Distribution of coating thickness applied by magnetron sputtering

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Abstract. The Danilin model for flat ring evaporator was studied and used to calculate the thickness distribution of the coating. The calculations for different types of the cathode current density variations (uniform, triangle and third-degree polynomial) were made. Relation between the magnetron sputtering system parameters providing the most uniform coating was analysed. Research of the target sputtering profile with nonzero cone angle was performed. It was established that in case of the cone angle increasing in the areas of substrate situated under the cathode the sputtered coating becomes thicker. Also at the center and on the edges of the substrate the coating thickness is decreased due to the redistribution of thickness.

1. Introduction
In the magnetron sputtering systems (MSS) [1, 2] can be used targets of different shapes, but the flat and conical targets are used most often. At the initial moment of sputtering the ions bombard the smooth surface, and over time the target become V-shaped. Herewith the cavity inside the target is constantly increasing and the deposition rate of the sputtering material is reduced. The deposition rate depends on the design of MSS and the discharge current value [3, 4]. Longer deposition process compensates the decreasing in deposition rate. The accuracy of the deposition mode correction can be increased if the deposition rate dependence on the target operation time at a fixed discharge current is known [5].

2. The Danilin model
In case of the MSS with a flat cathode the Danilin model can be used to calculate the thickness distribution of the film or coating [6]. The Danilin model for a flat ring evaporator is a special case of the model for a cone evaporator (the angle of the cone target in this case will be zero). The free path of the sputtered atoms shouldn’t be less than the distance from the cathode to the substrate (straight-span mode); the distribution of material in space occurs according to cosine law; the distribution rate is proportional to the density of the ion current.

When the target of MSS is an axially symmetrical body, on its surface there is a narrow annular sputtering zone with following dimensions: width l, internal radius \( R_1 \), external radius \( R_2 \) and average radius \( R_{\text{avg}} \). The drawing of the MSS with annular-shaped target is presented in figure 1. From the drawing follows:

\[
H_1 = H + \left( R_2 - R_1 \right) \gamma; \quad \cos \varphi(R, \alpha) = \frac{1}{r} \left[ H_1 \cos \gamma + \left( R - R_{\text{cond}} \cos \alpha \right) \sin \gamma \right];
\]

\[
\cos \theta(R, \alpha) = H_1 / r; \quad r(R, \alpha) = \left( H_1^2 + R_{\text{cond}}^2 + R^2 - 2R_{\text{cond}} R \cos \alpha \right)^{0.5}.
\]
The general formula for calculating the film thickness \( h(R_{cond}) \) in this case is

\[
h(\text{R}_{\text{cond}}) = \frac{R_{2}^{2}\pi \cos \phi(R, \alpha) \cos \theta(R, \alpha) R \Pi(R)}{\int_{R_{1}}^{R_{2}} \frac{R_{2}^{2}}{R_{1}^{2}} (R, \alpha) \cos \gamma dR},
\]

where \( \Pi(R) \) is the Lagrange polynomial. If the target cone angle is zero, these expressions take the following form:

\[
H_{1} = H \; ; \; \cos \theta(R, \alpha) = \cos \phi(R, \alpha) \; ; \; \cos \phi(R, \alpha) = \frac{H}{R} \; ; \; r(R, \alpha) = (H^{2} + R_{\text{cond}}^{2} + R^{2} - 2R_{\text{cond}}R \cos \alpha)^{0.5}.
\]

Thus the formula for the film thickness calculation is

\[
h(\text{R}_{\text{cond}}) = \frac{R_{2}^{2}\pi \cos \phi(R, \alpha) \cos \theta(R, \alpha) R \Pi(R)}{\int_{R_{1}}^{R_{2}} \frac{R_{2}^{2}}{R_{1}^{2}} (R, \alpha) \cos \gamma dR} = \frac{H^{2}R \Pi(R)}{\int_{R_{1}}^{R_{2}} (H^{2} + R_{\text{cond}}^{2} + R^{2} - 2R_{\text{cond}}R \cos \alpha)^{2} dR}.
\]

To simplify the calculation, take typical values as the size of the sputtering system. The diameter of the target can vary within 0.005…5 m [7]. However, the MSS is most effective when the target has a relatively small diameter – 50…75 mm. The ratio \( R_{\text{cond}}/R_{\text{avg}} \) varies in the range of 0.2…1; the ratio \( H/R_{\text{avg}} \) varies in the range of 0.6…2. Therefore it can be assumed that \( l = 36 \) mm, \( R_{1} = 32 \) mm, \( R_{\text{avg}} = 50 \) mm, \( R_{2} = 68 \) mm, \( H = 20…100 \) mm, \( R_{\text{cond}} = 100 \) mm [6].

The current density distribution was studied by two methods: using a target consisting of seven isolated rings, each of which was removed from the share of the total current on the target, as well as by measuring the profile of the target spraying zone after a long time of the MSS operation at constant parameters. The obtained data were approximated by the Lagrange polynomial \( \Pi(R) \), which takes into account the real radial distribution of the current density. There are three types of the radial current density distribution for consideration.

**Uniform current density distribution.** The polynomial describing the uniform current density distribution over the target radius is

\[
\Pi_{1}(R) = \begin{cases} 
0, & \text{when } R \leq R_{1}; \\
1, & \text{when } R_{1} \leq R \leq R_{2}; \\
0, & \text{when } R \geq R_{2}.
\end{cases}
\]

In this case, the general formula for calculating the film thickness become

\[
h(\text{R}_{\text{cond}}) = \frac{R_{2}^{2}\pi \cos \phi(R, \alpha) \cos \theta(R, \alpha) R \Pi_{1}(R)}{\int_{R_{1}}^{R_{2}} \frac{R_{2}^{2}}{R_{1}^{2}} (H^{2} + R_{\text{cond}}^{2} + R^{2} - 2R_{\text{cond}}R \cos \alpha)^{2} dR}.
\]
The dependence of the thickness distribution of the inflicted film on the substrate $h(R_{\text{cond}})$ at different values of the distance $H$ from the substrate to the target, if the current distribution over the radius of the target is uniform, is presented in figure 2(a).

Figure 2. Film thickness distribution in case of: (a) – uniform current density over the target radius; (b) – triangle-shaped current density; (c) – current density approximated by third-order polynomial. The curve 1 is the spray profile directly from the target (excluding $H$), $2 - H = 30$ mm, $3 - 40$ mm, $4 - 80$ mm.

Triangle-shaped current density distribution. In this case, the polynomial describing the current density distribution is given by the expression

$$
\Pi_2(R) = \begin{cases} 
\frac{R - R_1}{R_{\text{avg}} - R_1}, & \text{when } R_1 \leq R \leq R_{\text{avg}}; \\
\frac{R_2 - R}{R_2 - R_{\text{avg}}}, & \text{when } R_{\text{avg}} \leq R \leq R_2.
\end{cases}
$$

The general formula for the film thickness calculation is

$$
h(R_{\text{cond}}) = \frac{R_2 2\pi}{R_1} \int_{R_1}^{R_2} \frac{H^2 R \Pi_2(R)}{(H^2 + R_{\text{cond}}^2 + R^2 - 2R_{\text{cond}} R \cos \alpha)^2} dR.
$$

The radial thickness distribution of the inflicted film is presented in figure 2(b), in comparison with the case of uniform current density distribution (figure 2(a)) the film thickness decreases slightly when $H = 0$ (ceteris paribus) and then the decreasing become stronger as the distance from the target to the substrate increases. This is due to the fact that now the cathode is sprayed unevenly across its surface – the nature of the distribution has become such that the current density is maximal at $R = R_{\text{avg}}$, and decreases linearly as $R$ to $R_1$ on the one hand, and to $R_2$ on the other hand relative to $R_{\text{avg}}$.

Current density distribution is approximated by third-order polynomial. This case describes the current density distribution over the target radius most close to the real situation. The Lagrange polynomial for this type of current density distribution is

$$
\Pi_3(R) = \begin{cases} 
0, & \text{when } R \leq R_1; \\
-0.24 \left| R - R_{\text{avg}} \right| 10^{-1} + 0.44 \left| R - R_{\text{avg}} \right| 10^{-1} - 0.64 \left| R - R_{\text{avg}} \right| 10^{-1} + 1, & \text{when } R_1 \leq R \leq R_2; \\
0, & \text{when } R \geq R_2.
\end{cases}
$$

The general formula for the film thickness calculation is
h(R_{\text{cond}}) = \int_0^{2\pi} \int_{R_1}^{R_2} R^2 R \Pi_3(R) \left( R^2 - 2R_{\text{cond}} R \cos \alpha \right)^2 d\alpha dR.

The radial thickness distribution of the film is presented in figure 2(c), the film thickness when the real radial current density distribution is taken into account is somewhat “sagging” compared to the case of uniform current density distribution. However, the thickness of the film in this case is more than with the triangular-shape current density distribution.

3. Investigation of the film thickness uniformity in different conditions
In order to determine the geometric parameters of the film deposition system in the MSS, it is necessary to study the uniformity of the film thickness on flat surfaces depending on the cone angle of the target and the $H/R_{\text{cond}}$ ratio.

It is assumed that the cone angle of the target is zero (a flat disk) and the current density distribution over the target radius is constant ($\Pi(R) = 1$). Determine the value of $H/R_{\text{cond}}$, in which the thickness of the coating on the maximum area will not change with an accuracy of ±2 %. To do this, it is necessary to find the film thickness in the center of the substrate (at $R_{\text{cond}} = 0$), as well as the ratio of the film thickness at $R_{\text{cond}} \neq 0$ to the film thickness in the center of the substrate. The ratio of $R_{\text{avg}}$ and $H$ in which the quotient of the film thickness distributed over the substrate to the film thickness in the center of the substrate will be close to 100 % can be found further by fixing the $R_{\text{avg}}$ and varying $H$.

The following expression is used for determination of the film thickness in the substrate center:

$$h|_{R_{\text{cond}}=0} = H^2 \int_0^{R_2} \frac{R \Pi(R)}{R_1 \left( R^2 + R_{\text{cond}}^2 \right)^2} dR.$$

The general formula for the film thickness calculation is

$$h(R_{\text{cond}}) = \int_0^{2\pi} \int_{R_1}^{R_2} \frac{H^2 R \Pi(R)}{(R^2 + R_{\text{cond}}^2 + R^2 - 2R_{\text{cond}} R \cos \alpha)^2} d\alpha dR.$$

Thus it is necessary to provide the validity of expression $h/h_0 \rightarrow 100\%$. The film thickness distribution for the annular evaporator is shown in figure 3.

Figure 3. Film thickness uniformity vs. distance from the substrate center. Curve 1 is for the conditions $H = 30 \text{ mm}$, $R_{\text{avg}}/H = 1.6$; $2 - H = 40 \text{ mm}$, $R_{\text{avg}}/H = 1.25$; curve $3 - H = 50 \text{ mm}$, $R_{\text{avg}}/H = 1.0$; curve $4 - H = 60 \text{ mm}$, $R_{\text{avg}}/H = 0.83$; curve $5 - H = 65 \text{ mm}$, $R_{\text{avg}}/H = 0.77$; curve $6 - H = 100 \text{ mm}$, $R_{\text{avg}}/H = 0.5$.

The graph in figure 3 shows that the maximum average uniformity of the film thickness distribution obtained in the range $H = 60...65 \text{ mm}$ under condition of $R_{\text{avg}} = 50 \text{ mm}$. Thus, $R_{\text{avg}}/H$ is in the range of $(50/65)\ldots(50/60)$, $R_{\text{avg}}$ – in the range of $0.77H\ldots0.83H$. Consequently $R_{\text{avg}} = 0.8H$, $H = 1.25R_{\text{avg}}$ – the distance from the target to substrate should be equal to $1.25R_{\text{avg}}$ for the maximum uniformity of the film thickness distribution. As mentioned earlier, only at the initial moment of sputtering the target surface is flat, and later the surface profile become V-shaped at that the profile depth is constantly...
increasing. In this case, the cone angle of the sputtered target $\gamma \neq 0$; this kind of MSS is shown in figure 4.

Two areas of sputtering are arising during the MSS functioning. The overall film thickness will be equal to the sum of the thicknesses resulting from the combined evaporation of these areas. It is assumed that the current density distribution over the target radius is uniform. The formulas characterizing the obtained areas are written below. The expressions for the first sputtering area are

$$H_1 = H + (R - R_1) \tan(\gamma);$$

$$r(R, \alpha) = \sqrt{[H + (R - R_1) \tan(\gamma)]^2 + R_{\text{cond}}^2 + R^2 - 2R_{\text{cond}}R \cos \alpha};$$

$$\cos \varphi(R, \alpha) = \frac{[H + (R - R_1) \tan(\gamma)] \cos(\gamma) + (R - R_{\text{cond}} \cos \alpha) \sin(\gamma)}{H + (R - R_1) \tan(\gamma)};$$

$$\cos \theta(R, \alpha) = \frac{[H + (R - R_1) \tan(\gamma)]^2 + R_{\text{cond}}^2 + R^2 - 2R_{\text{cond}}R \cos \alpha}{H + (R - R_1) \tan(\gamma)}.$$

The thickness of the film deposited from the first sputtering area is

$$h_1(R_{\text{cond}}) = \int_{R_1}^{R_{avg}} \frac{2\pi}{R_{avg}} [H + (R - R_1) \tan(\gamma)] R \cos(\gamma) \cos \varphi_1(R) \cos \theta_1(R) dR.$$

The expressions for the second sputtering area are

$$H_2 = H + (R_2 - R) \tan(\gamma);$$

$$r(R, \alpha) = \sqrt{[H + (R_2 - R) \tan(\gamma)]^2 + R_{\text{cond}}^2 + R^2 - 2R_{\text{cond}}R \cos \alpha};$$

$$\cos \varphi(R, \alpha) = \frac{[H + (R_2 - R) \tan(\gamma)] \cos(\gamma) + (R - R_{\text{cond}} \cos \alpha) \sin(\gamma)}{H + (R_2 - R) \tan(\gamma)};$$

$$\cos \theta(R, \alpha) = \frac{[H + (R_2 - R) \tan(\gamma)]^2 + R_{\text{cond}}^2 + R^2 - 2R_{\text{cond}}R \cos \alpha}{H + (R_2 - R) \tan(\gamma)}.$$

The thickness of the film deposited from the second sputtering area is

$$h_2(R_{\text{cond}}) = \int_{R_1}^{R_{avg}} \frac{2\pi}{R_{avg}} [H + (R_2 - R) \tan(\gamma)] R \cos(\gamma) \cos \varphi_2(R) \cos \theta_2(R) dR.$$
The thickness of the coating deposited on the substrate will be determined by the total impact on it of both areas of the target:

$$h(R_{\text{cond}}) = h_1(R_{\text{cond}}) + h_2(R_{\text{cond}}).$$

Consider the effect of the distance from the target to the substrate on the nature of coating distribution in the case where the target is sputtered over time and takes the form of a V-shaped groove. Let the cone angle $\gamma$ be as small as $\pi/15$, and the expression describing the current density distribution over the target radius is approximated by a triangle. Film thickness distribution of for the annular evaporator at different target-substrate distances is presented in figure 5.

![Figure 5](image_url)

**Figure 5.** Film thickness distribution of for the annular evaporator at different distances to target. Curve 1 is for the condition $H = 40$ mm, 2 – $H = 50$ mm; 3 – $H = 60$ mm; 4 – $H = 80$ mm.

It was taken in the calculations that $R_{\text{avg}} = 50$ mm. The maximum uniformity of the film thickness distribution is observed at $H = 1.25$, $R_{\text{avg}} \approx 60$ mm. The influence of the cone angle on the profile of the deposited coating at $R_{\text{avg}} = 50$ mm, $H = 1.25R_{\text{avg}} \approx 60$ mm is shown in figure 6.

![Figure 6](image_url)

**Figure 6.** Cone angle impact on the deposited coating profile. Curve 1 is for condition $\gamma = 0^\circ$; 2 – $\gamma = 15^\circ$; 3 – $\gamma = 30^\circ$; 4 – $\gamma = 45^\circ$.

It can be seen from figure 6 that the achievement of the maximum uniformity of the film thickness distribution occurs at small values of the cone angle $\gamma < 30^\circ$. With increasing $\gamma$ in the substrate areas directly above the cathode, there is a strong thickening of the deposited film, but the thickness in the center and at the edges of the substrate is significantly reduced (thickness redistribution occurs). The MSS is already inoperative when $\gamma > 30^\circ$. Therefore, to obtain the maximum area with a high uniformity of the film thickness distribution, it is necessary to avoid large values of $\gamma$ and adhere to the ratio $R_{\text{avg}} \approx 0.8H$.

4. Conclusion

The study of changes in the profile of the sputtered cathode-target surface on the coating thickness distribution [8] allows to determine a number of parameters of the MSS requiring experimental determination, which have a significant impact on the deposited coating profile.

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