Computation of Optogeometric Properties of Thin Films Optical Waveguides using the Newton-Raphson Method

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ABSTRACT

There are numerous methods for calculating refractive index and thickness of dielectric and polymer thin film coating materials used in optical waveguide applications. This paper reports the use of the Newton-Raphson method, based on results obtained from m-line spectroscopy, to simulate zero function equations derived from defined combinations of the conventional mode dispersion equations using the Fortran 77 high level language.

The solution for three transverse electric modes and five transverse magnetic modes of propagation were analyzed using a 632.8nm laser beam. The m-line angles studied for the 3TE modes are -2.490^o, -3.885^o, and -5.230^o using Polymethyl-Methacrylate films and -19.8^o, -21.7^o, -24.8^o, -29.3^o, and -32.2^o for the 5TM modes using Germanium Sulphide film in a planar waveguide.

The results obtained for refractive index and thickness were found to be 1.554±0.002 and 2.284±0.007µm respectively for the 3TE modes and 2.0558±0.0002 and 1.85±0.01µm respectively for the 5TM modes. The results generally showed a higher uncertainty in determining film thickness than the refractive index for both polarizations.

(Keywords: waveguide, dielectric, refractive index, thickness, dielectric and polymer thin films)

INTRODUCTION

Thin film materials whose particles are seemingly dispersed in a matrix with properties notably different from that of the bulk material are called thin films of the material. Their nature is such that, highly sensitive and non-destructive techniques are increasing being required in order to understand their microstructure [1]. Thin dielectric and polymer films find applications as planar wave guides in various experiments in integrated optics [2].

Considering their relevance in integrated optics and microelectronic industry, the fabrication and characterization of polymer thin films has been gaining enormous attention for many decades now [3]. Aside from other properties such as the bandwidth and extinction coefficients, the characteristic of the films could be traced to the refractive index and thickness of the materials since they characteristically account for the properties of the films [2]. Evidence of the calculation of these parameters for the zero order mode (TE_0, TM_0), 2TE, and 2TM modes simulated graphically have been reported [4].

This paper explores the use of a numerical methods based on the Newton-Raphson algorithm to do the simulation of some well defined zero function mode dispersion combination equations to determine the refractive index parameter and a subsequent substitution to compute the thickness of the thin film in a two-dimensional (2D) step-index waveguide.

PLANAR DIELECTRIC WAVEGUIDE

In a planar dielectric waveguide, dielectrics are used as guides for electromagnetic energy. We assumed an asymmetric waveguide composed of three layers that include (i) the substrate, (ii) the thin film, and (iii) the cladding layer.

Figure 1 is a simple illustration of the planar waveguide.

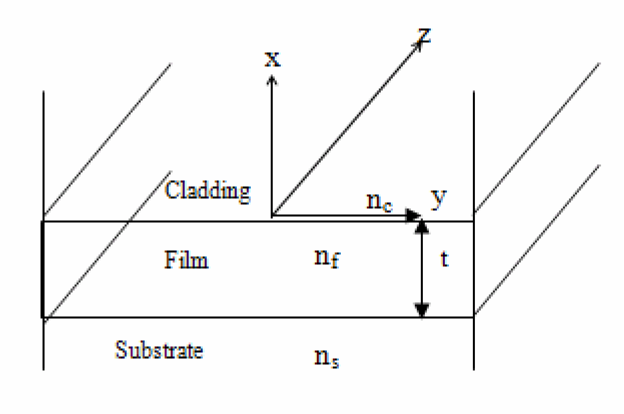

Figure 1: Schematic Illustration of a Planar Dielectric Waveguide (slab).

Wave propagation in the waveguide due to total internal reflection is sustained only if the refractive index of the thin film is greater than the index of substrate and the cladding layer. That is $n_f > n_s > n_c$.

Given this condition, a planar dielectric waveguide can guide waves, with the fields of these waves occupying the space within and around the dielectric structure. Waveguides that use dielectric films find good application in the realization of integrated optical devices [5]. The non-destructive determination of thickness and refractive index of transparent films on reflective substrates, which is in line with this work, has been reported [6].

In propagating a stable electric and magnetic field pattern that is periodic along the waveguide with negligible attenuation, two types of modes (TE and TM) are usually observed. The TE modes are generated when the electric field is transverse or perpendicular to the direction of propagation of the electromagnetic wave in the waveguide light confinement is observed to be only along the x-axis. For an infinitely extended upper and lower cladding layer, in addition to light confinement in the +z direction which is equally infinite in the ±y-direction, the electric and magnetic fields show no dependence in the ±y-direction. Hence for the TE mode $\mathrm{E}_z = 0$.

Similarly, the TM mode contains no magnetic field in the $z-$direction, making $\mathrm{H}_z = 0$.

The field components for both polarizations are given as: $E_y, H_x, andH_z$ for the TE polarization, and $H_y, E_x, andE_z$ for the TM polarization.

THE THEORETICAL FORMULATION

Electromagnetic energy, or a wave propagating in a planar dielectric waveguide, is described by the following Maxwell's equation:

$$\nabla \times E = \frac{\partial B}{\partial t} \text{ ------------------------------------ } \mathbf{(1)}$$

$$\nabla \times B = \frac{\partial D}{\partial t} + J \text{ --------------------------------} \mathbf{(2)}$$

$$\nabla . B = 0 \quad \text{--} \mathbf{(3)}$$

$$\nabla . D = \rho \quad \text{--} \mathbf{(4)}$$

From these equations, the TE and TM eigenvalue equation could be derived such that:

For the TE mode,

$$\frac{\partial^2 E_y}{\partial t^2} + \left(k_o^2 n_i^2 - \beta^2\right) E_y = 0 \text{ ---------------} \mathbf{(5)}$$

For the TM mode,

$$\frac{\partial^2 H_y}{\partial t^2} + \left(k_o^2 n_i^2 - \beta^2\right) H_y = 0 \text{ ---------------} \mathbf{(6)}$$

Doing a dispersion analysis for guided wave modes based on the principle of total internal reflection already described [4], the defining equation used for the simulation of the numerical results is a zero function equation of the form,

$$\Psi_{m\rho}(N_m, n)\xi_{f(m+1)\rho} - \Psi_{(m+1)\rho}(N_m, n)\xi_{fm\rho} = 0 \text{----} \mathbf{(7)}$$

Where,

$$\xi_{fmp}(N_m, n) = \left\{ \frac{\Phi_{fc}(N_m, n) + \Phi_{fs}(N_m, n) + m\pi}{k_0 t} \right\} \text{ ---- } \mathbf{(8)}$$

and

$$\sum_{i=1}^{2}\left(\frac{\Psi_{imp}(N_m,n)}{\xi_{fmp}(N_m,n)}\right)-\sum_{i=3}^{q}\left(\frac{\Psi^{q}{}_{imp}(N_m,n)}{\xi_{fmp}(N_m,n)}\right)=0 \text{----} \textbf{(9)}$$

i =1,2…q.

Hence, q is the total number of propagated modes in the film of the waveguide. The equation was solved for the refractive index using the Newton-Raphson algorithm which has the form:

$$n_{q+1}=n_q-\frac{f(n_q)}{f^{1}(n_q)} \text{------------------------} \textbf{(10)}$$

For a relatively accurate solution, the zero function equations for particular mode combination and polarization were linearized to obtain the starting guesses for the different iteration schemes. This method offers a simple and elegant means of determining the roots (refractive index) of the functions [7]. The possible cases of failure have also been discussed elsewhere [8].

RESULTS AND DISCUSSION

The Newton-Raphson simulation of the zero function equation was done for the 3TE and 5TM modes of the m-lines report of Agan *et al*. (2005) for the 3TE modes [3] and Huang *et al.* (2004) for the 5TM modes [9] at a wavelength of 632.8nm. These results are presented in Table 1.

Table 1: Refractive Index and Thickness for the 3TM and 5TM Modes.

Parameter	**Results for 3TE**	
	Numerical	**Experimental**
Refractive Index	1.554±0.002	1.4869
Thickness of Film	2.28±0.07µm	2.300
Parameter	**Results for 5TM**	
	Numerical	**Experimental**
Refractive Index	2.0558±0.0002	2.09±0.08
Thickness of Film	1.85±0.01µm	1.83±0.08

In Table 1 the numerical approach using Newton-Raphson algorithm gave index and thickness values of 1.554±0.002 and 2.28±0.07µm for the 3TM mode. This result is in agreement with the graphical result earlier obtained [4].

Applying the same numerical scheme to the zero order (TE, TM), 2TE, 2TM modes, the uncertainties in the refractive index measurements were in the range of 0.0002 to 0.01, while thickness values were in the range of 0.0005 to 0.03nm. The results obtained for PMMA film using three observed TE modes was found to be in very acceptable agreement with those obtained experimentally [3].

Using the same numerical scheme for the 5TM modes, the results gave a refractive index of 2.0558±0.0002 and thickness of 1.85 ± 0.01µm respectively for the films. The result was found to within the limits of experimental errors confirm the experimental result [9]. The result in this and those earlier investigated reveal that the numerical scheme with a good starting guess and step size will produce results that are in better agreement with experiments that those obtained graphically. The sample of the program simulation for the 5TM modes is presented in the appendix.

CONCLUSION

The difference in the experimental values from those of the theoretical values is attributable to a number of factors; these may include factors such as stress [3] which is quite probable, since the method does not work contact-less [2]. Other factors may include any deviations from the conditions for accurate measurements of these parameters such as (i) a good knowledge of the prism's characteristic, (ii) accurate measurement of angles, and (iii) taking into account the distance between the prism and guide i.e. the air-layer-thickness (ALT) [10].

The model prism waveguide coupler system with variable air-gap thickness from 0 to 0.5µm have been reported and is linked to the discrepancy between the effective indices values predicted by the conventional prism waveguide coupler and those of thin-film optics [11]. The choice of the method to adopt for the computation of these parameters, either by graphical or numerical means, depends on interest. However, the numerical technique using the Newton-Raphson algorithm presented in this work is recommended since the results obtained using this method show a closer agreement with those obtain from experiments than those obtained graphically.

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APPENDIX

NUMERICAL SOLUTION PROGRAM SIMULATION FOR 5TM MODES

```
    PROGRAM ESAN8
    PARAMETER(NMAX=100)
    COUNT=1
    READ(*,*)A,B,CV,CW,CX,CY,
         G,Y,Eo,E1,E2,E3,E4,Xo,R
    PA=SIN(CV)/A
    PB=ASIN(PA)
    PC=B+PB
    PD=SIN(PC)
    DV=A*PD
    QA=SIN(CW)/A
    QB=ASIN(QA)
    QC=B+QB
    QD=SIN(QC)
    DW=A*QD
    RA=SIN(CX)/A
    RB=ASIN(RA)
    RC=B+RB
    RD=SIN(RC)
    DX=A*RD
    SA=SIN(CY)/A
    SB=ASIN(SA)
    SC=B+SB
    SD=SIN(SC)
    DY=A*SD
    DV=2.0491
    P=Xo
    OPEN(2,FILE='RES2.DAT')
    DO 20 I=1,NMAX

AA=ATAN((P/F)**2*SQRT(ABS((DV*
         DV-F*F)/(P*P-DV*DV))))

AB=ATAN((P/G)**2*SQRT(ABS((DV*
         DV-G*G)/(P*P-DV*DV))))
    AC=4.*ATAN(1.)*(Eo)
```

```
AD=8.*ATAN(1.)*SQRT(ABS((P*P-
            DV*DV)))

AW=ATAN(((P+R)/F)**2*SQRT(ABS((
            DV*DV-F*F)/((P+R)**2-
            DV**2))))

AX=ATAN(((P+R)/G)**2*SQRT(ABS((
            DV*DV-G*G)/((P+R)**2-
            DV**2))))
      AY=8.*ATAN(1.)
     * *SQRT(ABS((P+R)**2-DV*DV))
      AZ=((AW+AX+AC)/AY)
      AT=Y*((AA+AB+AC)/AD)
      AXA=(AZ-AT)/R
      BA=ATAN((P/F)**2
     * *SQRT(ABS((DW*DW-F*F)
     */(P*P-DW*DW))))
      BB=ATAN((P/G)**2
     * *SQRT(ABS((DW*DW-G*G)
     */(P*P-DW*DW))))
      BC=4.*ATAN(1.)*(E1)
      BD=8.*ATAN(1.)
     * *SQRT(ABS((P*P-DW*DW)))
      BW=ATAN(((P+R)/F)**2
     * *SQRT(ABS((DW*DW-F*F)
     */((P+R)**2-DW*DW))))
      BX=ATAN(((P+R)/G)**2
     * *SQRT(ABS((DW*DW-G*G)
     */((P+R)**2-DW*DW))))
      BY=8.*ATAN(1.)
     * *SQRT(ABS((P+R)**2-DW*DW))
      BZ=((BW+BX+BC)/BY)
      BT=Y*((BA+BB+BC)/BD)
      BXB=(BZ-BT)/R
      CA=ATAN((P/F)**2*
     * SQRT(ABS((DX*DX-F*F)
     */(P*P-DX*DX))))
      CB=ATAN((P/G)**2
     * *SQRT(ABS((DX*DX-G*G)
     */(P*P-DX*DX))))
      CC=4.*ATAN(1.)*(E2)
      CD=8.*ATAN(1.)
     * *SQRT(ABS((P*P-DX*DX)))
      CW=ATAN(((P+R)/F)**2
     * *SQRT(ABS((DX*DX-F*F)
     */((P+R)**2-DX*DX))))
      CX=ATAN(((P+R)/G)**2
     * *SQRT(ABS((DX*DX-G*G)
     */((P+R)**2-DX*DX))))
      CY=8.*ATAN(1.)
     * *SQRT(ABS((P+R)**2-DX*DX))
      CZ=((CW+CX+CC)/CY)
      CT=Y*((CA+CB+CC)/CD)
      CXC=(CZ-CT)/R
      DA=ATAN((P/F)**2
     * *SQRT(ABS((DY*DY-F*F)
     */(P*P-DY*DY))))
      DB=ATAN((P/G)**2
     * *SQRT(ABS((DY*DY-G*G)
     */(P*P-DY*DY))))
      DC=4.*ATAN(1.)*(E3)
      DD=8.*ATAN(1.)
     * *SQRT(ABS((P*P-DY*DY)))
      DWW=ATAN(((P+R)/F)**2
     * *SQRT(ABS((DY*DY-F*F)
     * /((P+R)**2-DY*DY))))
      DXX=ATAN(((P+R)/G)**2
     * *SQRT(ABS((DY*DY-G*G)
     */((P+R)**2-DY*DY))))
      DYY=8.*ATAN(1.)
     * *SQRT(ABS((P+R)**2-DY*DY))
      DZZ=((DWW+DXX+DC)/DYY)
      DT=Y*((DA+DB+DC)/DD)
      DXD=(DZZ-DT)/R
      EA=ATAN((P/F)**2
     * *SQRT(ABS((DZ*DZ-F*F)
     */(P*P-DZ*DZ))))
      EB=ATAN((P/G)**2
     * *SQRT(ABS((DZ*DZ-G*G)
     */(P*P-DZ*DZ))))
      EC=4.*ATAN(1.)*(E4)
      ED=8.*ATAN(1.)
     * *SQRT(ABS((P*P-DZ*DZ)))
      EW=ATAN(((P+R)/F)**2
     * *SQRT(ABS((DZ*DZ-F*F)
     */((P+R)**2-DZ*DZ))))
      EX=ATAN(((P+R)/G)**2
     * *SQRT(ABS((DZ*DZ-G*G)
     */((P+R)**2-DZ*DZ))))
      EY=8.*ATAN(1.)
     * *SQRT(ABS((P+R)**2-DZ*DZ))
      EZ=((EW+EX+EC)/EY)
      ET=Y*((EA+EB+EC)/ED)
      EXE=(EZ-ET)/R
      RT=(AT+BT-CT-DT-ET)
      FT=((AZ+BZ-CZ-DZZ-EZ)
     * -(AT+BT-CT-DT-ET))
      QT=FT/R
      PX=P-(RT/QT)
      GK=PX-P
      IF(GK.LT.10E-10)THEN
      GO TO 60
      END IF
      P=PX
      COUNT=COUNT+1
   20 CONTINUE
   60 TY=ATAN((P/F)**2
     **SQRT(ABS((DV*DV-F*F)
     */(P*P-DV*DV))))
      BY=ATAN((P/G)**2
```

```
* *SQRT(ABS((DV*DV-G*G)
*/(P*P-DV*DV))))
 BT=4.*ATAN(1.)*E1
 SR=SQRT(ABS(P*P-DV*DV))
 tTM=Y*((TY+BY+BT)
* /(8.*ATAN(1.)*SR))
 PRINT*,P,tTM,COUNT
 WRITE(2,*)P,tTM,COUNT
 STOP
 END
```

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