Sculptured thin films as versatile photonic structures

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Sculptured thin films are nanoengineered to meet the requirements of a variety of applications such as optical filters, sensors, and waveguides by exploiting controllable porosity, 3D periodicity, and chirality.

Commercialization of a technology requires tight integration of the fabrication process with model-based approaches to the material design that cover all essential aspects, including deviations from ideal performance. Sculptured thin films (STFs) lend themselves well to this purpose. They are characterized by having 1-, 2-, or 3D periodicity with tailorable porosity and chirality (‘handedness’). STFs are relatively easy to make using a two-stage process of lithography and deposition. Theoretical work has outlined a whole host of possible applications for STFs, such as filters, sensors, and 3D photonic crystals (3DPCs) with integrated waveguides, revealing their impressive scientific and economic potential.

The primary impetus for STF research has been provided by the sensor and filter design possibilities identified using an inhomogeneous continuum model (ICM) approach. This model focuses on structural chirality and vertical periodicity (that is, in the thickness direction). The lateral periods (LPs) are assumed to be much smaller than the incident light wavelength. However, a more complete understanding of the optical response of STFs is required to quantitatively understand the impact of deviations from ideal. In addition, not all the parameters needed for the ICM model are easily accessible experimentally. This presents a gap that needs to be closed before commercial success can be achieved.

We have developed a model that considers the key structural parameters, allowing us to draw quantitative insights into critical conditions for 1D photonic structures and to design materials with a desired performance. We can also explore applications exploiting full-3D periodicity. We employed an input set that is commonly used to evaluate the output of a fabrication process. The model could therefore also serve as the basis for appropriate production monitoring and control methods to ensure high yields.

Figure 1. (a) Example of a chiral sculptured thin film (STF) made of parylene. (Courtesy: Mark Horn, Penn State University.) (b) Reconstructed profile of a chiral STF using the pile-of-discs model: for a stack of sufficiently thin cylinders, the resulting structure closely approximates an array of helices with lateral periods (LPs) $D_x$, columnar inclination $\chi$, and fill-factor $f$ (not indicated on the diagram). Successive higher layers are systematically offset such that the centers of the cylinders trace out a circle of radius $R$, the helical sweep radius, over one full vertical period, $\Omega$.

Figure 1(a) shows the helical-shaped STFs we have focused on. We used the classical differential theory of gratings to model a chiral STF as a 3D-periodic structure. The base unit is established using a 2D Fourier representation of a stack of cylinders.
arranged on a simple rectangular lattice. Figure 1(b) illustrates this model. Successive higher layers are systematically offset such that the centers of the cylinders trace out a circle of over one full vertical period. For sufficiently thin cylinders, the resulting structure closely approximates an array of helices. The structural parameters and bulk refractive index of the columnar material form the input set for the model and are identical to those used to evaluate a fabricated structure. The diffraction efficiencies can be determined for excitation by left- and right-circularly polarized (LCP and RCP) plane waves to completely characterize the chirality.

The most striking optical phenomenon exhibited by chiral STFs is the circular Bragg phenomenon (CBP), the focus of the majority of device applications proposed and realized thus far. The CBP causes high reflectance in a certain spectral region when the handedness and half-structural period of the film match the handedness and wavelength of the incident plane wave inside the film. From the traces for $D_{x,y} = 200\text{nm}$ in Figure 2(a) and (b), it is clear that there are two distinct high-reflectance bands. The band centered at $\sim 400\text{nm}$ is a manifestation of the CBP as it shows up very strongly only for the co-handed RCP case. The second band, centered at $\sim 280\text{nm}$, is polarization-independent and associated with the LP. The stop band due to the LP cannot be predicted by the ICM. The equivalence of the grating theory and the ICM is seen in the convergence of the traces for progressively smaller LPs. The remaining structural parameters offer additional degrees of freedom for the design process, within limits. Figure 2(c) and (d), for example, shows that as $f$ increases, the stop band locations show a red-shift. In addition, we see that the peak reflectance in the CBP region and the polarization discrimination decrease substantially for very high $f$. Varying both $\chi$ and $D_{x,y}$ (relative to $\Theta$) also has a strong effect on the location and width of the stop bands. Non-specular propagating orders have a significant effect up to the cutoff wavelength $D_{x,y} \leq \lambda_{\text{cutoff}} \leq 2D_{x,y}$. Taken together, our findings help us assess the viability of proposed applications for STF in a way that cannot be done with the ICM. Rules of thumb derived from numerical experiments also greatly simplify the design process for specific applications.

STFs engineered to have structural periodicity in 3D are obvious candidates for applications such as waveguides. Here, up to 100% reflectance within a spectral band is required, independent of the angle of incidence and polarization state. We explored the feasibility of using continuous helical STFs rather than square spiral STFs, which were previously studied extensively using an FDTD (finite-difference time-domain) approach. Our motivation for using helical STFs was their rotational near-symmetry, and the simplicity and robustness of the deposition process involved. The highlighted regions in Figure 3 show modestly high reflectance ($\geq 60\%$) in a narrow band of...
wavelengths for $0^\circ < \theta < 80^\circ$. The potential for designing 3DPCs using continuous helical STFs is evident. However, further design optimization is required to meet the target of complete confinement.

In conclusion, we have presented an approach to modeling STFs as 3D periodic structures. This model provides a common, easily accessible set of parameters to evaluate the deposition process and optical response of such films. The model is a valuable tool in studying the spectral characteristics of STFs over a far wider parameter space of interest than possible with the ICM. We have also made an encouraging first attempt at designing a 3DPC using a helical STF. More extensive numerical investigations will provide us with a better understanding of how to engineer the stop bands and work toward an improved chiral STF-based 3DPC design.

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Vijayakumar Venugopal is the sole proprietor of Fiat Lux Technologies, a consulting firm offering services in optical metrology, data analytics, and design and development of sensors and model-based approaches for manufacturing process control. Areas of application include thin-film optics, semiconductor manufacturing, solar cell device optimization, and building technology.

References