Mathematical modeling of island films growth initial stages

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Abstract. Applications of the metal island nanostructures in science and technology are presented. Experimental studies using the UVN-1M vacuum unit were carried out to test the metal thin films formation modes. The growth the initial stages control on the tunnel current change is carried out. Thicknesses of obtained samples were measured using an atomic-force microscope as well as growth of thin films and island nanostructures 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, helioenergetics etc.

Recent studies have revealed that island thin films can be used in the solar panels and devices based on that 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 in 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 a basis for new variations how to make a MOS transistor.

Gold-based island thin films (ITF) allow to create high-efficiency photoelectric converters [1]. 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 significance increase of the photocell efficiency.

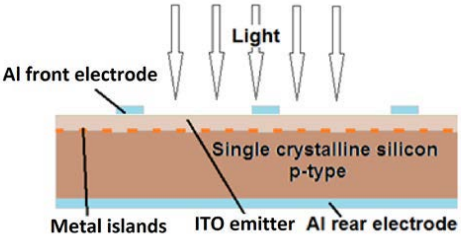


Figure 1. A photoelectric converter based on the golden island nanostructure [2].

Island nanostructures in microelectronics have become extremely popular in 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 accessible 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 getting such unique covers.

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 (BMSTU).

2.1 Thermal evaporation

It is well known that the thin films deposition by thermal evaporation in vacuum occurs by summing energy to the evaporated material by resistive heating. When evaporation temperature was 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. In addition, 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 vacuum can be chosen as an alternative method of obtaining non-continuous metal films. The process is carried out at Ar atmosphere, which the ions are formed in the gas discharge and accelerated due to the negative potential application to the target. High-energy argon ions sputter material atoms (copper or aluminum) from the surface layers of target. Then the atoms are deposited on the substrate [3]. The main advantages of this method are adjustable deposition rate and the possibility of applying dielectric, metals, semiconductor films.

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

Figure 2. Experimental stand of current control during thin film growth.

3. Unit of the discontinuous thin films and nanostructures control

Cover was carried out on a small modular vacuum installation UVN-1 M, designed for research in the field of thin films and nanostructured cover formation in vacuum [4].

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

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

To perform the experiment, it is necessary to connect the picoammeter to the dielectric substrate 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 ~~from~~ against possible damage [5]. 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.

4. Formulation and perform of research

The process of thin metal film deposition was carried out on the installation UVN-1M. In the vessel 1 (Fig. 3) the thin film is sprayed by thermal evaporation. On the substrate holder 2, a substrate 3 is placed on which the evaporated material 4 is deposited (in the first case – copper, in the second - aluminum). 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).

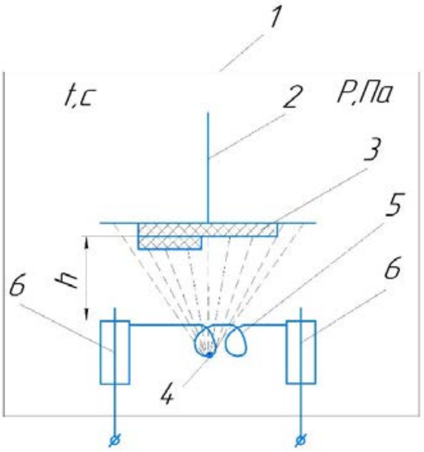


Figure 3. Scheme of thermal evaporation process in vacuum.

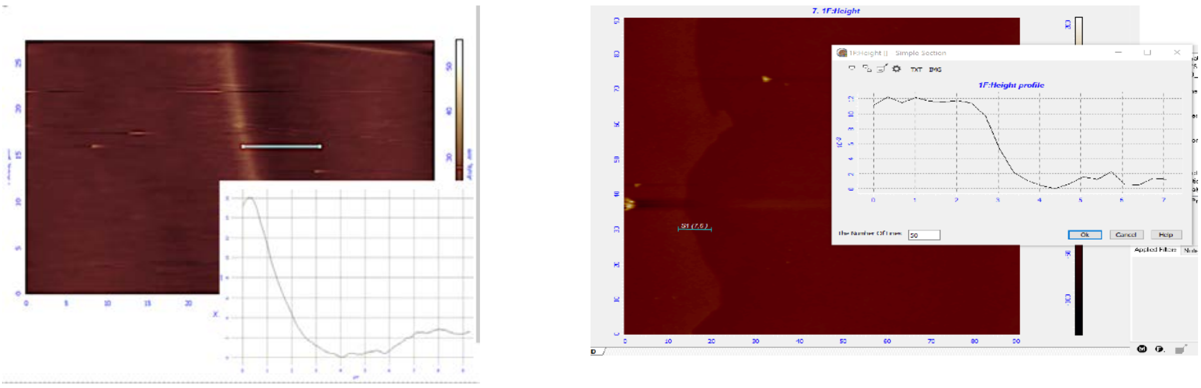
By varying the distance from the evaporator to the substrate (30 mm and 60 mm), as well as the process time (30 s and 60 s), experiments on copper (Figure 4) and aluminum (Figure 5) deposition were carried out on a substrate of sitall.

Figure 4. Sitall substrate samples with copper cover.

Figure 5. Sitall substrate samples with aluminum cover.

The obtained samples were measured on AFM at three points in the scanning area of 90x90 mkm (Figure 6). As experimental samples a measurements result, the dimensions of the thicknesses of copper and aluminum covers depending on the process parameters were obtained (table).

It was decided to calculate 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 factorial experiment.



a) b)

Figure 6. Step AFM-image and its measurement chart for copper (a) and aluminum (b) thin films.

Table 1. Experimental data.

Material	The distance from the evaporator to the substrate h (mm)	Deposition process time t (s)	The thin film thickness y (nm)
Cu	30	30	40
Cu	30	60	800
Cu	60	30	180
Cu	60	60	583
Al	30	60	37
Al	30	30	25
Al	60	30	13
Al	60	60	17

5. Elaboration and discussion of the experimental results

5.1 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:

$$Y_{Cu} = 400 + 292X_2 - 89X_1X_2, \tag{1}$$

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, that 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, as variation of two parameters can affect the output parameter – the film thickness.

5.2 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:

$$Y_{Al} = 23 - 8X_1 + 4X_2, \tag{2}$$

where X_1- distance, [non-dimensional]; X_2- 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, as 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 ~~as~~ 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 in 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 ~~arrive on~~ 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, which means the cover growth is faster.

As recommendations for obtaining nanoscale thicknesses cover of copper and aluminum on sitall substrates is 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. References

[1] Axelevitch, A. International Journal of Renewable Energy Sources // Application of Embedded Metal Nanostructures for Solar Cells, 2016.

[2] Kreibig, U. Optical Properties of Metal Clusters / U. Kreibig, M. Vollmer. – Berlin: Springer, 1995.

[3] Panfilov, Yu.V. Thin films deposition in vacuum // Technology in the electronics industry. – 2007. – Vol. 3. – P. 76-80. (in Russian).

[4] Sidorova, S. International Russian Automation Conference / S. Sidorova, M. Pronin, A. Isaeva // IEEE Automated Unit for Control of Initial Stages of Metal Islands Thin Films and Nanostructures Growth, 2018.

[5] Isaeva, A.A. Stand of the initial growth stages control of metal island thin films and nanostructures and their formation modes development / A.A. Isaeva, M.A. Pronin, S.V. Sidorova // Vacuum science and technology. Materials of the XXV scientific and technical conference with the participation of foreign experts, 2018. – P. 181-186. (in Russian).