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Optical spectra of graded nanostructured TiO_2 chiral sculptured thin films

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ABSTRACT

The optical properties of graded chiral sculptured TiO_2 thin films in axial and non-axial excited states are calculated using the rigorous coupled wave analysis method (RCWA) in conjunction with the Bruggeman homogenization formalism. The filtering frequency and polarization selectivity of these graded nanostructured TiO_2 sculptured thin films showed dependence on both structural and deposition parameters. The results achieved are consistent with the experimental data [K. M. Krause and M. J. Bret, Adv. Funct. Mater. 18 (2008) 3111].

1. Introduction

Chiral thin films or chiral sculptured thin films (CSTFs) are columnar (range between 1 and 100 nm) thin films deposited on substrate with a tilt angle, α, by a method known as oblique-angle deposition (OAD) and controlled azimuthal rotation, φ of the substrate. The columnar structure of thin film can be designed in nano and micro scale 3D for use in optical, chemical, mechanical, biological, electrical and magnetic applications [1]. The above mentioned method can be used to produce 3D photonic crystals that depending on their nano-structural dimensions they prohibit the propagation of a certain bands of electromagnetic frequency through macroscopic (Bragg) and microscopic scattering resonances [2].

The most important optical feature of chiral sculptured thin films is the circular Bragg phenomenon that unlike ordinary thin films occurs in chiral sculptured thin films. This phenomenon is studied extensively both theoretically [3–11] and experimentally [12–15]. If the handedness of the chiral sculptured thin film is the same as that of the polarization of the incident circular plane wave, then nearly all the incident light will be reflected in a narrow region of the wavelength (this is called the Bragg regime), otherwise nearly all the incident light will be transmitted. In these films (chiral sculptured thin films grown normal to the substrate surface) the helical axis or the axis of non-homogeneity is normal to the substrate surface (z-axis). These films can be used to discriminate the right-handed circular polarization (RCP) from the left-handed circular polarization (LCP). There is another group of chiral sculptured thin films called slanted chiral sculptured thin films in which the helical axis is tilted with respect to the normal to the substrate surface. In this kind of thin films due to the periodicity of structural parameters in both normal and parallel directions to the substrate surface, the interaction between circular Bragg phenomenon (specular diffraction) and non-specular diffraction (Rayliegh-Wood anomalies) occurs which can be related to the diffraction gratings [16–19]. The study on the slanted chiral sculptured thin films is of importance in understanding the optical ray diffraction by sculptured thin films [20]. In addition, many applications have been proposed for slanted chiral sculptured thin films, such as optical beam splitters, couplers, nano-band and sub nano-band spectral-hole filters and biosensors [21–24].

A third group of chiral sculptured thin films has been introduced by Krause and Brett [25], so called graded chiral sculptured thin films which are similar to the slanted chiral sculptured thin films with a gradient in their thickness in their nano-column structural assembly (Fig. 1). The graded chiral sculptured thin films are produced using selected fixed oblique deposition angles with a shadowing block positioned at the center of the rotating substrate. This shadowing object modulates the microscopic structure of the thin film and produces spatially graded chiral sculptured thin film with graded optical properties. In these films it is possible to distinguish both polarization and frequency selection simultaneously. This technique can be used to produce polarization responsive and tunable frequency optical filters, sources, and detectors for applications such as multichannel light wave systems as well as providing a graded scaffolding to support liquid crystals [25].

Optical devices with tunable optical functions (refractive index, absorption and extinction coefficient, optical activity and other functions) have always been of interest and desire in different areas

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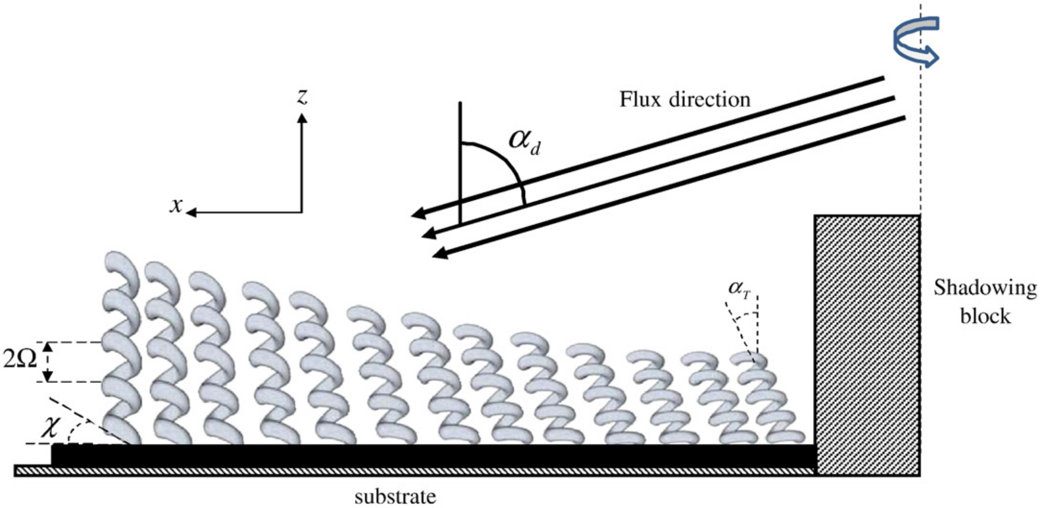

Fig. 1. Schematic of graded nanostructured chiral thin films. α_d, α_T, Ω and χ, are deposition angle, tilt angle, half structural period and rise angle, respectively.

of science and industry. A large body of the recent research in the field of thin films and nano-structures is devoted to the production of optical devices with filtering frequency [26,27 and references therein] and polarization selectivity properties [28 and references therein]. However building of a device, that can have both of these properties simultaneously have been a difficult task. Similar films exist in the nature, such as animals with skins, feathers, wings of varying thickness and chiral structure which while shows different colors it also changes the polarization of the incident light [29–31]. Thin films with variable structural characteristics and filtering frequency at varying frequency along their length have already been produced using different techniques [32–35]. Bragg reflection from gratings is also a method for producing optical components with tuneable characteristics [36,37]. Cunningham et al. [33] also reported a guided-mode resonance filter (GMRF) photonic crystal which can separate the reflection of specific wavelength bands across the width of the component. On the other hand, liquid crystals with helical molecular structures can distinguish the circular polarization of the incident light [38]. Production of nano-structures with sensitivity to the circular polarization of the incident light has also been achieved by means of OAD with azimuthal rotation, φ of the substrate in recent years. Krause and Brett [25] who inspired from the nature used the above combination of OAD and substrate azimuthal rotation as well as fixing a macroscopically shadowing block in the center of the rotating substrate holder to produce thin films with both frequency filtering property and sensitivity to the polarization of the light.

In this work the rigorous coupled wave analysis (RCWA) proposed and extended by Lakhtakia [20] for slanted chiral sculptured thin films is applied to graded chiral sculptured thin films using a computer code written in Mathematica 5.2. Reflection, transmission and circular polarization selectivity for graded chiral sculptured thin films are calculated and compared with the experimental results reported in Ref. [25]. A good agreement between our theoretical results and those of Krause and Brett is achieved.

In Section 2 the finalized formalism of the rigorous coupled wave analysis is given. The numerical results are reported, discussed and compared with Krause and Brett's experimental results in Section 3.

2. Theory

The rigorous coupled wave analysis (RCWA) method was first proposed by Moharam and Gaylord in 1981 [39] in order to obtain a near-exact solution to Maxwell equations for periodic diffracting structures. Wang and Lakhtakia [20] formalized the rigorous coupled wave analysis for the slanted chiral sculptured thin films and obtained the following final algebraic equation:

$$\begin{bmatrix} e^{-id\left[\underline{\underline{\tilde{D}}}_1\right]}\left[\underline{\underline{U}}_T\right] & \left[\underline{\underline{U}}_R\right] \\ \left[\underline{\underline{V}}_T\right] & e^{id\left[\underline{\underline{\tilde{D}}}_2\right]}\left[\underline{\underline{V}}_R\right] \end{bmatrix} \begin{bmatrix} \left[\underline{T}\right] \\ \left[\underline{R}\right] \end{bmatrix} = \begin{bmatrix} \left[\underline{\underline{U}}_A\right] \\ e^{id\left[\underline{\underline{\tilde{D}}}_2\right]}\left[\underline{\underline{V}}_A\right] \end{bmatrix} \left[\underline{A}\right] \tag{1}$$

where,

$$[\underline{A}] = \begin{bmatrix} a_L^{(n)} \\ a_R^{(n)} \end{bmatrix}, [\underline{R}] = \begin{bmatrix} r_L^{(n)} \\ r_R^{(n)} \end{bmatrix}, [\underline{T}] = \begin{bmatrix} t_L^{(n)} \\ t_R^{(n)} \end{bmatrix} \tag{2}$$

where, $\{a_L^{(n)}, a_R^{(n)}\}$, $\{r_L^{(n)}, r_R^{(n)}\}$, $\{t_L^{(n)}, t_R^{(n)}\}$ are the nth order harmonic complex amplitudes of the incident, and reflection and transmission of left- and right-handed circularly polarized light, respectively. The rest of the parameters in Eq. (1) are described in detail in Section 2-2 of reference [20].

Once all $\{a_L^{(n)}, a_R^{(n)}\}$, $\{r_L^{(n)}, r_R^{(n)}\}$, $\{t_L^{(n)}, t_R^{(n)}\}$ for all n orders have been determined using the RCWA, the nth order reflection and transmission coefficient can be obtained from:

$$r_{\sigma\sigma'} = \frac{r_\sigma^{(n)}}{a_{\sigma'}^{(0)}},\ t_{\sigma\sigma'} = \frac{t_\sigma^{(n)}}{t_{\sigma'}^{(0)}},\ \sigma, \sigma' = L,R \tag{3}$$

The nth order harmonic reflection and transmission are:

$$R_{\sigma\sigma'}^n = \frac{Re\left[k_z^{(n)}\right]}{Re\left[k_z^{(0)}\right]}\left|r_{\sigma\sigma'}^{(n)}\right|^2,\ T_{\sigma\sigma'}^n = \frac{Re\left[k_z^{(n)}\right]}{Re\left[k_z^{(0)}\right]}\left|t_{\sigma\sigma'}^{(n)}\right|^2,\ \sigma,\sigma' = L,R \tag{4}$$

The first subscript shows the polarization state of the reflected or transmitted and the second subscript indicates the polarization state of incident light and Re[ ] is the real part. $k_z^{(n)}$ is the z component of the wave vector for the nth order harmonic ($K_\pm^{(n)} = k_x^{(n)}u_x + k_y^{(0)}u_y \pm k_z^{(n)}u_z$):

$$\begin{cases} k_z^{(n)} = +\sqrt{k^2 n_{hs}^2 - \left(k_{xy}^{(n)}\right)^2} \\ k_{xy}^{(n)} = +\sqrt{\left(k_x^{(n)}\right)^2 + \left(k_x^{(0)}\right)^2} \\ k_x^{(n)} = k_x^{(0)} + nk_x \\ k_x = \frac{\pi}{\Omega}\left|\sin\alpha_T\right| \end{cases} \tag{5}$$