Modeling of a profile of a PbTe semiconductor nanofilm

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Abstract. The results of experiments on the production of plumbum telluride semiconductor films are given. The models of ballistic and random deposition describing the profile of the films obtained are proposed. The performed simulation qualitatively correctly reflects the relief of the obtained films.

Introduction
Today, semiconductor plumbum telluride (PbTe) nanofilms are often used in various fields of nano- and microelectronics. This situation is associated with their unique electrical and optical properties, which are largely due to the peculiarities of the surface structure of their surface. For example, the presence of a certain surface relief of a nanofilm leads to an increase in the actual contact area in a semiconductor device [1]. The actual area may significantly exceed the area of the visible contact window, which in turn may affect the electrical parameters of the contact and the characteristics of the devices. In this regard, the study of surface growth processes is an important task.

The results of experiments
The initial PbTe heteroepitaxial structures were grown by molecular beam epitaxy in the ETH laboratory (Zurich). For laser irradiation of the samples, an experimental setup described in [2] was used. 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.

Nanofilm profile model

Studying the processes of film formation during molecular beam epitaxy and precipitation from solution demonstrates the appearance and growth of inhomogeneous three-dimensional surface structures [3]. Competing diffusion processes of precipitated particles over the surface, which allow smoothing out the inhomogeneities that form, form a real surface that may contain significant inhomogeneities with the presence of three-dimensional irregular structures.

Today, the concept of scaling is used to study the various processes of appearance of heterogeneity and surface roughness. [3] Theoretical consideration of the instability of surface growth in various deposition processes (molecular beam epitaxy (MBE), chemical precipitation from solution) indicates that the scaling transformation method or scale invariance should be universal and most convenient [3]. In various processes it was obtained [1] that the process of formation of irregular structures on the surface is described by the power law $K \sim t^n$, where K is the scale of non-uniformity, which is indicative of fractions the mechanism of this process. [3] Confidently identifying the fractal growth of the surface allowed the use of an atomic force microscope (AFM). The resolution of the microscope from $\sim 10 \mu m$ to $\sim 5 \text{ nm}$ made it possible to observe the hierarchy of structures on four orders of magnitude (scale from 10 nm to 100 µm) (Fig. 1).

In this regard, to calibrate the method of obtaining nanofilms and predict their properties, we simulated the relief of their surface in the framework of the scaling approach. To describe the scaling functions, random and ballistic deposition models were used [4, 5]. In the proposed models, the computational domain is represented in the form of a rectangular lattice of size $M \times L$, and particles according to specified rules are deposited along the vertical direction on the previously formed structure, fixing themselves at the nodes of the square lattice. Thus, over time, a cluster or aggregate with a specific geometry is formed. Two functions are used to describe the process: the average surface height $\bar{h}(t)$ which determines the position of the baseline for the surface of the sample and the roughness $W(t)$.

In the random growth model, all columns are filled randomly (Fig. 2a). Then, after random deposition of N particles, it is possible to calculate the height of the deposited structure $h$ from the relation $h = \sqrt{Nf(1-f)} + (Nf)^2$, where $f = 1/L$ is the probability of filling an arbitrary column, $L$ is the width of the calculated areas, i.e. $h(i) = h(i) + 1$, where $i$ is the number of the time step. [6] The model allows to estimate the surface roughness $W(t)$ as $W^2(L, T) = \bar{h}^2(t)$, where $\bar{h}(t) = Nf = t$ is the average surface height formed during time $t$. In the deposition model, the particle is fixed at the point of the first contact with an already deposited structure (the nearest
neighbor rule) (Fig. 2b). Thus, during the deposition, the height of the nearest left and right columns is taken into account as: \( h(i) = \text{MAX}(h(i-1), h(i) + 1, h(i + 1)) \) [7]. In contrast to the previous model, a particle can thus adhere by its side surface to an already formed structure [8], i.e. the possibility of growth along the local normal to the surface is taken into account, which may lead to the expansion of local protrusions on the front surface, and hence to an increase in the growth of the surface in the lateral direction.

![Fig. 2. Scheme of random (a) and ballistic (b) deposition](image)

**Nanofilm profile simulation results**

The proposed models were used to calculate reliefs and roughness in relative units, and the effect of the width of the scan area on the roughness was also evaluated.

Fig. 3a shows the image of a modeled profile (side section) of a h (i) nanofilm 100 rel. Wide. units in time \( T = 100 \) relative units, at a deposition rate of 30 particles per unit time. Fig. 3b - roughness graph for the above parameters.

![Fig. 3. Random deposition model: relief (a), roughness (b).](image)

Fig. 4a shows the image of the modeled profile (side section) of the nanofilm and roughness within the framework of the ballistic deposition model.
From Figures 3 and 4, it is obvious that the ballistic deposition model generates a more heterogeneous and rough structure with a higher average height, which corresponds to the initial stages of obtaining nanofilms with a small number of laser passes on the surface (5-10 passes). Such a model describes qualitatively thermal diffusion processes with a high probability of sticking of particles at high temperature. The random deposition model allows us to obtain more homogeneous structures with less roughness. Unlike structures after ballistic deposition, random structures generally have a less inhomogeneous front, which corresponds to the final stages of the experiment, when a well-formed nanofilm is obtained after a larger number of laser passes (15-20 passes) with a lower thermal diffusion intensity. By setting the value of the model particle, the proposed models allow us to calculate the magnitude of the inhomogeneities and the film thickness. For example, for a lead telluride nanofilm, with a block size from 10 nm to 30 nm for a ballistic deposition model, we obtain an average film thickness of 65 - 190 μm, for a random model from 30 to 160 μm. The calculated differences in height are left on average for ballistic deposition without taking into account very deep valleys of the order of 20-30 nm, for a random 35-50 nm.

Consider the effect of the width of the scan area on the amount of roughness, based on Fig. 1 and 5, 6. From a comparison of the surface profiles it can be seen that, regardless of the width of the scanning area, the maximum height difference over the surface profile is approximately 35 nm. Obviously, with an increase in the width of the scanning area at a constant value of the number of measurement points, some of the information about the surface that is between the measurement points is lost. This means that the microscope needle does not fully measure the profile of an individual grain on the surface, as a result, the surface relief becomes smoother and the roughness decreases. As the width of the scanning area increases, macroscopic growth islands are also drawn on the surface relief, which are not visible when the scanning area is less than 10 μm. This effect is clearly seen from the comparison of AFM images of the surface morphology obtained by varying the width of the scan area. [9] Therefore, for a complete analysis of the surface roughness, it is necessary to study the statistical parameters of the surface in a wide range of magnifications.

In fig. 5.6 shows a family of dependences of the surface roughness of PbTe epitaxial films obtained with different growth models. In fig. 5 - in the framework of the random deposition model, in fig. 6 - ballistic.

The dependence of roughness on the width of the scanning area for a film generated on the basis of a random deposition model with parameters similar to Fig. 3, is shown in Fig. 5. For this case, the roughness has the following maximum values: 12 nm, 8 nm, 5.9 nm, 4.7 nm, 4.5 nm with a scan area width of 25 μm, 50 μm, 75 μm, 100 μm and 125 microns respectively. This picture indicates a decrease in roughness.
Fig. 5. Dependence of roughness of random deposition structures on the size of the scanning area: 25 μm (a), 50 μm (b), 75 μm (c), 125 μm (d).

As you can see, all these dependencies have a similar appearance and are close to exponential.

Figure 6 shows the dependence of roughness on the size of the scan area for structures modeled within the ballistic deposition model, with parameters similar to Figure 4. For this case, the roughness has the following maximum values: 8 nm, 4.95 nm, 5.02 nm, 3.99 nm, 4.99 nm with a scan area width of 25 μm, 50 μm, 75 μm, 100 μm and 125 μm, respectively.

In the first temporary area to 10 rel. unit when there is a slow increase in roughness. This is explained by the fact that at the initial stage there are not many islands of the emerging film and they have a fairly simple relief. In the second area from 10 to 100 relative units there is a sharp increase in surface roughness. This is due to the fact that for a given time interval there is a rapid growth of the film and the complication of the relief of its surface.
Fig. 6. Dependence of the roughness of the ballistic deposition structures on the size of the scanning area: 25 μm (a), 50 μm (b), 75 μm (c), 125 μm (d).

In this case, the dependencies are of a fairly non-monotonic nature, and for small values of the scan area (Fig. 6 a, b), it tends to a sinusoid with increasing amplitude and proceeds to exponential behavior. In the case of ballistic deposition, the maximum roughness values, depending on the size of the scanning area, decrease not so monotonously than for the random one (Fig. 6 b, c), but still tend to decrease. For large values of the scanning area, the dependence becomes monotonous and tends to exponential. In our opinion, such a picture can be explained by the more chaotic nature of the structures of ballistic deposition than by chance.

Conclusion

The results obtained qualitatively correspond to the data of the relief study and the structure of the films by the methods of AFM microscopy. [9] The simulation allows, in the first approximation, to estimate the structure of plumbum telluride nanofilms, as well as to evaluate the experimental conditions for their preparation.

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