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To cite this article: A E Komlev et al 2018 IOP Conf. Ser.: Mater. Sci. Eng. 387 012038

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Features of magnetron sputtering of a doubled Ta/Ti target

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Abstract. In this work, investigation of magnetron sputtering process of the doubled Ta/Ti target is presented. Such a construction allows to simultaneously sputter two materials, forming complex film structures on a substrate. The results of computer simulation and experimental investigation of the thermal behavior of the target, current-voltage and spectral characteristics of discharges, and characterization of the fabricated coating samples are given.

1. Introduction
The modern development of micro- and nanotechnologies opens new perspectives and possibilities for creating multicomponent film structures that significantly expand the functionality of the raw materials. Adding to a TiN film materials such as Si, Al [1] makes it possible to increase microhardness by more than 3 times, to the value of 42 GPa [2]. Heusler’s alloys such as Fe₃NbSn, Co₂Cr₁₋ₓFeₓₐₓAl, PtMnSb, Co₂FeSi, Co₂FeAl [3] are actively created and studied, as they define a new stage of spin electronics development.

One of the traditional ways of forming such structures is the method of magnetron sputtering by several confocal sources. Schematically, this process is shown in figure 1. The method of co-sputtering allows to accurately control the elemental composition of the deposited films.

As an alternative method, a number of authors consider the possibility of magnetron sputtering of composite (“mosaic”) targets [4–6]. The mosaic target is a matrix of a water-cooled cathode made from a material A (figure 2), in which the body has varying geometry inserts made of matter B (figure 2). The dimensions of the target (radius Rₜ), insert parts (radius Rₛ) and their relative positions, e.g., circle radius Rᵥ, are determined based on the requirements to the structure and composition of the coating. Using reactive gases makes possible to form films compounds, for example, metal oxides (Ti-VO [7]), which are actively used in optoelectronics.

![Figure 1. Sputtering scheme with two sources.](image1)

![Figure 2. Geometric model of the "mosaic" target.](image2)

The application of such structures is challenging because of the need for accurate preliminary selection of the geometry of the insert parts to achieve the required composition of the deposited film. In the article [4], authors state that properly selected materials and their parameters allow to obtain uniform coatings over a large area. The advantage of using a "mosaic" target is especially evident in cases where it is necessary to obtain films containing elements with low mutual solubility or a large difference in the melting points.

As an alternative to the "mosaic" target the authors [8] suggest using a more efficient and simple doubled-target design: bottom water-cooled target of material A and the top one made of material B with apertures of a predetermined size and geometric shape in the erosion zone. This design allows the simultaneous sputtering of two materials. By varying the gap between the targets, it is possible to vary the temperature of the top plate, thereby realizing the "hot" target mode, which leads to an increase in the effects of thermionic emission and evaporation.

2. Investigation of the gas discharge emission and volt-ampere characteristics during sputtering of the hot double target in an inert medium

To study the physico-chemical processes that occur during sputtering a double target with a hot top cathode, a magnetron sputtering system was developed (figure 2). To implement the hot regime, the bottom target, made from tantalum sheet (99.99 %) with a diameter of 130 mm and 1 mm thickness, was fixed with a gap of 0.2 mm on a metal water-cooled base. The top target, which was a titanium sheet with 130 mm diameter and 1 mm thick, was fixed above the tantalum sheet with a gap of 1 mm. To realize the possibility of simultaneous sputtering of 2 targets, 8 holes with a diameter of 17 mm were cut out in a titanium disk and located along a radius of 29.2 mm corresponding to the middle of the erosion zone with an internal diameter of 40 mm and an external one of 76.6 mm. The experimentally determined ratio of the sputtered areas of the bottom tantalum (2054 mm²) and the top titanium target (1786 mm²) is 1.15 to 1. The sputtering coefficients of the selected metals are close to each other: 0.69 for tantalum and 0.71 for titanium.

The residual pressure in the chamber was less than 10⁻² mtorr, the argon pressure during sputtering was 1 mtorr, the current density varied from 13 to 123 mA/cm².

As a result of studying the composition of the discharge, emission spectra were obtained by sputtering the target in an inert argon atmosphere. During the processing of these spectra, the most informative lines of the emission spectrum of the discharge were chosen and their intensity was measured. The dependence of the emission line intensity on the current density is shown in figure 3a. The corresponding I-V characteristics are given in figure 3(b).

![Graph](image_url)

**Figure 3.** Dependence of the intensity lines of 1 – Ar, 2 – 656.2 nm line, 3 – Ti, 4 – Ta on the discharge current density (a); I-V characteristic upon sputtering of the doubled Ta + Ti target (b).

The obtained I-V characteristic corresponds to the standard form of the curve when a hot metal target is sputtered in an argon atmosphere. When the current density exceeds 80 mA/cm², the voltage
decreases, which is possibly due to the increase in thermionic emission. The gas composition of the discharge, which can be characterized by the results of optical emission spectroscopy (figure 3(a)), also has peculiarities at 80 mA / cm² current density. If the intensity of the neutral argon, tantalum and titanium emission lines increases gradually with increasing current density from 13 to 80 mA/cm², after reaching 80 mA/cm² saturation of the Ta line with a simultaneous decrease in the intensity of the Ti line is observed. When analyzing the emission spectra of the discharge, a line with a sharp increase of intensity in the current density range of 70–123 mA/cm² was observed at 656.2 nm. According to the reference data, this wavelength corresponds to neutral hydrogen, which can be present in the chamber in minimum volumes in the form of residual gases. Therefore, the observed effect requires further detailed study.

Thus, the analysis of the gaseous atmosphere composition through the results of the optical emission spectroscopy and the I-V characteristics of the discharge indicates the characteristic features observed in a gas discharge at a current density of more than 80 mA/cm² and reaching an top target temperature of 1400–1500 K.

3. Modeling of the thermal regime of the "hot" composite target
At the initial stage, the modeling of thermal processes during sputtering of a doubled target in the COMSOL Multiphysics software package was performed. This software allows to consider the dependence of the material parameters from temperature in the form of analytical, piecewise continuous functions, as well as interpolation of a number of data during the calculation.

Figure 4 shows a general view of the developed 3D model of the magnetron. The main elements are:

- the top titanium target of a given thickness with holes in the erosion zone;
- bottom tantalum target of a given thickness, with an annular zone of erosion;
- cooled stainless steel base;
- stainless steel fasteners (screws and washers that determine the size of the gap).

Figure 4. 3D model of a magnetron with a hot composite target.

A one-dimensional problem is described by a system of homogeneous differential equations:

\[
\rho_i c_i \frac{\partial T(x, t)}{\partial t} = \lambda_i \frac{\partial^2 T(x, t)}{\partial x^2}, \quad i = 1, 2, 3, 4
\]

where: \(T\) – temperature; \(c_i, \rho_i, \lambda_i\) – heat capacities, densities and coefficients of thermal conductivity of the target materials \((i = 1, 2)\), cooled base \((i = 3)\), fastener and chamber elements \((i = 4)\), and \(x\) is the spatial coordinate. For calculations were used material parameters from the embedded library.

The problem was solved for various values of the discharge current density taken from the experimental I-V characteristic. One of the boundary conditions implies a cooled wall of the base \((T = 283 \text{ K})\). A typical example of the calculation result for the target is shown in figure 5. The maximum target temperature is reached at a current density of 123 mA/cm² and is 1631 K (figure 6).

4. Experimental determination of target temperature
The target temperature was determined experimentally from the results of measuring the total emission spectrum of a gas discharge and the radiation from a heated target.
The ISM3600 spectrometer was used to measure the emission spectra of a gas discharge. As can be seen from figure 7, when the power is increased, the spectrum of the gas discharge undergoes a significant change. The detected optical spectrum recorded by sputtering a "hot" target is a combination of the spectra of glow discharge and thermal radiation of a target, the intensity of which increases with increasing current density.

Temperature calculation method is based on comparison of the theoretical emission spectrum of an absolutely black body at a given temperature with the position of minima on the total spectrum. Calculation of the temperature is carried out according to the well-known Planck’s formula:

\[
I(\lambda) = \frac{2\pihc^2}{\lambda^5 \exp\left(\frac{hc}{\lambda kT}\right) - 1},
\]

where \(I(\lambda)\) – spectral intensity at the given wavelength \(\lambda\); \(h\) – Plank’s constant; \(k\) – Bolzmann’s constant; \(T\) – object’s temperature (K); \(c\) – speed of light in vacuum.

The results of determining the temperature from the discharge emission spectra are given in figure 6. The discrepancy between the calculated and experimental data does not exceed 6%, which indicates the adequacy and correctness of the developed model.
Figure 8 shows the XRD spectra of the manufactured coating sample. It has one broad maximum near $2\theta = 38$ deg. This angle corresponds to the cubic body-centered modification Ta with the preferential orientation (110) at 37.6 degrees and to the hexagonal Ti with orientation (111) at 38.0 degrees, coherent-scattering region compile 4.5 nm. The width of the peak does not allow one to give an uniquely identify one or two phases are present in the sample. The data of the electron probe X-ray spectral analysis was used to determine the ratio of titanium and tantalum in the deposited films: 45 atomic % of Ti and 55 atomic % of Ta). Taking into account the similarity of the sputtering coefficients of the selected materials, which should ensure the deposition of the film on the substrate at the same speed, the result obtained is well correlated with the ratio of the areas of the sputtered surfaces.

5. Conclusions
The studies carried out by the authors demonstrated the possibility of practical application of a doubled target. Change of the gap between the targets allows to change the mode of operation of the magnetron sputtering system, switching it to the "hot" mode. Nevertheless, the peculiarities of the behavior of the I-V characteristic and the spectra of the gas-discharge emission detected by the authors during the sputtering of the "hot" doubled Ta/Ti target require additional investigation.

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