Program Calculation of Thin Film Thickness in Case of Parallel Arranged Target – Substrate

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Abstract – It's important to forecast the characteristics of thin solid layers before doing experiments. Among them two quantities – film thickness and its uniformity – are very essential.

According to the arrangement of the magnetron sputtering system built in the vacuum chamber (parallel disposition between cathode and substrate) we predict the above mentioned parameters. Some mathematical models for sputtering from different kinds of targets are applied.

We calculate film thickness with software program MAPLE, but for special cases we developed and used our own one, based on the program language DELPHI.

Keywords – film thickness, magnetron sputtering, mathematical models, MAPLE, program language DELPHI.

I. INTRODUCTION

In the thin film technology the **thickness** d of the layer is of significant importance. This quality influences in most cases the electrical, optical, mechanical and other properties of the film [1,2,3]. In order to achieve the same quality of the film all over the substrate we need an equal **thickness uniformity**. The most usefull quantity for us in this case would be not the absolute value of the film thickness d [*nm*] in a point at distance l from the center of the substrate, but the dimensionless ratio d/d_0 , where d_0 is the thickness of the film in the center of the substrate (l=0) and where in most cases the thickness has the highest value.

We have a magnetron sputtering system consisting of 4 targets with $\phi = 7,6$ cm each (Fig. 1) built in a vacuum chamber. Three of the cathodes maximum can operate simultaneously with constant power during the whole process. Here we introduce m_1 - the mass of the sputtered material with density ρ , produced from one very little sputtered surface unit in one second, that is so to say the mass velocity (intensity) of sputtering.

The substrate holder ($\phi = 30$ cm) contains 10 substrates (6.0 cm x 4.8 cm). It is motionless or rotates **parallel to the plane of the targets**. To calculate *d* or d/d_0 two main cases are considered (d_0 and *d* are here the thickness in the center and at distance *l* from the substrate center respectively):

1. Film deposition from **only one sputtered target** on a substrate holder, which center lies on the same vertical *Z* axis as the center of the first target (Fig. 1).

2. Film deposition from one or two targets. The substrate holder is again parallel to the targets, but its center projects on the connecting line between the centers of the two emitting sources. We'll name this case removed substrate holder.

We regard in both cases (1. and 2.) three different kinds of sputtered targets: thin *Ring*, *Ideal Disk* and *Real Disk*.

The first two cases are well described in the literature [], the last one gives an account of the different sputtered speed over the disk in our **real** experimental conditions [4].

Our aim is to make choice between different evaporation models and to predict thickness distribution of the film, in dependence of the distance target- substrate holder.

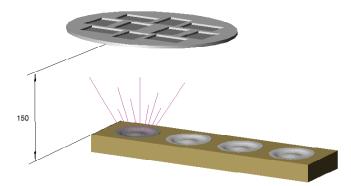


Fig.1: Drawing of the arrangement substrate: holder-sputtered target (150 mm distance between both of them)

II. ONE SPUTTERED TARGET. WORKING WITH MAPLE

The arrangement here is shown in Fig.1. The two centers – of substrate holder and of the sputtered target lay on one and the same perpendicular. Three parameters are important in the mathematical models below:

l- *distance* from substrate holder center to the considered point, h - height between target plane and the parallel to it substrate plane and *s* - *radius* of the sputtered ring ore disks. For simplicity new arguments: $\frac{l}{h}$ - *relative distance* instead

of l and $\frac{s}{h}$ - relative radius of the ring (disk) instead of s

are introduced. Assuming a plain substrate holder, motionless and parallel to the emitting surface (target- and substrate holder center lay on h), without more considerations we show the expressions which one need to

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introduce in a software program in order to calculate d, d_0 and d/d_0 :

$$d = \frac{M_r}{\pi \rho h^2} \frac{1 + (l/h)^2 + (s/h)^2}{\left\{ \left[1 - (l/h)^2 + (s/h)^2 \right]^2 + 4(s/h)^2 \right\}^{3/2}},$$

$$d_0 = \frac{M_r}{\pi \rho h^2} \frac{1}{\left[1 + (s/h)^2 \right]^3} - (Ring) \qquad (1)$$

$$d = \frac{M_d}{2\pi\rho s^2} \left\{ 1 - \frac{1 + \left(\frac{l}{h}\right)^2 - \left(\frac{s}{h}\right)^2}{\sqrt{\left[1 + \left(\frac{l}{h}\right)^2 + \left(\frac{s}{h}\right)^2\right] - 4\left(\frac{s}{h}\right)^2}} \right\},$$

$$d_0 = \frac{M_d}{2\pi\rho s^2} \cdot \frac{2\cdot\left(\frac{1}{h}\right)}{1+\left(\frac{s}{h}\right)^2} - (Ideal Disk) \quad (2)$$

$$d = \frac{2\tau}{\rho h^2} \int_{s=0}^{3.8} \frac{m_1(s) \cdot (1 + \left(\frac{l}{h}\right)^2 + \left(\frac{s}{h}\right)^2)}{\left[\left(1 - \left(\frac{l}{h}\right)^2 + \left(\frac{s}{h}\right)^2\right)^2 + 4 \cdot \left(\frac{l}{h}\right)^2\right]^{3/2}} s \cdot ds$$
$$d_0 = \frac{2\tau}{\rho h^2} \int_{s=0}^{3.8} \frac{m_1(s) \cdot s}{\left[\left(1 + \left(\frac{s}{h}\right)^2\right)\right]} ds - (\text{Real Disk}) \quad (3)$$

Here
$$M_r = 2\pi s.ds \int m_1 dt = 2\pi sds \tau$$
, and

$$M_d = \pi s^2 \int_t m_1 dt = \pi s^2 m_1 \tau$$
 are the total amount of

sputtered material during the whole time of evaporation τ in the case of *Ring* and *Ideal Disk* evaporators.

In (1) and (2) we assume $m_l = const(t)$ and $m_l \neq m_l(s)$. In (3) $m_{l=}m_l(s)$ and with $m_l(s) = (a + b.s + c.s^2 + d.s^3 + e.s^4)^{-1}$ we give an account of the different speeds of sputtering over the surface of the target in our experiments [], so we have to integrate over *s* with respect to $m_l(s)$.

The above written expressions (1), (2) and (3) has to be solved numerically and presented graphically. An appropriate program for this purpose is the program **MAPLE**. The lather is a mathematical software for researches, teachers and students. It uses over 3500 commands, which are spread from the elementary arithmetic and algebra till calculations which include differential equations, program modules, Fourier transformations and et. **MAPLE** offers good visualization possibilities.

Using **MAPLE** the problem was solved for each of the equations - (1), (2) and (3). We use a substrate holder with $R = l_{\text{max}} = 15$ cm. The upper limit of $\frac{l}{h}$ will vary with h. So the range of the new argument $\frac{l}{h}$ will be $\left(0 \div \frac{R}{h}\right)$. For our calculations the common used distances between target and substrate holder are h = 2;5;7;10;15;20 and 40 cm. These are the standard values on the x axis when plotting only one dependence $\frac{d}{d_0}$ on the graph. This gives for the upper limit of $\frac{l}{h}$ the values - 7.5;3;2.14;1.5;1;0.75 and 0.375 respectively. These are the standard values on the x axis when plotting only one dependence $\frac{d}{d_0}$ on the graph the lower limit for x is chosen. By plotting more than one on the graph the lower limit for x is chosen.

Below we show also a graphic comparison (h=2 cm.) performed by **MAPLE** for the above mentioned three cases.

Film Thickness from a Ring-, Ideal and Real Disk Evaporator, h=2cm

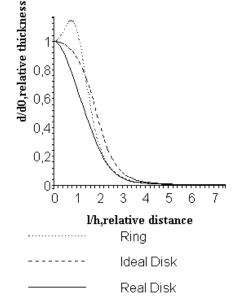


Fig. 2: Comparison : d/d_0 for the three evaporating models of evaporations by short distance *h*

Because of the *spherical symmetry* of the evaporating arrangement and if $m_1 \neq m_1(s)$ the results we will get for a motionless substrate holder will be the **same for a rotating** one.

III. REMOVED SUBSTRATE HOLDER. A DELPHI BASED PROGRAM

MAPLE is very convenient program for symbolic transformation, but it is not good for numerical calculations, which include sophisticated expressions. We can give an example on hand of equation (3) in the case of a removed substrate holder, that is when the centers of the sputtered target and the substrate holder **didn't lay** on one perpendicular to the parallel plains. The integral (3) is counted by **MAPLE** as **unsolvable** because of the complexity of

$$m_{I}(s) = (a+b.s + c.s^{2} + c.s^{3} + c.s^{4})^{-1}, \text{ where}$$
(4)

$$a = -1,0284864, b = -1,715905, c = 0,0036083349$$

$$d = 4,3724109^{*}exp(-9), e = -4,3472891^{*}exp(-6)$$

By our new vacuum arrangements, according to the practice [5,6] we use one or two simultaneously emitting cathodes. In both cases the holder center project lays on the connection line of the two target centers (Fig. 3).

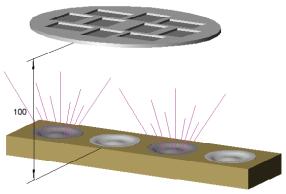


Fig. 3. Two emitting cathodes and a substrate holder above them in 100 mm. distance

The change in the experimental conditions (Fig.3) and the impossibility of **MAPLE** to give an account of them, forced us to develop our own program. The new experimental conditions complicate the development of an adequate theoretical model and appropriate applied program. Here one has to take in account the new technological parameters, such as the disposal between the targets and substrate holder, especially when targets are more than one and the substrates rotate. In this case the model is described with more sophisticated formulas than (1), (2) and (3).

For this purpose we chose the software language **DELPHI**.

DELPHI is based on the program language Pascal and is an environment for programming in Windows.

There are built in components in **DELPHI**, which save our efforts to create a convenient interface. *String Grid* is used for introducing input – and getting the output dates, not important if these are text, numbers or tables. The component *Image* is convenient for getting out graphics and images.

Fig. 4 represents the geometry, used in evaporation from 2 sources.

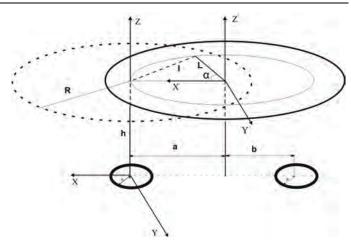


Fig. 4. Geometrical notations for evaporation from two sources, used for creating a theoretical model and a software program

In the component *StringGrid* (Fig. 5) we introduce the input data: height h, distance between center of rotation of substrate holder -L, the distances a and b between the cathode centers and the projection of the rotation center.

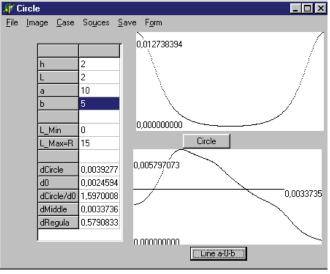


Fig. 4. Interface of the first form of the program

Case from the menu give us the possibility to change the kind of evaporation source: thin ring with radius *s* (*Ring*), ideal disk evaporator (*Ideal*) and a cathode from the experiments (*Real*) with the same radius.

With the option *Source* we can choose one or two identical sources and предлага избор между един и два еднотипни изпарителя a *Save* makes possible to save the results – in the form of tables or graphics.

Using the button *Circle* a graphic image of the thickness d over a circle with radius L is created. The average thickness value over the same circle is given in *dCircle*, and this in the centre of the holder in the row d0. The next row gives the ratio between the two values - *dCircle/d0*.

The button *Line a-0-b* creates a graphical presentation of the thickness *d* over the line, which connects the projects of the two evaporators on the holder's plane and passing through the centre of rotation *O*. *dMiddle* represents the average value of thickness over the mentioned line.

As we already pointed out that a very important characteristic is the thickness uniformity of the layer. It is reported in the row *dRegula*, and is defined by

$$dRegula = \mathbf{p} \cdot \mathbf{s}/\mathbf{p} + \mathbf{s}, \ \mathbf{p} = \int_{0}^{L_{-Ma}} d(x) dx, \qquad (5)$$

where

$$\mathbf{s} = \frac{1}{2} \int_{0}^{L_{-Ma}} abs(p/L_Max - d(x)) dx.$$
 The meanings

of **p** and **s** from *dRegula* is shown on Fig. 5.

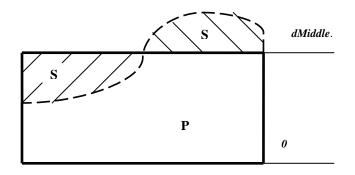


Fig.5. Geometric sense of **p** and **s** from *dRegula*

Using the option *Form* from the menu of the first form we go to the screen on Fig. 6.

The values of $C1^*dRegula+C2^*dMiddle$ for different *h*, *a* and *b* are shown here. The coefficients C1 and C2 are introduced in the lower part of the form and are responsible for the relative part of these two characteristics (*dRegula* and *dMiddle*) in the produced layer.

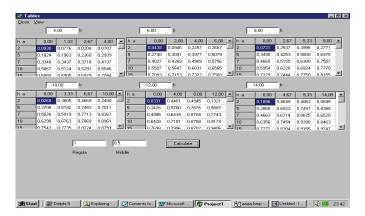


Fig.6. Interface of the second form of the program

Fig. 7 shows an quality picture of the thickness distribution over the substrate holder, which is produced by the same program. The darker parts of the picture corresponds to thicker parts of the film.

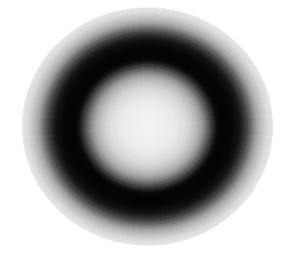


Fig.7. Thickness distribution over the substrate holder

IV. CONCLUSIONS

The problem, set in this work was to find the thickness distribution in a thin film produced by magnetron sputtering. Three different kind (*Thin Ring, Ideal Disk* and *Real Disk*) of targets were used in order to make a mathematical model of evaporation. The two varieties of one basic arrangement between the plain substrate holder and the target plane, namely parallel to each other need different software programs In the first case we used a commercial one (**MAPLE**), in the second (removed disk) we had developed an **own program** on hand of the program language **DELPHI**.

The problem, announced at the beginning of the work has been is solved, using the advantages of the two programs.

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