Percolation model of electric properties of laser modified PbTe film

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Abstract. The results of experiments on obtaining and studying the electrical properties of semiconductor films of PbTe are presented, and a model of current-voltage characteristics in the percolation approximation is proposed. The simulation performed qualitatively correctly reflects the current-voltage characteristics of the obtained films.

1. Introduction
The electrophysical properties of nanostructured semiconductor island lead telluride (PbTe) films are of scientific interest in the field of creating new unique materials based on well-known ones that can be used to develop innovative technologies of modern electronics and photonics.

2. Description of experimental studies on obtaining PbTe nanofilms and their electric properties
To obtain semiconductor island PbTe nanofilms, the action on the epitaxial PbTe structures from the side of the lead telluride film of cw YAG: Nd³⁺ - a laser with a wavelength of 1.06 μm and a power of 5-10 W was applied, while the laser beam was moving at a speed of 80 μm / s. [1] The obtained nanostructures were investigated using a Quanta 200 3D SEM and an Integra-Aura probe nanolaboratory. Detailed studies of the obtained nanofilms, performed using MATLAB tools, demonstrated their fractal nature. The surface of the films was characterized by a granular structure with a bimodal distribution function for the lateral sizes of granules of 1-3 μm and a relief height difference of 30-40 nm.

The electrical conductive properties of the obtained nanofilms were studied by measuring the current-voltage characteristics (CVC) using a four-probe circuit with a linear arrangement of contacts [2]: two end contacts provided direct current supply using a stabilized power source and were located at the same distance from each other equal to 6 mm. The I - V characteristics of the initial and modified PbTe films are shown in Fig 2. The voltage was varied from 0.1 to 1 V. The resistance value in the investigated range was about 10⁷ Ohm. The current strength was on the order of 10⁻⁶ A, depended directly on the size of the granules and was, on average, linear in the voltage intervals (0.1; 0.4) V and (0.65; 1). For average voltage values in the interval (0.4; 0.65), a resonant current surge was observed (Fig. 1).
Fig. 1. $I - V$ characteristics of the initial (1) and modified (2-5) island PbTe films for different granule sizes: 2 - $5.17 \times 10^8$ cm$^{-2}$, 3 - $5.25 \times 10^8$ cm$^{-2}$, 4 - $5.38 \times 10^8$ cm$^{-2}$, 5 - $5.46 \times 10^8$ cm$^{-2}$, when measured in the longitudinal direction (a), in the transverse (b).

The appearance of a resonant burst is considered as a result of the participation in the surface electrical conductivity of weakly and strongly bound electrons, which are initially at the size quantization levels in nanodots [3].

3. Model of the electric properties

To explain the obtained experimental results, as well as to calibrate the experimental conditions and predict the electrophysical properties of island nanofilms, the apparatus of mathematical modeling was used, within the framework of the percolation conductivity approach, when the sample was presented in the form of a percolation cluster or a system of percolation clusters. Within this model, individual percolation clusters or parts of a common cluster model the conductivity of islands as a system of conductors. In our approach, to estimate the electrical conductivity, we distinguished and calculated the length of the continuous shortest path of current flow inside the cluster (fig.2).

Fig. 2. Model diagram: conductive islands marked with color, substrate - white, voltage is applied to boundaries A and B, conductive elements form a conduction track.

Fig. 3. Percolation cluster construction scheme (a) cell marking: 1 - occupied cells(b); 0 - free; marking of adjacent clusters according to the Hoshen-Kopelman algorithm [6] (c) the skeleton of a percolation cluster at $p = 0.58$ [5] (d).
To construct a percolation cluster, the cell percolation model [4], implemented by the Monte Carlo method, was used (Fig. 3 a).

Within the framework of this model, a uniform grid is superimposed on the square computational domain, for the cells of which the value of the probability of its employment \( p \) is set. If the constructed common cluster connects two opposite sides of the system, then it is percolation and conduction paths are distinguished in it. For this, the Hoshen - Kopelman algorithm was used [5] (Fig. 3b, c). In addition, this algorithm made it possible to estimate the size distribution of clusters of the general percolation cluster. To estimate the shortest distance of current flow, we used the algorithm for isolating the skeleton of the percolation cluster [6]. To estimate the \( I - V \) characteristic, a classical model according to Ohm's law was used [4].

![Fig. 4. Percolation clusters and possible paths of conduction for permeabilities a) 0.6 b) 0.65 c) 0.7 d) 0.75 e) 0.8 f) 0.85 g) 0.9.](image)

According to the above algorithm, calculations of the percolation surface and electrical conductivity were carried out. The computational area was selected with a size of 100 * 100 relative units. The computational grid consisted of 10,000 cells. In modeling, the main parameter was the degree of permeability \( p \), which varied from 0.6 to 0.9. Fig. 4 shows the structures of the percolation surfaces. The percolation probability was considered as the probability of finding continuous horizontal paths. The calculation showed that for a permeability of 0.6 (Figure 4a) there are horizontal paths that do not completely intersect the computational domain, which indicates the absence of percolation. For such a case, the hopping conductivity model [7] is more applicable, for which, after clustering, it becomes possible to reveal clusters containing the maximum number of particles, which, in our opinion, make the maximum contribution to the total conductivity of the film. For example, a cluster with a number of particles equal to 1877 is the maximum. Its permeability is 0.571. It is also possible to distinguish a cluster with a number of particles equal to 1800, with a permeability of 0.125. In addition, it is possible to distinguish clusters with 420 particles, 0.125 permeability, 380 particles, 0.039 permeability. An experimental study has shown that percolation conductivity was observed at a value of the probability of permeability starting from 0.65 -0.9 (Fig. 4 b-g.). For example, Fig. 4a shows the structure of the percolation surface at \( p = 0.65 \). Of the entire set of clusters, a single maximum cluster is distinguished, containing 5936 particles, which provides conductivity.

The selection of the conduction tracks and the estimation of their length made it possible to calculate the resistance (Fig. 5 a) and electrical conductivity as \( \sigma = 1 / R \), which made it possible to simulate the \( I - V \) characteristic (Fig. 5 b) of the nanotape (2) from Fig. 2b depending on the permeability.
The calculated I – V characteristics are directly proportional to the permeability. Comparison of the calculated parameters with the measurement data for the film showed a relative simulation error of the order of 12%, which, in our opinion, fully satisfies the errors for the model of the electrical conductive properties of nanostructures.

![Fig 5. Resistance (a) and IV-characteristics (b) depending on the permeability.](image)

4. Conclusion
Thus, using the proposed approach, it is possible to simulate the electrical properties of island lead telluride nanofilms in the percolation approximation.

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