode. Data processing" and "Assisted mode. KWW-function parameters" (Fig. 3) are design to switch to intermediate windows of the same name, contain drop-down menus of the following three items that initialize the following:

"Assisted mode. Data processing" and "Assisted mode. KWW-function parameters" "Test" – call the window of the Mathcad package with a test case (does not allow any changes);

"My program" call of the window of the Mathcad package with a similar file used for processing the experimental data loaded for processing with the participation of the operator and allowing to make changes (modify the algorithm);

"Description" for opening files of the .pdf type, which contained information about the calculation algorithms used in the software modules of the Mathcad package.

The first of these algorithms provides a processing process with the participation of the operator of the data entered at the previous step by the operator. The purpose of the second algorithm is to fix and accumulate an array of values of the parameters of the Kohlrausch-Williams-Watts function, approximating the observed kinetics of changes in the resistance of the sensor under study, with subsequent visualization of their dependences on a given factor.

The main window also contains a toolbar with two buttons "Menu" and "Help". The Menu button contains two items. When you select the first of them, "Open Mathcad", Mathcad will be launch or a prompt will appear on the screen to select the Mathcad startup file yourself. When you select the second item "Exit", the application will be close. The Help button also contains a two-item menu. The "User's Manual" item opens a document with a user's manual. The "Workshop" item launches a browser to access the Internet.

It should be note that before using the described software product on a specific computer, it is necessary to install it together with the standard mathematical package Mathcad, Excel, a browser and .pdf file reader. The configuration of the product presented here is reduce to prescribing in the Visual Studio environment the corresponding file addresses in its monitor, which contain specific software implementations of computational algorithms from its library.

4. Algorithm for computer processing and data analysis

The maintenance algorithm provided by the IS for processing experimental data for measuring and controlling the parameters of gas sensors includes the following operations:

1. Preparation of the measuring setup for the specific conditions of the experimental study (placement of the sensor sample in the chamber, setting the physical parameters of the experiment: temperature, partial pressure, holding a variable interval to achieve a steady state, etc.).

2. Transfer (movement) of the sensor sample into an air atmosphere that does not contain active gas and launch the program for digitization and input of measurement data into the PC memory.

3. After generating a text file containing the experiment data, click the Entering the Experiment Date Argument button on the main menu of the data processing and analysis program. In the new menu, select and run the "Auto Program". In the window that opens, in the first column of a new row in the Excel table, load the value of the factor whose influence on the relaxation dependences of the resistance response

of the sensor under research is the purpose of the research. The results are the temperature, the partial pressure of the active gas, or the physical parameter of the sensor under research (Fig. 4). In the remaining 3 fields of the columns (values of the parameters of the KWW function), enter "0" (they will be filled as a result of the processing process).

4. Activate and click on the button labeled "Automated mode. KWW Function Parameters" (launching the software in automated mode). In the window that opens in the form of a document of the mathematical package Mathcad, the results of processing presented in graphical and textual form (values of the parameters KWW of the function β , S_0 and τ corresponding to the accepted value of the studied influence factor and other experimental conditions).

5. For data processing and data analysis of the next measurement in accordance with paragraph 3, enter the new value of the factor, the influence of which is the purpose of the study, in the next line of the table (Fig. 4c). The file containing the specified.

5. Results of testing

The results of testing the IMS under consideration for computer processing of measurement data of gas sensor parameters in automatic mode are shown in Fig. 5. The effect of temperature on the kinetics of the response of conductivity to methane in ZnO-Ag ceramics was investigate.

The results presented on the presence of the temperature of the maximum sensitivity of the sensor (near 500 K), on the decrease in the characteristic time and the duration of the relaxation process, are in accordance with the available ideas and specific literature data [13].

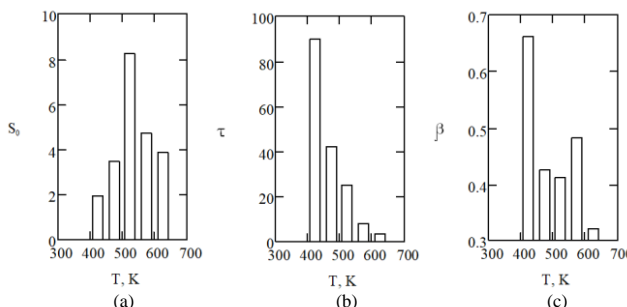


Fig. 5. Diagram of the influence of temperature (T , K) on the stationary (maximum) value of the response S_0 (a). The parameters that determine the relaxation process: the time characteristic τ , c (b) and the index of the extension of the duration of this process β (c) of a sample of zinc oxide ceramics with the addition of silver oxide (1.5 wt.%) after exposure to methane (relative concentration in air 0.005%)

6. Conclusions

A variant of the implementation of a specialized information system for computer data processing in measuring and controlling the parameters of gas sensors based on experimental studies of the kinetic dependences of the response of gas-sensitive sensors, and their approximation by the well-known model of the stretched Kohlrausch-Williams-Watts function is present.

The system provides the following service functions for processing and analyzing the specified data:

- automated digitization and input of measurement data into the EOM memory in the form of text files directly from the measurement or control hardware;
- primary processing and analysis of data within the framework of the extended exponential function model, in particular, to determine its parameters and plot their dependences on various factors (temperature, partial pressure of the detected gas, structural features and chemical composition of the sensor used, etc.).

Data processing and analysis software is based on the integrated use of heterogeneous software products and provides the following service functions:

- data entry using Excel spreadsheets;
- calculations in the mathematical package "Mathcad" given parameters;
- visualization of the obtained dependencies in the form of graphs;
- providing the necessary textual information about the calculation algorithms used and test examples of their use;
- Internet access, if necessary, to obtain additional information.

Prospects for further developments and research are in the improvement of software and hardware. The presented results can be extended to studies of a wider class of relaxation processes that can be described by means of an extended Kohlrausch-Williams-Watts exponential function.

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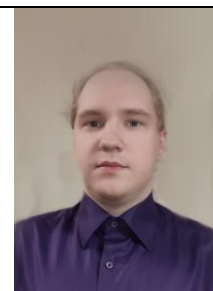
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