Spectral Remittances of Chiral Nano - Sculptured TiO$_2$ Thin Films

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Abstract

The transmission and reflection spectra from a right-handed chiral sculptured TiO$_2$ thin film are calculated using the piecewise homogeneity approximation method and the Bruggeman homogenization formalism by considering that the propagation of non-dispersive dielectric function occurs for non-axial states. The results show that the characteristic circular Bragg phenomenon in co-handed circular reflectance is more pronounced and the observed consecutive peaks and troughs in circular remittances are representative of the influence of azimuthal and polar angles on these spectra.

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Keywords: Chiral sculptured thin films; Bruggeman formalism; Piecewise homogeneity approximation method

1. Introduction

The Sculptured thin films (STFs) are columnar thin films that their columnar growth direction can change suddenly during their growth [1]. When the columnar thin films with a diameter of 10 to 300 nm are deposited at oblique incident and the two principal axes of rotation can change separately or together, then many kinds of morphologies in nano-scales can be produced [2-4]. The optional rotation of these two principal axes results in two groups of sculptured thin films, namely sculptured nematic thin films (SNTFs) [5] and thin film helicoidal bianistropic media (TFHBM) [6]. The SNTFs are two dimensional nano-structures with simple shapes such as oblique columns, chevrons, zig-zags, and complex morphologies including shapes such as C, S and many other shapes. The TFHBMs are three dimensional nano-structures including morphologies from simple helicoids to super helicoids [7].

In this paper we report on the circular reflectance and transmittance from a right handed TiO$_2$ CSTF using the Bruggeman homogenization formalism [8-13] and the piecewise homogeneity approximation method [11,12] in non-axial propagation state. The theory of the work is explained in section 2 and the numerical results are given in section 3.

2. Theory

Consider that a region \((0 \leq z \leq d)\) in space is occupied by a chiral sculptured thin film (CSTF) and that this film is being excited by a plane wave which propagates with an angle \(\theta_{inc}\) relative to z axis and angle \(\psi_{inc}\) relative to x axis in xy plane. The phasors of incident, reflected and transmitted electric fields are given as [11, 12]:

\[
\begin{align*}
E_{inc}(r) &= \left( \frac{i s - p}{\sqrt{2}} a_L - \frac{i s + p}{\sqrt{2}} a_R \right) e^{i \omega z}, z \leq 0 \\
E_{ref}(r) &= \left( -\frac{i s - p}{\sqrt{2}} r_L + \frac{i s + p}{\sqrt{2}} r_R \right) e^{i \omega z}, z \leq 0 \\
E_{tra}(r) &= \left( \frac{i s - p}{\sqrt{2}} t_L - \frac{i s + p}{\sqrt{2}} t_R \right) e^{i \omega (z - d z)}, z \geq d
\end{align*}
\]

(1)

The magnetic field’s phasor in any region is given as:

\[
H(r) = (i \omega \mu_0)^{-1} \nabla \times E(r)
\]

Where \((a_L, a_R), (r_L, r_R)\) and \((t_L, t_R)\) are the amplitudes of incident plane wave, and reflectance and transmittance waves with left- or right-handed polarizations. We also have;

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Fig. 1. Reflectance and transmittance spectra from a right-handed TiO$_2$ CSTF as functions of wavelength $\lambda_0$ and $\theta_{inc}$ at $\psi_{inc} = 0^\circ$. 
\[ \mathbf{E} = x\mathbf{u}_x + y\mathbf{u}_y + z\mathbf{u}_z, \]
\[ K_0 = K_0 (\sin \theta_{\text{inc}} \cos \psi_{\text{inc}} \mathbf{u}_x + \sin \theta_{\text{inc}} \sin \psi_{\text{inc}} \mathbf{u}_y + \cos \theta_{\text{inc}} \mathbf{u}_z) \]  
\[ (2) \]

where \( K_0 = \omega \sqrt{\mu_0 / \varepsilon_0} = 2\pi / \lambda_0 \) is the free space wave number, \( \lambda_0 \) is the free space wavelength and \( \varepsilon_0 = 8.854 \times 10^{-12} \text{F/m} \) and \( \mu_0 = 4\pi \times 10^{-7} \text{H/m} \) are the permittivity and permeability of free space. The unit vectors for linear polarization parallel and normal to the incident plane, \( \mathbf{s} \) and \( \mathbf{p} \), respectively are defined as:

\[ \mathbf{s} = -\sin \psi_{\text{inc}} \mathbf{u}_x + \cos \psi_{\text{inc}} \mathbf{u}_y, \]
\[ \mathbf{p} = + (\cos \theta_{\text{inc}} \cos \psi_{\text{inc}} \mathbf{u}_x + \cos \theta_{\text{inc}} \sin \psi_{\text{inc}} \mathbf{u}_y) + \sin \theta_{\text{inc}} \mathbf{u}_z \]  
\[ (3) \]

and \( \mathbf{u}_{x,y,z} \) are the unit vectors in Cartesian coordinates system. The reflectance and transmittance amplitudes can be obtained, using the continuity of the tangential components of electrical and magnetic fields at two interfaces, \( z = 0 \) and \( z = d \), and solving the algebraic matrix equation [12]:

\[
\begin{bmatrix}
    i(t_L - t_R) \\
    -i(t_L + t_R) \\
    0 \\
    0
\end{bmatrix} = \begin{bmatrix}
    -\sin \psi_{\text{inc}} & -\cos \psi_{\text{inc}} \cos \theta_{\text{inc}} & -\sin \psi_{\text{inc}} & \cos \psi_{\text{inc}} \cos \theta_{\text{inc}} \\
    \cos \psi_{\text{inc}} & -\sin \psi_{\text{inc}} \cos \theta_{\text{inc}} & \cos \psi_{\text{inc}} & \sin \psi_{\text{inc}} \cos \theta_{\text{inc}} \\
    -\eta_0^{-1} \cos \psi_{\text{inc}} \cos \theta_{\text{inc}} & \eta_0 \sin \psi_{\text{inc}} & \eta_0^{-1} \cos \psi_{\text{inc}} \cos \theta_{\text{inc}} & \eta_0 \sin \psi_{\text{inc}} \\
    -\eta_0^{-1} \sin \psi_{\text{inc}} \cos \theta_{\text{inc}} & -\eta_0^{-1} \cos \psi_{\text{inc}} \cos \theta_{\text{inc}} & -\eta_0^{-1} \sin \psi_{\text{inc}} \cos \theta_{\text{inc}} & -\eta_0^{-1} \cos \psi_{\text{inc}}
\end{bmatrix} \]
\[ \begin{bmatrix}
    -\sin \psi_{\text{inc}} & -\cos \psi_{\text{inc}} \cos \theta_{\text{inc}} & -\sin \psi_{\text{inc}} & \cos \psi_{\text{inc}} \cos \theta_{\text{inc}} \\
    \cos \psi_{\text{inc}} & -\sin \psi_{\text{inc}} \cos \theta_{\text{inc}} & \cos \psi_{\text{inc}} & \sin \psi_{\text{inc}} \cos \theta_{\text{inc}} \\
    \eta_0 \sin \psi_{\text{inc}} & \eta_0 \sin \psi_{\text{inc}} & \eta_0^{-1} \cos \psi_{\text{inc}} \cos \theta_{\text{inc}} & \eta_0 \sin \psi_{\text{inc}} \\
    \eta_0^{-1} \sin \psi_{\text{inc}} \cos \theta_{\text{inc}} & \eta_0^{-1} \cos \psi_{\text{inc}} \cos \theta_{\text{inc}} & \eta_0^{-1} \sin \psi_{\text{inc}} \cos \theta_{\text{inc}} & -\eta_0^{-1} \cos \psi_{\text{inc}}
\end{bmatrix} \]
\[ (4) \]

and:

\[ B(z, \Omega) = \begin{bmatrix}
    \cos(\pi z / \Omega) & -\sin(\pi z / \Omega) & 0 & 0 \\
    \sin(\pi z / \Omega) & \cos(\pi z / \Omega) & 0 & 0 \\
    0 & 0 & \cos(\pi z / \Omega) & -\sin(\pi z / \Omega) \\
    0 & 0 & \sin(\pi z / \Omega) & \cos(\pi z / \Omega)
\end{bmatrix} \]
\[ \eta_0 = \sqrt{\frac{\mu_0}{\varepsilon_0}} \text{ is the intrinsic impedance of vacuum.} \]

The 4 x 4 matrix \([M'(z, \Omega, \kappa, \psi_{\text{inc}})]\) satisfies the differential matrix equation [11, 12]:

\[
\frac{d}{dz} [M'(z, \Omega, \kappa, \psi_{\text{inc}})] = i[R'(z, \Omega, \kappa, \psi_{\text{inc}})] [M'(z, \Omega, \kappa, \psi_{\text{inc}})] \quad 0 < z < d
\]  
\[ (7) \]
<table>
<thead>
<tr>
<th>a) Reflectance</th>
<th>b) Transmittance</th>
</tr>
</thead>
<tbody>
<tr>
<td>$R_{LL}$</td>
<td>$T_{LL}$</td>
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<td>$R_{RL}$</td>
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<td>$R_{LR}$</td>
<td>$T_{LR}$</td>
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<tr>
<td>$R_{RR}$</td>
<td>$T_{RR}$</td>
</tr>
</tbody>
</table>

Fig. 2. Reflectance and transmittance spectra from a right-handed TiO₂ CSTF as functions of $\theta_{inc}$ and $\psi_{inc}$ for $\lambda_0 = 600nm$. 
where:

\[
\begin{bmatrix}
0 & -i \frac{\pi}{\Omega} & 0 & \omega \mu_0 \\
\frac{i \pi}{\Omega} & 0 & -\omega \mu_0 & 0 \\
0 & \omega \epsilon_0 \epsilon_c & 0 & i \frac{\pi}{\Omega} \\
\omega \epsilon_0 \epsilon_b & \tau & 0 & i \frac{\pi}{\Omega}
\end{bmatrix}
\]

(8)

\[
\begin{bmatrix}
-A \cos \xi \sin 2\chi & 0 & -B \sin \xi \cos \xi & -B \cos^2 \xi \\
A \sin \xi \sin 2\chi & 0 & B \sin^2 \xi & B \sin \xi \cos \xi \\
C \sin \xi \cos \xi & C \cos^2 \xi & 0 & 0 \\
-C \sin^2 \xi & -C \sin \xi \cos \xi & -A \sin \xi \sin 2\chi & -A \cos \xi \sin 2\chi
\end{bmatrix}
\]

where in these equations, \(A = \kappa (\epsilon_b - \epsilon_a)/2 \epsilon_c \tau\), \(B = \kappa^2/2 \omega \epsilon_0 \epsilon_c \tau\), \(C = \kappa^2/\omega \mu_0\), \(\xi = (\pi z/\Omega) - \psi_{inc}\) and \(\tau = \cos^2 \chi + (\epsilon_c/\epsilon_a) \sin^2 \chi\). \(\kappa = K_0 \sin \theta_{inc}\) and \(\Omega\) is the half of the periodical structure and \(\epsilon_{a,b,c}\) are the relative permittivity scalars and \(\chi\) is the rise angle for the CSTF.

In order to obtain \([M'(d,\Omega,\kappa,\psi_{inc})]\) the piecewise homogeneity approximation method is used. In this method the CSTF is divided into \(N\) (a big enough number) very thin layers with a thickness of \(\frac{h = d}{N}\) (5 nm will suffice). Using the equality of the tangential components of fields at interfaces the matrix \([M'(d,\Omega,\kappa,\psi_{inc})]\) can be estimated [12]:

\[
[M'(d,\Omega,\kappa,\psi_{inc})] \approx [M_{PH}^{N}], [M_{PH}^{N-1}], ..., [M_{PH}^0]
\]

(9)

where:

\[
[M_{PH}^j] = e^{i \Delta z P(z_j + 1/2, \Omega, \kappa, \psi_{inc})}
\]

\[
= [M^0] + \lim_{r \to \infty} \sum_{n=1}^r \frac{(ih)^n [P(z_{j+1/2}, \Omega, \kappa, \psi_{inc})]^n}{n!}
\]

(10)

The number of terms in Eq. (10) can be determined from two converging conditions [12]:

\[
\begin{align*}
\text{Re} \{ [(ih)^{\alpha+1} ] P(z_{j+1/2}, \Omega, \kappa, \psi_{inc}) ]^{\alpha+1} (r+1)! \}_{\alpha\beta} & \leq 10^{-12} \\
\text{Re} \{ \sum_{n=0}^r (ih)^n P(z_{j+1/2}, \Omega, \kappa, \psi_{inc}) ]^n / n! \}_{\alpha\beta} & \leq 10^{-12} \\
\text{Im} \{ [(ih)^{\alpha+1} ] P(z_{j+1/2}, \Omega, \kappa, \psi_{inc}) ]^{\alpha+1} (r+1)! \}_{\alpha\beta} & \leq 10^{-12} \\
\text{Im} \{ \sum_{n=0}^r (ih)^n P(z_{j+1/2}, \Omega, \kappa, \psi_{inc}) ]^n / n! \}_{\alpha\beta} & \leq 10^{-12}
\end{align*}
\]

(11)

\[
\frac{\chi}{\pi}, \frac{\kappa}{\omega}, \frac{\epsilon}{\epsilon_c}, \frac{\tau}{\Omega}, \frac{\psi_{inc}}{\pi}, \frac{\Omega}{\pi}
\]

In order to obtain \([M'(d,\Omega,\kappa,\psi_{inc})]\) the piecewise homogeneity approximation method is used. In this method the CSTF is divided into \(N\) (a big enough number) very thin layers with a thickness of \(\frac{h = d}{N}\) (5 nm will suffice). Using the equality of the tangential components of fields at interfaces the matrix \([M'(d,\Omega,\kappa,\psi_{inc})]\) can be estimated [12]:

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\text{Im} \{ [(ih)^{\alpha+1} ] P(z_{j+1/2}, \Omega, \kappa, \psi_{inc}) ]^{\alpha+1} (r+1)! \}_{\alpha\beta} & \leq 10^{-12} \\
\text{Im} \{ \sum_{n=0}^r (ih)^n P(z_{j+1/2}, \Omega, \kappa, \psi_{inc}) ]^n / n! \}_{\alpha\beta} & \leq 10^{-12}
\end{align*}
\]

(11)
Fig. 3. Reflectance and transmittance spectra from a right-handed TiO₂ CSTF as a function of wavelength $\lambda_{\text{inc}}$ at $\psi_{\text{inc}} = 0^\circ$ and $\theta_{\text{inc}} = 20^\circ$. 
when transmittance and reflectance amplitudes are obtained from Eq. (4), then we can obtain the reflectance and transmittance coefficients as:

\[
\begin{align*}
    r_{i,j} &= \frac{r_i}{a_j}, & i, j = L, R \\
    t_{i,j} &= \frac{t_i}{a_j}
\end{align*}
\]  

(12)

The transmittance and reflectance are obtained from:

\[
\begin{align*}
    R_{i,j} &= \left| r_{i,j} \right|^2, & i, j = L, R \\
    T_{i,j} &= \left| t_{i,j} \right|^2
\end{align*}
\]  

(13)

3. Numerical results and discussion

We consider that a right-handed TiO2 sculptured thin film with a thickness \( d \) in its bulk state has occupied the free space. The relative permittivity scalars \( \varepsilon_{a,b,c} \) in this sculptured thin film were obtained using the Bruggeman homogenization formalism. In this formalism, the film is considered as a two phase composite, vacuum phase and the inclusion phase. These quantities are dependent on different parameters, namely, columnar form factor, fraction of vacuum phase (void fraction), the wavelength of free space and the refractive index \( n_s \) of the film’s material (inclusion). Each column in the STF was assumed to consist of a string of small and identical ellipsoids and are electrically small (i.e., small in a sense that their electrical interaction can be ignored). Therefore [10,12]:

\[
\varepsilon_\sigma = \varepsilon_\sigma(a_0, f_v, \gamma^e_a, \gamma^e_b, \gamma^e_c),
\]

(14)

where \( f_v \) is the fraction of void phase, \( \varepsilon_s = n_s^2 \) is the relative dielectric permittivity, \( \gamma^{e,a}_a \) is one half of the long axis of the inclusion and void ellipsoids, and \( \gamma^{e,b}_b \) is one half of the small axis of the inclusion and void ellipsoids.

The homogenization was performed using \( \lambda_0 = 591.82 \text{ nm}; n_s(\lambda_0) = 2.759 \) [14] and then from the Bruggeman formalism the relative permittivity scalars with values of \( \varepsilon_a = 3.34, \varepsilon_b = 4.91, \varepsilon_c = 3.72 \) were obtained. These values are constant at all wavelengths and the dispersion of the dielectric function is not included in the calculations. In all calculations the values of \( f_v = 0.4, \gamma^e_a = 10, \gamma^e_b = 2, \gamma^e_c = 20, \chi = 30^\circ, \Omega = 160 \text{ nm}, d = 40 \Omega \) were fixed.

In each plot of Figs. 1 the circular reflectance and transmittance (circular remittances) are plotted as functions of the wavelength \( \lambda_{inc} \) and \( \theta_{inc} \) for \( \psi_{inc} = 0 \), while in Fig.2 the circular remittances are given as functions of \( \theta_{inc} \) and \( \psi_{inc} \) for \( \lambda_{inc} = 600 \text{ nm} \) for a right-handed TiO2 CSTF.

In Fig. 1 it can clearly be observed that in \( R_{LL} \) plot, because of none similarity of the handedness of the CSTF and the direction of the polarization of the circular plane wave, the reflectance is negligible and at \( \theta_{inc} = 90^\circ \) it assumes a value of unity, for in this case the reflectance becomes zero (\( T_{LL} \)). In the \( R_{RR} \) plot, owing to the same handedness of the structural direction in the thin film and the polarization of the incidence plane wave, the circular Bragg phenomenon is clearly distinguishable, and the central wavelength for the Bragg peaks can be estimated from:

\[
\lambda_{inc} \approx \Omega(\sqrt{\varepsilon_a + \sqrt{\varepsilon_b}}) \cos^{1/2} \theta_{inc}.
\]

In the \( T_{RR} \) plot the corresponding trough to this peak can be observed. When the cross-polarized remittances, \( R_{LR} \) and \( T_{LR} \) are compared with \( R_{RL} \) and \( T_{RL} \) plots it can be vividly observe that in non-axial propagation unlike the axial propagation, the cross polarized remittances depend on the polarization state.

In Fig. 2 the influence of the azimuthal and polar angles on the remittances from the CSTF in form of peaks and troughs/valleys can be distinguished. At \( \theta_{inc} < 60^\circ \) it can be seen that there is no considerable change in the values of circular remittances by increasing the azimuthal angle. However, for \( \theta_{inc} \geq 60^\circ \) any increase in the azimuthal angle affects the values of circular remittances considerably.

In Fig. 3 the reflectances and transmittances from a right-handed TiO2 CSTF are given as function of wavelength \( \lambda_{inc} \) at \( \theta_{inc} = 20^\circ \) and \( \psi_{inc} = 0 \). These results can be explained with the interpretation of the results given for Fig. 1.

In summary, in this work by using the Bruggeman homogenization formalism and the piecewise homogeneity approximation method we have been able to obtain the reflectance and transmittance spectra from a right-handed TiO2 CSTF. The occurrence of the circular Bragg phenomenon due to the same handedness of the structural direction in the thin film and the polarization of the incidence plane wave (i.e., \( R_{RR} \) plot)
was clearly observed and it was possible to conclude that the circular remittances depend on the polar and azimuthal angles. It was also shown that the variation of the polar angle changes the values of these remittances and there exists an order in these remittances for $\theta_{inc} < 60^\circ$ as function of $\psi_{inc}$, and there is a disorder for $\theta_{inc} \geq 60^\circ$.

4. Conclusions

The influence of the polar and azimuthal angles on the remittances spectra of circularly polarized plane waves from a right-handed TiO$_2$ CSTF in the non-axial propagation state is reported, using the piecewise homogeneity approximation method and the Bruggeman homogenization formalism at a single wavelength of $\lambda_0 = 591.82 \text{nm}$. The results show that the appearance of the circular Bragg phenomenon in $R_{RR}$ plot is due to the same handedness of the structural direction in the thin film and the polarization of the incidence plane wave. It is also shown that the incident angle of the plane wave on the CSTF affects the circular reflectance and transmittance and for incidence angles farther away from surface normal the influences of the polar and azimuthal angles on the remittances spectra are more pronounced.

Acknowledgements

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References: