Method for Designing Coating Thickness Uniformity Shadow Masks for Deposition Systems with a Planetary Fixture

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ABSTRACT

A numerical model is presented incorporating coating thickness uniformity averaging from the double rotation of a planetary substrate fixture. The model converges on an optimal shadow mask shape much more rapidly than when using simpler empirical models, reducing the number of coating runs required. Detailed knowledge of the coating plume distribution across the planetary is not needed as the model assumes perfect averaging of the planetary motion and incorporates the measured coating flux variation across the mask. Shadow masks are designed using the model in an iterative process. With measured uniformity data from a run without any mask and from a run with a mask of known mask shape, it is shown that the desired uniformity can be obtained in a few iterations. A total thickness variation of less than 0.5 % across a four 333 mm diameter planetary is achieved in an ion beam deposition (IBD) system. Although the method is demonstrated using IBD, it is equally valid for other deposition technologies such as e-beam evaporators with a planetary fixture.

INTRODUCTION

High precision optical coatings require tight layer thickness control during deposition to meet optical requirements. There are multiple factors in the deposition process that result in deviations in layer thickness from the desired design thickness. Precise determination of the deposition end point of each layer is essential and is typically achieved with time control for processes with stable deposition rates, quartz crystal microbalance (QCM) sensors or optical monitoring during the deposition.

In addition to controlling the layer endpoints, it is also important to have a uniform coating thickness distribution over the substrates being coated. Deposition systems do in general have a spatially non-uniform coating flux. This makes some form of substrate motion necessary for improving the thickness uniformity across the substrate area. The simplest type of motion is a single rotation of the substrate fixture which ensures averaging of the coating thickness along a given radius from the center of rotation. This presupposes that the fixture completes sufficient rotations during the deposition of each layer.

The single rotation provides thickness averaging for an annulus around the center of rotation. However the width of the annulus having the desired thickness variation is limited which reduces the useful area for yielding parts. The area can be increased by using a mechanical shadow mask to even out the coating thickness distribution over a larger annulus [1, 2]. The useful coating area can be further increased by the use of a double rotation/planetary motion fixture. The additional motion increases the averaging during deposition and can typically give thickness uniformity variation in the 1-2 % range across each planet of the planetary [3].

Mechanical shadow masks can be used for planetary fixtures also to further improve the coating thickness uniformity. Numerical models used for designing shadow masks can become quite complicated as the distribution of the coating plume and the chamber geometry as well as the motion of the substrate fixture needs to be included. This is particularly true for the case of planetary motion as the model needs to integrate the coating flux over the complex trajectory followed by each point on the planetary coating fixture [3-5]. It can be difficult to get good agreement between the calculated coating flux distribution predicted by numerical models and the actual flux distribution. These discrepancies are due to factors such as topography changes of the material in e-beam evaporation and the extended spatial distribution of the sources in sputtering processes. It is often necessary to add free parameters to the model to match the calculations to the measured coating flux. The mapping of the coating flux across the fixture plane is time consuming, particularly if the flux does not have circular symmetry so that a full two dimensional mapping is necessary. This is usually the case for sputtering processes [6, 7] as the coating plume is a result of the sputtering of an extended target surface by an inhomogeneous and often asymmetric ion beam or plasma. In addition, the ion beam profile in an ion

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beam deposition (IBD) process will vary between different ion source grid sets. It is impractical in a production setting to map the coating plume for each of the grid sets.

As a result it is desirable to develop a model that can predict the required mask shape and quickly iterate to the desired thickness uniformity. Ideally, this model would be based on only the measured radial uniformity variation across a planet without any additional knowledge of the coating plume. Such a model is presented in this work.

THEORETICAL MODEL

It is useful to build a model for planetary rotation by first considering a single rotation fixture. Figure 1 shows a sketch of such a fixture. The coating flux across the fixture tooling plate is in general non-uniform and therefore a function of both r_p and θ. If the fixture rotates many times during the deposition of a layer, the coating thickness along a circle of radius r_p gets averaged over θ. The resulting coating thickness is only a function of r_p.

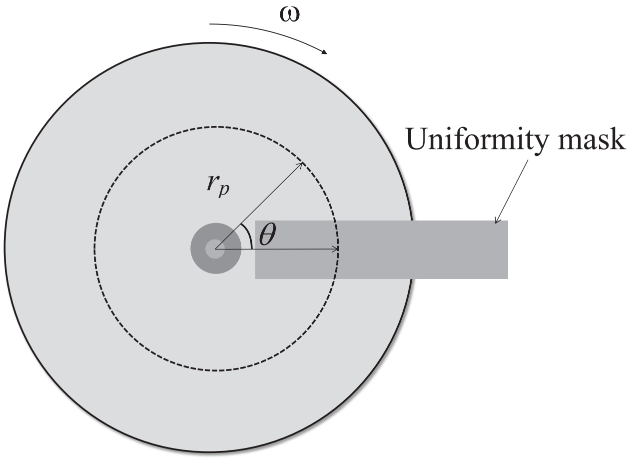

Figure 1: Single rotation fixture. A point at radius r_p passes under a uniformity mask which blocks the coating flux over the arc length covered by the mask during the rotation.

The coating thickness uniformity can further be improved by covering a portion of the fixture plane with a shadow mask. If the functional shape of the coating flux, $F(r_p,\theta)$, is known, the reduction in coating thickness can readily be calculated. This is accomplished by simply taking the fraction of the integrated coating flux in the arc section covered by the mask to the integrated flux of the full rotation without any mask. If $F(r_p,\theta)$ is not known, the effect of covering a section of the arc by a mask of known arc length can be measured experimentally. The desired shape of the mask can be found with an iterative design process.

The process starts by first measuring the coating thickness as function of r_p without a mask. A trial mask of known arc coverage calculated from the measured uniformity variation without a mask is introduced and the resulting coating thickness is measured. A linear interpolation between the measured changes in coating thickness vs. mask coverage can then be used to calculate the adjustment to the arc coverage needed to obtain the desired coating thickness. 1-2 iterations of the mask design and coating thickness measurements are typically needed to obtain the desired coating variations when using this method. An advantage of this iterative method is that only the coating thickness uniformity variation as a function of radius needs to be measured and no additional information about the coating flux distribution is needed. It is desirable to expand this iterative method to also work for planetary rotation fixtures.

An illustration of a planetary fixture is show in Figure 2. The motion is assumed to give perfect averaging during the deposition so that azimuthal variations in coating thickness can be ignored for both the rotation of the main planetary gear (sun rotation) as well as the individual planet rotation. This is a reasonable assumption since azimuthal variations cannot be compensated for by adjusting the shape of the shadow mask but need to be addressed by adjusting factors such as rotation speed vs. deposition rate and gearing ratio between the sun and planet rotation. It is also assumed that the shadow mask is close enough to the coating plane to form a sharp shadow onto the coating fixture and that the outline of the edge of the mask and the resulting shadow cast onto the coating plane coincides.

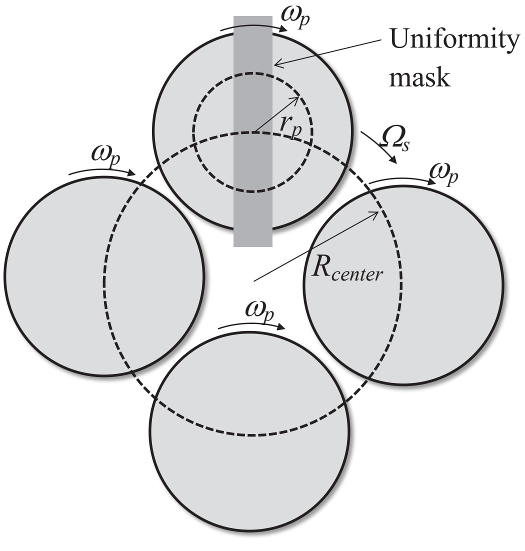

Figure 2: Planetary rotation fixture. All four planets rotate around themselves (planet rotation) as well as around the center (sun rotation). A stationary uniformity mask covers a fraction of the rotational arc around the sun.

The effect of the sun rotation can be thought of as averaging each planet through the coating flux around the sun radius in the same way as for a single rotation fixture. The planetary motion will average the coating flux that a point on the planets at radius r_p sees over different sun radii. This motion will range from R_{center}-r_p to R_{center}+r_p as it completes multiple iterations of the sun rotation. As a result, the point on the planet will pass under the uniformity mask in different locations depending on the orientation of the planet as it passes the mask. It is useful to consider a stationary planet spinning under the uniformity mask and separately consider the effect of the sun rotation averaging.

The contribution to the coating flux reduction for a point at radius r_p from each section of the mask between sun radii $(R_{center} - r_p)$ and $(R_{center} + r_p)$ is proportional to the time the point at r_p spends under each mask section. The planet rotational speed, ω_p, is assumed to be constant. The sun radius component of the rotation point at planetary radius r_p can then be written as:

$$R(t) = R_{center} + r_p \bullet cos(\omega_p \bullet t) \tag{1}$$

The uniformity is typically measured at discrete locations across the planets at radii $r_1, r_2, \ldots r_N$ as illustrated in Figure 3. Since the planet is symmetric from the center and out, it is in principle only necessary to measure the uniformity along a radius from the center to the edge. However, factors such as planetary rotation run-out, thermal variations and measurement errors introduce variations in the measured uniformity. It can therefore be beneficial to measure the uniformity across the full planet (edge to edge) and/or multiple planets and use the average. Note that the spacing between the measurement points across the planet needs to be small enough to give a smooth representation of the uniformity variation.

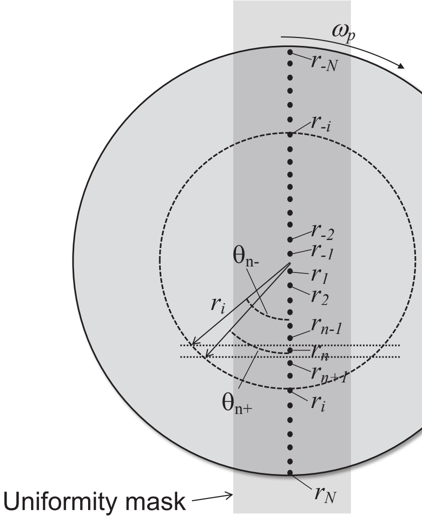

Figure 3: Layout of the measurement points across the planet at the moment they align with the mask axis. θ_{n-} *and* θ_{n+} *denotes the angle between the rotational vector at radius* r_i *and the mask axis when the vector is projected at* $(r_n+r_{n-1})/2$ *and at* $(r_n+r_{n+1})/2$ *respectively.*

Figure 3 illustrates the mirrored measurement points about the center of rotation denoted by a negative index which is convenient when calculating the contributions across the full shadow mask. It is assumed that Figure 3 illustrates the moment when the measurement points are aligned along the axis of the stationary mask. The time spent, Δt, by a point at radius r_i in the projection of the mask from the measurement point r_n half way to its nearest neighboring points r_{n-1} and r_{n+1}, is proportional to the angle swept out along the arc (see Figure 3). It can be expressed as:

$$\Delta t_{n,i} = [\theta_{n-} - \theta_{n+}] \cdot \frac{1}{\omega_p} = \left[\cos^{-1}\left(\frac{r_{n-1}+r_n}{2r_i}\right) - \cos^{-1}\left(\frac{r_{n+1}+r_n}{2r_i}\right)\right] \cdot \frac{1}{\omega_p} \tag{2}$$

where ω_p is the angular velocity for the planet rotation.

Since points on the planet rotating away from sun center vs. rotating towards sun center are averaged the same under the mask, only one half of the rotation needs to be considered. If full averaging is assumed in the deposition of a layer, the planetary rotation speed is arbitrary. The total effect of the shadow mask becomes a sum of the contributions for all the time segments as the point passes under the mask. Since only the relative uniformity is of interest, the expressions can be normalized as long as all the points on the planet are normalized in the same way.

Using equation (2) modified for the inner and outermost points, the contributions from the rotational averaging under the mask for a point at radius r_i on the planet can be written as:

$$a_{1,1} = \frac{\pi}{2}$$

$$a_{1,i} = \frac{\pi}{2} - \cos^{-1}\left(\frac{r_2+r_1}{2r_i}\right) \text{ for } i > 1$$

$$a_{n,i} = \left[\cos^{-1}\left(\frac{r_{n-1}+r_n}{2r_i}\right) - \cos^{-1}\left(\frac{r_{n+1}+r_n}{2r_i}\right)\right] \text{ for } i > 2 \text{ and } n = 2 \text{ to } i\text{-}1$$

$$a_{i,i} = \left[\cos^{-1}\left(\frac{r_{i-1}+r_i}{2r_i}\right)\right] \text{ for } i > 1 \tag{3}$$

The factor ω_p has been dropped as it will be normalized out in the equations below. Two weight factors, P_n and S_n, are introduced to allow the model to be adjusted to fit measurements. P_n weights the contributions from each section of the mask to take into account coating flux variation along the length of the mask. S_n accounts for the azimuthal flux variation along a circle around the sun rotation. It is equivalent to the ratio between arc coverage and coating thickness reduction used for the single rotation iterative process described above. The sum of all the mask contributions for a point at radius r_i across the mask from sun radius R_{center} - r_i to R_{center} + r_i can then be written as:

$$C_i = \frac{\sum_n (M_n \cdot P_n \cdot S_n + M_{-n} \cdot P_{-n} \cdot S_{-n}) \cdot a_{n,i}}{\sum_n (P_n + P_{-n}) \cdot a_{n,i}} \tag{4}$$

where C_i is the effective average mask coverage at planetary radius r_i, M_n is the fractional mask arc coverage of the circle at sun radius $R_{center} + r_n$ for $n < 0$ and $R_{center} - r_n$ for $n > 0$. n is summed over all planetary positions ranging from $n = 1$ to $n=i$. Note that the sum covers one half of the planet rotation. Due to symmetry, the geometric factors, $a_{n,i}$, are the same for both quadrants of the sum (n and $-n$). The sum has been normalized by dividing by the sum of all the un-weighted geometrical factors times the P_n weight factors, which are the two factors that sets the weight of each mask contribution along the length of the mask.

P_n can be left as a fitting parameter together with S_n. However, P_n can relatively easily be determined empirically by mounting slides along the length of the coating mask and depositing a single layer coating onto the slides. The relative coating flux profile along the mask can then be measured by fitting the coating thickness to the measured spectra of points along the slides. In this work, the flux for a single Ta_2O_5 layer along the mask was measured once. Although this flux will have variations from material to material and grid set to grid set in the IBD deposition, it was found that this variation was accounted for by the second weight factor, S_n. P_n could be left fixed to the values from this single measurement even for different coating materials. This is thought to be because the main variation in P_n is caused by the geometry of the deposition system.

For a known mask coverage profile, M_n, the relative coating thickness (hereafter referred to as "uniformity"), U_i, at planet radius r_i is given by:

$$U_i = N_i \bullet (1 - C_i) \tag{5}$$

where N_i is the uniformity without any shadow mask (zero percent coverage), and C_i is the effective coverage for radius r_i calculated using equation *(3)* and *(4)*. Since the center point of the planet is the only point that is affected by the mask coverage at a single sun radius, it is necessary to start at this point and then perform the calculation for increasing planetary radius, r_i. It is convenient to normalize the calculated and measured thickness profiles to 100% in the middle of the planet.

Two additional simplifications are introduced in the model. The restriction $M_{-n} = M_n \cdot (R_{center}-r_i)/(R_{center}+r_i)$ is imposed. This sets the arc length of the mask at sun radii $R_{center} + r_i$ equal to the arc length of the mask at $R_{center}-r_i$ which makes the mask approximately symmetrical about the planet rotation center. To reduce the number of variables further, the weight factor S_{-n} is set equal to S_n. This is an approximation, as in general the coating flux will not have the same distribution around the sun rotation at radius $R_{center}+r_n$ as for radius $R_{center}-r_n$. However this approximation has been found to work well for our system in part due to the fact that the coating flux is much higher towards the middle of our planetary ($R < R_{center}$) so that the mask coverage at $R < R_{center}-r_n$ is weighted more by the P_n factors than the mask coverage at $R > R_{center}+r_n$.

The iterative design procedure outlined above for the single rotation fixture can now be used. The distribution of the uniformity without any shadow mask, N_i, is measured first. The weight factors, S_n, can be set to 1 as a starting point. This is equivalent to assuming that the coating flux is uniformly distributed along a circle around the sun rotation. Using equation (3), (4) and (5), the required mask coverage, M_n, can be calculated starting in the middle at r_1 and outwards that results in an even 100 % uniformity across the planets. The arc coverage of the mask at the center of the planets is empirically picked. If the coating thickness is thinnest in the middle of the planet, it is set to be as small as possible and still maintain a mechanically rigid mask. If the coating thickness is thickest in the middle, a trial coverage is picked. If 100 % uniformity cannot be obtained across the planets without the mask coverage going to zero as the calculation progresses outwards, the center coverage has to be increased and the calculation restarted. The physical mask shape is generated based on the arc coverage obtained in the calculation.

Note that initially setting the values of S_n to 1 will in general lead to an initial mask design that is relatively far from the final mask shape. If a previous mask design has been established with known arc coverage (for example for a different coating material), the number of iterations needed can be reduced by using the S_n values established in this mask design rather than setting the S_n values to 1.

The first generated mask is used for another coating run and the resulting uniformity across the planets is again measured. The coverage for the current mask, M_n, is used with equation 3, 4, and 5 to calculate the S_n factors that makes the model fit the resulting measured uniformity. The calculation is again performed by iterating from the middle of the planet and out. S_1 is kept equal to 1 through all iterations since the calculated and measured uniformity is being normalized to 100 % in the middle of the planet. The newly obtained weight factors that make the model fit the measurement are used to calculate an adjusted mask arc coverage, M_n, which will result in 100 % uniformity across the planets. A new mask is generated from the adjusted arc coverage and the process is repeated until the desired uniformity is achieved.

It should be noted that although the procedure is typically used for generating a coating thickness distribution with equal thickness across the planets, the model can also be used to generate a non-uniform coating thickness profile by changing the targets for the desired coating thickness from 100 % to the new targeted thickness values. This might be useful for creating a linear thickness slope along a radius on the planets or to adjust the coating uniformity to account for curvature of the coating plane across the coating fixture.

EXPERIMENTAL RESULTS

Mask generation was performed in a Veeco SPECTOR-HT™ IBD System with a 4 planet fixture. Each planetary fixture had a diameter of 333 mm. The deposition system was equipped with an optical monitoring system (OMS) creating additional shadowing in front of the planetary fixture. The no mask run used for the mask design was performed with the OMS hardware in place and the resulting change in coating flux was treated as part of the variation in the coating plume when designing the mask.

The uniformity was measured for a single ~500 nm thick Ta_2O_5 layer deposited with a deposition rate of ~4.3 Å/s on glass microscope slides placed across one of the planetary fixtures. The relative coating thickness variation was determined by fitting a model to the measured spectral scans across the glass slides using the Swanepoel method [8, 9].

The unmasked uniformity was measured to have a variation of ~3.2 % across a 330 mm diameter (see Figure 4). An initial uniformity mask was designed based on the measured no mask uniformity using the method described above. In this case, weight factors previously determined for another set of ion source grids were used as the starting weight factors, S_n, rather than setting them equal to one. This ensured that the first iteration of the mask included coarse adjustments for chamber geometry and coating plume distribution.

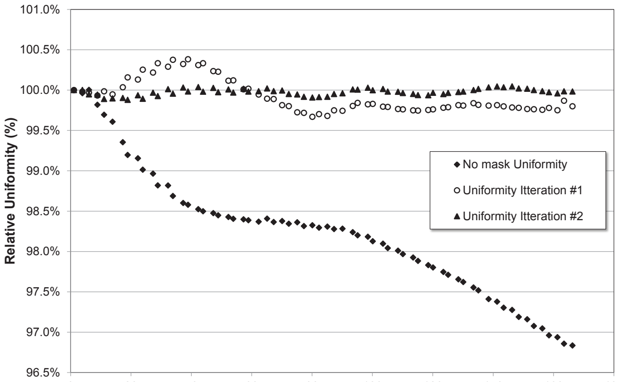

Figure 4: Measured relative coating thickness uniformity for a single Ta_2O_5 layer as function of planetary radius for no mask, mask iteration #1 and mask iteration #2.

The calculated shape of the designed mask is shown in Figure 5 (dashed outline). The resulting measured uniformity variation was reduced to ~ 0.7 % (see Figure 4). The weight factors of the model, S_n, were adjusted to fit the new measurement. A second mask was designed with the new weight factors and a third run deposited. The shape of the second mask is shown in Figure 5 (solid outline). The resulting uniformity was measured to be ~ 0.2 % across the fixture (see Figure 4). This was within the desired uniformity and no further iterations were necessary.

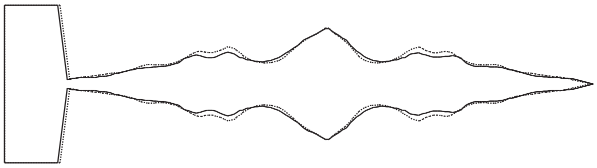

Figure 5: Physical shape of Ta_2O_5 mask for iteration #1 (dotted line) and iteration #2 (solid line). The sharp end of the mask is mounted pointing inwards towards the center of the sun rotation. The wide section in the middle aligns with the middle of the planet fixtures.

The Veeco SPECTOR-HT IBD system used in this work is equipped with selectable uniformity masks for individual coating materials that are rotated into position for the deposition of each coating layer. This is necessary due to the difference in sputtering plume for the materials in the IBD process. As a result, the mask design procedure is performed independently for the different coating materials. The above method has been used with similar result to the Ta_2O_5 results shown here for several coating materials including SiO_2, Nb_2O_5, and Si_3N_4. Uniformity results for these materials are shown in Figure 6. Typical thickness variation across the planets is ~ 0.5 % for all the materials. Further improvement can be achieved with further iterations of the mask shape.

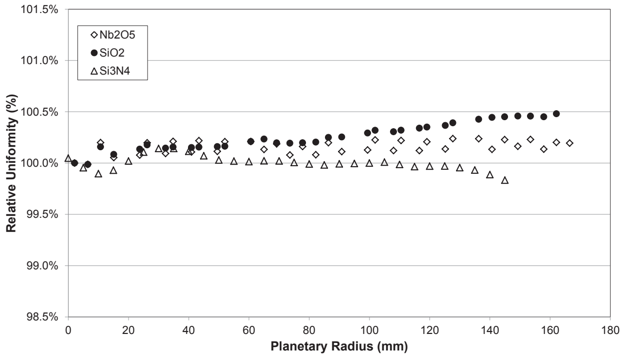

Figure 6: Measured relative coating thickness uniformity for single layer Nb_2O_5, SiO_2 and Si_3N_4 coatings as function of planetary radius.

CONCLUSIONS

This work has presented an iterative model for designing uniformity shadow masks for deposition systems with planetary fixtures. The model is based on only measuring the radial coating thickness variation across the deposition fixture without any other knowledge of the coating flux across the planetary fixture. The contributions for a point on the planet from different mask segments are summed up taking into account the geometrical averaging over the mask resulting from the planetary motion. Weight factors are introduced to account for the non-uniform coating flux. Adjusting the weight factors to match the model to the measured uniformity with a known mask shape yields rapid convergence in an iterative process. Experimental results for IBD deposited Ta_2O_5, SiO_2, Nb_2O_5, and Si_3N_4 coating layers show that thickness uniformity below 0.5% is obtained across a 333mm diameter fixture.

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