Investigation on the optical properties of ZnS nano-rod and chiral sculptured thin films using experimental and theoretical approaches

A Siabi-Garjan\textsuperscript{1}, H Savaloni\textsuperscript{1}, F Abdi\textsuperscript{1}, A Ghaffal\textsuperscript{1} and F Placido\textsuperscript{2,3}

\textsuperscript{1} Department of Physics, University of Tehran, North-Kargar Street, Tehran, Iran
\textsuperscript{2} Thin Film Centre, University of West of Scotland, Paisley, High Street, UK
\textsuperscript{3} Scottish Universities Physics Alliance (SUPA), UK

E-mail: savaloni@khayam.ut.ac.ir

Received 6 March 2013
Accepted for publication 8 April 2013
Published 29 April 2013
Online at stacks.iop.org/PhysScr/87/055705

Abstract

ZnS thin films with nano-rod and chiral sculptured structures of different thicknesses were deposited on glass substrates. Nano-structure of the films was obtained, using field emission scanning electron microscopy (FESEM). Their optical properties were measured by spectrophotometry in the spectral range of 350–1000 nm for both s- and p-polarizations at different incident light angles. The concept of local homogenization proposed by Bruggeman is used by estimating the permittivity dyadics of ZnS in the form of thin films with nano-rod and chiral sculptured structures. Making use of a simulation program, the influence of different deposition parameters on the optical spectra of the above-mentioned sculptured thin films is investigated. It is found that film thickness plays a major role in affecting the optical spectra of thin films and variation of other parameters results in a shift in the position (wavelengths) of the peaks. It is shown that the simulation results may be used for prediction of optical spectra of these sculptured thin films and can particularly be useful in the case of chiral sculptured thin films whose production can be a cumbersome task.

PACS number: 78.20.

(Some figures may appear in color only in the online journal)

1. Introduction

Introductory electromagnetic theory provides a simple approach for analyzing the optical properties of homogenized thin films [1, 2]. However, when the layers deviate from homogenized structure and contain a certain amount of voids in their structure, an accurate solution of Maxwell’s equations for these structures is either impossible or very difficult. Such layers with a variable amount of voids and shapes can be produced using either oblique angle deposition (deposition angle $<85^\circ$) or glancing angle deposition (deposition angle $>85^\circ$) techniques [3–5] and are called sculptured thin films that have columnar structure (range between 1 and 100 nm) [6–8]. In order to obtain optical properties of these sculptured thin films, it is assumed that the evaporant in its bulk form is isotropic and any sculptured thin film is a composite material consisting of two phases, namely evaporant and void [5]. The Bruggeman formalism is used to homogenize the composite media of the thin-film helicoidal bianisotropic media (TFHBM) and deduce the effective constitutive properties of dielectric TFHBM [9–12]. The most important parameters in the homogenization technique are the volumetric fraction of material particles, local direction of the film material and film thickness. The first two parameters are important in defining the local dielectric permittivity and the last parameter is the most important one in defining the optical spectra [11].

The aim of this work is to produce ZnS nano-rods at different oblique angles and chiral sculptured thin films with different structural parameters and obtain their structural
and optical properties, and then compare the latter with those calculated using the Bruggeman local homogenization method for both of these sculptured structures. Good agreement with experimental results is obtained. It is also deduced that the most significant parameter in performance of these films is the film thickness which affects the optical response of the film due to impedance mismatch at different interfaces and the cavity effect within the film confinement. On the other hand, the characterization wavelengths in this work are larger than the film thicknesses. This may cause deviations on strict analytical models. In addition, as the film thickness increases, the size and the number of grains and voids within the film structure vary causing adjustment on the optical response of the sample.

2. Theory

The homogenization process in the simulation work is based on the Bruggeman formalism [9–11]:

$$f_v A_v + (1 - f_v) A_s = 0,$$

$$A_{x,v} = \varepsilon_0 (\varepsilon_{x,v} I - \varepsilon_{ref}) \left[I + i \omega \varepsilon_0 D_{s,v}(\varepsilon_{x,v} I - \varepsilon_{ref})\right]^{-1},$$

$$D_{s,v} = \frac{2}{i \pi \omega \varepsilon_0} \int_0^{\pi} \int_0^{2\pi} \sin \theta \left[\frac{(\sin \theta \cos \psi)^2 u_{33} u_{11} + (\cos \theta)^2 u_{33} u_{11}}{\gamma_0^2} + \frac{\sin \theta \sin \psi}{\gamma_0} \right] \times \frac{(\sin \theta \cos \psi)^2 \varepsilon_{a} + (\cos \theta)^2 \varepsilon_{b} + (\sin \theta \sin \psi / \gamma_0)^2 \varepsilon_{c}}{2} d\theta d\psi.$$  

$A_{x,v}$ is the polarization density tensor of material (void), $D_{s,v}$ is the depolarization tensor of material (void), $f_v$ is the void fraction, $\varepsilon_{x,v}$ is the dielectric constant of material (void), $\varepsilon_{ref}$ is the Bruggeman reference dielectric constant, and $\gamma_0$ is the Bruggeman parameters defined in figure 1 that will be further discussed in the following paragraph.

In this formalism the sculptured thin film is considered as a two-phase composite, namely the void phase and the material (inclusion) phase. Both of these are dependent on the column form factor, the fraction of void phase, free-space wavelength and the refractive index of the material. In addition, each column in the sculptured thin film structure is considered as a string of identical long ellipsoids (figure 1). The ellipsoids are considered to be electrically small (i.e. small in a sense that their electrical interaction can be ignored) [13–15]. In addition, the ratio of the ellipsoid’s diameters is arbitrary (they are dimensionless and usually one of them is taken as unity and the other two are valued relative to the one taken as unity). Therefore, for this ellipsoid the dielectric constant and hence the electrical permittivity is given by a dyadic in the form of

$$\varepsilon_{ref} = \begin{pmatrix} \varepsilon_b & 0 & 0 \\ 0 & \varepsilon_c & 0 \\ 0 & 0 & \varepsilon_d \end{pmatrix}.$$  

For any arbitrary orientation of an ellipsoid in space, this dyadic undergoes two rotations and changes to a dyadic of nine elements in the form of

$$\varepsilon_{T}^{TF} = S_z(\beta (z)) S_y(\chi) \varepsilon_{ref} S_y^T(\chi) S_z^T(\beta (z)).$$  

$S_{z,y}$ matrices are rotation matrices about the z- and y-axis, and the amount of rotation is equal to their arguments and $S_{z,y}^T$ matrices are their transpose matrices.

$\chi$ (i.e. $\chi = 90 - \beta$, where $\beta$ is the column’s growth angle relative to the surface normal) is the angle of rise and $\psi(z)$ is the local azimuthal angle whose value shows the amount of rotation of the ellipsoid about the z-axis. In effect, the thin film is considered as a few thinner layers that are arranged on top of each other in the z-direction and to each layer a permittivity constant in matrix form is attributed. Then by solving the Maxwell’s equations and implementing the boundary conditions to each layer, a transfer matrix can be obtained. By multiplying these transfer matrices, a total transfer matrix can be achieved. The use of this matrix allows us to obtain scattering matrices that give us transmission and reflection coefficients for the whole thin film (e.g. linear and circular polarizations) [11]. The important point in these calculations is the use of a dyadic instead of a scalar (number) in the Maxwell’s equations:

$$D(r, \omega) = \varepsilon_{T}^{TF} E(r, \omega), \quad B(r, \omega) = \mu_{0} H(r, \omega).$$  

3. Experimental details

ZnS sculptured thin films were deposited on glass substrates (microscope slide) by electron beam evaporation. An Edwards (Edwards E19 A3) coating plant with a base pressure of $2 \times 10^{-7}$ mbar was used. The deposition angle was fixed at 75° (oblique angle) and a substrate azimuthal rotation speed of 0.06 rpm was chosen. A deposition rate of 0.8 Å/s was used for production of the chiral sculptured thin films. The deposition rate was measured by a quartz crystal deposition rate controller (Sigma Instruments, SQM-160, USA) positioned close to the substrate and at almost the same

![Figure 1](image-url)
the values of the growth angles

azimuthal angle as that of the substrate. This was corrected by obtaining the film thickness using the field emission electron microscope.

Figure 2 shows the schematic representation of the deposition process and rotation for oblique deposition. ZnS chiral thin films with three and five pitches were produced by rotation of the substrate holder about its surface normal three times and five times, respectively, while the deposition rate was kept fixed at 0.8 Å s⁻¹. The thickness of each pitch was 80 nm (i.e. half structural period Ω = 40 nm). The movement of the stepper motor and its speed of revolution as well as facility for dividing each revolution into different sectors are controlled through the interface to a computer in which the related software is written and installed. All these are domestic made.

ZnS nano-rod-shaped thin films were produced by deposition at different oblique angles of 15°, 30°, 45° and 60° with different thicknesses in the range of 60–80 nm and 0°, 15°, 30° and 45° with a thickness of 210–240 nm with a deposition rate of 0.8 Å s⁻¹. Hence, the deposition time for the deposition of thicker films was about three times that of the thinner films. As mentioned above in the case of the oblique angle deposition, the film thickness was also monitored by a quartz crystal deposition rate controller positioned close to the substrate and at almost the same azimuthal angle as that of the substrate in which its angle with respect to the deposition source (crucible) was adjusted for different deposition angles.

Prior to deposition, all glass substrates were ultrasonically cleaned in heated acetone and then ethanol. The surface roughness of the substrates was measured by a Talyurf profilometer and an atomic force microscope (AFM) and the rms substrate roughness Rq obtained using these methods was 0.3 and 0.9 nm, respectively.

The deposition process was repeated a few times and the reproducibility of the results was confirmed.

The film thicknesses and column shapes and sizes were measured by a field emission electron microscope (FESEM) (Hitachi S-4100 SEM, Japan). The FESEM samples were coated with a very thin layer of gold to prevent the charging effect. The reflectance and transmittance spectra of the samples were obtained using a single-beam spectrophotometer (Aquila nkd-8000) in the spectral range of 350–1000 nm and both s- and p-polarizations in steps of 5 nm wavelength at different incident light angles.

<table>
<thead>
<tr>
<th>Deposition angle, α (°)</th>
<th>Growth angle, β (°)</th>
<th>Growth angle (tangent rule) (°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>15</td>
<td>6.0</td>
<td>7.5</td>
</tr>
<tr>
<td>30</td>
<td>12.0</td>
<td>16.1</td>
</tr>
<tr>
<td>45</td>
<td>24.0</td>
<td>26.7</td>
</tr>
</tbody>
</table>

4. Results and discussion

4.1. Experimental results of ZnS thin films with nano-rod structure

As mentioned in section 3, ZnS thin films with nano-rod structure were deposited at different deposition angles with two different thicknesses of 60–80 and 210–240 nm. It is well known that the growth angle for these films is smaller than the deposition angle [16] and generally the tangent rule (tan β = ½ tan α, where α and β are the deposition and the growth angles, respectively) [17] applies for the deposition angles smaller than 60°, while at higher deposition angles the Tayt [17] formula (β = α − sin⁻¹ (1/cosα)) is more appropriate [18]. The growth angles of our thicker ZnS films (210–240 nm) are compared with those of the tangent rule and reasonably good agreement is obtained. The same measurements on thinner films of 60–80 nm thickness due to thinness of the films may not be as reliable as those of thicker films, although the typical FESEM of these samples given in figure 3(a) for a deposition angle of 15° shows the same growth angle as that observed for thicker films (i.e. 6° given in table 1). Hence it can be assumed that the growth angle for the thinner films is the same as that of the thicker films.

It should also be noted that by increasing the deposition angle both the film thickness and the void fraction in the structure of the film increase [18–20]. Figures 3(a) and (b) show typical FESEM images of ZnS thin films with nano-rod structure.

Optical spectra obtained for these films are given in figure 4. Tns, Tps and Rns, Rps define the transmittance and the reflectance for s- and p-polarizations, respectively. A near-normal incident light angle (10°) was used for collection of these spectra.

In figure 4, column II (films of 240 nm thickness), it can be seen that by increasing the deposition angle up to 30° the position of peaks for both transmittance and reflectance spectra is shifted to larger wavelengths (red shift), while at a higher deposition angle of 45° this is changed to the opposite direction (i.e. blue shift). The variation of spectral features of thinner films of 80 nm (figure 4, column I) is not as obvious as that of thicker films. This can be due to the thinness of these films and may possibly be due to the formation of a dense bottom layer in these sculptured thin films [21, 22] which can be of ~ 40–50 nm thickness. Hence with regard to the film thickness, particularly in the case of our thinner films, this bottom layer in fact is competing with the upper porous layer of the film. The effect of this dense bottom layer reduces as the film becomes thicker.
Figure 3. Typical FESEM images of ZnS thin films of different thicknesses with nano-rod structure: (a) 80 nm and (b) 240 nm.

Figure 4. Optical spectra of ZnS thin films with nano-rod structure grown at different oblique angles ($\alpha$). Column (I) 80 nm thickness and column (II) 240 nm thickness.

4.2. Simulation results for ZnS thin films with nano-rod structure

The angle used in the simulation program is the rise angle ($\chi = 90 - \beta$, where $\beta$ is the growth angle). Figure 5 shows the simulation results for ZnS thin films with nano-rod structure and with 240 nm thickness for different rise angles ($\chi$) and volumetric fraction of the evaporant material ($f_v$). Results of the simulation program indicate that the most influential parameter on the optical spectra is the film thickness and the rest of the parameters mostly cause a shift in the peak position. The contribution of the film thickness in the optical spectra of thin films may be considered from either the optical or material perspective. From the optical perspective, the thickness will affect the transmittance and reflectance response of the thin film due to the impedance mismatch at different interfaces (film/glass, film/air) and the cavity effect within the film confinement. On the other hand, the film thicknesses in this work are much smaller than the wavelengths of the incident light used for their optical characterization. This may cause deviations on strict analytical models.

From the material perspective, the effective medium theory can be used to estimate the bulky optical parameters that affect optical response. By increasing the film thickness, the size and number of grains/voids within the constructed...
thin film vary [20] which will cause the filling factor (packing density) to change, which in turn influences the optical response of the produced sample.

However, the effective medium theory mentioned in the above paragraph is a simple way of taking an average between the dielectric constants of the material inclusion and the void part of the thin film, while the film structure and orientations are not considered in the formalism. In the Bruggeman homogenization formalism used in this work (section 2), a more accurate method of obtaining an average is considered.
while the effect of both structure and orientation is also included in the calculation. The results given below clearly show the effect of these parameters in the optical response of the sculptured thin films produced in this work which cannot be observed when the effective medium theory is used.

In figure 5, the shift in the position of peaks in both transmittance and reflectance spectra with variation of the rise angle \( \chi \) and the volumetric fraction of the evaporant material \( f_s \) can be clearly observed, while the change in the intensity is not significant. It should also be pointed out that the most affected spectrum belongs to the case of \( \chi = 75^\circ \) (i.e. \( \beta = 15^\circ \)), \( f_s = 0.75 \). Therefore, considering these results and the significant influence of thickness on the results as mentioned above, these two parameters were fixed and only the film thickness was varied in the following calculations. Figure 6 shows the reflectance and transmittance spectra of thin films with nano-rod structure and different thicknesses with fixed values for \( \chi = 65^\circ \) (i.e. \( \beta = 25^\circ \)) and \( f_s = 0.75 \). Similarities can be observed between these results and the experimental ones presented in figure 4. For example, there is reasonably good agreement between figures 6(b) and 4(b)(I), while one can also observe similarities between figure 6(c) (100 nm) and that of the experimental one (figure 4(c)(I)). The intriguing point is that the latter experimental case (i.e. figure 4(c)(I)) is obtained for the deposition angle of \( \alpha = 45^\circ \) and the growth angle of \( \beta = 24^\circ \) (see table 1). The growth angle is almost the same as that used for the simulation work (i.e. \( 25^\circ \)) and presented in figure 6. In addition, it may be concluded that the thickness of the experimental sample as measured during the deposition is also consistent with that of the simulation work. The remaining parameter to be clarified for consistency with the experimental results is the material inclusion (void fraction) in the body of the thin film structure. As mentioned above, the simulation work was carried out with a material inclusion of 75% (\( f_s = 0.75 \)) or a void fraction of 25%. In order to obtain a value for this parameter from the experimental results, AFM analysis was performed on the produced samples. From the AFM images of the samples, one may obtain the surface void fraction. The AFM images of the samples (two-dimensional (2D) and three-dimensional (3D)) together with the fraction of void images obtained from the above-mentioned experimental samples (i.e. figures 4(b)(I) and (c)(I)) are given in figure 7. The surface void fractions obtained from these figures are 18 and 27%, respectively. These values are in close agreement with the value used for the simulation results (i.e. 25%) although one should keep in mind that the value used for simulation reasons is the bulk void fraction. Therefore, all of the parameters used in the simulation results presented in figure 6 are consistent with those of experimental work (i.e. growth angle, film thickness and material inclusion/void fraction). This clarifies that our selection of parameters for simulation purposes is their consistency with the experimental observations.

In the case of comparing the thicker experimental results with those of simulation work, it can be seen that the thicker experimental films of 240 nm thickness (i.e. figure 4(II)) show a similar trend. Among the simulated results, figure 6(g) shows the highest degree of agreement with the experimental results in figure 4(II) of the same thickness. In order to investigate further the consistency of the simulation results with that of experimental ones, in figure 8 the experimental results of figure 4(c)(II) are compared with those of simulation (figure 6(g)). In order to improve the quality of fitting of the simulation work to that of the experimental one, as mentioned above a search procedure was carried out with a fixed value for film thickness (240 nm) while the rise angles \( \chi \) and the volumetric fraction of material particles \( f_s \) were the adjustable parameters. The result of this search is given in figure 8(b).

It can be seen that the volumetric fraction of material remains unchanged, while the rise angle \( \chi \) is increased from 65° to 80°. This means that the growth angle \( \beta \) of the nano-rods is decreased from 25° to 10°. This in fact is in very good agreement with our experimental observation as given in table 1. This change in the rise angle has improved the fitting of these two sets of data particularly
at wavelengths above 500 nm for both transmittance and reflectance spectra, while the matching of the position of peaks is also improved. Experimental reflectance and transmittance spectra show peaks at 385 and 565 nm, and 450 and 825 nm, respectively; similar peaks can be observed in the simulation results with some shifts at 400 and 590 nm, and 490 and 830 nm (figure 8(b)), respectively, while the intensity of all experimental peaks for both transmittance and reflectance spectra is greater than the simulation results, particularly the transmittance peak at 450 nm and the reflectance peak at 385 nm. The differences observed between the experimental and the simulation results in this work and in particular in figure 8 can be attributed to the following reasons: in the experimental results the sum of transmittance and reflectance within the wavelength range of 450–490 nm is almost unity. Therefore, it may be concluded that in the experimental measurements absorption is negligible, while this sum in the simulation results is less than unity; hence there should exist absorption. Considering the significant influence of the imaginary part of the refraction coefficient on the absorption, it may be suggested that there may be a difference between the refraction coefficients used in the simulation work (simulation calculations were carried out, using the optical constants of the bulk ZnS from those reported in [23]) and those involved in the experimental results; hence this difference between the two approaches may be the cause of observed differences in the presented results in this work. In order to obtain some insight into the effect of these parameters on the simulation results, we have calculated the refraction constants of our films by the method described in the following section.

4.3. Refraction coefficient of ZnS thin films with nano-rod structure

In order to obtain the refraction coefficient \(n_f\) of the ZnS thin films with nano-rod structure, we have used the prescription given in [24, 25] where it is suggested that the following equation may be used to obtain the optical constants of low absorption thin films without considering their geometry (structure):

\[
T = \frac{16n_0n_fn_s^2\alpha_{\text{ext}}}{C_1^2 + C_2^2\alpha_{\text{ext}}^2 + 2C_1C_2\alpha_{\text{ext}}\cos(4\pi nfd/\lambda)},
\]

\[
C_1 = (n_0 + n_f)(n_f + n_s),
\]

\[
C_2 = (n_0 - n_f)(n_f - n_s),
\]

\[
\alpha_{\text{ext}} = \exp(-4\pi kd/\lambda).
\]
Figure 10. Typical FESEM images of ZnS thin films with chiral structure with different number of pitches: (a) three pitches and (b) five pitches.

Figure 11. Comparison of simulation results with experimental results for ZnS thin films with chiral structure and three pitches: \( \Omega = 40 \text{ nm}, L = 240 \text{ nm}, R_c = 75 \text{ nm} \) and \( f_s = 0.55, h = 1 \).

In equation (5), \( n_0, n_s, n_f \) are real parts of the refraction indices of the thin film, the substrate and the air, respectively. \( d \) is the film thickness and \( k \) is the imaginary part of the refraction index of ZnS nano-rod thin films. It is worthwhile to mention here that although we have attempted to calculate the refraction indices of our films using the above equation it does not exactly provide accurate values for our films due to lack of inclusion of film structure parameters in the formalism. However, it should give data which in our opinion may be closer to the real values than the bulk.

In order to calculate the refraction index of our ZnS thin films with nano-rod structure using equation (5), we first obtained the imaginary part of the refraction index \( k \), using the extinction coefficient \( (\alpha_{\text{ext}}) \) equation as [2]

\[
\alpha_{\text{ext}} = \exp \left( -\frac{4\pi k d}{\lambda} \right) = \frac{T}{1 - R}.
\]

while the film thickness \( d \) was obtained from the predictions of our simulation results that showed good agreement with the experimental measurements (section 4.2, i.e. 80 and 240 nm for low and high film thicknesses, respectively). Then equation (5) was numerically solved with \( n_s = 1.52, n_0 = 1 \). The results are given in figures 9(a)(I) and (b)(I) (for ZnS films of lower thickness) and figures 9(a)(II) and (b)(II) (for ZnS films of higher thickness) while those of [23] that are used in our simulation work are also included in these figures for comparison.

The results in figure 9 show that the real part of the refraction index for both thicknesses varies between 1.9 and 2.5, which is in agreement with the data (values) reported in [24, 25]. However, there exists a minimum at wavelengths between 600 and 800 nm in figures 9(a)(II) while for lower thicknesses in figure 9(a)(I) this minimum is observed for films produced at deposition angles of 15° and 60°. The data of [23] used in this work for simulation purposes decrease with increasing wavelength. Hence, considering these results, we may attribute the differences observed in figure 8 between our experimental results and those obtained from simulation.
Comparison of simulation results with experimental results for ZnS thin films with chiral structure and five pitches: \(\Omega = 40\) nm, \(L = 400\) nm, \(R_c = 75\) nm and \(f_s = 0.55, h = 1\).

by using the refraction indices of [23] to the differences between the refraction index obtained in figure 9 and those of [23]. Comparison of the optical constants obtained using the procedure in this section with those of Palik [23] clearly shows that the imaginary part of the refraction coefficient of [23] is much higher than our results at the wavelength region between 350 and 600 nm. This is almost exactly the main region of difference between our simulation results and those of experimental data (see figure 8). In addition, the real part of the refraction coefficient obtained here (figures 9(a)(I) and (a)(II)) also shows clear deviation from that of [23] at the higher wavelength region (above 500 nm). This may be the cause of damping of reflectance at this region in our simulation work (compare figures 4(b)(I) and (c)(I) with figures 6(b) and (c)).

As mentioned above, we emphasize again that the results of this section may not be the correct values for our films because the film structure parameters are not included in the formalism.

In addition, we wish to mention that our aim in this work has been to obtain optical spectra of our thin films by an independent simulation approach using the homogenization formalism with some available parameters such as film thickness, geometrical shape, void fraction and refraction indices and compare the results with experimental spectra. Therefore, the use of refraction indices obtained in this section (although not being the correct values but somewhat closer to the real values than the bulk) instead of bulk values would not be a logical way of simulating the optical spectra of the same samples. Hence our approach has been independent of the parameters of the produced samples.

### 4.4. ZnS thin films with chiral sculptured structure

Figure 10 shows the FESEM images of chiral ZnS sculptured thin films with 3 (240 nm thickness) and 5 (400 nm thickness) pitches, while the pitches and their rotation directions are shown on a column by arrows. In figures 11 and 12 the experimental and the simulated optical spectra of these chiral sculptured thin films obtained for different incident light angles and for both s- and p-polarizations are compared. The important parameters of the chiral thin films are film thickness \(L\), half structural period \(\Omega\), radius of the chiral cross-section \(R_c\) and handedness of the chiral \(h\). Since our experimental chiral films were produced as right-handed chiral, this parameter is set at \(h = 1\) for the simulation reason.

The other parameters mentioned above in the simulation work were set at the following values: \(\Omega = 40\) nm, \(R_c = 75\) nm and \(f_s = 0.55\). It should be mentioned that these parameters were chosen according to the measurements performed on the FESEM images. It can be observed that the simulated spectra are in good agreement with experimental ones, in a sense that the position of peaks and their variations are very similar.

Finally, one may seek the origin of the peaks and valleys in the optical spectra presented throughout this work that are most affected by the film thickness as discussed above. Referring to equation (5) it can be seen that the only oscillatory term in this equation is the cosine term in the denominator \((\cos(4\pi n_d/\lambda))\). Considering that transmittance is dependent on wavelength and that the variation of refraction index is small compared with that of film thickness, then on increasing the film thickness the oscillation period decreases, which in turn produces the peaks and valleys in the optical
spectra. The other parameter that strongly affects the optical spectra and in particular causes the difference between s- and p-polarization results (e.g. spectra in figures 4 and 6 for ZnS nano-rod structures and figures 11 and 12 for ZnS chiral nano-structure (section 4.4)) is the incident light angle which is used as near normal (10°) in the case of ZnS nano-rod structures (figures 4 (experimental) and 6 (simulation)) while in the case of chiral nano-structure higher incident angles are also used (figures 11 and 12). In all these figures it can be seen that at a low incident angle of 10°, the difference between s- and p-polarization spectra is either negligible or non-existent, while this difference becomes more distinguishable by increasing the incident light angle (figures 11 and 12). It can be seen that by increasing the incident light angle the reflectance of p-polarized light decreases and its transmittance increases. The variation of s-polarized light with the incident light angle is opposite to that of p-polarized light. This is due to the incident light angle approaching the Brewster angle [1, 2], which is 67.38 for the bulk sample, and a wavelength of 600 nm [23]. In figures 11 and 12 it can clearly be observed that at an incident light angle of 60° the reflectance of p-polarized light is very close to zero while it must be noted that the Brewster angle for thin films may vary from that of the bulk.

5. Conclusions

ZnS sculptured thin films in shapes of oblique nano-rods with different thicknesses and chiral shaped with three and five pitches were produced using oblique angle deposition in conjunction with rotation of the substrate holder with an electron beam source. Their nano-structure was analyzed using FESEM and AFM and their optical spectra were obtained using spectrophotometry for both s- and p-polarizations. The Bruggeman local homogenization formalism was implemented by estimating the permittivity dyadics of ZnS in the form of thin film nano-rods and chiral sculptured thin films. The homogenization results showed good agreement with the experimental results for both ZnS nano-rods and ZnS chiral thin films produced with different deposition parameters. The results also showed the significance of film thickness in the optical performance of these thin films, which can be due to the impedance mismatch at different interfaces and the cavity effect within the film confinement. On the other hand, since the characterization wavelengths are larger than the film thicknesses in this work, this causes deviations on strict analytical models. In addition, as the film thickness increases, the size and the number of grains and voids vary causing adjustment on the optical response of bulky material. The simulation method described in this work may, in particular, be used for the prediction of the optical spectra of chiral sculptured thin films whose production involves a complex procedure.

Acknowledgments

This work was carried out with the support of the University of Tehran and the Iran National Science Foundation (INSF). HS is grateful to the Centre of Excellence for Physics of Structure and Microscopic Properties of Matter, Department of Physics, University of Tehran for partial support of this work.

References

[18] Savaloni H and Gholipour Shahrahi M 2004 Nanotechnology 15 311