

Представлено методику та розроблено комп'ютерні засоби автоматизованого вимірювання електричних параметрів та обробки отриманих експериментальних даних із врахуванням моделей опису фізичних процесів, які визначають експлуатаційні характеристики напівпровідникового матеріалу. Реалізована можливість автоматизованого дослідження якості та омичності контактів, що значно підвищує надійність отриманих даних.

Розглянуто методи і особливості програмної обробки результатів автоматизованих досліджень за допомогою моделей, які дають можливість врахувати вплив поверхні та структури і товщини зразка на електричні властивості напівпровідникових плівок.

Проведено експериментальні дослідження серії тонких плівки n-PbTe та показано ефективність розроблених засобів і методик обробки наукових даних із застосуванням описаних методик аналізу експериментальних даних. На основі моделювання визначено електричні параметри приповерхневих шарів, розділено вплив поверхневого та зернограничного механізмів розсіювання носіїв заряду на електричні параметри плівки. При цьому поверхнева рухливість носіїв заряду приблизно в 3 рази менша рухливості в об'ємі матеріалу, що, незважаючи на високий коефіцієнт дзеркальності (0,4), вказує на домінування дифузного розсіювання носіїв заряду на поверхні досліджуваних тонкоплівкових зразків. Врахування впливу поверхні та меж зерен дає можливість вибрати технологічні режими та тривалість наплення для отримання напівпровідникового матеріалу з потрібними властивостями.

В результаті використання розроблених засобів вдалося значно зменшити трудомісткість процесу вимірювання основних електричних параметрів напівпровідникових матеріалів, обробки отриманих експериментальних результатів, підвищити точність отриманих результатів

Ключові слова: комп'ютерні засоби, автоматизація, алгоритми мінімізації, контакти, електричні властивості

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METHODS OF COMPUTER TOOLS DEVELOPMENT FOR MEASURING AND ANALYSIS OF ELECTRICAL PROPERTIES OF SEMICONDUCTOR FILMS

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1. Introduction

The rapid development of computer technology in recent decades has led to the fact that today the computer has become a major tool in the initial processing of scientific experiments. A number of versatile computer applications and environments have been developed, including Maple, MathCAD, LabView, Origin, etc. These tools are versatile enough, but they need sufficient time for their study, writing

of programs for the implementation of certain models. Many difficulties also arise with the integration of such tools into existing laboratory complexes for rapid data analysis in the measurement process. Therefore, the development of specialized computer tools for the study of the electrical properties of thin-film semiconductor materials, methods of processing, software filtering and data approximation, taking into account models of physical processes and effects that determine the material properties, remains relevant.

2. Literature review and problem statement

A number of methods have been developed to investigate the properties of semiconductors. Among the theoretical methods, the modeling methods and numerical quantum mechanical calculations used for modeling the electronic structure of molecules and condensed phases of matter should be noted [1, 2]. With properly selected models, these methods allow obtaining a great deal of information about semiconductor properties by computer calculations, including the effect of surface and alloying impurities on the electrical properties of the material. But the main disadvantage of these methods is the need for large computing power and long calculations. With regard to experimental methods, a large amount of data, methods of their statistical and mathematical processing have been accumulated in the field of semiconductor materials science. Recently, much attention has been paid to experimental studies of the properties of A^{III}B^V [3] and A^{IV}B^{VI} [4] semiconductor compounds, in particular in the form of thin films and nanostructures. Such studies are time-consuming and require automation of both the measurement process and the subsequent computer data processing. The problem of computer data processing is partially described in [5, 6], where the parameters and characteristics of semiconductor devices using modern technologies are explored. Electronic tools of current-voltage characteristics research are described by the authors [7]. These works mainly relate to computer research tools for semiconductor devices and modules and only partially affect semiconductor materials research.

In order to develop computer analysis tools, it is important to correctly select the basic parameters that determine the electrical properties of semiconductor materials, the response function, and the mathematical model. The electrical properties of thin-film semiconductor materials are determined by kinetic parameters. In particular, a model describing the mechanisms of charge carrier scattering is presented in [8], and the authors [4, 9] described methods for considering the effect of intergranular grain boundaries on the electrical conductivity of a polycrystalline film. Thus, a barrier theory of conductivity is presented in [4], which considers the intercrystalline boundary as a potential barrier that leads to the charge carrier scattering. In addition to grain boundaries, the free surface of the film has an important effect in the thin-film material. A method for taking into account the influence of surface effects is described in [10]. Despite a large number of simplifications and assumptions, taking into account the effect of the surface and intergranular boundaries by methods and models described in [4, 8–10] allows determining the scattering of charge carriers that have a dominant effect on the electrical properties of the material. The authors of [11] have developed a technique for computer simulation of ready-made instrument structures, which demonstrates the powerful capabilities of modern computer research tools.

When applying these methods, there is a need to process large arrays of data, use various mathematical methods of analysis, which are mainly realized with the use of complex mathematical software packages, and are quite time-consuming.

The literature review has shown that there are a sufficient number of methods and models that well describe the electrical properties of thin-film semiconductor materials. But there are virtually no specialized computer tools for their rapid application, especially during the experiment.

Therefore, the development of such tools can greatly simplify experimental studies.

3. The aim and objectives of the study

The aim of the work is the selection of methods and development of computer tools for the investigation of the electrical properties of thin-film semiconductor materials based on models of physical processes and effects that determine the properties of the material.

To achieve the aim, the following objectives were accomplished:

- to determine the basic parameters and models that describe the properties of thin-film semiconductor materials;
- to present algorithms for creating tools of automated measurement and preliminary processing of experimental data taking into account the selected models for describing physical processes that determine the operating characteristics of the semiconductor material;
- to investigate the electrical parameters of a series of n-PbTe thin semiconductor films and to estimate the efficiency of the tools developed.

4. Selection of models and parameters describing the properties of thin-film semiconductor materials

The choice of models, factors and methods for processing the experimental data was realized based on those physical processes of charge carrier transfer in thin films that make the major contribution to the operational properties of the semiconductor material.

The basic physical models were chosen for further analysis of the accumulated experimental data. These models describe the basic electrical properties of the semiconductor and give the possibility to determine the parameters that are not directly measurable, to evaluate the mechanisms of conductivity and charge carrier scattering.

The parameters of the surface layer are very different from the bulk ones in thin films. Therefore, to estimate the electrical properties of the surface layer in films, it is advisable to use a two-layer Petritz model [7]. Thin film in this model is composed of two layers: the surface (s) one (surface space charge region) with the thickness d_s , the concentration of current carriers p_s , and their mobility μ_s , and the bulk (b) one, characterized by similar values (d_b, p_b, μ_b), which are connected in parallel. The thickness of the film is $d = d_s + d_b$.

In this case, according to [7]:

$$\sigma = \frac{\sigma_s d_s + \sigma_b d_b}{d}; \quad (1)$$

$$R = \frac{R_s \sigma_s^2 d_s + R_b \sigma_b^2 d_b}{(\sigma_s d_s + \sigma_b d_b)^2} d; \quad (2)$$

$$\mu = \sigma R = \frac{\sigma_s^2 d_s R_s + \sigma_b^2 d_b R_b}{\sigma_s d_s + \sigma_b d_b}; \quad (3)$$

$$S = \frac{S_s \sigma_s d_s + S_b \sigma_b d_b}{\sigma_s d_s + \sigma_b d_b}. \quad (4)$$

If the experimental (σ, R, μ, S), bulk ($\sigma_b, R_b, \mu_b, S_b$) values and the total film thickness d are known, then it is

possible to determine approximately the thickness d_s and the parameters of the surface layer (σ_s , R_s , μ_s , S_s) from the above relations.

The least-squares method was used to determine the surface coefficients. When approximating the conductivity by the formula (1), one can obtain the function of two variables d_s and σ_s , the minimization of which is realized using the algorithm of minimization of the functions of many variables by the deformed polyhedron method (by Nelder and Mead). The block diagram of this algorithm is given in [12]. Although this technique is simple enough, its realization has shown good efficiency – finding a minimum occurs in 80–100 iterations and takes part of a second.

A more accurate model describing kinetic processes in thin films is the Fuchs-Sondheimer model [8]. This model describes well the thickness dependences of the electrical parameters of thin films and allows determining the dominant scattering mechanisms of charge carriers, taking into account the dimensional effects associated with scattering on the outer surfaces of the film. The film conductivity σ is determined from the Boltzmann kinetic equation [8, 13] and for the limiting case $k \gg 1$ (thick films) is equal:

$$\sigma = \sigma_b \left(1 + \frac{3}{8k} (1-p) \right)^{-1}, \quad k \gg 1. \quad (5)$$

For very thin films ($k \ll 1$)

$$\sigma = \sigma_b \frac{3}{4} \frac{1+p}{1-p} k \ln \frac{1}{k}, \quad k \ll 1, \quad (6)$$

where σ_b is the electric conductivity of the bulk sample, the dimensionless thickness $k = d/l$, l is the electron mean path length, p is the reflectance coefficient (mirror reflection probability, $0 \leq p \leq 1$). If $p = 0$, then there is a diffuse scattering, when $p = 1$ – pure mirror reflection.

According to the Sondheimer model, the manifestation of the dimensional effect in the dependence of the Hall coefficient R_H on the film thickness for the case of a magnetic field directed perpendicular to the surface can be determined from the equation [8]:

$$R_H = R_{Hb} \frac{4}{3} \frac{1-p}{1+p} \frac{1}{k (\ln k^{-1})^2}, \quad k \ll 1. \quad (7)$$

The current carrier mobility in the case of diffuse scattering on the surface is defined as [14]:

$$\mu = \mu_b \left(1 + \frac{d}{l} \right)^{-1}, \quad (8)$$

where μ_b is the current carrier mobility in bulk material.

For polycrystalline films, except the free surface, the electronic transport of current carriers is determined by both the crystallites themselves and the intergranular barriers [4]. If the structure of crystallites is ordered, then the intergranular boundaries are disordered. Given the nature of the grain boundary region, according to the model [15], the electronic properties of polycrystal are determined by the charge carrier capture by dangling bonds of atoms, localized at the intergranular boundaries. Two main mechanisms of charge transfer are considered for the barrier region: thermoelectron overbarrier emission and subbarrier tunnel transport. In this case, the conductivity of a polycrystal with size L will be determined as [15]:

$$\sigma = \frac{Lq^2 p}{\sqrt{2\pi m^* kT}} e^{-\frac{qV_b}{kT}}. \quad (9)$$

Taking into account that

$$\sigma = q\mu p, \quad (10)$$

the effective value of mobility in this case will be

$$\mu = \frac{Lq}{\sqrt{2\pi m^* kT}} e^{-\frac{E_b}{kT}}, \quad (11)$$

where $E_b = qV_b$, V_b – barrier potential, q – electron charge, T – absolute temperature, k – Boltzmann constant, m^* – effective mass of the charge carrier, p – concentration of current carriers.

5. Development of algorithms and tools for automated measurement of electrical parameters of semiconductor films and processing of experimental data

When studying the electrical properties of semiconductors, such basic parameters as the specific conductivity, the Hall coefficient, the thermoelectromotive force are measured, based on which the concentration and mobility of charge carriers are determined. The latter determine the basic operational characteristics of semiconductors. For thin films, the key role is played by the influence of structure and surface effects, which are not directly measurable but are well described by the theoretical models discussed above.

Selected models take into account the basic physical processes that contribute to the operational properties of the semiconductor material and allow selecting the necessary experimental parameters for analysis, taking into account the thickness and structure of the material studied, and developing computer automated tools to determine the predominant mechanism of carrier scattering, estimate the parameters of the surface layers and intergranular boundaries, which are not directly measurable.

Since the process of measuring electrical parameters is rather time-consuming, a method and an automated hardware-software measurement complex were first developed to obtain both electrical and thermoelectric parameters of semiconductor materials [16]. As a result, there is a need to process a large amount of experimental data. It is also convenient to make express data analysis already during the experiment. The reliability and ohmicity of the electrical contacts in the measurements are important, as their violation leads to large errors and faults. Contact analysis in the measurement process greatly improves the certainty and reliability of the results obtained, excluding incorrect data, such as contact breaks or microcracks in the film, which may result from thermal or mechanical stresses. Therefore, the developed hardware-software complex was substantially modified, which is shown in the block diagram (Fig. 1), in particular, the analytical module and the self-diagnostics module were added. The analytical module can use a database of previous experiments, which enables the efficient analysis of the data obtained for one series samples that differ, for example, in thickness.

To study the quality of ohmicity of contacts, it is convenient to analyze the current-voltage characteristic for linearity and symmetry in both directions of current flow. Since the electrical resistance at small test currents (when the sample is not

substantially heated) is constant, the current dependence on voltage is linear $I=GU$. The analysis of this characteristic makes it possible to estimate the quality of contacts and the correct choice of contact material. The conductivity G is also required to analyze the measurement results for the contact integrity and absence of sample damage during the experiment.

The least-squares method was applied for the automated analysis, which analytically resolves for one parameter. The mean square deviation of the obtained results s in both directions of the current would not exceed some value, which is determined by the instrumental and methodological measurement error. A simplified algorithm for measuring of voltage-current characteristics and analysis of contact quality is shown in Fig. 2.

Computer analysis and simulation software module was written in the Delphi environment. Not very popular at the moment, the development environment is used to be fully compatible with a previously developed control program and visualization module. To implement all three models, it is necessary to approximate the data with different dependencies with a different number of parameters. With this in mind, the procedure that implements the least-squares method using the algorithm for minimizing the functions of many variables by the deformed polyhedron method is made parameterized one. It is possible to choose both the type of function and the number of variables, as well as adjust the approximation parameters. The program has a convenient graphical interface presented in Fig. 3.

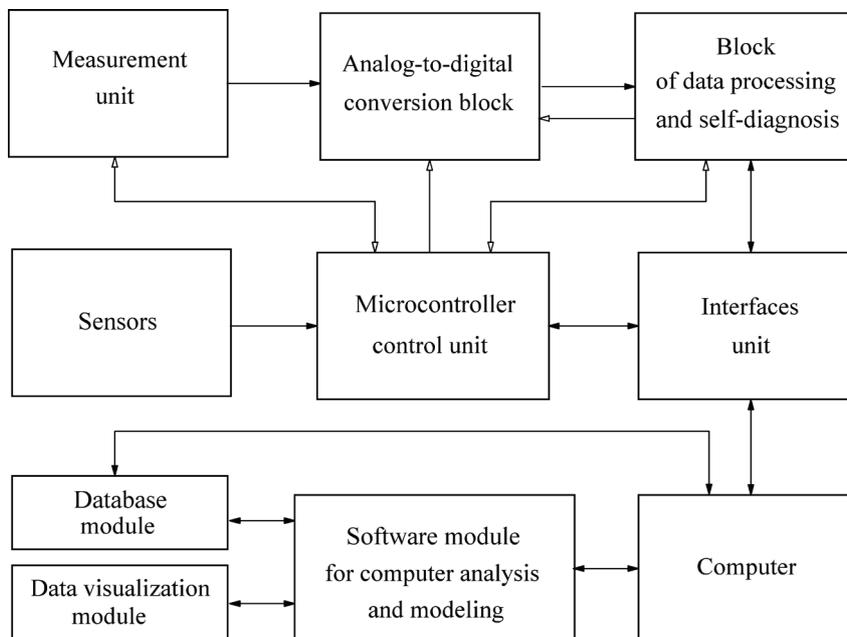


Fig. 1. Block diagram of a specialized software-hardware system for the investigation and modeling of the electrical properties of thin-film semiconductor materials (black arrows are informative, transparent ones are control).

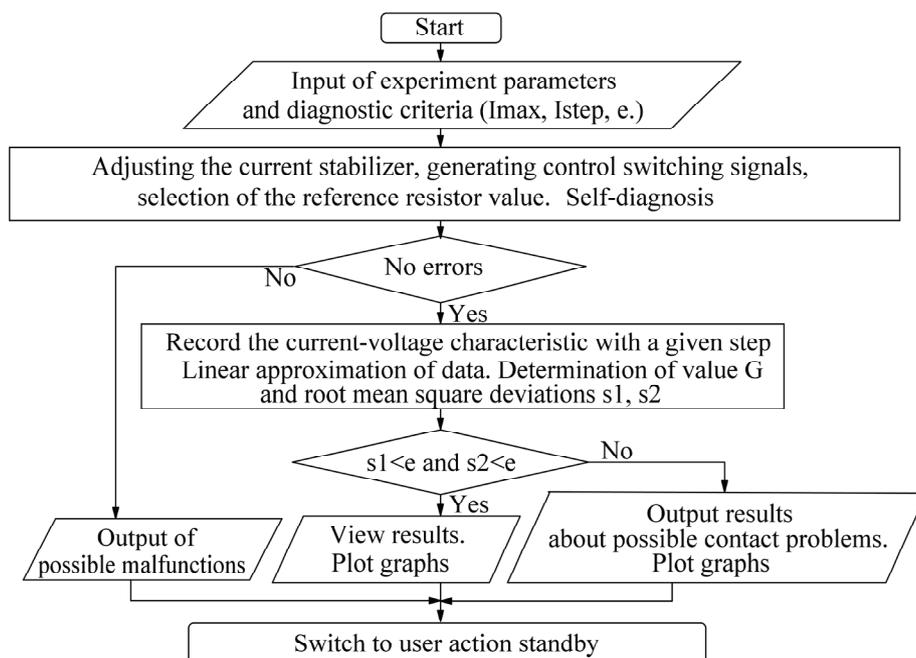


Fig. 2. Algorithm for measurement of voltage-current characteristics and analysis of contact quality

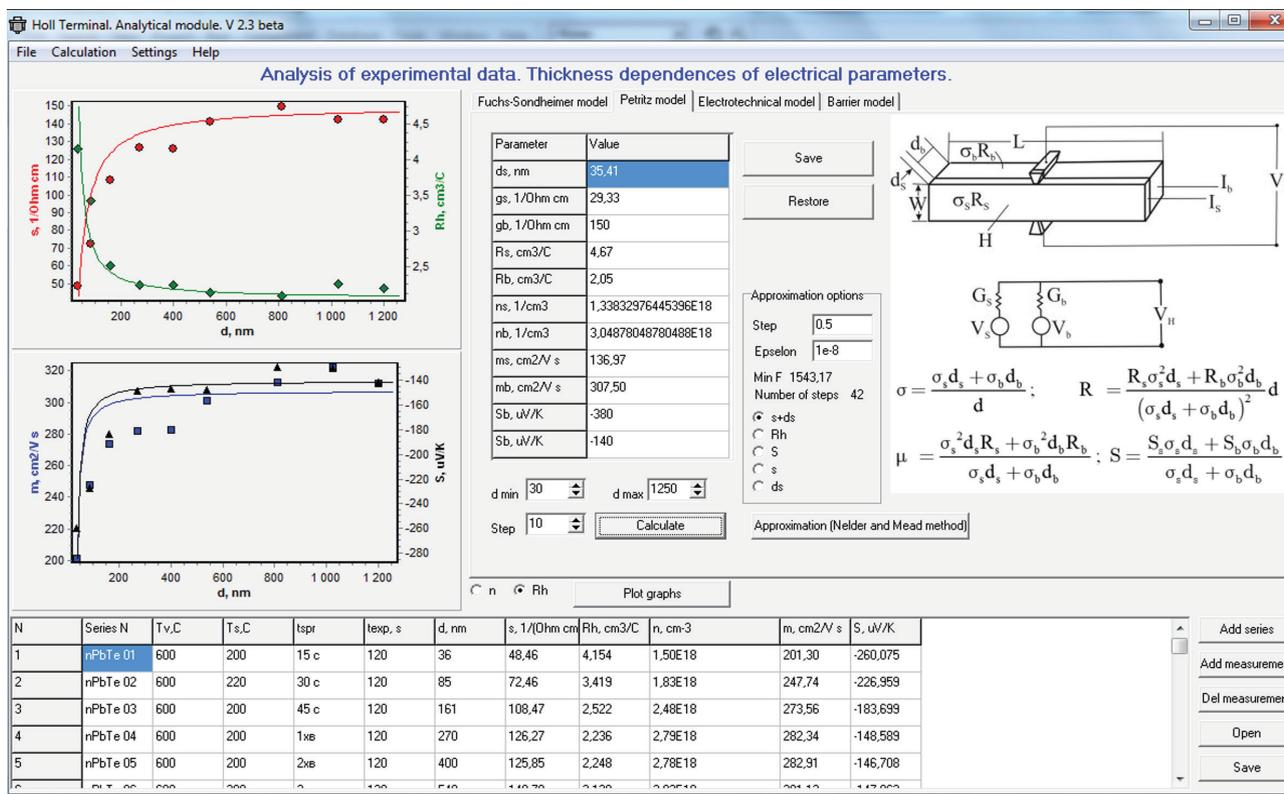


Fig. 3. General view of the program analytic module window

For each of the models discussed above, the program has a separate insert (tabs) with the possibility to set known parameters and to choose analysis modes and parameters approximation. At the bottom of the program, the table shows systematic experimental data, and the left part of the program window displays the parameters obtained in the form of graphs.

The calculation results according to the Petritz model are presented in Fig. 3. The calculation uses information about the electrical parameters of the bulk material and the results of experimental measurements that determine the electrical parameters of the surface layer. Approximating the results of the experiment by dependencies (5)–(7), one can obtain the charge carrier scattering coefficient by the film surface from the Fuchs-Sondheimer model. Using the dependency (11), one can obtain the mobility of charge carriers, which is related to the effect of intergranular boundaries. Development of software using fairly simple approximation algorithms with data visualization allows preliminary analysis of the obtained data already during the experiment.

6. Experimental research and data analysis

Consider the work of the computer data analysis module based on real investigation of the n-PbTe thin semiconductor film series. Films were obtained by the thermal vacuum method from pre-synthesized n-PbTe material on fresh split (0001) mica-muscovite substrates. The film thickness was set by the deposition time within (0.25–9) min and measured using an MII-4 microinterferometer. The thickness of the films was entered into the program database manually.

Electrical parameters were measured for 9 samples of different thicknesses. The general view of the analytical module

of the program with the processed data for the considered series of samples according to the Petritz model is presented on the screenshot (Fig. 3).

Fig. 4 shows the experimental data for the specific conductivity and Hall coefficient for the obtained series of samples, as well as compares the calculation results according to the Petritz and Fuchs-Sondheimer models. As can be seen, both models describe the experiment well.

In Fig. 4, curves 1 are calculated from equations (1), (2), and curve 2 is calculated for thin films ($k < 1$) from equations (5)–(7). Here only experimental data that satisfy this condition are considered. Table 1 summarizes all simulation results. Also, the effect of grain boundaries, which create a potential barrier, was calculated. The activation energy of electrical conductivity was 0.08-0.1 eV, which indicates a relatively small effect of grain boundaries on the overall electrical conductivity of the material. It should be noted that the obtained mirror coefficient of 0.4 and the free path length of 260 nm are in good agreement with the data of similar investigations. The result is explained by the fact that the films obtained on mica are characterized by a mosaic structure, which provides a thin-film material with a sufficiently high structural perfection.

Table 1

Electrical parameters of surface layer of n-PbTe thin films

| Surface layer parameters | |
|--|----------------------|
| $\sigma_s, \text{Ohm}^{-1}\cdot\text{cm}^{-1}$ | 21.21 |
| $R_{Hs}, \text{cm}^3/\text{C}$ | 4.67 |
| n_s, cm^{-3} | $1.34 \cdot 10^{18}$ |
| $\mu_s, \text{cm}^2/\text{V}\cdot\text{s}$ | 99.05 |
| $S_s, \mu\text{V}/\text{C}$ | -380 |
| d_s, nm | 35.18 |

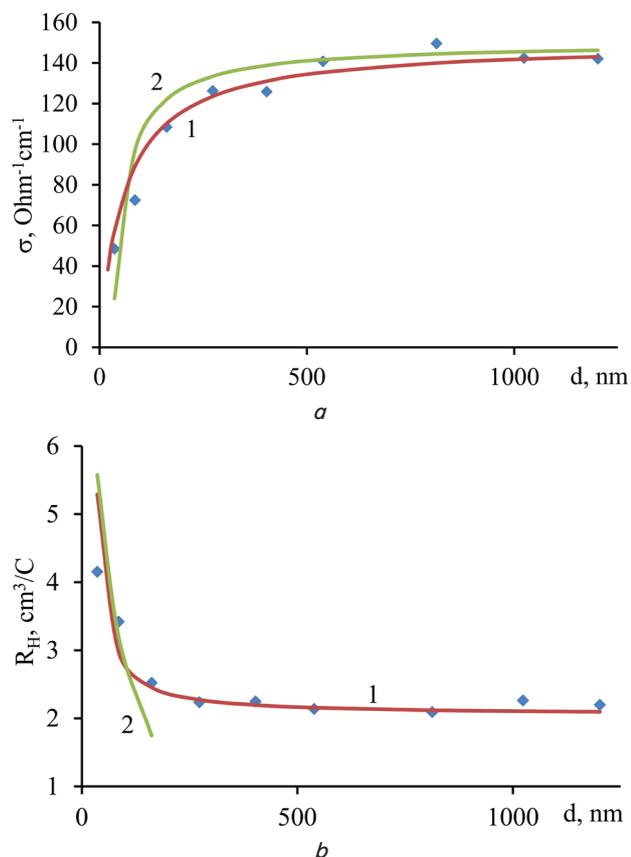


Fig. 4. Thickness dependences of electrical parameters for PbTe samples: a – specific conductivity; b – Hall coefficient; \blacklozenge – experiment; curve 1 – calculation according to the Petritz model; 2 – calculation according to the Fuchs-Sondheimer model

7. Discussion of results of using the developed computer tools

The analysis of the obtained results and the comparison of the calculation results with the experimental measurements (Fig. 4) showed that the selected models well describe the experimental data. In particular, the parameters of the surface layer are obtained from equations (1)–(4), which are presented in Table 1, and the coefficient of surface reflectance and the length of free path of charge carriers are determined from equations (5)–(7). Despite the relative simplicity of the realized algorithms, the automated computer tools developed have shown high performance. For example, checking the linearity of a current-voltage characteristic does not increase the time of the experiment, but makes it possible to estimate the quality of the contacts and immediately identify the problem in the event of defects appearance.

The advantage of the realized research method is the automation of both the measurement process and the

pre-processing of the result already in the process of the experiment according to the selected models, depending on the material studied. This makes it possible to determine the basic electrical characteristics of the material, such as the concentration and mobility of charge carriers, the effect of the surface, and the dominant conductivity mechanisms. The visualization of the results obtained in the form of graphical dependences gives an opportunity to visually detect errors and defective samples already in the measurement process. Compared to universal tools and mathematical software packages that provide much greater data processing capabilities, the development of specialized tools, despite the limited set of models, is well integrated into the developed measurement complex and provides information about the electrical properties of thin-film semiconductor material with minimal time and labour required for measurement and processing.

The use of sufficiently simplified models that take into account only classical effects and well describe the properties of thin-film material imposes some limitations on the application of the developed tools for the analysis of nano- and 2D structures, where quantum effects play a major role. In order to further improve the developed tools, work is underway to add models to the analytical module that would take into account quantum-size effects, statistical data processing capabilities and algorithms for calculating a minimum sufficient number of measurements, taking into account already available data.

8. Conclusions

1. Models and basic parameters are determined, which allow calculating the concentration and mobility of charge carriers and taking into account the effect of the surface and film structure and determining the dominant scattering mechanisms.

2. Methods, algorithms, block diagrams are presented, and computer tools for the automated measurement and processing of experimental data are developed, taking into account models for describing physical processes that determine the operating characteristics of semiconductor material, which significantly reduced the time spent conducting and processing the experiment.

3. Experimental studies of a series of n-PbTe thin films were carried out using the developed tools, the electrical parameters of the surface layers were determined. In this case, the surface mobility of charge carriers is about 3 times less than the mobility in the bulk material, which, despite the high reflectance coefficient (0.4), indicates the dominance of the diffuse scattering of charge carriers on the surface of the thin-film samples studied. High efficiency of the developed tools for carrying out such researches is shown.

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