Graph-analytical model of the electrical conductivity of a semiconductor island plumbum telluride nanofilm

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Abstract. This article presents the results of experimental studies on obtaining and measuring the electronically conductive properties of island semiconductor plumbum telluride nanofilms, as well as modeling their conductive properties within the hopping conductivity model and the classical model taking into account the structure within the DLA model using graph theory methods.

Introduction

Today, new unique materials using plumbum telluride (PbTe), structured by nanoparticles into the main matrix of the substance and / or on the surface, form the basis for the development of promising materials with predetermined properties that can be widely used in various fields of nanoelectronics and photonics as a new elemental bases, for example, information and energy storage elements, thermoelectric sensors, detectors, radiation sources, solar batteries, etc.

The electrical properties of PbTe island nanofilms on substrates of various nature are of scientific interest from the point of view of modifying the properties of the medium, in essence creating new materials based on well-known ones. The physicochemical and especially electrically conductive properties of such materials substantially depend on the location of the structural features on the surface, which makes it possible to control their properties.

In this regard, the development of methods for managing the placement of nanoscale elements on a solid substrate becomes a very urgent task. Existing methods of substance transfer are technologically complex and expensive, and so impose significant restrictions on the choice of working material used.

For these reasons, the methods of laser-controlled synthesis of nanostructured surfaces discussed in this article are among the most rapidly developing instruments of modern micro-nanoelectronics and photonics, which make it possible to obtain a wide class of nanostructured materials with the required surface topology, due to the controlled motion of the laser beam.

To calibrate and clarify the conditions for the experimental acquisition and prediction of the conductive properties of PbTe island nanofilms, it is proposed to use a mathematical modeling tool. At the moment, there are no universal mathematical models of electrical conductivity for the obtained nanofilms; therefore, this paper proposes an approach to modeling their properties within the framework of combining the graph and classical models, which allows describing the properties of both the island and the film as a whole.

Description of experimental studies
The initial PbTe heteroepitaxial structures were grown by molecular beam epitaxy in the ETH laboratory (Zurich). The features of the deposition of lead telluride layers and the parameters of the films under study are described in detail in [1].

The surface of the films was characterized by a block structure with a bimodal distribution function for lateral block sizes of 1-3 μm and an average elevation difference of 10-20 nm (Fig.1). The film thicknesses ranged from 1 to 6 μm.

Fig. 1. AFM image of PbTe film surface. The field of laser modification passes diagonally, the original surface (right upper and lower left corners). Laser exposure parameters: power 6 W, beam diameter 30 μm, scanning speed 80 μm / s.

A 4-pin circuit was used to study the current-voltage characteristics (Fig. 2), the two extreme contacts were made in the form of clamping areas, and the two internal contacts are the needles of an atomic-force microscope that allow measurements at a distance of up to 100 μm between the needles. The resulting value is obtained by averaging 10 measurements in one position, the total measurement time at one point is 1 minute. As part of the research, measurements were carried out in the longitudinal and transverse directions with respect to the modification area, and the pressure contacts in both cases were located at a distance of 1 cm from each other along the laser modification area.

Fig. 2. Four pin circuit

The current-voltage characteristics of the original and modified PbTe films are shown in Fig. 1. The voltage ranged from 0.1 to 1 V. The current strength was about 10^-6 A and wore an average linear character with small deviations in the middle of the interval. The resistance for such a current strength was about 10^9 Ohms.
Model of conductive properties

As a model of the electrical conductivity of a semiconductor island plumbum telluride nanofilm, taking into account the interposition of islands and temperature conditions, consider the graph model of electron hops, the totality of which will determine the conduction path between the islands, and in the framework of the island we will use the classical Ohm's law.

In the framework of inter-island conduction, we assume that the electron jump is possible when the relative value of the potential well does not exceed $d_{rel}$. Thus, the model will show only the set of all possible jumps, which will significantly save computational costs in the calculation.

The simulation algorithm consists of several steps:

1. Construction of a random weighted graph $G(V, E)$, in which the vertices $V = (v_1, v_2, ..., v_m)$ correspond to the islands of the nanofilm, and the edges $E = (e_1, e_2, ..., e_n)$ correspond to electron jumps, and the weights $W = (w_1, w_2, ..., w_n)$ from $[0; d]$ set the relative value of the potential well through the probability of overcoming it. Vertices and weights are represented as uniformly distributed random variables. [2]

2. The choice of a pair of vertices of the graph to which the voltage is applied. Calculation of the shortest path between them taking into account the weights using the Dijkstra algorithm, when the shortest path with the least weight is chosen. [3]

   Within the framework of this algorithm, each vertex of the graph is assigned a label — the minimum known distance from this vertex to the current vertex $a$. The algorithm works step by step - at each step it “visits” one vertex and tries to reduce marks. The operation of the algorithm is completed when all vertices are visited.

   In the process of initialization of the algorithm, the label of the vertex $a$ itself is set equal to 0, the labels of the other vertices are infinity, i.e. distances from $a$ to other vertices are still unknown. All vertices of the graph are marked as unvisited.

   At the step of the algorithm, the vertices are visited. If all vertices are visited, then the algorithm terminates. Otherwise, the vertex $u$ having the minimum mark is selected from the nodes that have not yet been visited, and all possible routes are considered, in which $u$ is the penultimate point. The vertices connected to the vertex $u$ by edges are considered neighbors of this vertex. For each neighbor, a new path length is considered as the sum of the current label $u$ and the length of the edge connecting $u$ with this neighbor. If the resulting length is less than the neighbor label, then replace the current label with this length. Having considered all the neighbors, mark the vertex $u$ as visited and repeat the step of the algorithm. [4]

3. Calculation of conductive characteristics.
To model the electrical conductivity, the Miller-Abrahams network [5] was used, which formed the graph G. The edge of the graph between vertices i and j is a conductor with resistance $R_{ij}$, which is calculated by the formula:

$$R_{ij} = R_0 e^{u_{ij}}, \quad u_{ij} = \frac{2\tau_{ij}}{\alpha_B} + \frac{\varepsilon_{ij}}{T},$$

(1)

where $r_{ij} = w_{ij}(T)$ is the distance between nodes i and j of the network, $u_{ij}$ is the length of the edge of the graph, which depends on the temperature of the system, $R_0 = \frac{1}{\alpha_B}$, where $\alpha_B$ is the Bohr radius, $\varepsilon_{ij}$ is some characteristic energy that was represented through the number of graph edges incident to a given vertex, and $T$ is the system temperature.

The network conductivity was calculated by the formula:

$$\sigma_{ij} = e^{-2\alpha_B R_{ij} - \frac{\varepsilon_{ij}}{kT}},$$

(2)

where $k$ is the Boltzmann constant.

Then amperage is calculated as:

$$I_{ij} = \frac{U_i - U_j}{R_{ij}},$$

(3)

where $U_i - U_j$ is the voltage drop, which is represented as $U \cdot r_{ij}$, where $U$ is the voltage supplied to the system.

In addition to the graph model proposed above, we consider the conductive properties of a film island. Such a model, in our opinion, makes it possible to take into account the structural features of the island topography, which significantly affect the electrical conductivity.

Consider the island formation model and on its basis we describe the conductive properties.

To describe the structure of the island film aggregates, the model of diffusive limited aggregation (DLA) was chosen [6]. This choice was due to a number of reasons: firstly, from the results of experimental studies it is obvious that thermal diffusion takes place, which is quite well modeled in the proposed approximation, and secondly, the islands of the resulting film are visually similar to fractal clusters (dendrites) generated by the algorithm DLA.

The algorithm consists of steps:

1) on a square two-dimensional lattice, a germ structure is specified;
2) far from the cluster (from the nucleus) in the nucleation region of the computational domain $R_p$ a new particle is generated;
3) a new particle wanders randomly;
4) if a particle comes to a busy cell, then it sticks with a given probability;
5) if the particle moves far enough away from the cluster, outside the external sphere $R_e$ it is destroyed;
6) repeat, starting from step 3, until the particle sticks with a given probability, after which a new particle is launched.

In the simulation, the initial concentration of the aggregation centers and the probability of sticking of particles and the viscosity parameter were varied within the von Neumann two-dimensional neighborhood of order 1 [7] (Fig. (b)).
Fig. 4. Island model: DLA scheme (a), von Neumann neighborhood (b).

It should be noted that the proposed model is used in relative units and is imitative. The characteristics of the conditions under which film aggregates are formed are veiled in the adhesion probability parameter, which allow for thermal diffusion processes or the lifetime of moving particles to be taken into account. The probability of a free particle sticking to an aggregate is a numerical characteristic of the structured, modeled structure. Thus, the larger the given parameter of the sticking probability, the more intense the thermal diffusion proceeds, which means, obviously, the system temperature is also higher.

Thus, the simulated island is represented as a fractal cluster along which the directed motion of electrons takes place. In this connection, to describe the electrical conductivity through volt-ampere characteristics, it is necessary to single out the paths of the electrons and, taking into account their length, calculate the resistance and amperage.

It is assumed that the voltage is applied to the most distant points of the cluster, so the length of the conduction path is calculated as the diameter of the minimum coverage area $R_b$ [8]:

$$l = \sqrt{(x - x_c)^2 + (y - y_c)^2}, \quad (4)$$

where $x, y$ are the current coordinates of the particle in the cluster, $x_c, y_c$ are the coordinates of the center.

Resistance was calculated as:

$$R_{PbTe} = \rho_{PbTe} \frac{l}{S}, \quad (5)$$

where $\rho_{PbTe}$ is the electrical resistivity of plumbum telluride, $l$ is the length of the conducting track, $S$ is the cross-sectional area of the conducting track, $L$ is the total length of the conduction track.

Volt-ampere characteristics $I$ were calculated according to Ohm’s law:

$$I = \frac{U}{R}, \quad (6)$$

where $U$ is the voltage.

**Simulation of conductive properties**

According to the proposed models, a random graph was constructed that describes the motion of an electron between islands and the construction of an island structure with an estimate of the conductivity track size.

We simulate the case of a sufficiently rarefied island film with 10 islands and estimate its volt–ampere characteristics at a voltage in the range of 0.1–1 V, at a temperature of 300 K or 1 in relative
units. For such a temperature, we set the maximum jump between neighboring islands $d_{\text{max}} = 1$ relative units or 10 nm in absolute units.

Fig. 5 (a) shows a random weighted graph with 10 vertices. Voltage is connected to peaks 5 and 2. The shortest path, taking into account weights, includes vertices 5, 7, 6, 1, 2, and the total weight of the path is $d_s = 1.0940$ relative units. Then the absolute length of the total path consisting of jumps will be 10.940 nm.

Thus, by varying the length of the jump in the model, one can take into account the influence of the topological characteristics of the film on the conductive properties.

In addition, the length in the jump is influenced by the temperature in the simulated system [5]. This dependence is directly proportional.

Fig. 5. Random graph with 10 vertices: sparse island film (a), well-formed film (b).

Fig. 6 shows an island film pattern with 10 islets within the DLA model with different parameters sc and viscosity $p$. As from the drawings, these parameters significantly influence the film structure. At small values (Fig. (A) - (d)), a rarefied island film with the prevailing hopping conductivity mode is modeled; at medium values, hopping conductivity is an equivalent contribution to the total conductivity; at large values, the island film tends to solid and the islands merge and here prevail already conduction along the island (rice (e), (f)). Obviously, the diameter of the minimum coverage area also increases from 5 rel. units (fig. a) to 30 relative units. Taking the average cell size of 10 nm, we obtain the frame absolute lengths of the conduction paths $l$ in the interval from 50 to 300 nm.
Fig. 6. The structure of the island film is the DLA model for 10 islands (a) $sc = 0.01$, $p = 0.01$, (b) $sc = 0.1$, $p = 0.1$, (c) $sc = 0.5$, $p = 0.1$, (d) $sc = 0.9$, $p = 0.1$, (e) $sc = 0.2$, $p = 0.2$, (f) $sc = 0.9$, $p = 0.5$.

Estimating the electrically conductive properties with the parameters for plumbum telluride by the formulas (1) - (6) for voltages from 0.1 to 1 V, we obtain the frame limits for film resistance of the order of 109 Ohms, current strengths from $0.15 * 10^{-6}$ to $6 * 10^{-6}$ A and conductivity of about $10^{-6}$.

In fig. Figure 7 shows the calculated PtTe ampere characteristic, the graph of which was obtained using the approximation by splines. [9] The dependence obtained is on average linear, with minor deviations in the middle of the interval. The error of the simulation was about 30%, which at the qualitative level corresponds to the experimental dependencies.

Fig. 7. PbTe rated volt ampere characteristic

**Conclusion**

The results obtained at a qualitative level correspond to the data of an experimental study of the current-voltage characteristics of lead telluride nanofilms. The simulation allows, in the first approximation, to obtain a framework estimate of the electrically conductive properties of islet lead telluride islet nanofilms, as well as to estimate the experimental conditions for obtaining them for given volt-ampere characteristics.

This work was partially supported by the Ministry of Science and Higher Education project 16.1123.2017/4.6 and RFBR project 18-32-20006 mol_a_ved.

This work was partially supported by the Ministry of Science and Higher Education and FSRC «Crystallography and Photonics» RAS.

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