Simulation of the electrical conductivity of island-type thin films and nanostructures

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Abstract. Areas of application of islet thin films in science and technology are described. Experiments on the formation of metal island nanostructures are performed. The principle of calculating the size of islands at different stages of growth is presented. The function of the tunneling current between islet nanostructures versus the deposition time is empirically deduced.

1. Introduction

The growth process of a continuous thin film can be divided into the following steps (figure 1):
1. Nucleus formation
2. Nucleus growth, islet formation
3. Coalescence of islets
4. Channel formation
5. Hole formation
6. Continuous film formation

Figure 1. Stages of film growth: a – nucleus formation; b - nucleus growth, islet formation; c, d - coalescence; d - channel formation; e - hole formation; g - continuous film formation [5]

Islet nanostructures or island-type thin films (ITF) are films whose formation was completed at the stage of island formation [1].
They arouse interest in themselves because of the special properties associated with the nano-
dimension of these structures in all three directions. A striking representative of such effects is the
dimensional quantization of the energy levels of an electron located inside an island.

The literature discusses methods for modeling ITF. The authors show the importance of the various
characteristics of these methods, because each of them has its own particular qualities, both the
application and the results obtained.

Among these methods, molecular beam epitaxy (MBE), gas phase epitaxy (GPE), ion beam etching
(IBE), lithography and many others are often distinguished.

One of the most promising and modern technological methods is the MBE method. Its principle of
operation is based on the growth of single crystal layers due to reactions between thermally generated
molecular or atomic beams of the corresponding components and the surface of a substrate located in
ultrahigh vacuum at elevated temperature [1,2,3].

Scientists note that new methods for obtaining ITF can make a huge breakthrough in
instrumentation at almost all of its sections. For example, ITF can be used to increase the operability
of a transistor - a device that converts electrical signals [2,5-11]. If quantum dots are formed in the
channel of such a device, then quantum effects such as tunneling and dimensional quantization of the
energy spectrum of charge carriers can significantly improve the characteristics of the element.

Also, islet structures can be used in medicine. Some scientists believe that by applying gold
nanoparticles to a surface immobilized by a dye, the sensitivity of giant Raman spectroscopy (GRS)
can be significantly increased [2].

It is also indisputable that the development of methods for obtaining ITF will coordinately affect
nano-electronics itself. One of the arguments is the fact that island-type structures are used as catalytic
seeds to produce carbon nanotubes (CNTs) [6].

It should also be noted that quantum dots (islands of semiconductor materials 2–10 nm in size) are
one of the methods for implementing qubits in quantum computers [19].

Based on the results of the literature review, it becomes clear that island-based nanostructures are
an integral part of the future of mankind, and new ways of creating ITF, as well as modernization of
existing ones, can play a key role in the development of technologies!

The work is devoted to the development of a mathematical model for the formation of an island-
type film, with the help of which it will be possible to determine the size of structures obtained from
various materials.

The aim of the study is to build a mathematical model of the conductivity of electric current
through an island-type thin structure based on previously obtained experimental data.

2. Methods and materials
The method of thermal evaporation is based on the heating of substances in special evaporators to a
temperature at which a noticeable evaporation process begins, and the subsequent condensation of the
vapor in the form of thin films on the treated surfaces located at some distance from the evaporator
[5].

When thin films are deposited in vacuum by thermal evaporation (figure 2), energy is supplied to
the substance being evaporated by resistive (direct and indirect) and / or high-frequency heating,
electron bombardment, heating using laser radiation or using an electron beam.

![Figure 2. The scheme of the method of thermal evaporation [5]](image-url)
When the temperature of the evaporated substance rises to a temperature equal to or higher than the evaporation temperature, particles of the evaporated substance leave the evaporator, are transferred to the substrate in vacuum, and condense on its surface, forming a thin film [5].

The current flows over the substrate surface either by direct tunneling (figure 3), or by tunneling through stable energy impurity states.

![Figure 3. Particle tunneling through a potential barrier [5]](image)

Hill also proposed a model [7], in which the participation of the substrate in the conduction mechanism between the islands was taken into account. In this case, the magnitude of the current increases, since the height of the potential barrier is less than the thermodynamic work function of the electron. In addition, the transparency of the potential barrier increases even more if there are free alkali metal ions on the surface of the substrate, which form surface electronic states in the substrate itself [8, 12].

Based on the experimental data, an empirical dependence of the current flowing on the substrate between the contacts on the film deposition time was obtained [12]. In this paper, this result will be the main one - most arguments will be based on it.

3. Vacuum processing equipment

In this work, for the formation of island nanostructures, a small-sized modular type vacuum installation was used (UVN-1M), which is intended for research in the field of thin film deposition in vacuum (figure 4).

![Figure 4. The basic vacuum circuit of the initial installation; P1, P2 - a wide-range sensor and a Pirani sensor, respectively; CV1 - a vacuum chamber; VE1, V1 - angular solenoid valve and butterfly valve, respectively; NR1 - turbomolecular pump; NI1 - spiral pump](image)

Installation specifications:
- ultimate pressure: $10^{-3}$-10$^{-6}$ Pa;
- working gas pressure: 0.1–100 Pa;
- film deposition rate: $10^{-3}$-15 nm/s;
• etching rate of layers: 10^{-2}–50 nm/s;
• power consumption: 1.5–5 kW;
• overall dimensions: 500×1100×1600 mm;
• weight: 90 kg.

4. Solution
The tunneling current between islands of the same material depends on the applied potential and the
distance between islands [9, 10, 11]. Known view for the dependence of the density of the tunneling
current:
\[ j_t = e^2 V (2m \varphi)^{1/2} (4\pi^2 h^2 \vartriangle z)^{-1} e^{-2h \Delta z (2m \varphi)^{1/2}}, \]

\( m \) – electron mass;
\( \Phi \) - electron work function of the film material;
\( \hbar \) – reduced Planck constant;
\( V \) – applied external potential;
\( \vartriangle z \) – distance between the islands;
\( e \) – electron charge;

Let’s consider the basic experiment: a substrate was prepared from ceramic with pre-formed
contact pads on it (figure 5). Let’s place it in the working chamber and pump out this volume up to 10^{-3}
Pa (working pressure). After heating to 80\(^\circ\), we begin to evaporate copper from a tungsten spiral.

\[ \varphi = \text{const}; \]
\[ \frac{e^2 V (2m \varphi)^{1/2} (4\pi^2 h^2 \vartriangle z)^{-1} e^{-2h \Delta z (2m \varphi)^{1/2}}, \text{where}}{\text{}} \]

Then, in equation (1) we get:
\[ \varphi = \text{const}; \]

Thus, from equation (1) we obtain:
\[ j_t = A V (\vartriangle z)^{-1} e^B \Delta z, \text{where} \]

\[ A = e^2 (2m \varphi)^{1/2} (4\pi^2 h^2)^{-1} = \text{const} > 0; \]
\[ B = -2h (2m \varphi)^{1/2} = \text{const} < 0; \]

Let’s assume that the voltage is constant \( (V = \text{const}) \), then equation (2) will simplify to:
\[ j_t = \frac{C}{\Delta z} e^B \Delta z, \text{where} \]

\[ C = e^2 V (2m \varphi)^{1/2} (4\pi^2 h^2)^{-1} = \text{const}; \]

With the growth of the film, the diameter of the islands changes according to the following law
determined experimentally [6]:
\[ D = (175 + 27x_1 - 22x_2 - 8x_3 + 10x_1x_2 \Delta t) \in [20; 35] 498 + 134x_1 - 59x_2 - 8x_3 + 36x_1x_2 \Delta t \in [40; 65] 880 + 41x_1 - 14x_2 \Delta t, \text{ where} \]
\[ x_1, x_2, x_3 \] – are dimensionless magnitudes of factors: application time — \( x_1 \), evaporator — substrate
distance — \( x_2 \), substrate temperature — \( x_3 \).

Interestingly, the selected time intervals are characterized by various physical processes occurring
on the substrate, in terms of the number \( (N, \text{pcs} / \mu \text{m}^2) \) of islands and their size \((D, \text{nm})\): from 20 to 35 s
- $N$ and $D$ increase; from 40 to 65 s - $N$ is stable, $D$ grows; from 70 to 85 s - $N$ decreases, $D$ grows. Let’s turn to dimensionless quantities of factors. In this case, the upper level of the factor is “1”, and the lower is “–1”. The coordinates of the center of the plan are zero.

From this expression we will consider only the average time interval $t \in [40; 65]$ s, since it is on this interval that the number of islands on the substrate is already stabilized and only the distance between them will affect the tunneling current [6].

Now, let’s connect the distance between the islands with their diameter. Let’s assume that the change in the interval between the islands is proportional to the change in the remaining free area on the substrate (figure 6).

![Figure 6. The process of island growth at $t=40..65$ s](image)

Let the number of islands per unit area is $N$ ($N = \text{const}$ in our time interval). The area $S_1$ occupied by one island will be equal to:

$$S_1 = \frac{\pi D^2}{4}, \text{where}$$

$D$ - is the average diameter of the island;

Then the area $S_\Sigma$ occupied by all structures will be equal to:

$$S_\Sigma = S_1 \cdot N = N \frac{\pi D^2}{4};$$

Let the substrate area be $S$, then the time dependence of the distance between the islands is proportional to $S \cdot S_\Sigma$. We get:

$$j_t = \frac{C_1}{S - S_\Sigma} e^{C_2(S - S_\Sigma)}; \text{where}$$

$$C_1 = e^{2V(2m\varphi)^{-1/2}} (F4\pi^2\hbar^2)^{-1}; \quad C_2 = -2Fh(2m\varphi)^{-1/2},$$

$F$ - is the dimensional constant characterizing the transition from the distance between the islands to the difference between the areas.

Let’s us depict the dependence for the diameter for the selected interval in the following graph (figure 7).

![Figure 7. Graph of the island diameter versus time](image)

Let’s convert this graph to the equation:
\[ D = 10.72t - 64.8 \text{ [nm]}, \text{ where } t \in [40; 65] \text{ s} \]  
(5)

Now, let's substitute equation (5) in equation (3) and picture the resulting graph (figure 8):

\[ j, 10^9, \text{ A} \]

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Figure 8. Characteristic dependence of current strength on time, calculated according to the model

Let's compare this dependence with that obtained in the course of a real experiment (figure 9).

\[ j, 10^9, \text{ A} \]

\[ j, 10^9, \text{ A} \]

Figure 9. Characteristic dependence of current strength on time, obtained experimentally (1) and calculated according to model (2)

One of the basic assumptions of why real dependence behaves in this way may be the property of the islands themselves. The islands grow in pulses, in particular, the total surface area of two islands differs from the area of one obtained when they merge [6, 15-16]. Because of this phenomenon, “jumps” may appear inside the dependence of the tunneling current on time, since the tunneling current depends on the distance between the islands, which, in turn, is associated with their area.

The second important fact is the influence of the characteristics of the vacuum installation on the course of the experiment. In a real experiment, the compact modular vacuum installation uses the Edwards nEXT 75D turbomolecular pump as the final pump, with the help of which an operating pressure of \(10^{-3}\) Pa is reached during the experiment. At such pressures, the concentration of molecules in the volume can be calculated from the equation of state of an ideal gas:

\[ P = nkT \Rightarrow n = \frac{P}{kT}, \text{ where} \]

\[ k \text{ – Boltzmann coefficient} = 1.38 \times 10^{-23} \text{ J/K}; \]
$T$ – working temperature $= 363$ K [5];
We get:
\[ n = 2.05 \times 10^{17} \text{pcs/m}^3 \]
This means that during the entire experiment, quite a few gas molecules remained inside the setup, which could get on the substrate during film growth and cause sharp increases in resistances between the islands, which could cause the value of the tunneling current between them to drop.

5. Work results
As a result of the review of information sources, the advantages of instruments and devices on the islet nanostructures are considered and substantiated, the relevance of the study of ITF is determined.
A mathematical model of the dependence of the tunneling current on the geometric parameters of the ITF is developed.

6. Conclusion
The obtained mathematical model of the growth of an island thin film is idealized, since it contains some assumptions. However, even now it is capable of transmitting the correct nature of the change in the tunneling current during the formation of the ITF. In the future, the model will be finalized. Using it, it will be possible to determine not only the time of formation of islands from different materials, but also the parameters of the resulting substrate – island thin film system.

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