Mathematical modeling of geometrical and electrical characteristics of island films growth initial stages

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Abstract. The metal island nanostructures application fields in science and technology are presented. Experimental studies were carried out using the UVN-1M vacuum unit to test the metal thin films formation modes. Presents the control principle at the initial stages of growth of the tunneling current change between the island thin films. A series of copper and aluminum ITF samples were obtained. The derived samples thicknesses were measured using an atomic-force microscope, as a result, the dependence of the geometric and electrical characteristics of thin films and island nanostructures on the process parameters were simulated.

1. Introduction

Island thin films and nanostructures are in high demand in many fields of science: microelectronics and nanoelectronics, optics, photonics, laser technology, solar energy, etc.

Recent studies have revealed that island thin films can be used in the solar panels and devices based on those panels.

Moreover, island nanostructures make glasses of the optical instruments in space vehicles more transparent, island nanostructures are used in the digital and alphanumeric displays, and gas sensors for better sensibility.

Although, an aluminum island could be used as a base for the single-electron transistors, while a block of islands could be a basis for new variations of the creation MOS transistor.

Gold-based island thin films (ITF) allow creating high-efficiency photoelectric converters [1]. The efficiency of photoelectric converters is limited by the high electric and optic losses [2]. A golden island thin film (Figure 1) produced by the triode sputtering and built into the p-n-composition of the photovoltaic structure shows a significant increase of the photocell efficiency.

Island nanostructures in microelectronics have become extremely popular for creating memory elements. The main advantages of that memory are energy self-sufficiency, fast response time, small sizes of the data recording cells and low power consumption.

In microelectronics, aluminum and copper island nanostructures are of special interest because of their processing characteristics and reasonable price. Aluminum is characterized by the high oxidation susceptibility that makes it easy to create the oxide protection layers.
Today island thin films and nanostructures are highly popular, that is why this article and previous researches deal with the issue of creating such unique covers.

Figure 1. A photoelectric converter based on the golden island nanostructure [2].

2. Metal island thin films production methods
Thermal evaporation and magnetron sputtering methods were chosen based on the existing available methods for obtaining island nanostructures analysis. Mentioned below methods could be implemented using the laboratory vacuum modular type tool UVN-1M (located in BMSTU).

2.1 Thermal evaporation
It is well known that thin films deposition by thermal evaporation in vacuum occurs by summing energy to the evaporated material by resistive heating. When evaporation temperature has reached the particles leaving the evaporator and condensate on the substrate surface [3]. The main advantages of the method are high deposited material purity and relatively easy implementation. Also, the ability to control the thermal evaporation process allows to influence the initial cover growth stages (changing the source current) and to obtain discontinuous thin films with different structures.

2.2 Magnetron sputtering
The magnetron sputtering method in a vacuum can be chosen as an alternative method of obtaining non-continuous metal films. The process is carried out at the argon atmosphere, in which the ions are formed in the gas discharge and accelerated due to applying the negative potential to the target. High-energy argon ions sputter material atoms (copper or aluminum) from the surface layers of the target. Then the atoms are deposited to the substrate [3–5]. The main advantages of this method are adjustable deposition rate and the possibility of covering films of dielectric, metals, semiconductor materials.

This article describes experimental studies that have been carried out for the thermal evaporation method in a vacuum. In the future, it is planned to perform similar modeling of the magnetron sputtering method also.

3. Unit of the discontinuous thin films and nanostructures control
Special tooling for compact modular vacuum installation UVN-1M was designed for research in the field of thin films and nanostructured coatings formation under vacuum [6].

The vacuum system consists of a dry pump and a turbo molecular pump, which allowed to perform oil-free pumping. Different technological modules are used in a chamber to switch between the mentioned above methods. The exchange of the technological modules could be carried out very easy as they mounted using quick-release flange. It allows performing several experiments per working day.

The stand of the thin films initial stages control (Figure 2) is arranged on the UVN-1M installation basis (1) using picoammeter (2) and electric power supply (3).

To perform the experiment, it is necessary to connect the picoammeter to the dielectric substrate with a pre-formed area on its surface through the current leads installed in the upper flange. The electric power supply allows limiting the maximum current (short-circuit current), which protects the picoammeter against possible damage [7]. During the experiment, after the beginning of intensive evaporation, the operator simultaneously opens the flap and turns on the picoammeter. The data recorded by the device is transmitted to the PC. Figure 3 shows one of the graphs of ITF copper growth.
Figure 2. The experimental stand of tunnel current control during thin film growth.

Figure 3. Diagram of the change in the tunneling current overtime during the copper coating process.

Of particular interest are the characteristic peaks depending on the tunnel current process time. The current measurement starts when the damper is opened. Picoamperes captures the first signal after 1.5 seconds after coating starting. Obviously, the closer the evaporator is positioned to the substrate, the coating growth process is faster, and means, the record of changes in the value of the current starts earlier. The peaks of the diagram indicate multiple stages of island coalescence at the initial stages of thin-film coating growth [7].

4. Statement of problems of experimental researches

The process of thin metal film deposition was carried out using the installation UVN-1M. In the chamber 1 (Figure 4) the thin film is deposited by thermal evaporation. The substrate (3) is positioned on a holder (2). Evaporated material 4 is deposited (in the first case – copper, in the second - aluminum) to the substrate.

The material is located on the evaporator 5, which is heated by resistive heating through the current leads 6, located at a distance h (mm) from the substrate holder. The deposition process takes place during the time t (s) and under pressure P (Pa).

Experimental research will be divided into two stages. The first stage is the formation of ITF on dielectric substrates (made of sitall) to control the tunneling current during the deposition process and determine the initial stages of coating growth.

For the second stage, the substrate will be replaced by a silicon wafer. Silicon is the basis for the creation of a MOSFET. The modes of formation will be adjusted based on mathematical models created on the first stage.
5. Stage 1. Research of the copper and aluminum ITF

5.1 Reception of research results
By varying the distance from the evaporator to the substrate (30 mm and 60 mm), as well as the processing time (30 s and 60 s), experiments with copper (Figure 5) and aluminum (Figure 6) deposition were carried out on a substrate of sitall.

The obtained samples were measured by AFM at three points in the scanning area of 90x90 μm (Figure 7).

As experimental samples, measurement results, the dimensions of the thicknesses of copper and aluminum covers depending on the process parameters were obtained (table 1).

It was decided to investigate mathematical models of the thin film thickness dependence on the process parameters for processing the data and working out the nanoscale thin-film cover formation modes. The claimed math models were constructed by the method of full factor experiment.
Table 1. The results of experiments on the copper and aluminum formation for on the sitall substrate.

| Material | Substrate material | № sample’s | The distance from the evaporator to the substrate h (mm) | Deposition process time t (s) | The thin film thickness y (nm) |
|----------|--------------------|------------|--------------------------------------------------------|-----------------------------|-------------------------------|
| Cu       | Sitall             | 1          | 60                                                     | 30                          | 40                            |
| Cu       | Sitall             | 2          | 30                                                     | 60                          | 800                           |
| Cu       | Sitall             | 3          | 30                                                     | 30                          | 180                           |
| Cu       | Sitall             | 4          | 60                                                     | 60                          | 583                           |
| Al       | Sitall             | 1          | 30                                                     | 60                          | 37                            |
| Al       | Sitall             | 2          | 30                                                     | 30                          | 25                            |
| Al       | Sitall             | 3          | 60                                                     | 30                          | 13                            |
| Al       | Sitall             | 4          | 60                                                     | 60                          | 17                            |

5.2 A mathematical model for the copper thin film covers

The experiment has revealed a mathematical model of the thickness dependence of the thin-film cover formed by evaporation:

\[ Y_{Cu} = 400 + 292X_2 - 89X_1X_2, \]  

(1)

where \( X_1 \) is the distance, [non-dimensional]; \( X_2 \) is time [non-dimensional].

The analysis of the obtained data results showed that the experiments became reproducible, the model validity was confirmed.

It is needed to mention that the distance was not relevant, which may be due to the small variation interval. Maybe it is necessary to lower the bottom. The time factor had a significant impact as with the time increased the film thickness increases. This fact correlates to the physics of the received mathematical model. The interaction of the distance and time is also relevant, the variation of two parameters can affect the output parameter – the film thickness.

5.3 A mathematical model for the aluminum thin-film covers

The experiment has revealed a mathematical model of the thickness dependence of the thin-film cover formed by evaporation:

\[ Y_{Al} = 23 - 8X_1 + 4X_2, \]  

(2)

where \( X_1 \) is the distance, [non-dimensional]; \( X_2 \) is time, [non-dimensional].

The analysis of the obtained data results showed that the experiments became reproducible, the model validity was confirmed.

It stands to mention that time and distance became relevant, as with the time increased or the distance shortened the film thickness increases that correlates to the physics of the mathematical model. The interaction of the distance and time is not significant, the variation of two parameters at the same time cannot affect the output parameter – the film thickness.

Comparing thickness dependence models on process parameters for copper (1) and aluminum (2), it seems to be interesting that the distance from the evaporator to the substrate does not affect the cover thickness. In this case, the time factor has a significant impact. However, for aluminum covers, the distance factor is twice important comparing the time factor. The distance from the evaporator to the substrate factor is responsible for the film growth rate.

This pattern may be related to the mechanisms of growth of covers from different materials on the initial stages, which in turn also affect the covers growth rate, and hence the thickness. Since aluminum is a lighter-melting material, aluminum particles reach the substrate surface at a lower temperature than copper particles. So, there is a growth of aluminum film by the vapor-crystal mechanism, the particles crystallize on the substrate, bypassing the liquid phase.

As recommendations for obtaining nanoscale thicknesses cover of copper and aluminum on sitall substrates are necessary to reduce process time up to 30 s, and the distance from the evaporator to the substrate to increase to 60 mm. In this case, the cover growth process will slow down slightly, i.e. the film growth rate will decrease. Then it will be possible to control more the growth initial stages.
process and to obtain island nanostructures arrays with specified geometric characteristics (island width and height and the distance between the islands)

6. Stage 2. Formation research of the ITF on a silicon substrate.

An aluminum ITF layer on a silicon substrate is conductive in the MOSFET (memory element). Tunnel current passes through the aluminum islands so that the transistor has a higher speed [8].

Based on the obtained formation mathematical model a series of experiments on the aluminum formation on a silicon substrate (figure 8). The experiments were carried out in the same way. After analyzing the mathematical models obtained at the first stage, the ITF formation modes – the distance from the evaporator to the substrate (30 and 40 mm) and the formation time (7 and 20 s) are corrected.

![Figure 8. Silicon substrate samples with aluminum cover.](image)

The samples were measured using an atomic force microscope, similar to the above technique. The size of the Islands is shown in table 2. Image 3 of the sample obtained by AFM is shown in figure 9.

| Material | Substrate material | № sample's | The distance from the evaporator to the substrate h (mm) | Deposition process time t (s) | The thin film thickness y (nm) |
|----------|--------------------|------------|---------------------------------------------------------|-----------------------------|-----------------------------|
| Al       | Silicon            | 1          | 40                                                      | 7                           | 3.5                         |
| Al       | Silicon            | 2          | 40                                                      | 7                           | 5.7                         |
| Al       | Silicon            | 3          | 30                                                      | 20                          | 11.7                        |
| Al       | Silicon            | 4          | 30                                                      | 20                          | 12.8                        |

![Figure 9. Sample 3 aluminum ITF on silicon.](image)

As a result of the experiments, a mathematical model of the aluminum ITF thickness dependence on silicon formed by thermal evaporation in a vacuum is obtained:

\[ Y = 8.4 - 0.8X_1 + 3.8X_2 \]  

(3)

where \( X_1 \) is the distance, [non-dimensional]; \( X_2 \) is time [non-dimensional].
The analysis of the obtained data results showed that the experiments became reproducible, the model validity was confirmed.

It stands to mention that time and distance became relevant, as with the distance increased or the time decreases the film thickness increases that correlates to the physics of the mathematical model. The interaction of the distance and time is not significant, as a variation of two parameters at the same time cannot affect the output parameter – the aluminum ITF thickness.

When comparing the mathematical models of aluminum ITF on sitall (2) and silicon (3), it is easy to notice that the same factors – distance and ITF formation time – are significant. However, in the second case, the coefficients before the parameters take smaller values, which indicates a lower rate of film growth.

7. Research realization of the aluminum ITF electrical characteristics on a silicon substrate

One of the important ITF characteristics as a conductive layer is resistance. To measure the resistance used LCR-station 1 (figure 10). Two probes 2 coming out of it should be applied to the test surface 3 at a certain distance from each other. To increase the measurement accuracy, each sample was measured three times. The resulting measurements of the samples are shown in table 3.

Figure 11 shows the known graph of the resistivity dependence on the thin metal film thickness. ITF are formed on the segment I, this section is linear [9]. Given this, it was decided to make the mathematical model also linear.

Segment I includes films less than 10 nm thick. Here \( \rho \) takes high values because in the early stages of the film is discontinuous. In this area, the resistance is determined by the resistance of the substrate sections.

As the coating thickness increases, its resistance decreases because the distance between the islands is reduced and there are no barriers to the flow of current through the sample. As a result of the research, a mathematical model of the dependence of the resistance of aluminum on a silicon substrate on the parameters of the formation is obtained. The coating is formed by thermal evaporation in a vacuum:

\[
Y = 750 + 185X_1 - 334.5X_2, \tag{4}
\]

where \( X_1 \) is the distance, [non-dimensional]; \( X_2 \) is time, [non-dimensional].

The analysis of the obtained data results showed that the experiments became reproducible, the model validity was confirmed. It stands to mention that time and distance became relevant, as with the distance increased or the time decreases the film thickness increases that correlates to the physics of
the mathematical model. The interaction of the distance and time is not significant, as a variation of two parameters at the same time cannot affect the output parameter – the film resistance.

Based on the measurement results, a graph of the resistance dependence on the aluminum ITF thickness on silicon was obtained (figure 12).

Figure 12. Experimental dependence of resistance on aluminum ITF thickness.

The nature of the change in resistance depending on the film thickness doesn’t contradict the physical meaning. It is obvious that with the increase of the film thickness (the size of the Islands), the distance between the islands decreases and the resistance of the metal coating decreases. As a result, the current conductivity of the film increases.

8. Conclusion
To create a conductive layer of the MOSFET material – aluminum, due to its high oxidability to create an insulating layer. As a method of forming the ITF of the aluminum method of thermal evaporation was selected, which correspond to the parameters of the purity of the deposited layer and the simplicity of the monitoring of the tunneling current. The experimental researches were reformed by using mathematical models of ITF size dependence. Based on modeling the technological modes of the process were selected. Processing the results of the study allowed us to evaluate the geometric and electrical characteristics of thin films.

9. References
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