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# The optical constants determination of thin-films

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**Abstract.** A method for calculating the optical constants of weakly absorbing homogeneous thin films of refractive index, n lower than substrate index, s (s < n) and extinction coefficient, k from the spectral Transmission information alone with no prior knowledge of their characteristics was studied. Initially the procedure uses transmission turning point data to estimate the refractive index, n and extinction coefficient, k by an analytical approach. The calculations are done from the knowledge of transmission turning point data, which was obtained from Shimadzu UV3100 spectrophotometer. The data are then fitted to a high order polynomial function that undergoes an iterative refinement routine by means of a goal seek routine to determine with good accuracy the film parameters as a function of wavelength.

**Keywords:** optical constants, refractive index, transmission, thin films, turning point and weakly absorbing.

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## 1. INTRODUCTION

In today's technological world, thin films are becoming increasingly importance for fundamental studies in different fields of physics, electronics and other numerous practical applications. The huge progress in thin film physics has been widened to the largest degree by the development of suitable vacuum and non-vacuum technologies, which thin film can be deposited with ease by such technology. Many workers and researchers are interested in fundamental properties of solids in thin film form, since they are differ from BULK material. Examples of such research include studies of optical, electrical and magnetic investigations of structural order, phase transitions and of different surface reactions and surface phenomena. The results obtained by such studies are great interest to those concerned with the practical and commercial applications of thin films. Examples of such applications which are very important for the fields of optics and electronics are: transmission and reflection type interference filters with wide and narrow bandwidths highly reflected coatings, anti-reflection films, beam splitters, polarizer and thin film circuits etc. The determination of optical constants is a subject which received much attention in the past fifty years or so, and there are many papers have published and widely dispersed in many journals on this subject, consequently there are many methods exist for this type of analysis. Many of these methods impose rather heavy computation and are now assisted by the availability of powerful computers to enable thin film scientists to solve iteratively even the most complicated transmission and reflection equations which are essential for the determination of optical constants. As mentioned above in the past fifty years great progress has been made both in theoretical understanding of thin film and in the experimental demonstration of validity of many features of thin film which predicted by theory [1]. Therefore, many procedures were proposed in the past by other researchers, this types of procedures can be applied to non-absorbing or weakly absorbing, homogenous films deposited on transparent substrate and to calculate the refractive index *n*, extinction coefficient *k* and thickness *d*, at all turning points [2, 3, 4, 5 and 6]. The routine described in this report, use's the Swanepoel's analytical method to obtain an initial approximation of *n* and *d*. these values are inserted into the

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required transmission equations and an approximated *k* is isolated numerically. Then an iterative refinement routine by means of a goal seek function was performed on the *k* set of data that was used to extract more precise results.

## 2. THEORETICAL BACKGROUND

There are many models have been developed to treat different type of thin film materials but they are unique to the type of thin film that can be analyzed. By considering a plane-parallel plate of refractive index, *n* and extinction, *k* sandwiched between two mirrors with reflectivities of $R_1$ and $R_2$ see figure 1. The cavity is regarded as radially infinite and has a transverse thickness, t. when irradiated with plane wave illumination of wavelength, $\lambda$ whose coherence length is greater than the path length *nt*, i. e. thin film, interference will occur in the beams transmitted and reflected by etalon. The fraction of the input intensity, $I_0$ that is transmitted, can be calculated by the summation of the individual beam amplitudes.

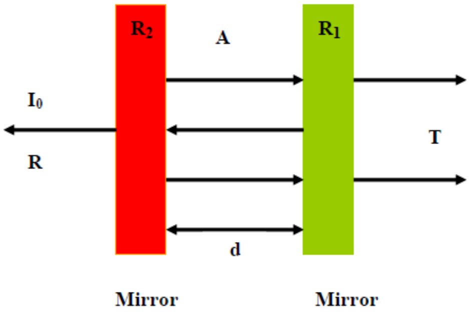


**Figure 1.** The representation of a Fabry-Perot cavity.

The method outlined in here is based upon the measurement of the transmission spectrum of thin film and substrate combination. When the turning point envelopes $T_{max}$ and $T_{min}$ are constructed, the wavelength position and transmission value of each peak and trough can be calculated by the following transmission equation:

$$T = \frac{(1-R_1)(1-R_2)\exp(-\alpha t)}{(1-R_\alpha)^2}\left(\frac{1}{1+F\sin^2\frac{\emptyset}{2}}\right) \tag{1}$$

If an infinite substrate approximation is used, the constants are given by:

$$\alpha = 4\pi\kappa/\lambda \tag{2}$$

$$R_\alpha = \sqrt{R_1R_2}\exp(-\alpha t) \tag{3}$$

$$F = \frac{4R_\alpha}{(1-R_\alpha)^2} \tag{4}$$

$$\emptyset = \left(\frac{2\pi}{\lambda}\right)\times Optical\ path\ difference = 4\pi nt/\lambda \tag{5}$$

And if the back substrate surface reflectivity is accounted for, then the constants are given by the following:

$$R = 1 - \frac{(1 - R_1)(1 - R_2)\exp(-2\alpha t)}{(1 - R_\alpha)^2}\left(\frac{1}{1 + Fsin^2\frac{\emptyset}{2}}\right) \tag{6}$$

$$A = 1 - R - T = 1 - \frac{(1 - R_1)(1 + R_2\exp{(-\alpha t)})(1 - \exp{(-\alpha t)})}{(1 - R_\alpha)^2}\left(\frac{1}{1 + Fsin^2\frac{\emptyset}{2}}\right) \tag{7}$$

$$f = \frac{\pi\sqrt{F}}{2} \tag{8}$$

The term $\frac{1}{1+\mathrm{Fsin}^2\frac{\emptyset}{2}}$ is known as the Airy function. The maxima and minima of the transmission and reflection equations correspond to the turning points of these functions. The reflectance transmittance vary periodically with wavelength due to the constructive and destructive interference of the waves reflected from front and rear number of half wavelengths, then destructive interference occurs, and a transmission minima results since $\sin^2\emptyset = 1$.

This can be written as: $nt = \frac{\mathrm{m}\lambda}{4}$. Where *m* is an even and odd integer for constructive and destructive interference respectively. The transmission of cavities with varying finesses corresponding to front and rear reflectivity of 0.5, 0.8 and 0.99 are shown in figure 2.

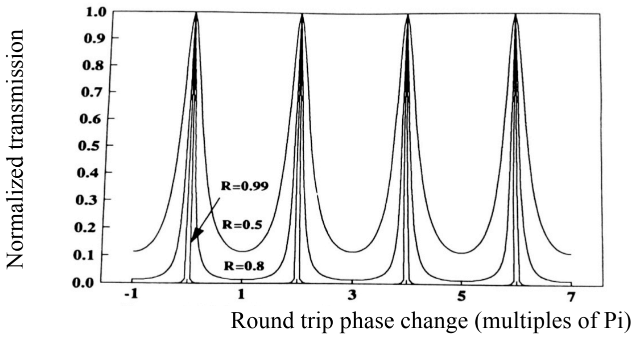


**Figure 2.** The Airy function of the normalized transmission of a Fabry-Perot etalon against the round trip phase change, $\emptyset$.

The transmission spectrum of a single layer thin film of refractive index *n*, extinction coefficient *k*, and thickness *d*, deposited on a non-absorbing substrate of refractive index, *s* can be characterized in terms of maxima and minima transmission values i.e. turning points. These turning points can be obtained when the optical thickness is equal to an even number of quarter wavelengths. Which correspond to maxima, where m is an even integer, these conditions yield the envelope functions which are assumed as:

$$T_{max} = \frac{16n_0s(n^2 + k^2)\alpha}{A + B\alpha^2 + 2C\alpha}) \tag{9}$$

$$T_{min} = \frac{16n_0s(n^2 + k^2)\alpha}{A + B\alpha^2 + 2C\alpha} \tag{10}$$

In the case of an optical thickness equal to an odd number of quarter wavelengths, which correspond to minima, in this case m is an odd integer; these conditions yield the envelope functions which are assumed as:

$$T_{max} = \frac{16n_0s(n^2+k^2)\alpha}{A+B\alpha^2-2C\alpha}) \tag{11}$$

$$T_{min} = \frac{16n_0s(n^2+k^2)\alpha}{A+B\alpha^2-2C\alpha} \tag{12}$$

In the case of weakly absorption, the constants A, B and C in the equations 9, 10, 11 and 12 are given by:

$$A = (n+n_0)^2(n+s)^2 \tag{13}$$

$$B = (n-n_0)^2(n-s)^2 \tag{14}$$

$$C = -(n^2-n_0)^2(n^2-s)^2 + 4n_0s \tag{15}$$

$$\alpha = \exp\left(-\frac{4\pi k t}{\lambda}\right) \tag{16}$$

From equations 9 to 12 an explicit expression for n as a function of $n_0$, s, Tmax and Tmin can be obtained by subtracting the reciprocals of Tmax and Tmin of equations 9, 12 or 10, 11 which given by:

$$n = [N \pm (N^2 - n_0^2s^2)^{\frac{1}{2}}]^{\frac{1}{2}} \tag{17}$$

Where

$$N = \frac{n_0^2+s^2}{2} + 2n_0s\frac{T_{max}-T_{min}}{T_{max}T_{min}} \qquad For\ n > s \tag{18}$$

and

$$N = \frac{n_0^2+s^2}{2} + 2n_0s\frac{T_{min}-T_{max}}{T_{max}T_{min}} \qquad For\ n < s \tag{19}$$

Similarly by taking the ratio of $T_{max}$ and $T_{min}$ the extinction coefficient, *k* can be derived.

$$n(\lambda), k(\lambda) = a + \sum_{i=1}^{m}\left(\frac{b_i}{\lambda^i}\right) \tag{20}$$

$$n^2(\lambda) - 1, k^2(\lambda) - 1 = a + \sum_{i=1}^{m}\left[\frac{b_i}{\lambda^i - c_i}\right] \tag{21}$$

In the two adjacent maxima and minima are selected of the order *m* and *m+1*, then the interference condition for even and odd can be written as:

$$n_1t = \frac{m\lambda_1}{4} \tag{22}$$

and

$$n_2t = \frac{(m+1)\lambda_2}{4} \tag{23}$$

Where $n_1$ and $n_2$ are the refractive indices at the turning points $\lambda_1$ and $\lambda_2$. Manipulation of equations 22 and 23 gives the following expression for the thickness, t of the cavity.

$$t = \frac{\lambda_1 \lambda_2}{2(\lambda_2 n_1 - \lambda_1 n_2)} \tag{24}$$

Where $\lambda_1$ and $\lambda_2$ are the wavelengths of adjacent maxima and minima at which the refractive indices have the values $n_1$ and $n_2$ respectively [7].

## 3. METHODS

The method for calculating the optical constants at first, required us to make wavelength scans of transmission. Once the transmission envelopes for maxima and minima at all tuning points were obtained from the spectrophotometer, the best maxima and minima values were selected and then inserted into a mathematical package call maple. Finally, three programs within the Excel's environment were used to complete the aim of the project. For further details see the following steps:

- Using the Shimadzu UV3100 spectrophotometer

A transmission spectrum of a low index film ($MgF_2$) on high substrate ($SF_6$) is taken by using the Shimadzu 3100 spectrophotometer. The wavelengths and transmission values i.e. $T_{max}$ and $T_{min}$ corresponding to all turning points are determined.

- Using the maple for the polynomial fitting

Polynomial have long been the functions of desires and most widely used to approximate other functions, mainly because they have the simplest mathematical properties and also because they furnish the best approximation of a function like $n(\lambda)$ and $k(\lambda)$. Therefore, to do the polynomial fitting for the completion, the spline function was used within the maple environment. The spline functions are fit polynomials between each data point, preserving continuity between neighboring polynomials. They also have very desirable characteristics as approximating and curve fitting functions. The spline function is defined by the following commands in the maple package.

```
>readlib(spline):
>spline([λ1 max/min , λ2 max/min ,.... λn max/min ],[ T1 max/min , T2 max/min ,... Tn max/min ],x);
```

This function gives as equation for the curve between each adjacent pair of points. In here also care must be taken, because maple for *n* number of wavelengths with corresponding transmission gives *n-1* points, each of these points must be entered into the spreadsheet plus the substrate values [7].

A method presented, for determining the optical constants of thin films and its application to molecular beam deposited polycrystalline layers [8]. The method calculates the optical constants of weakly absorbing, homogeneous layers from spectral transmission information alone, with no prior knowledge of their characteristics. The turning point envelopes $\boldsymbol{T_{max}}$ and $\boldsymbol{T_{min}}$ are constructed see figure 3.

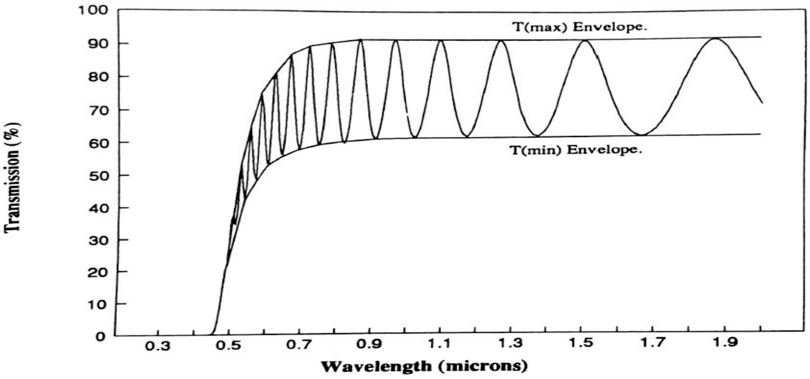


**Figure 3.** Construction of the transmission envelope functions for ZnSe grown at 0.5um/hr in room temperature.

## 4. DISCUSSION AND CONCLUSION

It can be emphasized that the thin films from the basis for many established and developing technologies. In the simplest case metal layers have always been important for optical and protective coatings for various materials. Furthermore, it is fair to say that besides being a field of great interest in modern physics, the study of thin films also has contributed vital elements to the most sophisticated commercial technologies. Therefore, the determination of the optical constants of thin films is a topic of fundamental and technological importance.

This report has examined the various published literatures in the field of thin film, with a view to a comparison of the techniques for calculating optical constants. The methods developed by other researchers were examined in great details [4, 5 and 6]. The latest method was found to be superior to the methods introduced by the previous two, due to having reduced errors in refractive index, *n* and extinction coefficient, *k* (see Table 1 & Figure 4). The results in table1 confirm that the new improved technique by Bennett et al. can provide higher accuracy in the calculation of the optical constants [6]. However, there is an experimental limitation to this technique but this is due to the instrumental accuracy.

To calculate the optical constants of a weakly absorbing homogenous thin-film ($MgF_2$) deposited on a transparent substrate ($SF_6$). The approach was based upon the transmission turning point data only and use's the equation developed by Manifacier et al. and an initial estimation of *n* and *t* were obtained from the method detailed by Swanepoel, then as iterative adjustment routines by means of a goal seek routine extract the calculated values of *n*, *k* and *t* to obtain a close match to the experimental data [4 and 5]. Fair results were obtained for the medium absorption region where the error on transmission was less than 1% see figure 3. But it breaks down in the low and high absorption regions. This is due to number of reasons, the calculated optical constants during the refinement process, which dependent on the of iterations performed and the weighted error function and also the results for the case of low index with high substrate will be more sensitive to errors in the transmission and in the substrate which can be neglected when the case is reversed. Finally, an extensive error analysis has been done, which confirms that the modified turning point technique can provide higher accuracy in the calculation of the optical constants.

**Table 1.** Shows the fractional errors obtained by the two different methods and the errors found in this report.

| Fractional error in % | Δt/t | Δn/n | Δk/k |
|---|---|---|---|
| Swanepoel's method | ±0.2 | ±1.5 | ±125 |
| Modified method | ±0.2 | ±0.4 | ±3.5 |
| Founded errors | ±0.1 | ±0.5 | ±1.6 |

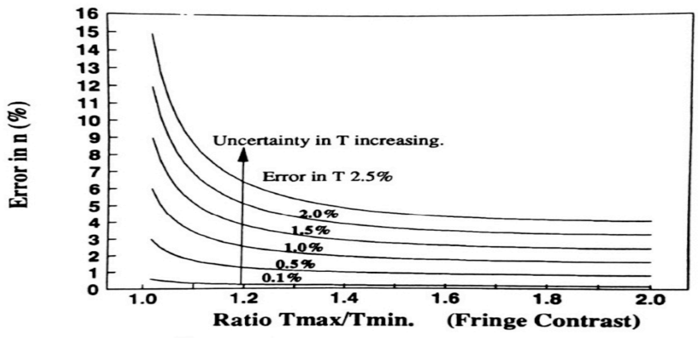
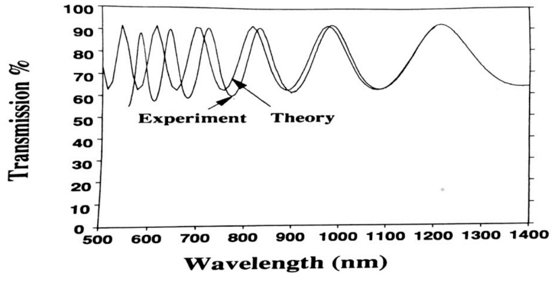


**Figure 4.** Calculated fractional error in Δn/n against fringe contrast for various Δt values, which shows a plot of fractional error versus the fringe contrast for various values of Δt.

It can be seen that the larger the fringe contrast the more precise the calculated value of $n$. And a matrix approach used to generate a theoretical spectrum from the calculated constants which is shown in figure 5. When compared to the original experimental transmission. A disagreement can be seen clearly from this graph even in the edge of weak region of the absorption. But when using the full modified turning point routine see figure 5 which can be seen that there is slight disagreement in the region of strong absorption wavelengths. For the above comparison they used a weighted error function below.

$$\omega = \sum_{i=1}^{p} \omega_i \left[T_{meas}(\lambda_{meas})_i - T_{calc}(\lambda_{calc})_i\right] \tag{25}$$

Where $\omega_i$ is the weighting factor for the *i*th turning point which occurs at a measured wavelength position $\lambda_{calc}$ and calculated position $\lambda_{calc}$ . Note must be taken that this comparison is best for odd integer quarter wavelength positions (for *n* > *s*).



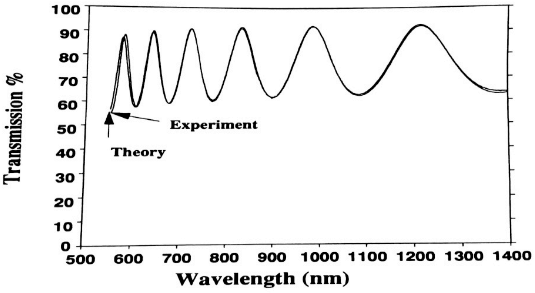


**Figure 5.** Comparison of experimental and theoretical spectra of a ZnSe layer deposited by Molecular Deposited Beam on a glass (BK7) substrate for R. Swanepeol data (up) and for the modified turning point method data (down).

The spectrum obtained from the turning method shows a much better agreement with the experimental values than that obtained from using R. Swanepeol method which breaks down considerably in the region of medium absorption. This result confirms that the new improved technique by Bennett et al. can provide higher accuracy in the calculation of the optical constants [6]. However, there is an experimental limitation to this technique but this is due to the limit of the instrumental accuracy.

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