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1983 J. Phys. E: Sci. Instrum. 16 1214

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Determination of the thickness and optical constants of amorphous silicon

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Received 27 May 1983

Abstract. The rigorous expression for the transmission of a thin absorbing film on a transparent substrate is manipulated to yield formulae in closed form for the refractive index and absorption coefficient. A procedure is presented to calculate the thickness to an accuracy of better than 1% with similar accuracies in the values of n . A method to correct for errors due to slit width is also given. Various formulae to calculate the absorption coefficient accurately over almost three orders of magnitude are discussed. Only data from the transmission spectrum are used and the procedure is simple, fast and very accurate. All formulae are in closed form and can be used on a programmable pocket calculator.

1. Introduction

Amorphous silicon or hydrogenated α -Si:H is an important material for photovoltaic devices. These devices consist of films with thicknesses of about $1\ \mu\text{m}$ and it is important to know the refractive index and absorption coefficient as function of wavelength to predict the photoelectric behaviour of a device. Knowledge of these optical constants is also necessary to determine the optical gap or to verify theoretical models of α -Si:H (Clark 1980).

The thickness of films can be determined using a surface-profiling stylus or by various interferometric methods (Bennet and Bennet 1967). A method is proposed in this paper to determine the thickness from the interference fringes of the transmission spectrum to an accuracy of better than 1%, provided the films are of good quality.

The refractive index and absorption coefficient are usually determined by elaborate computer iteration procedures (Lyashenko *et al* 1964, Wales *et al* 1967, Szczyrkowski *et al* 1977) using both the transmission and reflection spectra. A simple straightforward process has also been devised (Manifacier *et al* 1976) for calculating n and α but it will be pointed out in this paper that this process contains some mistakes. Methods are proposed in this paper to determine $n(\lambda)$ and $\alpha(\lambda)$ by simple straightforward calculations using the transmission spectrum alone. The accuracy is also of the order of 1% which is even better than the accuracy of the elaborate iteration methods.

In the discussion only the spectrum in the optical region is considered. All formulae are, of course, also valid in the near-infrared region and for films with small optical gaps it may be essential to do measurements in this region.

2. Theory

The practical situation for a thin film on a transparent substrate is shown in figure 1. The film has thickness d and complex refractive index $\mathbf{n} = n - ik$, where n is the refractive index and k the extinction coefficient which can be expressed in terms of the absorption coefficient α using equation (27). The transparent

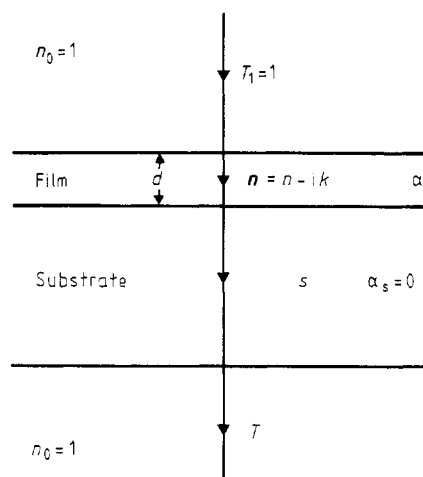


Figure 1. System of an absorbing thin film on a thick finite transparent substrate.

substrate has a thickness several orders of magnitude larger than d and has index of refraction s and absorption coefficient $\alpha_s = 0$. The index of the surrounding air is $n_0 = 1$. Rigorous analysis has to take into account all the multiple reflections at the three interfaces when calculating T .

If the thickness d is not uniform or is slightly tapered, all interference effects are destroyed and the transmission is a smooth curve as shown by the dotted curve T_s in figure 2. The spectrum can roughly be divided into four regions. In the transparent region $\alpha = 0$ and the transmission is determined by n and s through multiple reflections. In the region of weak absorption α is small but starts to reduce the transmission. In the region of medium absorption α is large and the transmission decreases mainly due to the effect of α . In the region of strong absorption the transmission decreases drastically due almost exclusively to the influence of α . The smooth transmission curve T_s is often used (Freeman and Paul 1979) to determine $\alpha(\lambda)$ in the optical and infrared region using a formula given in the appendix (A3).

If the thickness d is uniform, interference effects give rise to a spectrum shown by the full curve in figure 2. Far from being a nuisance, these fringes can be used to calculate the optical constants of the film as will be shown in this paper.

Considering the thick substrate alone in the absence of a film, the interference-free transmission is given by the well known expression

$$T_s = \frac{(1-R)^2}{1-R^2}$$

where

$$R = [(s-1)/(s+1)]^2$$

or

$$T_s = \frac{2s}{s^2 + 1} \quad (1)$$

and

$$s = \frac{1}{T_s} + \left(\frac{1}{T_s^2} - 1 \right)^{1/2} \quad (2)$$

The basic equation for interference fringes is

$$2nd = m\lambda \quad (3)$$

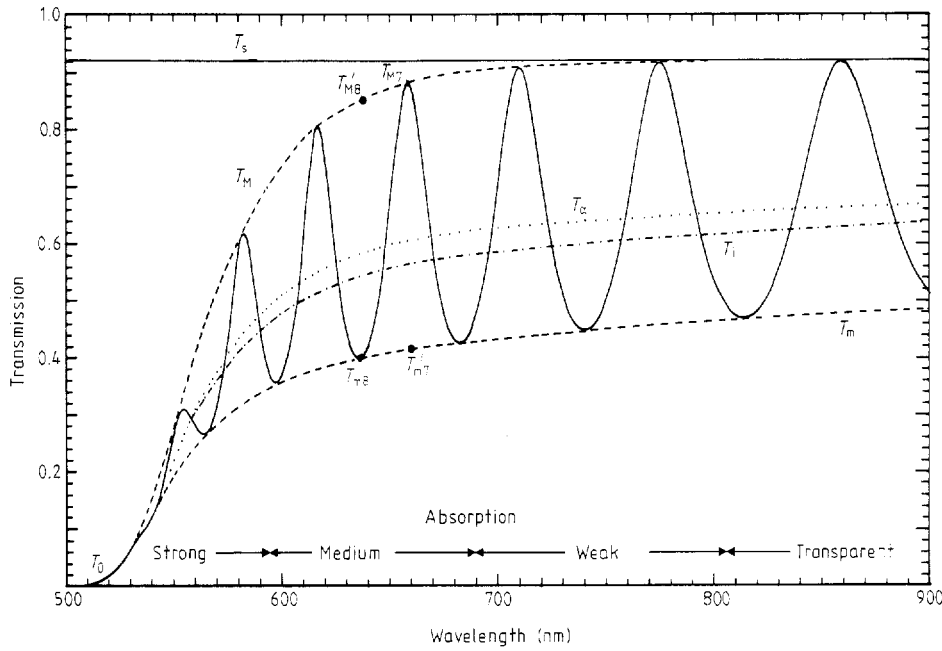


Figure 2. Simulated transmission spectrum (full curve) for a 1 μm film of α -Si:H on a finite glass substrate with transmission T_s . Curves T_M , T_α , T_i and T_m according to the text.

where m is an integer for maxima and half integer for minima. Equation (3) contains information on the product of n and d and there is no way of obtaining information on either n or d separately using this equation only.

The transmission T for the case of figure 2 is a complex function (Kerdec 1973, Mini 1982) and is given in the appendix (A1)

$$T = T(\lambda, s, n, d, \alpha).$$

If s is known it is convenient to write the above equation in terms of $n(\lambda)$ and the absorbance $x(\lambda)$, where x is defined in equation (5 f)

$$T = T(n, x).$$

The expression (A1) becomes much simpler if we put $k=0$, an approximation that is indeed valid over most of the region of the spectrum in figure 2. (A1) then becomes

$$T = \frac{Ax}{B - Cx \cos \varphi + Dx^2} \quad (4)$$

where

$$A = 16n^2s \quad (5a)$$

$$B = (n+1)^3(n+s^2) \quad (5b)$$

$$C = 2(n^2 - 1)(n^2 - s^2) \quad (5c)$$

$$D = (n-1)^3(n-s^2) \quad (5d)$$

$$\varphi = 4\pi nd/\lambda \quad (5e)$$

$$x = \exp(-\alpha d). \quad (5f)$$

The extremes of the interference fringes can be written as

$$T_M = \frac{Ax}{B - Cx + Dx^2} \quad (6)$$

$$T_m = \frac{Ax}{B + Cx + Dx^2} \quad (7)$$

For further analyses T_M and T_m are now considered to be continuous functions of λ and thus of $n(\lambda)$ and $x(\lambda)$ (Manifacier *et al* 1976), as is shown by the envelopes in figure 2. For any λ , T_M has a corresponding value T_m . In figure 2 for example T_{M7} has the corresponding value T_{m7} and T_{M8} has the corresponding value T_{m8} .

2.1. The transparent region

In the transparent region $\alpha=0$ or $x=1$ in equations (6) and (7). Substituting equations (5) into (6) yields

$$T_M = \frac{2s}{s^2 + 1} \quad (8)$$

Equation (8) is identical to equation (1) and the maxima of the interference fringes are a function of s only and coincide with T_s . When the maxima depart from T_s it denotes the onset of absorption. Equation (8) can be used to calculate s in the transparent region using the form of equation (2).

Substituting equation (5) in equation (7) for $x=1$ yields

$$T_m = \frac{4n^2s}{n^4 + n^2(s^2 + 1) + s^2}$$

or

$$n = [M + (M^2 - s^2)^{1/2}]^{1/2} \quad (9)$$

where

$$M = \frac{2s}{T_m} - \frac{s^2 + 1}{2}.$$

T_m is thus a function of both n and s , and n can be calculated from T_m using equation (9).

2.2. The region of weak and medium absorption

In this region $\alpha \neq 0$ and $x < 1$. Subtracting the reciprocal of equation (6) from the reciprocal of equation (7) yields an

expression that is independent of x

$$\frac{1}{T_m} - \frac{1}{T_M} = \frac{2C}{A}. \quad (10)$$

Substituting equation (5) into (10) and solving for n yields

$$n = [N + (N^2 - s^2)^{1/2}]^{1/2} \quad (11)$$

where

$$N = 2s \frac{T_M - T_m}{T_M T_m} + \frac{s^2 + 1}{2}.$$

Equation (11) can be used to calculate $n(\lambda)$ from T_M and T_m . It is identical to the formula derived by Manifacier *et al* (1976) using the theory for an infinite substrate.

Once $n(\lambda)$ is known, all the constants in equation (5) are known and x can be calculated in various ways. Both (6) and (7) are quadratic equations in x that can be solved for x and the results simplified using equation (5). Solving equation (6) gives

$$x = \frac{E_M - [E_M^2 - (n^2 - 1)^3(n^2 - s^4)]^{1/2}}{(n - 1)^3(n - s^2)} \quad (12)$$

where

$$E_M = \frac{8n^2s}{T_M} + (n^2 - 1)(n^2 - s^2).$$

Solving equation (7) gives

$$x = \frac{E_m - [E_m^2 - (n^2 - 1)^3(n^2 - s^4)]^{1/2}}{(n - 1)^3(n - s^2)} \quad (13)$$

where

$$E_m = \frac{8n^2s}{T_m} - (n^2 - 1)(n^2 - s^2).$$

Adding the reciprocals of equations (6) and (7) yields

$$\frac{2 T_M T_m}{T_M + T_m} = \frac{Ax}{B + Dx^2}. \quad (14)$$

Solving for x this gives

$$x = \frac{F - [F^2 - (n^2 - 1)^3(n^2 - s^4)]^{1/2}}{(n - 1)^3(n - s^2)} \quad (15)$$

where

$$F = \frac{8n^2s}{T_i}$$

and

$$T_i = \frac{2 T_M T_m}{T_M + T_m}. \quad (16)$$

From equation (14) and (4) it can be seen that T_i represents a curve passing through the inflection points of the fringes as shown in figure 2.

The interference-free transmission T_α can be calculated from the interference fringes by integrating equation (4) between a maximum and an adjacent minimum

$$T_\alpha = \frac{1}{\pi} \int_0^\pi \frac{Ax}{B - Cx \cos \varphi + Dx^2} d\varphi.$$

Assuming a narrow integration region where all parameters are constant, the integral yields

$$T_\alpha = \frac{Ax}{[(B - Cx + Dx^2)(B + Cx + Dx^2)]^{1/2}} \quad (17)$$

Substitution of equations (6) and (7) into (17) yields

$$T_\alpha = \sqrt{T_M T_m}. \quad (18)$$

T_α is thus just the geometric mean of T_M and T_m and equation (18) is a very useful relation. Solving equation (17) for x gives

$$x = \frac{\{G - [G^2 - (n^2 - 1)^6(n^2 - s^4)^2]^{1/2}\}^{1/2}}{(n - 1)^3(n - s^2)} \quad (19)$$

where

$$G = \frac{128 n^4 s^2}{T_\alpha^2} + n^2(n^2 - 1)^2(s^2 - 1)^2 + (n^2 - 1)^2(n^2 - s^2)^2.$$

Equation (19) is equivalent to a well known equation often used in optical and infrared studies, (A3). It can also be used to determine n from T_α in the transparent region where $\alpha = 0$. Putting $x = 1$ in equation (19) and solving for n gives

$$n = [H + (H^2 - s^2)^{1/2}]^{1/2} \quad (20)$$

where

$$H = \frac{4s^2}{(s^2 + 1) T_\alpha^2} - \frac{s^2 + 1}{2}.$$

Manifacier *et al* (1976) also derived an equation for x using the theory for an infinite substrate. Their formula is

$$x = \frac{(n + 1)(s + n)[1 - (T_M/T_m)^{1/2}]}{(n - 1)(s - n)[1 + (T_M/T_m)^{1/2}]} \quad (21)$$

Unlike the case with the refractive index, equation (21) is *not* equivalent to equations (12), (13), (15) and (19).

2.3. The region of strong absorption

In the region of strong absorption the interference fringes disappear. There is no way to calculate n and x independently in this region from the transmission spectrum alone. Values of n can be estimated by extrapolating the values calculated in the other parts of the spectrum. The values of x can then be calculated using any of the four formulae presented in the previous section with their appropriate curves. For very large α the four curves T_M , T_α , T_i and T_m converge to a single curve T_0 . If interference effects are ignored, equation (4) can be written for $x \ll 1$ as

$$T_0 \simeq Ax/B$$

or

$$x \simeq \frac{(n - 1)^3(n + s^2)}{16 n^2 s} T_0. \quad (22)$$

2.4. Numerical simulation

To test the accuracy of the theory presented here, a film with the following properties is postulated.

Substrate refractive index

$$s = 1.51 \quad (\text{constant})$$

Film thickness

$$d = 1000 \text{ nm}$$

Film refractive index

$$n = \frac{3 \times 10^5}{\lambda^2} + 2.6$$

Film absorption coefficient

$$\lg \alpha = \frac{1.5 \times 10^6}{\lambda^2} - 8 \quad (\alpha \text{ in nm}^{-1}).$$

The above values of $n(\lambda)$ and $\alpha(\lambda)$ represent typical values for α -Si:H (Freeman and Paul 1979). The spectrum in figure 2 is a plot of $T(\lambda)$ as calculated by (A1) using the above-postulated properties of the film. The true values of $n(\lambda)$, $\alpha(\lambda)$ and d can thus be used to determine the accuracy of calculated values. The smooth envelopes T_M and T_m are constructed on this simulated spectrum and the values from these 'experimental' envelopes are used in the calculation in the following sections. The width of the interference pattern ($T_M - T_m$) increases with increase in $(n-s)$ and statements about accuracy in the following sections refer to a typical spectrum of α -Si:H as in figure 2.

2.5. Infinite substrate approximation

Another expression for T , assuming an infinite substrate and thus ignoring the contribution of multiple reflections from the back of the substrate, has been used by many workers (Manifacier *et al* 1976, Lyashenko 1977, Hadley 1947). One equivalent form of this expression is given in the appendix (A2). A plot of T calculated from equation (A2) using the film properties given in the previous section is shown by the full curve in figure 3. The broken curve shows again the values of T calculated by equation (A1).

It can be seen that equation (A2) yields higher values for both T_M and T_m than equation (A1). A disturbing aspect is that equation (A2) predicts a transmission in the transparent region that is about 4% larger than the transmission of the substrate alone. This is impossible as can be verified experimentally. It is the author's opinion that calculated transmission curves using equation (A2) or equivalent forms should be regarded with suspicion; the equation does not represent the experimental values of T for real films on transparent substrates.

Equation (A2) can also be written in the form of equations (4) and (5) for the case of $k=0$. The only difference is in the expressions for B and D in (5b) and (5d), i.e. $B \equiv (n+1)^2(n+s)^2$ and $D \equiv (n-1)^2(n-s)^2$. Since the expression for n , equation (11), is independent of B and D it is valid for both (A1) and

(A2). The expressions for x do contain B and D and will thus be different for the two cases.

3. Determination of the refractive index

The refractive index of the substrate can be determined by measuring the transmission spectrum of the clean substrate alone and using equation (2) to calculate s . If significant dispersion is present the data can be fitted to a simple linear function to give $s(\lambda)$. In this work s is assumed to be constant at a value $s = 1.51$, yielding a transmission of 0.921, as shown by T_s in figure 2.

For the calculation of n in the region of weak and medium absorption the values of T_M and T_m at different λ must be obtained. The accuracy to which λ can be measured depends on the scale used and for the case of figure 2 the maximum accuracy is about ± 1 nm or about 0.1%. The maximum absolute accuracy of T_M and T_m is also about 0.001 or 0.1%. These two values set the limits for the accuracy of the calculated values of n and α .

Table 1 shows the values at the extremes of the spectrum of λ , T_M and T_m obtained from figure 2. The transmission values should be read on the curves of T_M and T_m at each wavelength and not on the actual spectrum. This procedure partly compensates for the approximations made in deriving equation (4) from equation (A1). If the intermediate values are to be calculated by computer, a parabolic interpolation between three nearest points should be done, since linear interpolation is not accurate enough. Attempts should not be made to fit T_M or T_m to some mathematical function since this leads to unacceptable errors and relevant physical information may be lost.

The values of refractive index n_1 as calculated from equation (11) is shown in table 1. There is a fair agreement with the true values n_{tr} . The accuracy can be improved after calculating d , as will be described in the next section.

A relative error in s of 1% leads to a relative error of about 0.5% in n over the whole spectrum. An absolute error of 1% in

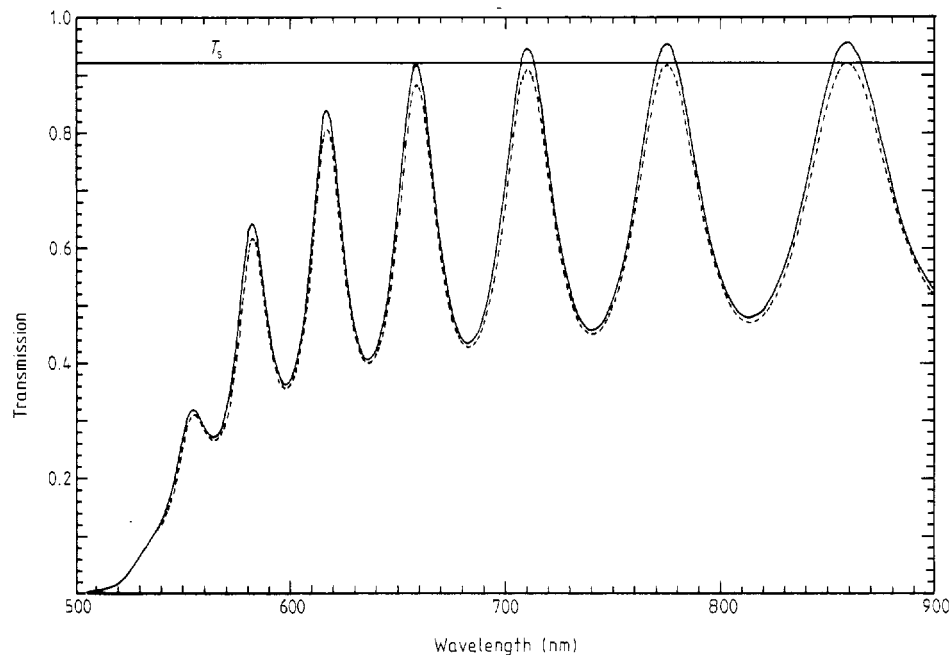


Figure 3. Simulated transmission according to the theory for an infinite substrate (full curve) in comparison with that of a finite substrate (broken curve).

Table 1. Values of λ , T_M and T_m for the spectrum of figure 2. Calculation of n and d .

| λ | T_M | T_m | n_1 | d_1 | m | d_2 | n_2 | n_{tr} |
|-----------|-------|-------|-------|----------------|------|-------|-------|----------|
| 859 | 0.919 | 0.478 | 3.015 | | 7 | 997 | 3.007 | 3.006 |
| 814 | 0.919 | 0.470 | 3.052 | | 7.5 | 1000 | 3.053 | 3.053 |
| 775 | 0.916 | 0.460 | 3.095 | 1035 | 8 | 1002 | 3.100 | 3.099 |
| 740 | 0.913 | 0.448 | 3.149 | 988 | 8.5 | 999 | 3.145 | 3.147 |
| 710 | 0.908 | 0.437 | 3.198 | 979 | 9 | 999 | 3.195 | 3.195 |
| 683 | 0.896 | 0.426 | 3.240 | 1023 | 9.5 | 1001 | 3.244 | 3.243 |
| 659 | 0.882 | 0.413 | 3.293 | 1013 | 10 | 1000 | 3.295 | 3.291 |
| 636 | 0.847 | 0.398 | 3.335 | 1002 | 10.5 | 1001 | 3.339 | 3.341 |
| 617 | 0.805 | 0.378 | 3.400 | 975 | 11 | 998 | 3.394 | 3.389 |
| 598 | 0.715 | 0.354 | 3.420 | 1049 | 11.5 | 1005 | 3.439 | 3.439 |
| 582 | 0.616 | 0.319 | 3.496 | 1006 | 12 | 999 | 3.492 | 3.484 |
| 564 | 0.433 | 0.256 | 3.570 | 819 | 12.5 | | | 3.542 |
| 555 | 0.328 | 0.210 | 3.668 | 830 | 13 | | | 3.573 |

$\bar{d}_1 = 1008; \sigma_1 = 25; \bar{d}_2 = 1000; \sigma_2 = 2$

T_M leads to a relative of about 0.5% in n in the region of weak absorption but increases to about 1% in the region of medium absorption. An absolute error of 1% in T_m yields a relative error of about 1.5% in n in the region of weak absorption and this increases to about 3% in the region of medium absorption. Equation (11) is thus more sensitive to errors in T_m than in T_M . To obtain 1% accuracy in n , T_M and T_m should be measured to about 0.2% absolute accuracy.

The values of n_1 in table 1 are calculated at the extremes of the spectrum only for illustrative purposes. It can of course be calculated at any value of λ using the smooth envelopes T_M and T_m .

4. Determination of the thickness d

If n_1 and n_2 are the refractive indices at two adjacent maxima (or minima) at λ_1 and λ_2 , it follows from equation (3) that the thickness is given by

$$d = \frac{\lambda_1 \lambda_2}{2(\lambda_1 n_2 - \lambda_2 n_1)}. \quad (23)$$

Equation (23) is very sensitive to errors in n and is not very accurate. The values of d calculated from equation (23) are shown as d_1 in table 1. There is some dispersion in the values of d_1 but the last two values deviate considerably from the other values. This deviation is an indication that n_1 as calculated from equation (11) and λ is not accurate enough and these values must be rejected. As a general rule the last two extremes of the spectrum should not be used in equation (11).

The average value of d_1 , ignoring the last two values, is $\bar{d}_1 = 1008 \pm 25$ nm. This value of \bar{d}_1 can now be used with n_1 to determine the order numbers for the extremes from equation (3). A big increase in accuracy now results in taking the exact integer or half-integer values of m for each λ and calculating the thickness d_2 from equation (3) using the values of n_1 again. If the values of m cannot be determined with certainty by inspection using equation (3), a few sets of values should be tried and d_2 calculated. The set of values of m that gives the smallest dispersion in \bar{d}_2 should be taken. The average value of d_2 in table 1 is $\bar{d}_2 = 1000 \pm 2$ nm. This is an accuracy better than 1%. Even if the values of λ are rounded off to even values and the values of T_M and T_m rounded off to 1% precision, the procedure still yields an answer of $\bar{d}_2 = 1000 \pm 3$ nm, illustrating the accuracy of the procedure to determine d .

Using the accurate values of m and \bar{d}_2 , n can again be calculated for each λ using equation (3). These values are shown as n_2 in table 1 and there is an excellent agreement with the true values n_{tr} . Now n_2 can be fitted to a function for extrapolation to shorter wavelengths. Using a function of the form $n = a/\lambda^2 + c$, a least-squares fit of the values n_2 in table 1 yields

$$n = 3.028 \times 10^5 / \lambda^2 + 2.595. \quad (24)$$

This is almost exactly the theoretical function used to generate the spectrum. Its form is a safe function to use for extrapolation, but a better fit to experimental values may be obtained by also including a term b/λ in equation (24).

The values of m and d can also be determined by a simple graphical method. Suppose the order number (integer or half integer) of the first extreme is m_1 . Equation (3) can now be

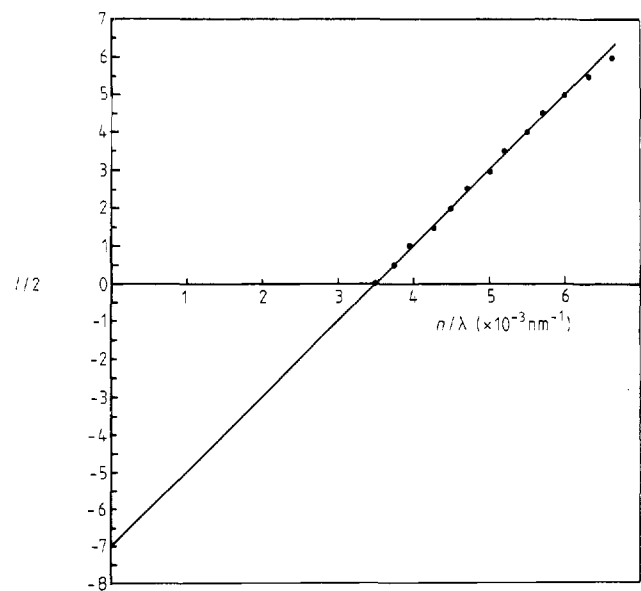


Figure 4. Plot of $l/2$ versus n/λ to determine the order number and thickness.

written for the extremes of the spectrum as

$$2nd = (m_1 + l/2)\lambda, \quad l = 0, 1, 2, 3 \dots$$

or

$$l/2 = 2d(n/\lambda) - m_1 \quad (25)$$

This is in the form of a straight line. If $l/2$ is plotted versus n/λ , a straight line will be obtained with slope $2d$ and cut-off on the y axis of $-m_1$. Figure 4 shows a graph of equation (25) for the values of λ and n_1 of table 1.

The straight line is now drawn such that the line through the points passes *exactly* through the nearest integer (or half integer) if the first extreme is a minimum) on the y axis. From figure 4 it follows that $m_1 = 7$. The slope of the line is exactly 2000, yielding a value for d of 1000 nm.

The graphical method has an appealing simplicity. In principle only the values of λ and n of two extremes are necessary to determine the order number m and the thickness d .

5. Corrections for slit width

In practice a spectrophotometer always has a finite spectral

width or slit width S and a band in the range $\lambda \pm S/2$ is incident on the film. The effect of this finite bandwidth on the transmission spectrum is to shrink the interference fringes: T_M becomes smaller and T_m larger. The effect can be minimised by experimentally reducing the slit S , but noise problems reduce the accuracy of T for small values of S . The effect of S becomes important when the width of the fringes is of the order of magnitude of S , as is the case for thicker samples, as is shown in figure 5.

Figure 5 shows a part of the spectrum on an expanded scale for a film with the same properties as that of figure 2, but with a thickness of $4 \mu\text{m}$. The full curve is the transmission simulated for a slit of $S = 4 \text{ nm}$ while the broken curve represents the spectrum that would have been obtained with essentially zero S . For these narrow fringes the change in T_M , ΔT_M , can be as much as 6%, which leads to serious errors, as shown in table 2.

Table 2 shows the values T_{MS} and T_{mS} for the extremes of the spectrum for $S = 4 \text{ nm}$. The values of the refractive index n_s as calculated by equation (11) from T_{MS} and T_{mS} is about 10% lower than the true values n_{tr} and n_s , even decreases for shorter wavelengths. If equation (23) is used to calculate d using n_s , a

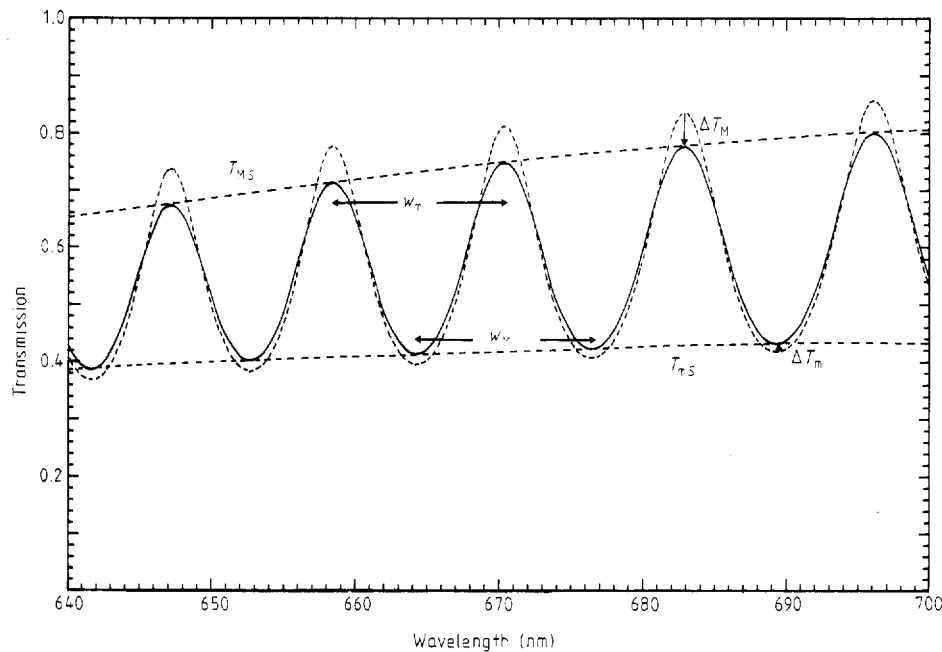


Figure 5. Simulated transmission for a slit width of 4 nm (full curve) compared to that of zero slit width (broken curve) for a film of $4 \mu\text{m}$ thickness.

Table 2. Transmission of a film of $4 \mu\text{m}$ with a slit of 4 nm and corrected values.

| λ | T_{MS} | T_{mS} | n_s | w_M, w_m | T_M | T_m | n_1 | n_{tr} |
|-----------|----------|----------|-------|------------|-------|-------|-------|----------|
| 696.0 | 0.802 | 0.436 | 3.057 | 13.6 | 0.857 | 0.420 | 3.226 | 3.219 |
| 689.4 | 0.790 | 0.432 | 3.059 | 13.2 | 0.847 | 0.415 | 3.236 | 3.231 |
| 682.8 | 0.778 | 0.428 | 3.061 | 13.0 | 0.835 | 0.410 | 3.247 | 3.244 |
| 676.4 | 0.764 | 0.424 | 3.061 | 12.4 | 0.822 | 0.405 | 3.259 | 3.256 |
| 670.4 | 0.749 | 0.419 | 3.062 | 12.2 | 0.810 | 0.400 | 3.270 | 3.268 |
| 664.2 | 0.732 | 0.414 | 3.062 | 12.0 | 0.793 | 0.395 | 3.278 | 3.280 |
| 658.4 | 0.715 | 0.408 | 3.062 | 11.6 | 0.776 | 0.389 | 3.290 | 3.292 |
| 652.6 | 0.695 | 0.402 | 3.061 | 11.2 | 0.755 | 0.381 | 3.303 | 3.304 |
| 647.2 | 0.674 | 0.395 | 3.060 | 11.0 | 0.734 | 0.374 | 3.313 | 3.316 |
| 641.6 | 0.650 | 0.387 | 3.057 | 10.8 | 0.709 | 0.367 | 3.322 | 3.329 |

value of $d \sim 6000$ nm is obtained — an error of 50%. The errors due to the effect of the slit s are thus very serious indeed, but can fortunately be corrected for.

The change in T , ΔT , is proportional to T and S and inversely proportional to the linewidth, w . Theoretical analyses show the proportionality dependence to be quadratic

$$\Delta T \propto (TS/w)^2.$$

The constant of proportionality depends on the way w is defined. If w is simply taken to be the width between the two extremes immediately adjacent to the one under consideration, the constant of proportionality is very close to 1 for a wide range of conditions, for both T_{MS} and T_{mS} . The correct values T_M and T_m can thus be calculated from the following equations

$$T_M = T_{MS} + (T_{MS}S/w_M)^2 \quad (26a)$$

$$T_m = T_{mS} - (T_{mS}S/w_m)^2 \quad (26b)$$

where

$$w_{M(i)} = \lambda_{m(i-1)} - \lambda_{m(i+1)}$$

and

$$w_{m(i)} = \lambda_{M(i-1)} - \lambda_{M(i+1)}.$$

The way of calculating w is shown in figure 5 and the values are given in table 2. The corrected values T_M and T_m using equation (26) are also shown as well as the refractive index n_1 calculated from equation (11) using the corrected values. There is a good agreement between n_1 and n_r . If the thickness is calculated from n_1 using the procedure shown in table 1, a value of $d = 4000 \pm 4$ nm is obtained with corresponding accuracies in the final values of n .

The use of the slit correction equation (26) thus transformed an error of 50% in d to an accuracy of 0.1%. Equation (26) is valid over a wide range of practical values of w , S and T . In practice the slit can be increased to reduce noise and equation (26) can be used to correct the experimental values of T , thus increasing the overall accuracy.

6. Determination of α

Since $n(\lambda)$ is known from equation (24), $x(\lambda)$ can be determined from any of the four curves T_M , T_α , T_i or T_m using their respective formulae. $\alpha(\lambda)$ can be calculated from $x(\lambda)$ and d using (5f). The values of α at the extremes are shown in table 3,

using the values of T_M and T_m from table 1. α is expressed in the commonly used units of cm^{-1} .

If the values n_1 of table 1 according to equation (11) are used in the calculations, all four formulae will of course give identical values. Equation (24) is used for n in the calculation of α in table 3. All four formulae yield values of α that are in very good agreement with the true values.

Table 4 shows the sensitivity of the various formulae to inaccuracies in the experimental parameters. The table shows the absolute change in the values of α of table 3, for small and large values of α , if the parameters are changed (by about 1%) as indicated.

From table 4 it is evident that formulae involving T_m are more sensitive to errors in s and n . α is also more sensitive to errors in T_m than in T_M . Equation (12) thus seems the best equation to use for calculating α . It can be shown however that the position of T_i in figure 2 is independent of errors due to slit width. Equation (15) may be used to calculate α without performing the slit correction with equation (26).

The values of α as calculated by equation (A3), using the value of T_α from equation (18), are also shown in table 3 and there is an excellent agreement with the other four formulae, thus verifying the correctness of the theory presented here.

The values of α calculated from equation (21) are also shown in table 3 and it can be seen that these values are much too high, especially in the region of weak absorption where the error is more than a factor of 10. This could be expected by considering the spectra of figure 3. The approximation assuming an infinite substrate thus leads to serious errors in determining α and k and the author maintains that the formula for α of Manifacier *et al* (1976) is wrong.

Table 5 shows the values for α in the region of strong absorption calculated from T_α extrapolated to T_0 in figure 2 and using equation (24) for the values of n .

The mistakes in the first few values of α calculated from T_M and T_m in table 5 are due to the fact that T_α was used in the calculation. If their appropriate curves are used better values are obtained. For values of $T < 0.05$ all curves converge to T_0 . The approximate formula (22) works well for values of $T < 0.2$ but becomes invalid for $T > 0.25$. Equation (19) can however not be used for values of $T < 0.01$ since due to its structure, round-off errors in calculations lead to errors. The values for α as calculated by equation (A3) again agree excellently with the other values.

A relative error of 1% in s leads to an absolute error of

Table 3. Values of α in units of 10^3 cm^{-1} calculated from the different formulae in the text.

| λ | True α | T_M (12) | T_α (19) | T_i (15) | T_m (13) | (A3) | (21) |
|-----------|---------------|---------------|--------------------|---------------|---------------|-------|-------|
| 859 | 0.011 | 0.013 | 0.033 | 0.042 | 0.070 | 0.047 | 0.241 |
| 814 | 0.018 | 0.013 | 0.011 | 0.010 | 0.006 | 0.026 | 0.308 |
| 775 | 0.031 | 0.036 | 0.026 | 0.022 | 0.008 | 0.043 | 0.349 |
| 740 | 0.054 | 0.058 | 0.062 | 0.064 | 0.070 | 0.078 | 0.329 |
| 710 | 0.094 | 0.095 | 0.101 | 0.105 | 0.115 | 0.119 | 0.356 |
| 683 | 0.165 | 0.183 | 0.177 | 0.174 | 0.164 | 0.195 | 0.480 |
| 659 | 0.286 | 0.287 | 0.291 | 0.294 | 0.301 | 0.310 | 0.552 |
| 636 | 0.508 | 0.555 | 0.542 | 0.534 | 0.514 | 0.561 | 0.870 |
| 617 | 0.877 | 0.890 | 0.912 | 0.924 | 0.957 | 0.912 | 1.111 |
| 598 | 1.575 | 1.686 | 1.652 | 1.634 | 1.581 | 1.669 | 2.082 |
| 582 | 2.644 | 2.712 | 2.732 | 2.741 | 2.770 | 2.748 | 2.951 |
| 564 | 5.115 | 5.277 | 5.316 | 5.329 | 5.381 | 5.329 | 5.446 |
| 555 | 7.349 | 7.428 | 7.544 | 7.575 | 7.720 | 7.553 | 7.217 |

Table 4. Change in values of α (cm^{-1}) due to changes in the parameters of the formulae.

| Change in parameters | $T_M(12)$ | | $T_\alpha(19)$ | | $T_i(15)$ | | $T_m(13)$ | |
|--------------------------|---------------|------|----------------|------|-----------|------|-----------|------|
| | $\alpha = 10$ | 5000 | 10 | 5000 | 10 | 5000 | 10 | 5000 |
| $s - 0.01s$ | +30 | +10 | -10 | -20 | -30 | -30 | -80 | -70 |
| $n - 0.01n$ | 0 | +40 | +60 | +80 | +100 | +100 | +200 | +180 |
| $T_M - 0.01$ | +80 | +180 | +50 | +110 | +40 | +90 | 0 | 0 |
| $T_m - 0.01$ | 0 | 0 | -100 | -180 | -140 | -240 | -280 | -500 |
| $T_M - 0.01, T_m + 0.01$ | +80 | +180 | -50 | -70 | -100 | -140 | -280 | -500 |

Table 5. Values of α in units of 10^3 cm^{-1} for the region of strong absorption using the different formulas in the text.

| λ | T_α, T_0 | True α | T_M (12) | T_α (19) | T_i (15) | T_m (13) | T_0 (22) | (A3) |
|-----------|-----------------|---------------|---------------|--------------------|---------------|---------------|---------------|-------|
| 550 | 0.223 | 9.09 | 10.61 | 9.09 | 8.93 | 6.90 | 9.00 | 9.10 |
| 545 | 0.179 | 11.22 | 12.48 | 11.21 | 11.10 | 9.49 | 11.14 | 11.21 |
| 540 | 0.135 | 13.93 | 14.96 | 13.95 | 13.89 | 12.69 | 13.92 | 13.96 |
| 535 | 0.095 | 17.40 | 18.14 | 17.40 | 17.37 | 16.52 | 17.38 | 17.40 |
| 530 | 0.060 | 21.88 | 22.42 | 21.93 | 21.92 | 21.39 | 21.92 | 21.93 |
| 525 | 0.034 | 27.68 | 27.84 | 27.55 | 27.54 | 27.24 | 27.55 | 27.55 |
| 520 | 0.016 | 35.26 | 35.17 | 34.95 | 35.02 | 34.89 | 35.02 | 35.03 |
| 518 | 0.011 | 38.93 | 38.85 | 38.66 | 38.75 | 38.66 | 38.75 | 38.75 |
| 516 | 0.007 | 43.02 | 43.31 | 44.39 | 43.25 | 43.19 | 43.25 | 43.25 |
| 514 | 0.005 | 47.60 | 46.64 | 45.46 | 46.59 | 46.55 | 46.59 | 46.59 |
| 512 | 0.003 | 52.73 | 51.70 | | 51.68 | 51.65 | 51.68 | 51.68 |
| 510 | 0.002 | 58.48 | 55.72 | | 55.71 | 55.70 | 55.71 | 55.71 |

about 20 cm^{-1} in α and a relative error of 1% in n leads to an absolute error of about 100 cm^{-1} in α over the whole region of strong absorption. From equation (22) it follows that an absolute error of ΔT in T_0 leads to an absolute error of $(1/d) \ln(1 + \Delta T T_0^{-1})$ in α . The accuracy of α thus decreases for $T < 0.01$.

In conclusion the author recommends that T_M with equation (12) be used to calculate α over the whole range of the spectrum. T_M is also the easiest curve to construct experimentally.

In cases where T_M cannot be constructed accurately, e.g. for very thick samples where slit errors may be present or very thin samples with a few fringes, T_i can be constructed and α be calculated from equation (15). α can be calculated with about 1% accuracy in the range of about 100 cm^{-1} to $5 \times 10^4 \text{ cm}^{-1}$ but the accuracy decreases outside this region.

Once $\alpha(\lambda)$ is known, $k(\lambda)$ can be calculated from the equation

$$k = \alpha\lambda/4\pi \quad (27)$$

which completes the calculation of the optical constants.

7. Conclusion

Formulae and procedures have been presented to calculate $n(\lambda)$, $\alpha(\lambda)$ and d for α -Si:H films to an accuracy of the order of 1% using data from the transmission spectrum alone. All formulae are in closed form and can easily be used on a programmable pocket calculator. The procedure has been used on a large number of α -Si:H films using a Varian DMS-90 spectrophotometer and the results showed that the accuracy claims are justified.

Appendix

The rigorous expression for the transmission T for a system as

shown in figure 1 is

$$T = \frac{A'x}{B' - C'x + D'x^2} \quad (A1)$$

where

$$A' = 16s(n^2 + k^2)$$

$$B' = [(n+1)^2 + k^2][(n+1)(n+s^2) + k^2]$$

$$C' = [(n^2 - 1 + k^2)(n^2 - s^2 + k^2) - 2k^2(s^2 + 1)]2 \cos \varphi$$

$$- k[2(n^2 - s^2 + k^2) + (s^2 + 1)(n^2 - 1 + k^2)]2 \sin \varphi$$

$$D' = [(n-1)^2 + k^2][(n-1)(n-s^2) + k^2]$$

$$\varphi = 4\pi nd/\lambda, \quad x = \exp(-\alpha d), \quad a = 4\pi k/\lambda.$$

In the case of an infinite substrate the transmission T is given by

$$T = \frac{A''x}{B'' - C''x + D''x^2} \quad (A2)$$

where

$$A'' = 16s(n^2 + k^2)$$

$$B'' = [(n+1)^2 + k^2][(n+s)^2 + k^2]$$

$$C'' = [(n^2 - 1 + k^2)(n^2 - s^2 + k^2) + 4k^2s]2 \cos \varphi$$

$$- k[2(n^2 - s^2 + k^2) + 2s(n^2 - 1 + k^2)]2 \sin \varphi$$

$$D'' = [(n-1)^2 + k^2][(n-s)^2 + k^2].$$

The absorbance x for a system as shown in figure 1 is given in

terms of the interference-free transmission T_α by

$$x = \{P + [P^2 + 2Q T_\alpha(1 - R_2 R_3)]^{1/2}\}/Q \quad (\text{A3})$$

where

$$Q = 2T_\alpha(R_1 R_2 + R_1 R_3 - 2 R_1 R_2 R_3)$$

$$P = (R_1 - 1)(R_2 - 1)(R_3 - 1)$$

$$R_1 = [(1 - n)/(1 + n)]^2$$

$$R_2 = [(n - s)/(n + s)]^2$$

$$R_3 = [(s - 1)/(s + 1)]^2.$$

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