

Characterizing Optical Thin Films (I)

Physical vapor deposition is the most common technique used to deposit optical thin films for a large variety of applications. This requires the ability to get a solid material into a vapor (gaseous) form, to transport it to a surface onto which the film is to be deposited, and to be able to control the physical and optical properties of the resultant film. Sputtering and evaporation in a vacuum are the prevalent techniques used to get solid materials into a vapor form. Regardless of the deposition technique used, it is necessary in the development of coating equipment and coating processes to have the ability to determine the physical and optical properties of the resultant films. There is a considerable range of equipment available to do this. However, all film Optical thin film manufacturers have to have the ability to measure the performance of finished devices. A recording spectrophotometer is the workhorse instrument to do this. Spectral measurements of single layer coatings and certain multi-layers structures can be used to extract optical properties of the films

Calculating the spectral performance of optical thin films on a surface is a very mature technology and has been widely published (1,2). It is then possible to take data from the spectral measurements of films and extract optical properties. It is the purpose of this article to discuss how this can be done, the validity of the results and then to discuss what we can further learn about the films from the results. To do so, we first look at using the optical properties of thin film materials to calculate the spectral performance.

What we want to do is to determine the amplitudes and intensities of light incident on a thin film and/or thin film system deposited on a surface. To do so is fairly straightforward however complex. One only has to set up Maxwell's equations, apply the appropriate boundary conditions to arrive at a solution. There are a variety of approaches that have been used based on this approach and, although seemingly different, eventually arrive at the same result. For this article I choose to use a convention as previously published by Heavens (1). Also, for simplicity I choose to pick up the calculations after the wave equations have been solved and we are at a position where the calculations have become relatively simple. That is, we assume all of the preliminary messy work has been done appropriately and we can go forward in a relatively easy manner. Also, we will reduce the complexity further by only considering light that is normally incident on the surface. This assumption is valid since oblique incidence is not needed in the examples that we will be considering later. Furthermore, we are going to assume that the materials are non-absorbing. This is not essential. However, if the materials were absorbing, the refractive index (n) would have to be replaced by the complex refractive index ($n-ik$). Once we have determined how to handle the non-absorbing situation, we will then allow for slightly absorbing films. The following derivation is also based on previously published material prepared by the author (3).

Consider light incident on a material with a smooth polished surface of refractive index n_1 (see Figure 1). Some of the light will be reflected at the surface and some of the light will be transmitted into the material. The Fresnel coefficients for the amplitudes of the reflected and transmitted light traveling from n_0 (the surrounding medium) to n_1 are given in equations 1 and 2 and for light traveling from n_1 to n_0 are given by equations 3 and 4.

$$r_1 = \frac{n_0 - n_1}{n_0 + n_1} \quad (1)$$

$$t_1 = \frac{2n_0}{n_0 + n_1} \quad (2)$$

$$r_1' = \frac{n_1 - n_0}{n_1 + n_0} \quad (3)$$

$$t_1' = \frac{2n_1}{n_0 + n_1} \quad (4)$$

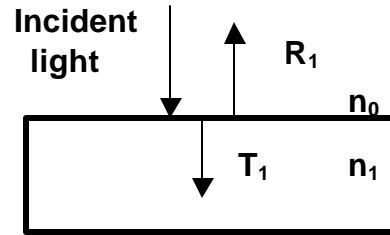


Figure 1. R and T of light incident on a surface.

As indicated previously, the above relationships are valid for light incident at normal incidences. For light obliquely incident on the surface it is necessary to consider the s and p polarizations, calculate R and T separately for each polarization and average them together. Although easy to do, this is a complication beyond what we need to consider at this point. The amount of reflected and transmitted light at the interface are given in equations 5 and 6 in terms of the Fresnel coefficients and the refractive indexes (where $r_1' = -r_1$):

$$R = r_1 r_1' = \frac{(n_0 - n_1)(n_0 - n_1)}{(n_0 + n_1)(n_1 + n_0)} = \left(\frac{n_0 - n_1}{n_0 + n_1} \right)^2 \quad (5)$$

$$T = t_1 t_1' = \left(\frac{2n_0}{n_0 + n_1} \right) \left(\frac{2n_1}{n_1 + n_0} \right) = \frac{4n_0 n_1}{(n_0 + n_1)^2} \quad (6)$$

If a thin film is deposited over the surface of the material there are now 2 interfaces where the light can be reflected and transmitted. Also, there will essentially be an infinite number of multiple reflection and transmissions that need to be summed to give the final amount of reflected and transmitted light. This sum is related to the optical properties of the film, the optical properties of the substrate, their relative values and the phase thickness of the film.

Consider the situation shown in Figure 2 for light incident at normal incidence on a coated surface (Note: although I had excluded oblique incidence, an angle is included in the figure so that the reflected and transmitted beams would be separated out and could be labeled. The calculations are for normal incidence.):

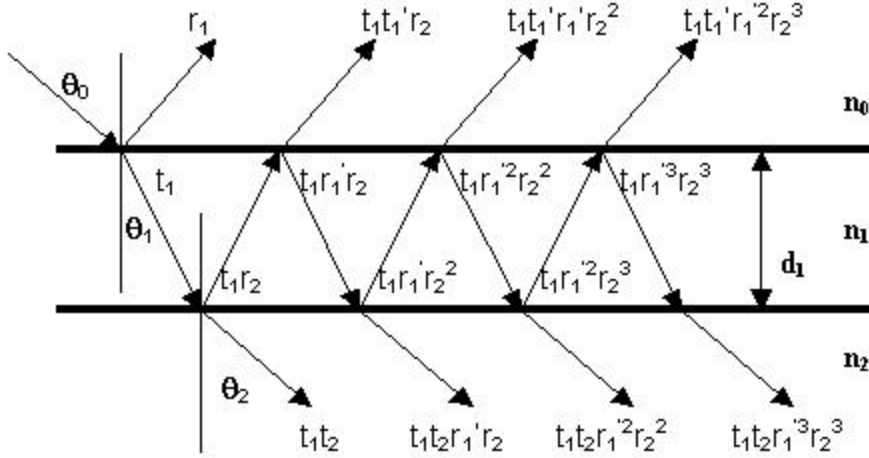


Figure 2. Showing a ray of light traveling in medium n_0 incident on film n_1 deposited over substrate n_2 .

The change in phase for the light traveling through the film is δ_1 given by:

$$\mathbf{d}_1 = \frac{2\mathbf{p}}{\mathbf{l}} n_1 d_1 \cos \mathbf{q}_1 \quad (7)$$

Therefore the sum of the reflected amplitude is given by:

$$\begin{aligned} R &= r_1 + t_1 t_1' r_2 e^{-2i\mathbf{d}} - t_1 t_1' r_1 r_2^2 e^{-4i\mathbf{d}} + t_1 t_1' r_1^2 r_2^3 e^{-6i\mathbf{d}} - t_1 t_1' r_1^3 r_2^4 e^{-8i\mathbf{d}} + \dots \\ &= r_1 + \frac{t_1 t_1' r_2 e^{-2i\mathbf{d}}}{1 + r_1 r_2 e^{-2i\mathbf{d}}} \end{aligned} \quad (8)$$

This expression can be simplified further by considering conservation of energy and the fact that if we are dealing with non-absorbing materials:

$$t_1 t_1' = 1 - r_1^2$$

so that equation 8 becomes:

$$R = \frac{r_1 + r_2 e^{-2i\mathbf{d}}}{1 + r_1 r_2 e^{-2i\mathbf{d}}} \quad (9)$$

It also follows that the sum of the transmitted amplitude is given by:

$$\begin{aligned}
T &= t_1 t_2 e^{-i\mathbf{d}} - t_1 t_2 r_1 r_2 e^{-3i\mathbf{d}} + t_1 t_2 r_1^2 r_2^2 e^{-5i\mathbf{d}} - t_1 t_2 r_1^3 r_2^3 e^{-7i\mathbf{d}} + \dots \\
&= \frac{t_1 t_2 e^{-2i\mathbf{d}}}{1 + r_1 r_2 e^{-2i\mathbf{d}}}
\end{aligned} \tag{10}$$

The above terms (R and T) are the amplitudes of the waves. What we are looking for is the ratio of the reflected and transmitted energies (\mathbf{R} and \mathbf{T}) to the incident energy. These are given by the product of each of the amplitudes with their complex conjugate of the amplitudes. When this is done, along with the appropriate calculations, the reflectance and transmittance become:

$$\mathbf{R} = n_0 R R^* = \frac{n_0 (r_1^2 + 2 r_1 r_2 \cos 2\mathbf{d}_1 + r_2^2)}{(1 + 2 r_1 r_2 \cos 2\mathbf{d}_1 + r_1^2 r_2^2)} \tag{11}$$

$$\mathbf{T} = n_0 T T^* = \frac{n_2 t_1^2 t_2^2}{(1 + 2 r_1 r_2 \cos 2\mathbf{d}_1 + r_1^2 r_2^2)} \tag{12}$$

The above term for the reflectance can be written as:

$$\mathbf{R} = \frac{A + B \cos C}{D + B \cos C} \tag{13}$$

where:

$$\begin{aligned}
A &= r_1^2 + r_2^2 && \text{Assuming } n_0 = 1 \text{ (the medium is air or vacuum)} \\
B &= 2r_1 r_2 \\
D &= 1 + r_1^2 r_2^2 \\
C &= 2\mathbf{d}_1 = \frac{4\mathbf{p}}{\mathbf{l}} n_1 d_1 && \text{Assuming the angle of incidence is 0 degrees}
\end{aligned}$$

If we now substitute the expressions for the Fresnel coefficient at the medium/film interface [equation 1] and the film substrate interface $[(n_1 - n_s)/(n_1 + n_s)]$ and the phase thickness into equation 13 we have the following expression for the reflectance of a single layer film (for normal incidence and non-absorbing):

$$\mathbf{R} = \frac{\left(\frac{n_0 - n_1}{n_0 + n_1}\right)^2 + \left(\frac{n_1 - n_2}{n_1 + n_2}\right)^2 + 2\left(\frac{n_0 - n_1}{n_0 + n_1}\right)\left(\frac{n_1 - n_2}{n_1 + n_2}\right)\cos\left(\frac{4\mathbf{p}}{\mathbf{l}} n_1 d_1\right)}{1 + \left(\frac{n_0 - n_1}{n_0 + n_1}\right)^2 + \left(\frac{n_1 - n_2}{n_1 + n_2}\right)^2 + 2\left(\frac{n_0 - n_1}{n_0 + n_1}\right)\left(\frac{n_1 - n_2}{n_1 + n_2}\right)\cos\left(\frac{4\mathbf{p}}{\mathbf{l}} n_1 d_1\right)}$$

The above expression can be rearranged to give (where $n_0=1$):

$$R = \frac{(1 + n_1^2)(n_1^2 + n_2^2) - 4n_1^2 n_2 + (1 - n_1^2)(n_1^2 - n_2^2) \cos \frac{4\mathbf{p}}{\mathbf{l}} n_1 d_1}{(1 + n_1^2)(n_1^2 + n_2^2) + 4n_1^2 n_2 + (1 - n_1^2)(n_1^2 - n_2^2) \cos \frac{4\mathbf{p}}{\mathbf{l}} n_1 d_1} \quad (14)$$

The above expression is accurate to calculate the reflectance of a single layer film of known refractive index n_1 and thickness d_1 where λ is a variable. Unfortunately nature is not as kind as we might wish. That is, n_1 is not a constant but varies as a function of the wavelength [$n_1 = f(\mathbf{l})$] and therefore the appropriate refractive index must be used in calculating R at each wavelength. Also it is not easy to solve equation 14 for n as a function of the measured reflectance at each wavelength. However, the cosine function is cyclical. This means that the value of the reflectance will increase and decrease in a regular manner as the thickness of the film increases. Consider the reflectance of films of magnesium fluoride ($n_1=1.38$) and aluminum oxide ($n_1=1.63$) on a glass substrate ($n_2=1.52$). Table I shows the values for the Fresnel coefficients and the terms A, B and D. Figure 3 shows a plot of the cosine function and the reflection of the two films as the thickness increases from zero to a thickness that corresponds to a full cosine cycle for each film.

Table I

TERM	$n_f = 1.38$	$n_f = 1.65$
r_1	-0.159663866	-0.245283019
r_2	-0.048275862	0.041009464
A	0.027823109	0.061845535
B	0.015415822	-0.02011785
D	1.0000594	1.00010118
R_{\max}	0.04258	0.080339
R_{\min}	0.0126	0.04258
$k = 0$	$n_o = 1$	$n_s = 1,52$

At zero thickness the reflectance is just that of the uncoated substrate (since it is uncoated) and the order is said to be 0. As the film grows, the reflectance will increase (film index > that of the substrate) or decrease (film index < that of the substrate) until reaching the first extreme, maximum and minimum respectively. This thickness corresponds to a quarter-wave optical thickness (QWOT) and is said to have an order of 1. As the film thicknesses increase further the reflectance of the films will then go in the opposite direction, decreasing for the high index film and increasing for the low index film until reaching that of the bare substrate. At this point the thicknesses correspond to a half-wave optical thickness (HWOT) and said to be absentee (as if there were no film) and an order of 2. Further increases in thickness will have the reflectance increasing and decreasing in the same pattern. Each successive extreme will be the next higher odd

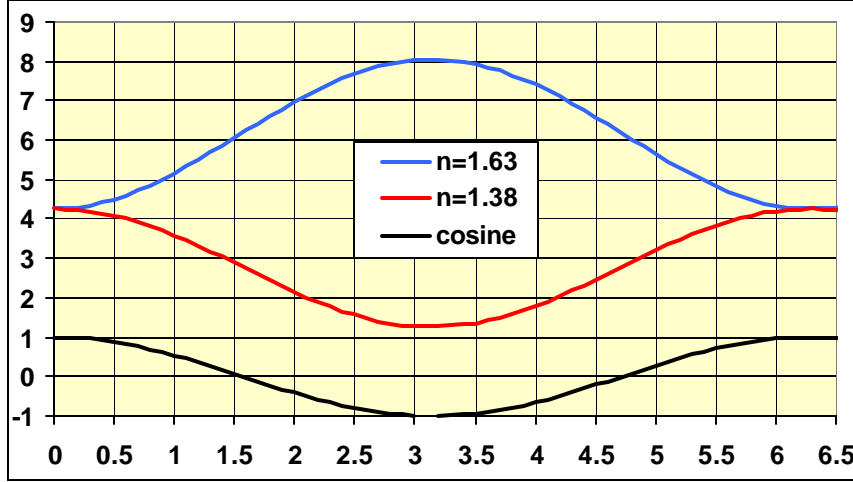


Figure 3. Reflectance of MgF₂ and Al₂O₃ films as the film thicknesses are increased.

order (3, 5, 7 etc.) and each successive value equal to that of the uncoated substrate will correspond to the next higher even order (4, 6, 8 etc.). At the QWOT the cosine is -1 and the expression for the reflectance becomes:

$$R = \frac{(1 + n_1^2)(n_1^2 + n_2^2) - 4n_1^2 n_2 - (1 - n_1^2)(n_1^2 - n_2^2)}{(1 + n_1^2)(n_1^2 + n_2^2) + 4n_1^2 n_2 - (1 - n_1^2)(n_1^2 - n_2^2)}$$

which can then be reduced to:

$$R = \frac{(n_1^2 - n_2)^2}{(n_1^2 + n_2)^2}$$

which is readily solved for n_1 :

$$n_1 = \left[n_2 \left(\frac{1 + \sqrt{R}}{1 - \sqrt{R}} \right) \right]^{0.5} \quad (15)$$

Equation 15 is a relatively simple and convenient expression that can be used to calculate the refractive index of any single layer film at QWOT films or odd numbered orders. Unfortunately the same can not be done at the HWOT films or the even orders since the cosine function is $+1$ and the expression reduces to one where there is no n_1 term left for which to solve. The expression is only in terms of the substrate refractive index and results in the reflectance of the uncoated substrate.

At the QWOT value (we refer to this as the first order or $m=1$) where the cosine is -1, the phase thickness is π radians. Therefore it follows that we can set the expression for the phase thickness equal to π and solve for the physical thickness of the film as follows:

$$\mathbf{p} = \frac{4\mathbf{p}}{\mathbf{I}_1} n_1 d \quad \text{or} \quad d = \frac{\mathbf{I}_1}{4n_1}$$

At each successively higher order the phase thickness is π radians thicker than at the previous order. Therefore, at the first order the above expression applies. At the second order the phase thickness is 2π or $4\pi n_2 d / \lambda_2$ and at the third order the phase thickness is 3π or $4\pi n_3 d / \lambda_3$. Therefore it follows that at any order m , the phase thickness is $m\pi$ or $4\pi n_m d / \lambda_m$ where λ_m and n_m are the wavelength and refractive index respectively of the m^{th} order and d is the film thickness. Therefore:

$$m\mathbf{p} = \frac{4\mathbf{p}}{\mathbf{I}_m} n_m d \quad \text{or} \quad d = \frac{m\mathbf{I}_m}{4n_m} \quad (16)$$

Equation 16 is valid at all orders, odd and even. Since for any specific film there is only one film thickness it follows that at any even order the refractive index can be calculated from an adjacent odd order in the interference pattern. Or, if x is an even order (2, 4, 6 . . etc.) then:

$$d = \frac{(x-1)\mathbf{I}_{(x-1)}}{4n_{(x-1)}} = \frac{x\mathbf{I}_x}{4n_x} = \frac{(x+1)\mathbf{I}_{(x+1)}}{4n_{(x+1)}} \quad \text{where } x-1 \text{ is the lower odd order}$$

and $x+1$ is the higher odd order.

Therefore it follows that the above expression can be solved for n_x two ways (where x is an even order) as follows:

$$n_x = \frac{n_{(x-1)}x\mathbf{I}_x}{(x-1)\mathbf{I}_{(x-1)}} \quad \text{or} \quad n_x = \frac{n_{(x+1)}x\mathbf{I}_x}{(x+1)\mathbf{I}_{(x+1)}} \quad (17)$$

We now have all the tools necessary to take reflection scans of a single layer material and extract the refractive index. As a first example, let us compute the theoretical performance of a hypothetical 400 nm TiO_2 film. If the film were non-absorbing and non-dispersive on a non-dispersive, we would have a trivially easy situation. For example consider the plot for a 400 nm TiO_2 film with a refractive index of 2.4 deposited on a glass substrate with a refractive index of 1.52 (see Figure 4). All of the reflectance peaks are of the same value 33.92% and the minima are 4.258%. The wavelengths of the maxima and minima are (Shown in Table II in order of decreasing wavelength – units are nm). The order of the interference pattern is easily determined. Starting at the longer wavelength, which is a minimum and therefore has to be even, we must determine an even number which multiplied by an even number will equal the product of the next

Non-dispersive TiO₂

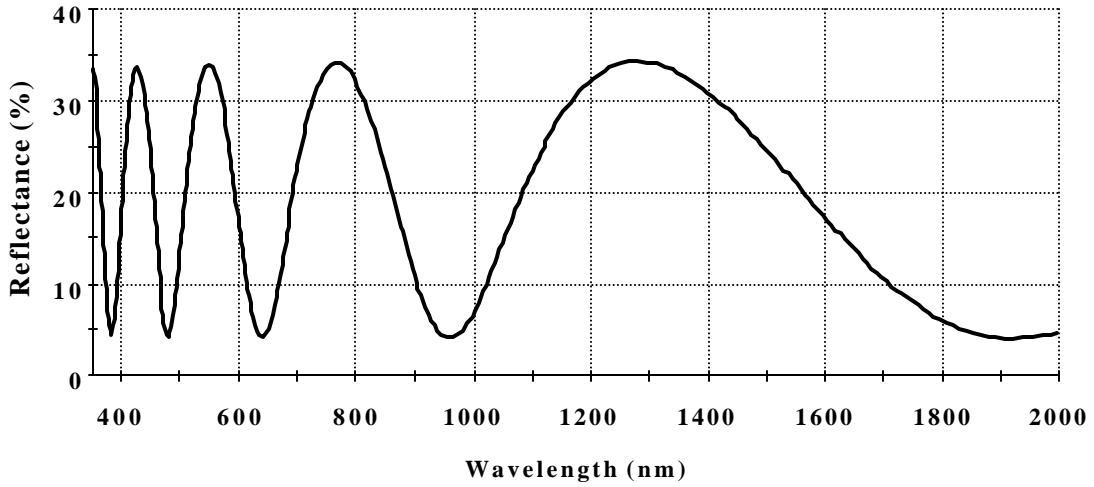


Figure 4. Reflectance of a 400 nm non-dispersive TiO₂ film on a non-dispersive glass substrate with $n_s = 1.52$.

higher integer times the next lower interference wavelength. If we start by trying 2, we see that 2×1920 (3840) does indeed equal 3×1280 (3840).

Table II

λ	1920	1280	960	768	640	549	480	427	384
order	2	3	4	5	6	7	8	9	10
product	3840	3840	3840	3840	3840	3840	3840	3840	3840

If we want to calculate the refractive index at the even orders, we can use equation 17. Let's take the 6th and 7th orders as an example.

$$n_x = \frac{n_{(x+1)} x \lambda_x}{(x+1) \lambda_{(x+1)}} = \frac{2.40 \times 6 \times 640}{7 \times 549} = 2.398$$

Of course we expected nothing less since the original calculation was based on an even refractive index of 2.40. The slight error is due to using wavelength data rounded off to the nearest integer. If we had used greater precision for the wavelengths, the refractive index calculation would have been even closer. Let's now consider a more complicated situation. We still have a 400 nm TiO₂ film over a glass substrate but both materials will be dispersive. Table III contains the dispersion data for the two materials and Figure 5 shows a computer generated reflection plot of the film (wavelength units are nm).

Table III

λ	1826	1234	936	753	640	558	498	451	416	386	361
n	2.283	2.320	2.339	2.358	2.400	2.442	2.492	2.539	2.596	2.652	2.708
k	0	0	0	0	0	.00023	.000420	.00044	.00286	.0054	.0079
glass	1.507	1.507	1.509	1.512	1.515	1.518	1.522	1.525	1.529	1.533	1.536

Dispersive IAD TiO₂

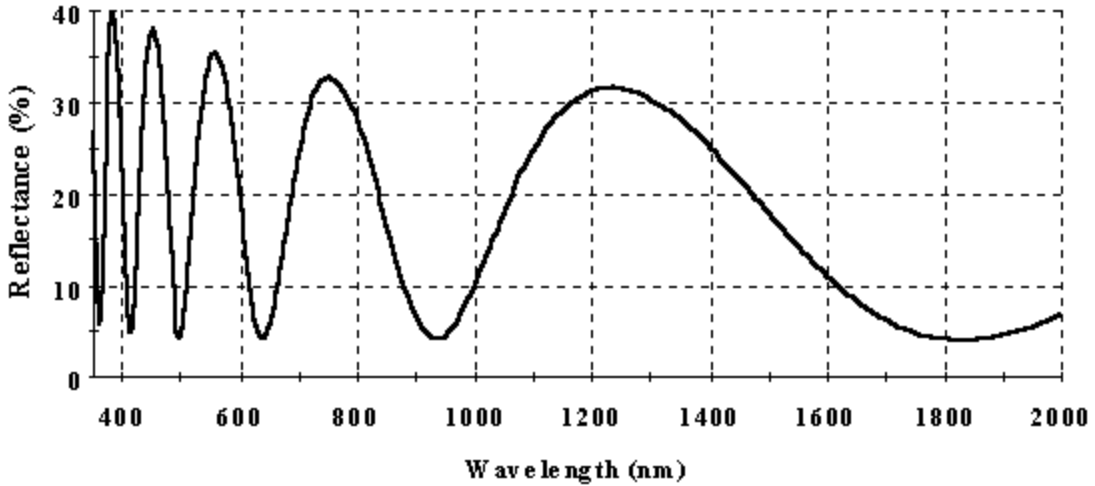


Figure 5. 400 nm dispersive TiO₂ film over a dispersive glass substrate.

The plot shown in figure 5 is significantly different than the one shown in Figure 4. In the first place, neither the maxima nor the minima are at the same value. Both are increasing as the plot goes from longer to shorter wavelengths. This is due to the fact that the refractive index of both materials (film and substrate) increases as one goes from longer to shorter wavelengths. The effect is further mitigated by the fact that the TiO₂ film becomes more and more absorbing starting at 451 nm and lower. Assume that the film is actually unknown. It is no longer as clear as to what the order is and we need to determine it. Again the order of the first minimum at 1826 must be an even order (2 or 4 or 6 - - - etc.) If we try 2, then $2 \times 1826 = 3652$ which is not quite the same as $3 \times 1234 = 3702$. However, $4 \times 1826 = 7304$ and $5 \times 1234 = 6170$ which are even further apart and therefore the first example is correct. As it turns out, in the real world of dispersive materials, the product of the order times the wavelength will be increasing (slightly) as we go to shorter wavelengths with greater refractive index. Table IV shows the wavelengths, orders and the products of the two for this example. Also shown in Table IV are the reflectance maxima and the calculation of the refractive index of the film using equation 15.

As a last step we can calculate the refractive index at the even orders by using equation 17. This is done from the the lower odd order in the row marked $n_{(n-1)}$ and from the higher order in the row marked $n_{(m+1)}$.

Table IV

λ	1826	1234	936	753	640	558	498	451	416	386	361
order	2	3	4	5	6	7	8	9	10	11	12
product	3652	3702	3744	3795	3840	3913	3984	4059	4160	4246	4732
max		.31648		.32801		.35329		.38101		.39751	
n		2.320		2.358		2.442		2.538		2.601	
$n_{(m-1)}$	2.289		2.326		2.405		2.491		2.548		-
$n_{(m+1)}$	-		2.345		2.401		2.486		2.601		2.654
average	2.289		2.336		2.403		2.489		2.577		2.654

As expected, the calculations for the refractive index are exactly the same as used from Table III to make the calculated plot **where the film material is non-absorbing**. Where the film is absorbing, the calculated refractive index is not the same as the example since equation 15 is based on the assumption that the film is non-absorbing. Absorption in the film reduces the value of the reflectance maxima that results in a lower than real refractive index. This is expected since in the derivation of equation 15 we assumed that the film material was non-absorbing. As indicated previously, if the film material is absorbing, it is necessary to replace the refractive index n_f with $n_f - ik_f$ where n_f is usually regarded as the real part of the refractive index and the extinction coefficient k_f is the imaginary part of the refractive index. Obviously the calculation of the film performance is much more complicated. Angus Macleod (2) has derived the following expression for the extinction coefficient:

$$k_f = \frac{I}{2\pi l_f \left(\frac{n_s}{n_f} + \frac{n_f}{n_s} \right)} * \frac{1 - R_f - T_f}{T_f} \quad (18)$$

The above expression is valid at the turning points of the film. One needs to know the reflection from a coating on a substrate, the transmission through the film into the substrate, the refractive index of the substrate the thickness of the film and the refractive index of the film. The reflectance of the film over the substrate can be measured directly from a sample with a frosted back or a wedged back that either scatters or reflects the back surface out of the aperture of the spectrophotometer. From this measurement the refractive index of the film can be calculated and the thickness of the film can be calculated (out at long enough wavelengths where the film is non-absorbing). The refractive index of the substrate is known. This leaves the transmission of the film into the substrate. We can measure the transmission of a thin parallel plate of glass coated on one side. Then knowing the reflectance of the uncoated side can calculate the transmission of the film into the substrate as follows:

$$T_f = \frac{T_p^2}{T_u - T_p + T_u T_p} \quad (19)$$

where T_p is the measured transmission of the plate
 T_u is the transmission through the uncoated side of the plate
 T_f is the transmission of the film side into the plate.

The thickness of the film could be measured directly or calculated using equation 16. Equation 16 is valid at QWOT where the film is non-absorbing. Thus a calculation of the thickness out at one of the longer wavelengths would be valid. If equation 16 is substituted in for the thickness in equation 18, the expression for the extinction coefficient becomes:

$$k_f = 0.6366 \bullet \frac{1 - T_f - R_f}{T_f \bullet m \bullet \left(\frac{n_s^2 + n_f^2}{n_s \bullet n_f^2} \right)} \quad (20)$$

To test the above equations (19 and 20), consider the previous 400 nm TiO₂ film. The computed transmission of a thin glass plate coated one side is shown in Figure 6 (the format of the plot is different in appearance than the previous plots since they were copied and pasted in directly from the software used to generate them). In this case the software was actually used to calculate the transmission through the film and we used Excel to calculate back to the measured transmission through the plate coated on one side.

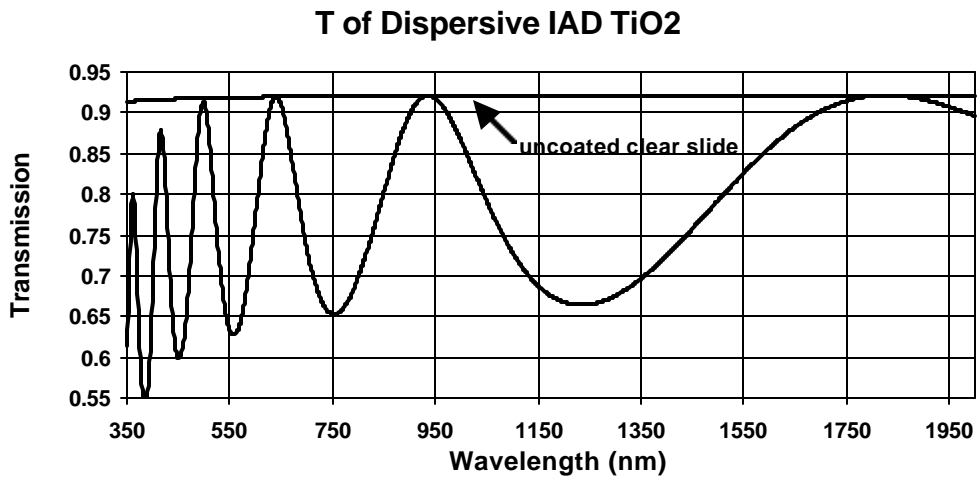


Figure 6. . 400 nm dispersive TiO₂ film over a dispersive glass substrate

The above film is non-absorbing at the maxima where the transmission is the same as that of the uncoated clear slide. The film is absorbing where the maxima are less than that of the uncoated clear slide. In order to calculate the extinction coefficient we must take the transmission data at the even orders (maxima in the transmission pattern and minima in the reflectance pattern) and calculate the transmission into the plate. The above data can

also be used to calculate the refractive index at the minima in the transmission pattern, if the film is non-absorbing, since the reflectance from the film side is just $1-T_f$. Data at the extrema for the above transmission scan and calculations made from that data is summarized in Table V. Included in the table is $1-T_f$ which will be the same as the reflectance in Table IV where the film is non-absorbing. Therefore, if the refractive index were calculated from the transmission data where the film is non-absorbing, it would be the same as the calculation from the measured reflectance data. Where the film

Table V

Order	2	3	4	5	6	7	8	9	10	11	12
l	1826	1234	936	753	640	558	498	452	416	385	361
T_n	0.92134	0.66414	0.92106	0.65298	0.91955	0.62734	0.91328	0.59895	0.87866	0.54133	0.79934
T_u	0.95906	0.95906	0.95981	0.95847	0.95809	0.95766	0.95721	0.95673	0.95625	0.95569	0.95259
T_r	0.95906	0.68352	0.95891	0.67199	0.95809	0.64524	0.95216	0.61563	0.91546	0.55526	0.8304
1-T_f	0.04094	0.31648	0.04109	0.32801	0.04191	0.35476	0.04784	0.38437	0.08454	0.44474	0.1696
R of R	0.04094	0.31648	0.04109	0.32801	0.04181	0.35329	0.04329	0.38096	0.04783	0.39751	0.05795
k	0	0	0	0	0.00001	0.00023	0.00042	0.00044	0.00289	0.00560	0.00821

is absorbing, the calculated refractive index will be different than that from the reflectance data, typically higher when calculated from the transmission data [compare row $1-T_f$ (=R if the film is non-absorbing) and R of R (reflectance as measured)]. The extinction coefficient k is calculated using equation 20 and recorded in the bottom row of the table. Note that this data is very close to the data used in calculating the reflection and transmission of the films (see Table III). The difference between the values used to calculate the film performance and the computed k from R and T data is due to rounding off the reflection and transmission measurements to 5 decimal places.

Remember that when calculating the refractive index the computed values were not the same as used to calculate the transmission and reflection of the film. Since we now know the extinction coefficient, it is possible to correct the refractive index calculations. A relationship to do this was reported by Macleod (see page 373 of reference 2) who credits Hall and Ferguson (4) for initially publishing the expression. The equation is:

$$n_c = \left[\frac{n_s(1 + \sqrt{R_f})}{1 - \sqrt{R_f}} \right]^{0.5} + \frac{\mathbf{p}k_f d_f}{\mathbf{I}} \left[\frac{1 + \sqrt{R_f}}{1 - \sqrt{R_f}} - n_s \right] \quad (21)$$

In the above equation, the first expression is just the refractive index as calculated from the reflection maxima (or therefore the refractive index) and the second expression is a correction factor. The thickness is the real thickness of the film and can be determined using an independent measurement or calculated from the optical data in a spectral region where the film is non-absorbing. In order to apply equation 21 to this example, we must first calculate the film thickness from an odd order and long wavelength using equation 16. Using the third order at 1234 nm with a refractive index of 2.32 we get 398.9 nm. Using this thickness and the Rand T film to substrate data, we get the following corrected refractive indexes:

Table VI

Order	2	3	4	5	6	7	8	9	10	11	12
design	2.283	2.320	2.339	2.358	2.400	2.442	2.492	2.539	2.596	2.652	2.708
n_r of R	2.289	2.325	2.336	2.358	2.403	2.442	2.489	2.538	2.577	2.601	2.654
n_c	2.289	2.325	2.336	2.358	2.403	2.444	2.491	2.544	2.592	2.698	2.705

The **design** row contains the refractive index at the wavelength of the specified order which was used in generating the reflection and transmission data. The **n_r of R** row contains the refractive index as calculated from the reflection maxima (n row from Table VI) and for the odd orders using equation 17 (average row from Table VI). Note again that where the material is absorbing, the refractive index is lower than the real design value. The **n_c** row contains the corrected refractive index using equation 21. Notice that this last row results in refractive index values very close to those used to prepare the example.

Therefore, we have demonstrated a technique which can be used to characterize single layer optical thin film that are non-absorbing or only slightly absorbing. The relationships developed herein are relatively simple and lend themselves to inclusion in various spreadsheets that would simplify analysis of multiple coating runs of materials. The relationships could also be used to setup worksheets in any one of many math programs to accomplish the same goal. The author routinely does this type of work using both a MathCad worksheet and an Excel spreadsheet.

In this article we have developed and demonstrated the tools necessary to take measured reflection and transmission data and extract the optical properties of a single layer thin film material. The example used herein was from precise computed data to demonstrate that the technique works well. In the real world the accuracy and precision of measured data is not as good as used for the example. Also, real films do not have perfect homogeneity as assumed and used in this example. In the next article in this series, we will discuss spectral measurement techniques, the nature and effect of inhomogeneous films and apply these relationships to real life film data.

References:

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- 3) D.E. Morton, copyrighted notes for "Preparation and Properties of Optical Thin Film Materials" - a short course prepared for the Society of Vacuum Coaters Education Program, 2001.
- 4) J. F. Hall and W. F. C. Ferguson, Optical properties of cadmium sulfide and zinc sulfide from 0.6 micron to 14 micron, *J. Opt. Soc. Am.*, **49** pp. 714-718, 1955.