Case study:

Numerical study of morphology and optical properties of coatings deposited by PVD on rotating gratings in a complex geometry

Production of modern advanced coatings by low pressure plasma deposition requires using a quite sophisticated technology and equipment. That may include deposition on a rotating or moving substrates, deposition on a non-flat substrates, multi-layer deposition etc. Development of such deposition techniques takes a lot of efforts and time. To reduce the time and cost of such development one can use computer simulations of the film growth and evaluation of the film properties.
In order to demonstrate the capabilities of ICS simulation offer, we simulated deposition of a multi-layer dielectrically enhanced Aluminum mirror on a moving grating (see Figure 1) in order to predict structural (density and roughness of the coating) and optical (effective refractive indices, reflectance,...) properties.

The simulation tools are the one offered by ICS: NASCAM and advanced optical plugin (see https://www.incosol4u.com/modeling-and-simulation).

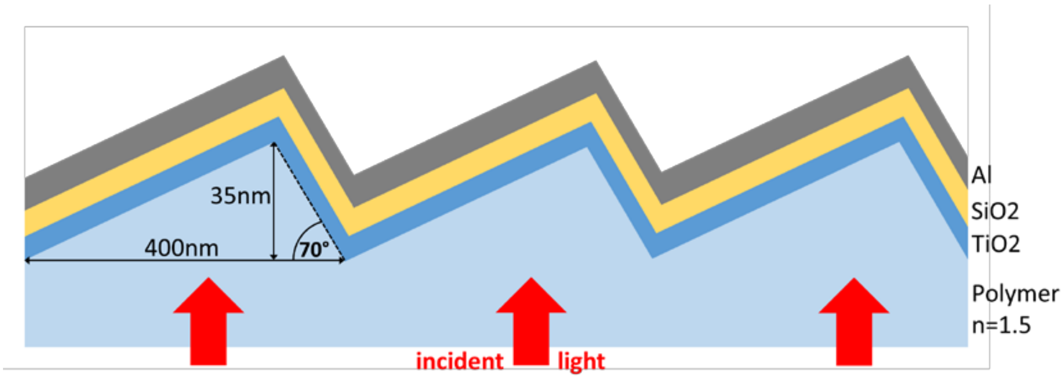

Figure 1: structure of the grating considered here for in-silico deposition and optical caracterisation

1 Deposition on gratings attached to a rotating holder.

The sketch of the deposition is shown in the Figure 2. A substrate is attached to a rotating substrate holder, called calotte, and is tilted with respect to the vertical axis. A point source of depositing atoms is located at the bottom and may be positioned as on-center as well as of-center. The position of the source is determined by its coordinate (x, y) in the bottom plane, and position of the substrate is characterized by its height H, distance from the center r, and its tilting with respect to the vertical θ.

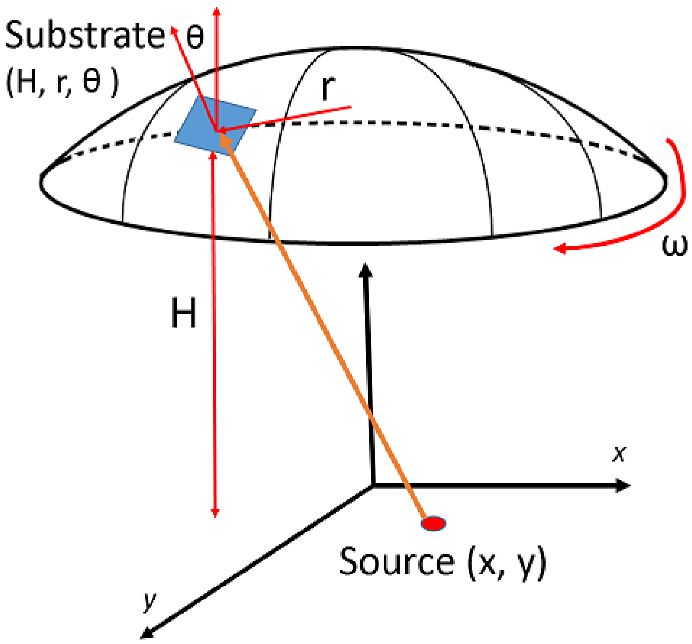

Figure 2: A sketch of the deposition process

The substrate is a grating with a large tilting angle of a smaller plane, in our case it is70 degrees.

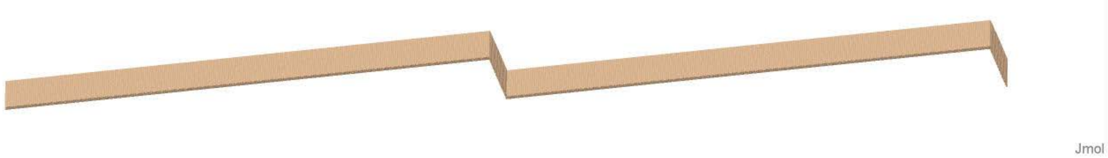

Figure 3: A sketch of a grating on which in-silico deposition will take place. The tilting angle of a smaller plane is 70 degrees.

As the substrate is not flat the properties of the coating may be different for different orientation of the grating lines with respect to their position on the substrate holder. For this reason, evaluation of film properties and optical performance of the coating was performed for the following cases: radial grating lines and tangential grating lines.

In addition, ICS made simulations for deposition with Ar^+ ion assistance for both cases.
We study the variation of the coating density for these cases and try to find deposition method that provides the best optical quality of the coating.
Each simulation consist of three consecutive steps, reactive depositions of TiO_2, SiO_2, and finally deposition of Aluminum. The thicknesses of the layers are 58 nm, 85 nm, and 80 nm respectively. The structure of the coating is shown in Figure 1.
The simulations with no ion assistance (see Figure 4 and Figure 5) reveal that because of the steep slope of one of the grating's plane, formation of pores in the coating occurs near the plane. Also the position of the top ridge (look at Al surface) is not the same for the two orientations. The local porosity is higher when the grating's lines are oriented radially. For the case of tangential orientation, the local porosity is lower.

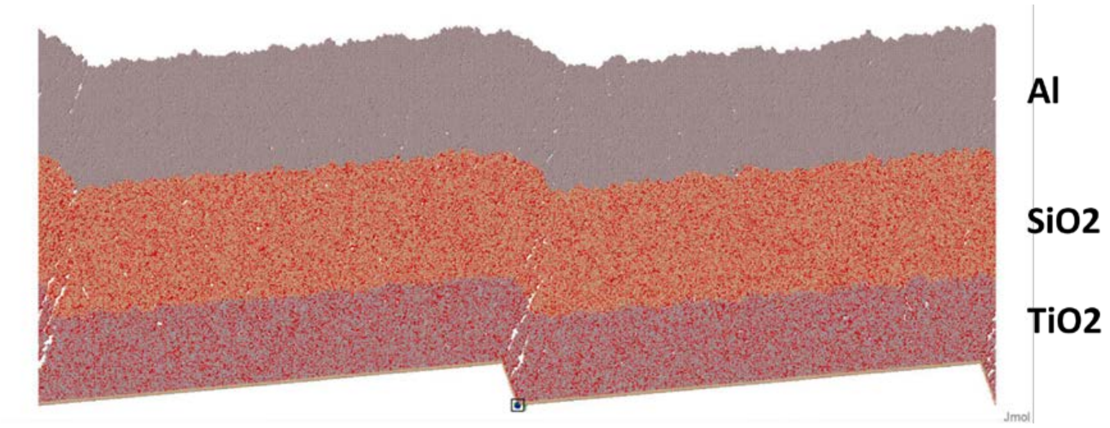

Figure 4: Radial orientation, no ion assisted deposition.

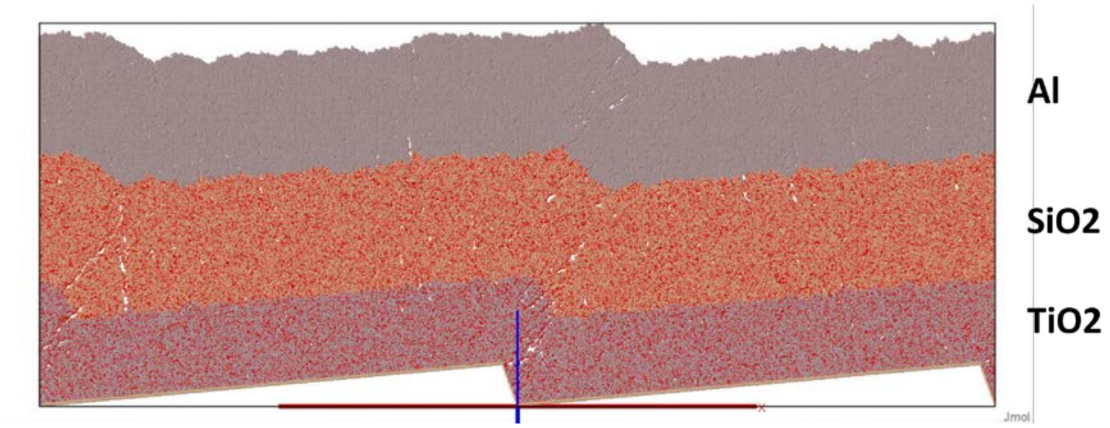

Figure 5: Tangential orientation, no ion assisted deposition.

Argon bombardment gives the possibility to reduce porosity of the coating. One can see in Figure 6 and Figure 7 that in this case for both tangential and radial orientations of the substrate porosity is significantly lower. Argon bombardment allows to obtain the coating with higher density and lower surface roughness. For the case of tangential orientation of the grating additional argon bombardment makes it possible to completely get rid of the pores.

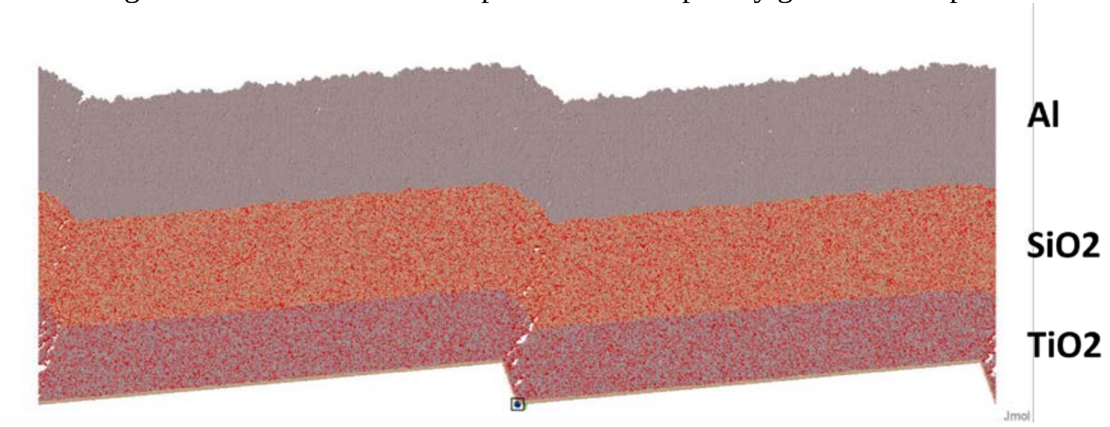

Figure 6: Radial orientation, ion assisted deposition.

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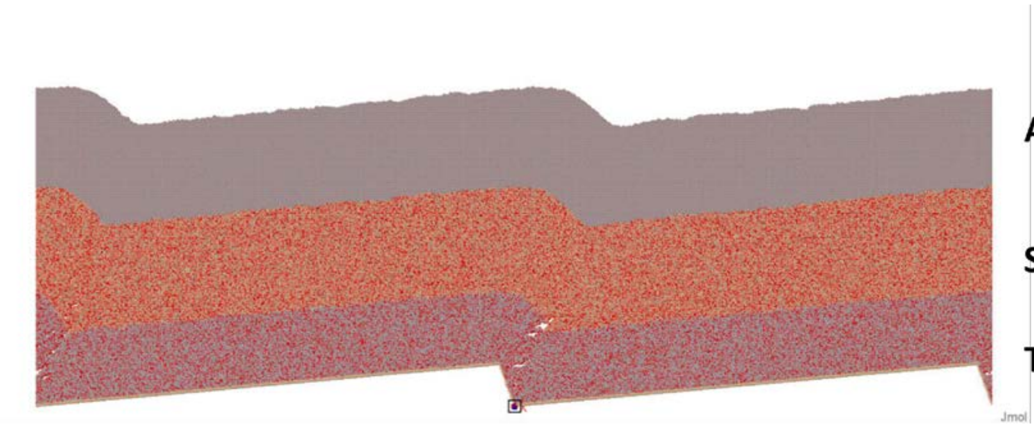

Figure 7: Tangential orientation, ion assisted deposition.

2 Optical modeling

The optical characterization of studied gratings concerned the computation of (1) the refractive indices of each deposited layers and (2) the optical response in far-field of the coated grating when illuminated by the substrate side in polymer (see Figure 1). This work has been done for UV, Visible and NIR light (100 nm < λ < 1 µm).

The first step consists in computing the effective refractive indices of the different layers of the coating. It is worth distinguishing two zones depending on the grating inclination angle as shown in Figure 8(a,b). Indeed, according to the simulation of coating morphology (see previous section), such difference in the inclination angle can drastically change the density of the film, and therefore its refractive index. Then, we computed the evolution of the refractive index in low and high density zones of the coating in the z direction (see Figure 8(c)).

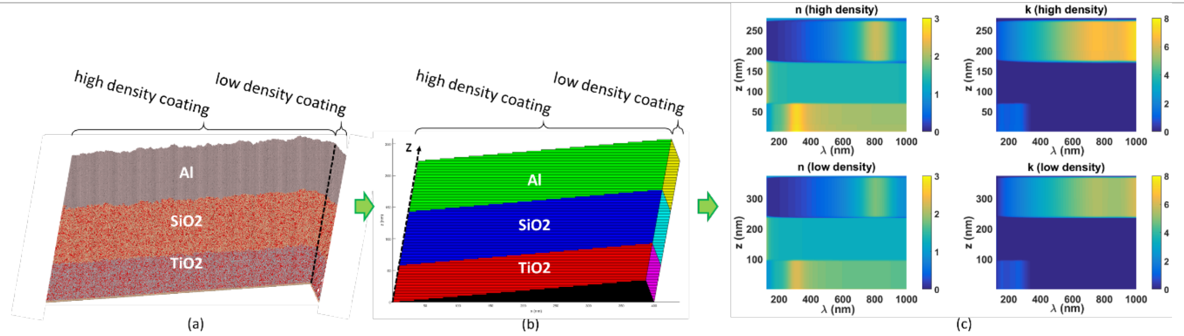

Figure 8: optical indices computations in low and high density zones of the coating (radial orientation, no ion assisted deposition)

These refractive indices have been directly used to compute the total reflectance, transmittance and absorbance (RTA) of the coated grating. The illumination was done from the substrate side. Due to the periodicity of the pattern with a period of the same order of magnitude as the studied wavelengths, it is not possible to use classical models dedicated to the optical modeling of coated flat substrates. In this study, ICS developed state of the art methods perfectly adapted to periodic patterns allowing modeling infinite structures (Figure 9-left). As an example, the RTA spectra of the grating coated with radial orientation and no ion assisted deposition is shown in Figure 9-right. We can notice that the light is mainly absorbed in UV. Moreover, the transmittance is totally negligible because of the aluminium back-reflector.

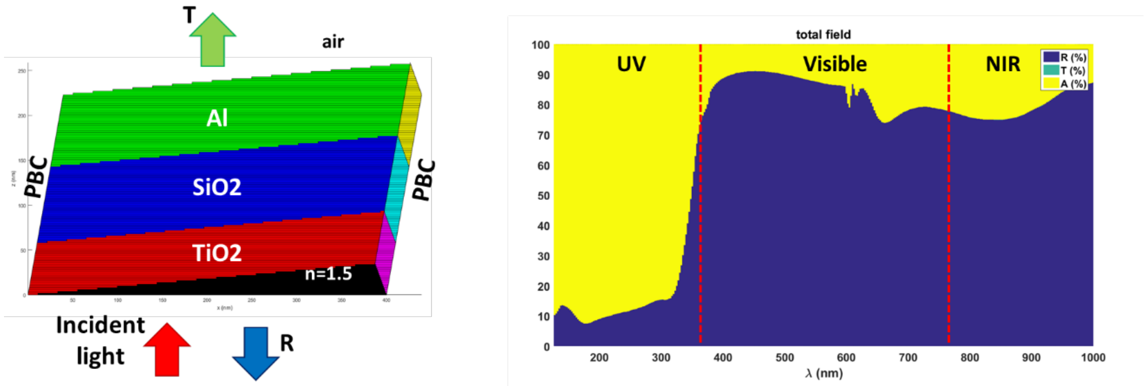

Figure 9: Left: optical grating adapted to ICS simulations. Right: reflectance, transmittance and absorbance of the grating (coating: radial orientation, no ion assisted deposition)

Moreover, such grating can present interesting diffraction effects due to the periodicity of the pattern (Figure 10-left). Fortunately, our simulations predict these diffractions orders defined by their own propagation directions (depending on the wavelength) and diffraction efficiency. Figure 10 (mid and right) shows the diffraction efficiency in reflection for a coating obtained with radial orientation and no ion assisted deposition. We can see that the light is mainly reflected in the diffraction order 0, which means that the reflection is mainly specular.

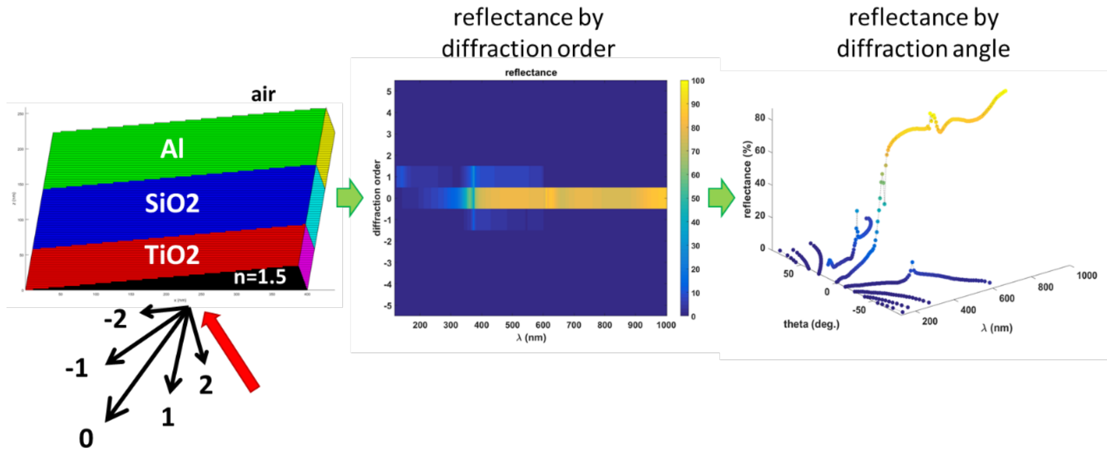

Figure 10: Left: optical grating sketch with diffraction orders in reflection. Middle: diffraction efficiency in function of diffraction orders. Right: diffraction efficiency in function of diffraction angle theta.

3 To go further

Our study can easily be extended by investigating the influence of different coatings or grating parameters, as shown in Figure 11. For example, it is possible to vary the light incidence angle (Figure 11(a,b)), the density of the coating (Figure 11(c)) which can be increased by ion assisted deposition, or the grating shape (Figure 11(d-f)). In this last case, it is interesting to notice that increasing the height of the grating can enhance drastically the diffraction efficiency for not-specular diffraction orders.

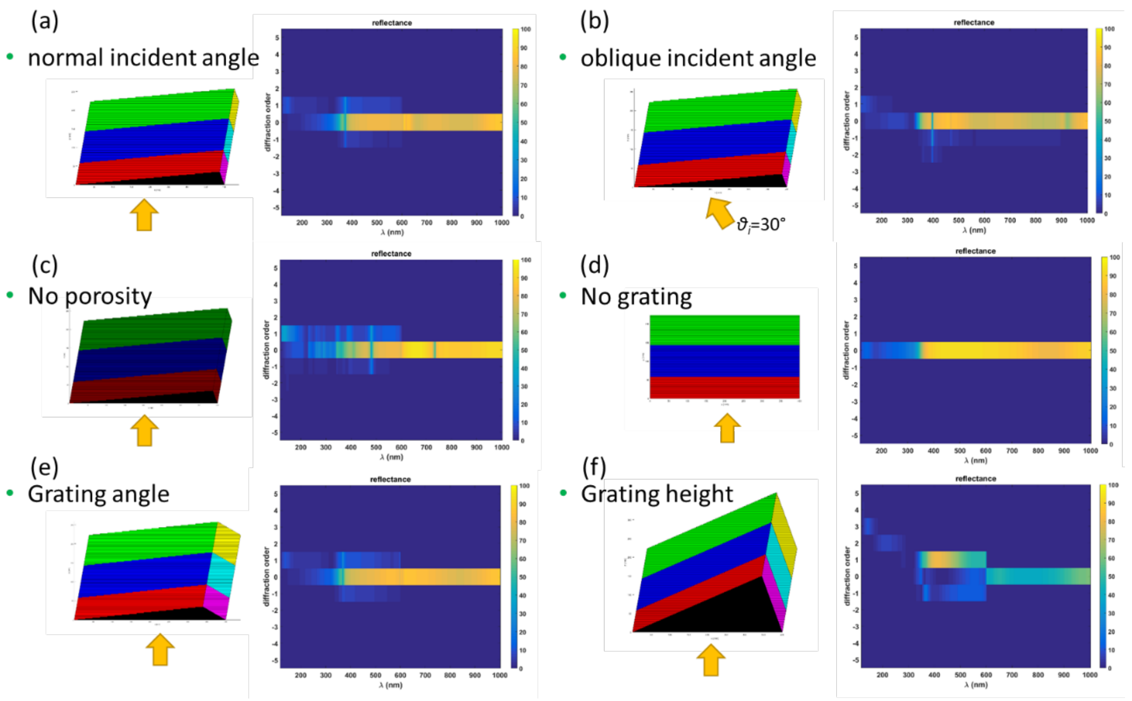

Figure 11: extended study by varying several coating and grating parameters.

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4 Conclusions

A full multi-model study has been performed to model patterned multi-layer dielectrically enhanced Aluminum mirror, from the atomic-scale deposition modeling to the prediction of structural and optical properties.
Morphology of the multi-layer coating deposited on a rotating grating was successfully studied for different deposition conditions. It was shown how orientation of the grating and additional assisted bombardment change the morphology of the coating. Then, an optical characterization was done, from the computation of refractive indices in each deposited layers, to the prediction of the optical response in far-field by ICS simulations. It allowed predicting the effect of deposition conditions on the reflectance and absorbance of light illuminating the mirror, and its diffraction efficiency.
Such kind of study can be improved by considering additional critical parameters like the grating shape (2D or 3D grating, influence of the grating period or height). Moreover, it is possible to investigate more complex optical phenomena (light trapping, local absorption, ...) for different specific applications like photovoltaic solar cells or structural colorations (photonic crystals). Finally, other domains of physics like electrical conductivity, thermal conductivity or elastic properties could be considered, depending on the desired application.

Should you be interested to get additional information or to know more about our offer in modeling or to buy a state of the art film growth simulation software that includes optical modeling, contact ICS.

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