

APPENDIX 1 . REFRACTIVE INDEX DETERMINATION

Figure 1A depicts the UV-Vis transmission spectrum of the cathode sample which was prepared with 5:1 ammonia to silane flowrate ratio and at substrate temperature of 250°C, i.e. Batch 1 sample. The envelope which coupled the interference fringes is formed between the respective maxima and minima of the fringes. 16 points from the envelope are utilized to generate up to 112 points using the Lagrange's Interpolating Polynomial.

The Lagrange fundamental polynomials of degree n based on $n+1$ distinct points $x_0 < x_1 < x_2 < \dots < x_n$ can be written in the form [1,2]

$$P_n(x) = \sum_{i=0}^{n} l_i(x)f(x_i) \quad (\text{A1.1})$$

$l_i(x)$ is itself a polynomial of degree $\leq n$ with the property

$$l_i(x) = \delta_{ij} = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases} \quad (\text{A1.2})$$

and

$$l_i(x) = \prod_{j=0, j \neq i}^n \left(\frac{x - x_j}{x_i - x_j} \right) \quad (0 \leq i \leq n) \quad (\text{A1.3})$$

which indicates that $l_i(x)$ is the product of n linear factor

$$l_i(x) = \left(\frac{x - x_0}{x_i - x_0} \right) \left(\frac{x - x_1}{x_i - x_1} \right) \dots \left(\frac{x - x_{i-1}}{x_i - x_{i-1}} \right) \left(\frac{x - x_{i+1}}{x_i - x_{i+1}} \right) \dots \left(\frac{x - x_n}{x_i - x_n} \right) \quad (\text{A1.4})$$

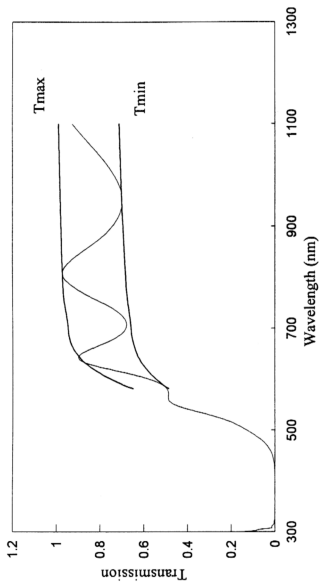


Figure 1.A. The application of envelope method utilizing the interference fringes appearing in the UV-Visible spectrum.

Lagrange Interpolation of degree 3 is used in this work, which gives the following equation (A1.5)

$$T = \frac{(\lambda - \lambda_1)(\lambda - \lambda_2)(\lambda - \lambda_3)}{(\lambda_0 - \lambda_1)(\lambda_0 - \lambda_2)(\lambda_0 - \lambda_3)}T_0 + \frac{(\lambda - \lambda_0)(\lambda - \lambda_2)(\lambda - \lambda_3)}{(\lambda_1 - \lambda_0)(\lambda_1 - \lambda_2)(\lambda_1 - \lambda_3)}T_1$$

$$+ \frac{(\lambda - \lambda_0)(\lambda - \lambda_1)(\lambda - \lambda_3)}{(\lambda_2 - \lambda_0)(\lambda_2 - \lambda_1)(\lambda_2 - \lambda_3)}T_2 + \frac{(\lambda - \lambda_0)(\lambda - \lambda_1)(\lambda - \lambda_2)}{(\lambda_3 - \lambda_0)(\lambda_3 - \lambda_1)(\lambda_3 - \lambda_2)}T_3$$

where T and λ are the transmission and wavelength respectively. Table 1A listed the T_{\max} and T_{\min} values obtained from the interpolation of the transmission spectrum displayed in Figure 1A. A typical tabulation used to calculate the refractive index is presented in Table 2A. Recall that the formulae employed are Equations 4.5 and 4.6

$$n = \left[N + (N^2 - S^2)^{\frac{1}{2}} \right]^{\frac{1}{2}} \quad (4.5)$$

$$N = 2S \left[\frac{T_M - T_m}{T_M T_m} \right] + \left[\frac{S^2 + 1}{2} \right] \quad (4.6)$$

In order to obtain the static refractive index n_0 , regression analysis is performed according to the the relation

$$n = \frac{a}{\lambda^2} + n_0 \quad (4.7)$$

The following result is obtained from data in Table 2A which gives n_0 value of 2.243.

Regression Output:	
Constant	2.243
Std Err of Y Est	0.002
R Squared	0.999
No. of Observations	113.000
Degrees of Freedom	111.000
X Coefficient(s)	82467.134
Std Err of Coef.	246.035

References

- [1] W.Cheney and D.Kincaid
Numerical Mathematics and Computing
Brooks/Cole Publishing Co.,California, 3rd., 1994, pg.134
- [2] M.K.Jain, S.R.K.Iyengar and R.K.Jain
Numerical Methods for Scientific and Engineering Computation
Wiley Eastern Ltd., New Delhi, 2nd ed., 1987, pg. 141-142

λ (nm)	Tmax	Tmin	λ (nm)	Tmax	Tmin	λ (nm)	Tmax	Tmin
500.000	0.907	0.845	688.530	0.965	0.898	926.813	0.973	0.907
502.781	0.910	0.847	695.735	0.965	0.898	930.609	0.974	0.907
505.563	0.912	0.849	702.940	0.966	0.899	934.406	0.974	0.907
508.344	0.914	0.851	710.145	0.966	0.899	938.203	0.974	0.907
511.125	0.916	0.853	717.350	0.967	0.900	942.000	0.974	0.907
513.906	0.918	0.854	724.555	0.967	0.900	949.531	0.974	0.907
516.688	0.919	0.856	731.760	0.967	0.901	957.063	0.974	0.907
519.469	0.921	0.858	738.965	0.968	0.901	964.594	0.974	0.908
522.250	0.923	0.859	746.170	0.968	0.901	972.125	0.974	0.908
525.031	0.925	0.861	753.375	0.968	0.901	979.656	0.974	0.908
527.813	0.926	0.862	760.580	0.969	0.902	987.188	0.974	0.908
530.594	0.928	0.864	768.122	0.969	0.902	994.719	0.974	0.908
533.375	0.930	0.865	775.664	0.969	0.902	1002.250	0.975	0.908
536.156	0.931	0.866	783.206	0.969	0.903	1009.781	0.975	0.908
538.938	0.932	0.868	790.748	0.970	0.903	1017.313	0.975	0.908
541.719	0.934	0.869	798.289	0.970	0.903	1024.844	0.975	0.909
544.500	0.935	0.870	805.831	0.970	0.903	1032.375	0.975	0.909
550.800	0.938	0.873	813.373	0.970	0.904	1039.906	0.975	0.909
557.100	0.941	0.875	820.915	0.971	0.904	1047.438	0.975	0.909
563.400	0.943	0.877	828.457	0.971	0.904	1054.969	0.976	0.909
569.700	0.945	0.879	835.999	0.971	0.904	1062.500	0.976	0.910
576.000	0.947	0.881	843.541	0.971	0.905	1064.844	0.976	0.910
582.300	0.949	0.883	851.083	0.971	0.905	1067.188	0.976	0.910
588.600	0.951	0.885	858.624	0.972	0.905	1069.531	0.976	0.910
594.900	0.952	0.886	866.166	0.972	0.905	1071.875	0.976	0.910
601.200	0.954	0.887	873.708	0.972	0.905	1074.219	0.976	0.910
607.500	0.955	0.888	881.250	0.972	0.906	1076.563	0.976	0.910
613.800	0.956	0.889	888.792	0.972	0.906	1078.906	0.977	0.910
620.100	0.957	0.890	896.334	0.972	0.906	1081.250	0.977	0.910
626.400	0.958	0.891	903.876	0.973	0.906	1083.594	0.977	0.910
632.700	0.958	0.892	911.418	0.973	0.906	1085.938	0.977	0.911
639.000	0.959	0.892	918.960	0.973	0.906	1088.281	0.977	0.911
645.300	0.960	0.893	926.502	0.973	0.906	1090.625	0.977	0.911
652.505	0.961	0.894	934.044	0.973	0.906	1092.969	0.977	0.911
659.710	0.962	0.895	941.586	0.973	0.906	1095.313	0.978	0.911
666.915	0.962	0.895	949.128	0.973	0.907	1097.656	0.978	0.911
674.120	0.963	0.896	956.670	0.973	0.907	1100.000	0.978	0.911
681.325	0.964	0.897	964.212	0.973	0.907			

Table 1A. Tmax and Tmin data generated from the Lagrange interpolation.

λ (nm)	Tmax	Tmin	$(1/\lambda)(1/\lambda)$	N	n
580.650	0.649	0.487	2.966E-06	3.272	2.486
584.519	0.672	0.499	2.927E-06	3.272	2.486
588.388	0.695	0.512	2.889E-06	3.270	2.485
592.256	0.715	0.524	2.851E-06	3.265	2.483
596.125	0.735	0.535	2.814E-06	3.259	2.480
599.994	0.754	0.545	2.778E-06	3.252	2.477
603.863	0.771	0.555	2.742E-06	3.244	2.474
607.731	0.788	0.564	2.708E-06	3.236	2.471
611.600	0.803	0.573	2.673E-06	3.228	2.467
615.469	0.818	0.581	2.640E-06	3.220	2.463
619.338	0.831	0.589	2.607E-06	3.211	2.460
623.206	0.844	0.596	2.575E-06	3.203	2.456
627.075	0.856	0.603	2.543E-06	3.196	2.453
630.944	0.866	0.609	2.512E-06	3.188	2.450
634.813	0.876	0.615	2.481E-06	3.181	2.447
638.681	0.885	0.620	2.451E-06	3.174	2.444
642.550	0.894	0.625	2.422E-06	3.167	2.441
646.575	0.902	0.629	2.392E-06	3.161	2.438
650.600	0.909	0.634	2.363E-06	3.154	2.435
654.625	0.915	0.637	2.334E-06	3.148	2.432
658.650	0.921	0.641	2.305E-06	3.143	2.430
662.675	0.926	0.644	2.277E-06	3.138	2.428
666.700	0.930	0.647	2.250E-06	3.133	2.425
670.725	0.934	0.649	2.223E-06	3.128	2.423
674.750	0.937	0.651	2.196E-06	3.123	2.421
678.775	0.940	0.653	2.170E-06	3.119	2.419
682.800	0.942	0.655	2.145E-06	3.115	2.418
686.825	0.944	0.656	2.120E-06	3.111	2.416
690.850	0.945	0.657	2.095E-06	3.108	2.414
694.875	0.946	0.658	2.071E-06	3.104	2.413
698.900	0.947	0.659	2.047E-06	3.101	2.411
702.925	0.947	0.660	2.024E-06	3.098	2.410
706.950	0.948	0.661	2.001E-06	3.094	2.408
713.253	0.950	0.662	1.966E-06	3.088	2.406
719.556	0.952	0.664	1.931E-06	3.082	2.403
725.859	0.955	0.666	1.898E-06	3.076	2.400
732.163	0.958	0.669	1.865E-06	3.070	2.398
738.466	0.960	0.671	1.834E-06	3.064	2.395
744.769	0.962	0.672	1.803E-06	3.058	2.392
751.072	0.964	0.674	1.773E-06	3.052	2.389
757.375	0.966	0.676	1.743E-06	3.046	2.387
763.678	0.967	0.678	1.715E-06	3.040	2.384
769.981	0.968	0.679	1.687E-06	3.035	2.382
776.284	0.969	0.680	1.659E-06	3.030	2.379
782.588	0.970	0.681	1.633E-06	3.025	2.377
788.891	0.971	0.682	1.607E-06	3.020	2.375
795.194	0.971	0.683	1.581E-06	3.015	2.373
801.497	0.972	0.684	1.557E-06	3.010	2.371
807.800	0.972	0.685	1.532E-06	3.006	2.369
812.151	0.973	0.686	1.516E-06	3.003	2.368
816.503	0.973	0.686	1.500E-06	3.001	2.366
820.854	0.974	0.687	1.484E-06	2.998	2.365
825.205	0.974	0.687	1.469E-06	2.996	2.364
829.556	0.974	0.688	1.453E-06	2.993	2.363
833.908	0.975	0.688	1.438E-06	2.991	2.362

Table 2A. Tabulation for the calculation of the refractive index.

Appendix 2. Error Analysis

Consider Z as a known function of several quantities A , B and C ,

$$Z = Z(A, B, C) \quad (\text{A2.1})$$

Let the standard error in variables A , B and C be ΔA , ΔB and ΔC respectively. Then the standard error in Z , ΔZ is given by [1]

$$(\Delta Z)^2 = (\Delta Z_A)^2 + (\Delta Z_B)^2 + (\Delta Z_C)^2 \quad (\text{A2.2})$$

where

$$\Delta Z_A = \left(\frac{\partial Z}{\partial A} \right) \Delta A ; \Delta Z_B = \left(\frac{\partial Z}{\partial B} \right) \Delta B ; \Delta Z_C = \left(\frac{\partial Z}{\partial C} \right) \Delta C \quad (\text{A2.3})$$

The standard errors of the quantities calculated in the present work shall be discussed precedingly. The details of the equations employed shall be referred to Chapter 4.

A2.1. Refractive index, n

The refractive index of the thin film was calculated using the following expressions

$$n = \left[N + (N^2 - s^2)^{\frac{1}{2}} \right]^{\frac{1}{2}} ; \quad N = 2s \left[\frac{T_M - T_m}{T_M T_m} \right] + \left[\frac{s^2 + 1}{2} \right] \quad (\text{A2.4})$$

Considering the refractive index of the substrate, s as a constant, the refractive index is a function of two variables

$$n = n(T_M, T_m) \quad (\text{A2.5})$$

Therefore the standard error in $n, \Delta n$ can be stated as

$$(\Delta n)^2 = (\Delta n_{T_M})^2 + (\Delta n_{T_m})^2 \quad (\text{A2.6})$$

where

$$\Delta n_{T_M} = \left(\frac{\partial n}{\partial T_M} \right) \Delta T_M \quad ; \quad \Delta n_{T_m} = \left(\frac{\partial n}{\partial T_m} \right) \Delta T_m \quad (\text{A2.7})$$

However the evaluation of the quantities $\left(\frac{\partial n}{\partial T_M} \right)$ and $\left(\frac{\partial n}{\partial T_m} \right)$ from Eq. A2.4 is quite laborious. Hence an alternative method which are less tedious and of equivalent accuracy, is utilized [1]. Consider the significance of Δn_{T_M} . It denotes the change in the value of n when T_M changes by an amount ΔT_M while T_m remaining constant, or may be written as

$$\Delta n_{T_M} = n(T_M + \Delta T_M, T_m) - n(T_M, T_m) \quad (\text{A2.8})$$

and similarly

$$\Delta n_{T_m} = n(T_M, T_m + \Delta T_m) - n(T_M, T_m) \quad (\text{A2.9})$$

Δn_{T_M} and Δn_{T_m} then combined as in equation A2.6 to evaluate the value of Δn . By taking $\Delta T_M = \Delta T_m = 0.5\%$, the standard error in the refractive index values obtained for all samples $\Delta n \leq 3\%$. Whereas the standard error in the static refractive

index n_0 was straightaway obtained from the least-squares fit to the Cauchy relation $n = \frac{a}{\lambda^2} + c$, hence $\Delta n_0 = \Delta c$ and $\Delta n_0 < 1\%$ for all samples.

A2.2 Film thickness, d

A graphical method was employed in determining the film thickness. From the relation

$$l/2 = 2d(n/\lambda) - m_1 \quad (\text{A2.10})$$

a least-squares method is performed on the plot $l/2$ vs. n/λ . Therefore the standard error in the film thickness, Δd is given by

$$\frac{\Delta d}{d} = \frac{\Delta m}{m} \quad (\text{A2.11})$$

where m and Δm are the gradient and standard error of the straight line respectively. Δd values for all samples are between 3% to 4%, except for samples R11 and R13 which register a slightly higher standard error of 10% and 6% respectively.

A2.3 Optical energy gap, E_g

The strong absorption region in an amorphous semiconductor can be expressed as

$$\alpha h\nu = A(h\nu - E_g)^2 \quad (\text{A2.12})$$

and hence the commonly used Tauc's plot of $(\alpha h\nu)^{1/2}$ vs. $h\nu$ was employed to deduce the E_g value.

Therefore E_g can be obtained as

$$E_g = \frac{c}{m} \quad (\text{A2.13})$$

where c is the intercept at the y-axis and m is the gradient of the slope. The standard error in E_g is hence given by

$$\left(\frac{\Delta E_g}{E_g}\right)^2 = \left(\frac{\Delta c}{c}\right)^2 + \left(\frac{\Delta m}{m}\right)^2 \quad (\text{A2.14})$$

It is found that the standard error in E_g as determined from the Tauc's plot, $\Delta E_g \leq 1\%$ for all samples.

A2.4 Film quantitative composition

The FTIR broad spectrum was reproduced by the superposition of Gaussian profiles

$$y = h \left\{ \exp\left[-\frac{4 \ln 2}{\omega^2} (p - x)^2\right] \right\} \quad (\text{A2.15})$$

and the area under a particular Gaussian profile S_{band} is given by

$$S_{band} = \int_{-\infty}^{+\infty} h \left\{ \exp[-A^2 (p - x)^2] \right\} dx = \frac{h \sqrt{\pi}}{A} \quad (\text{A2.16})$$

where $A = \frac{4 \ln 2}{\omega^2}$ and h are obtained from the least-squares fit of Eq. (A2.15).

Therefore

$$\left(\frac{\Delta S_{band}}{S_{band}}\right)^2 = \left(\frac{\Delta h}{h}\right)^2 + \left(\frac{\Delta A}{A}\right)^2 ; \quad \Delta A = \Delta m, \quad \Delta h = e^{\Delta c} \quad (\text{A2.17})$$

Here Δm and Δc are the standard error in the gradient of the y vs. $(p-x)^2$ graph and the standard error in the intercept at the y -axis of the graph respectively. Finally the integrated intensity of a particular bonding is estimated as

$$I_{bond(mode)} = \int_{\omega_0} \frac{\alpha(\omega)}{\omega_0} d\omega = \frac{2.303 S_{band}}{d\omega_0} \quad (\text{A2.18})$$

Hence

$$\left(\frac{\Delta I}{I}\right)^2 = \left(\frac{\Delta S_{band}}{S_{band}}\right)^2 + \left(\frac{\Delta d}{d}\right)^2 + \left(\frac{\Delta \omega_0}{\omega_0}\right)^2 \quad (\text{A2.19})$$

The standard errors in the integrated intensity of samples are all $\leq 17\%$.

References

[1] G.L.Squires

Practical Physics, McGraw-Hill Book Co., 2/e, 1976, pg. 36-37, 50-52