

The Colours of Thin Films and Stacked Layers

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(February 20, 2013)

The derivation of an expression for the reflectivity of transparent films or stacks of transparent films, free or on a substrate, is sketched. This can be used to compute the colours. First, the simplest case of a thin film (soap bubble) is considered. Then the transfer matrix method is applied to the general case, oblique incidence of light on stacks of layers with alternating index of refraction and absorption.

A Single Film

First a monolayer is considered, and normal incidence of the light. Assume that the z -axis is pointing to the right, the back side of the film is the plane $z = 0$, and the film has thickness D and refraction index n . The electric field to the left is that of the incoming and the reflected wave

$$E_x(z, t) = A_r(z)e^{-i\omega t} + A_l(z)e^{-i\omega t} = A_r(0)e^{i(kz-\omega t)} + A_l(0)e^{i(-kz-\omega t)} \quad (1)$$

where

$$k = \frac{2\pi}{\lambda}, \quad (2)$$

λ being the wavelength in air or vacuum.

A_r and A_l are assumed to be complex quantities, and here and in the following, the physical quantities are given by the real parts of the complex expressions.

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We are looking for the reflectivity which is given by

$$R = \left| \frac{A_1}{A_r} \right|^2 . \quad (3)$$

For the field in the dielectric layer we write

$$E_x(z, t) = A'_r e^{i(nkz - \omega t)} + A'_1 e^{i(-nkz - \omega t)} \quad (4)$$

and, finally, the outgoing wave to the right is

$$E_x(z, t) = e^{i(kz - \omega t)} \quad (5)$$

where the amplitude is arbitrarily taken to be real and equal to 1.

At the boundaries, the tangential components of the electric and of the magnetic field are continuous. For normal incidence, this simply leads to the continuity of E_x and its partial derivative $\frac{\partial E_x}{\partial z}$:

$$\begin{aligned} A'_r(0) + A'_1(0) &= 1 \\ nA'_r(0) - nA'_1(0) &= 1 \end{aligned} \quad (6)$$

at $z = 0$ and

$$\begin{aligned} A_r(-D) + A_1(-D) &= A'_r(0)e^{-iknD} + A'_1(0)e^{iknD} \\ A_r(-D) - A_1(-D) &= nA'_r(0)e^{-iknD} - nA'_1(0)e^{iknD} \end{aligned} \quad (7)$$

at $z = -D$. As in equation (3) only the ratio of A_1 over A_r occurs, we can omit constant overall factors. We thus get

$$\begin{aligned} A'_r(0) &\propto n + 1 \\ A'_1(0) &\propto n - 1 \end{aligned} \quad (8)$$

and

$$\begin{aligned} A_r(-D) + A_1(-D) &\propto A'_r(0)e^{-iknD} + A'_1(0)e^{iknD} \\ A_r(-D) - A_1(-D) &\propto nA'_r(0)e^{-iknD} - nA'_1(0)e^{iknD} \end{aligned} \quad (9)$$

Solving these equations we obtain

$$\begin{aligned} A_r(-D) &\propto 2 \cos(nkD) - i(n + n^{-1}) \sin(nkD) \\ A_l(-D) &\propto -i(n - n^{-1}) \sin(nkD) \end{aligned} \quad (10)$$

and

$$R = \left| \frac{A_l(-D)}{A_r(-D)} \right|^2 = \frac{(n - n^{-1})^2 \sin^2(nkD)}{4 + (n - n^{-1})^2 \sin^2(nkD)} \quad (11)$$

for the reflectivity.

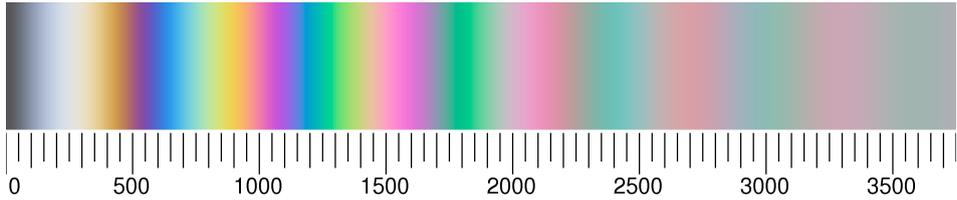


Figure 1: Reflection colours of a thin film with refractive index $n = 1.33$, computed for normal incidence. The scale gives the optical path difference between the rays reflected on the upper and the lower surface in nm (nanometers).

Dielectric Layers: the Transfer-Matrix Method

Assume dielectric layers on a substrate with index of refraction n_0 . The $z = 0$ plane is the boundary between the first layer and the substrate, and the layer is characterized by its refractive index n_1 , absorption coefficient κ_1 , and thickness D_1 . The layers are numbered consecutively in the order they are deposited.

Assume an incoming plane wave with the angle of incidence θ . We choose the coordinate system such that the plane of incidence is the x - z -plane. The wave vector in vacuum (or air) then is

$$\vec{k} = k(\sin(\theta), 0, \cos(\theta)), \quad (12)$$

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and the wave is

$$\vec{E}(\vec{r}, t) = \vec{A}e^{i(k \sin(\theta)x + k \cos(\theta)z - \omega t)}. \quad (13)$$

It is convenient to combine the absorption coefficient with the refractive index

$$\tilde{n} = n + i\kappa. \quad (14)$$

The boundaries between different layers are planes $z = z_b$. The boundary conditions can only be fulfilled if the exponential functions are continuous at the boundaries. Therefore, the frequency in all layers must be the same, and also the x -component of the wave-vector \vec{k}_j must be the same in all layers. This yields Snell's law of refraction when there is no absorption,

$$k_{j,x} = n_j k \sin(\theta_j) = k \sin(\theta). \quad (15)$$

With a complex refractivity \tilde{n} , we obtain

$$\sin(\theta_j) = \frac{\sin(\theta)}{n_j + i\kappa_j}, \quad \cos(\theta_j) = \frac{1}{n_j + i\kappa_j} \sqrt{(n_j + i\kappa_j)^2 - \sin^2(\theta)} \quad (16)$$

As complex angles are not particularly intuitive, in the following we prefer to use the components of the wave vector, which in the layer with number j is for the right-going wave

$$\vec{k}_j = k \left(\sin(\theta), 0, \sqrt{(n_j + i\kappa_j)^2 - \sin^2(\theta)} \right), \quad (17)$$

and for the left-going (reflected) wave

$$\vec{k}'_j = k \left(\sin(\theta), 0, -\sqrt{(n_j + i\kappa_j)^2 - \sin^2(\theta)} \right) \quad (18)$$

where the quantities k, θ without indices refer to the vacuum values of the incident wave.

To simplify the notation, we define

$$W_j = \sqrt{(n_j + i\kappa_j)^2 - \sin^2(\theta)}. \quad (19)$$

The two polarizations of the waves – orthogonal or parallel to the plane of incidence – have to be treated separately.

The s-polarization

In the layer with index j , the electric field orthogonal to the z - x -plane is

$$\vec{E}_{j,s}(\vec{r}, t) = S_r \vec{e}_y e^{i(\vec{k}_j \cdot \vec{r} - \omega t)} + S_l \vec{e}_y e^{i(\vec{k}'_j \cdot \vec{r} - \omega t)} \quad (20)$$

From Maxwell's equation $\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t}$, using $\frac{\partial \vec{B}}{\partial t} = -i\omega \vec{B}$, we obtain

$$\begin{aligned} \vec{B}_{j,s}(\vec{r}, t) &= S_r \frac{1}{c} (-W_j \vec{e}_x + \sin(\theta) \vec{e}_z) e^{i(\vec{k}_j \cdot \vec{r} - \omega t)} \\ &+ S_l \frac{1}{c} (W_j \vec{e}_x + \sin(\theta) \vec{e}_z) e^{i(\vec{k}'_j \cdot \vec{r} - \omega t)} \end{aligned} \quad (21)$$

As the factor $e^{-i\omega t}$ is the same in all terms, it is omitted in the following (which means that we consider only the time $t = 0$).

From Maxwell's equations it follows that at boundaries the tangential components of the electric field and of the magnetic field \vec{H} are continuous. We assume that for the dielectric layers $\mu = 1$ so that also the tangential components of \vec{B} are continuous. The x -component of \vec{B} is proportional to $\partial E_y / \partial z$. This leads to the boundary conditions. Denoting the z -coordinate of the boundary between layer i and layer j by z_b , we have

$$E_s^{(i)}(z_b) = E_s^{(j)}(z_b) \quad (22)$$

$$\frac{\partial}{\partial z} E_s^{(i)}(z_b) = \frac{\partial}{\partial z} E_s^{(j)}(z_b) \quad (23)$$

From equations (22, 23) we see that the quantities

$$F(z) := E_s(z) \quad \text{and} \quad G(z) := \frac{1}{k} \frac{\partial}{\partial z} E_s(z) \quad (24)$$

are continuous across the boundaries.

In the substrate, there is only an outgoing amplitude S_r which may be arbitrarily chosen and is given the value 1. We thus have the values of $F(0)$ and $G(0)$ on top of the substrate

$$F(0) = 1 \quad G(0) = iW_0 \quad (25)$$

and at the bottom of the first layer

$$\begin{aligned} F(0) &= S_r + S_1 \\ G(0) &= iW_1(S_r - S_1). \end{aligned} \quad (26)$$

From equation (20) we can get the values at $z = -D_1$.

$$\begin{aligned} F(-D_1) &= S_r e^{-ikW_1 D_1} + S_1 e^{ikW_1 D_1} \\ G(-D_1) &= iW_1(S_r e^{-ikW_1 D_1} - S_1 e^{ikW_1 D_1}). \end{aligned} \quad (27)$$

Expressing S_r and S_1 through $F(0)$ and $G(0)$

$$S_r = \frac{1}{2} \left(F(0) + \frac{G(0)}{iW_1} \right) \quad S_1 = \frac{1}{2} \left(F(0) - \frac{G(0)}{iW_1} \right) \quad (28)$$

we arrive at the following matrix equation:

$$\begin{pmatrix} F(-D_1) \\ G(-D_1) \end{pmatrix} = M_{1,s} \begin{pmatrix} F(0) \\ G(0) \end{pmatrix} \quad (29)$$

with

$$M_{1,s} = \begin{pmatrix} \cos(kW_1D_1) & -\frac{1}{W_1} \sin(kW_1D_1) \\ W_1 \sin(kW_1D_1) & \cos(kW_1D_1) \end{pmatrix} \quad (30)$$

The matrix is the transfer matrix which gives the name to the method. If there is a second layer with \tilde{n}_2, D_2 , the combined matrix is M_2M_1 , and so on. On top of the uppermost layer, at $z = -L$, there is air or vacuum, and

$$\begin{aligned} S_r(-L) &= \frac{1}{2}F(-L) + \frac{1}{2i \cos(\theta)}G(-L) \\ S_l(-L) &= \frac{1}{2}F(-L) - \frac{1}{2i \cos(\theta)}G(-L) \end{aligned} \quad (31)$$

The reflection coefficient is given by

$$R_s(\theta) = \left| \frac{S_l(-L)}{S_r(-L)} \right|^2. \quad (32)$$

The elements of the matrix (30) are complex numbers. In the PostScript language, complex algebra is not implemented. But it is easy to separate the real and imaginary parts of the matrix elements, using the addition theorems and

$$\cos(i\alpha) = \cosh(\alpha), \quad \sin(i\alpha) = i \sinh(\alpha) \quad (33)$$

The p-polarization

When the electric field is parallel to the plane of incidence, we can exploit the symmetry of the Maxwell equations with respect to electric and magnetic fields. For the electric field we make the ansatz (cf. eq. (21))

$$\begin{aligned}\vec{E}_{j,p}(\vec{r}, t) &= P_r (W_j \vec{e}_x - \sin(\theta) \vec{e}_z) e^{i(\vec{k}_j \cdot \vec{r} - \omega t)} \\ &+ P_l (W_j \vec{e}_x + \sin(\theta) \vec{e}_z) e^{i(\vec{k}'_j \cdot \vec{r} - \omega t)}\end{aligned}\quad (34)$$

Note that, since $W_j \vec{e}_x - \sin(\theta) \vec{e}_z$ is not a unit vector, the ‘‘amplitudes’’ P_r and P_l are only proportional to the true amplitudes. However, in the vacuum (or air) when $n = 1$ and $\kappa = 0$, $W = \cos(\theta)$, they are the correct amplitudes, and that is all what we need.

The quantities

$$\begin{aligned}F(z) &:= E_x = W_j (P_{r,j} + P_{l,j}) \\ G(z) &:= \frac{1}{k} \left(\frac{\partial E_x}{\partial z} - \frac{\partial E_z}{\partial x} \right) = i(n + i\kappa)^2 (P_{r,j} - P_{l,j})\end{aligned}\quad (35)$$

are continuous across the boundaries. Proceeding as before, one obtains

$$\begin{pmatrix} F(-D_1) \\ G(-D_1) \end{pmatrix} = M_{1,p} \begin{pmatrix} F(0) \\ G(0) \end{pmatrix}\quad (36)$$

with

$$M_{1,p} = \begin{pmatrix} \cos(kW_1 D_1) & -\frac{W_1}{(n_1 + i\kappa_1)^2} \sin(kW_1 D_1) \\ \frac{(n_1 + i\kappa_1)^2}{W_1} \sin(kW_1 D_1) & \cos(kW_1 D_1) \end{pmatrix}\quad (37)$$

The outgoing wave at $z > 0$ is assumed to be

$$\vec{E}_{0,p}(\vec{r}, t) = (W_0 \vec{e}_x - \sin(\theta) \vec{e}_z) e^{i(\vec{k}_0 \cdot \vec{r} - \omega t)},\quad (38)$$

yielding

$$F_0 = W_0, \quad G_0 = i(n_0 + i\kappa)^2\quad (39)$$

The amplitudes on top of the stack at $z = -L$ are recovered by

$$\begin{aligned} P_r(-L) &= \frac{1}{2\cos(\theta)}F(-L) - \frac{i}{2}G(-L) \\ P_1(-L) &= \frac{1}{2\cos(\theta)}F(-L) + \frac{i}{2}G(-L) \end{aligned} \quad (40)$$

The reflection coefficient is given by

$$R_p(\theta) = \left| \frac{P_1(L)}{P_r(L)} \right|^2. \quad (41)$$

Unpolarized Light

In this case, we have

$$R(\theta) = \frac{1}{2}(R_s(\theta) + R_p(\theta)). \quad (42)$$

Program Details and Special Cases

PostScript figures have been produced using the transfer matrix method, using the results of the preceding section. The method is very well suited to compute the reflectivity of large numbers of stacked layers of alternating refractive index; an example is given in the following figure.

The parameters have to be given in the first few lines of the program code. The following list holds for several different programs/pictures; not all of the parameters listed occur in each of them:

- $n_0, \kappa_0, n_1, \kappa_1, n_2, \kappa_2$, the refractive indices and absorption coefficients of the substrate and of the first and the second layer.
- N , the number of duplications. If there are only two layers on top of the substrate, this number is 0, the number of double layers is 2^N .

- $D_1n_1 + D_2n_2$, the optical periodicity interval
- `weight1`: the relative optical thickness of layer 1, i.e. $\text{weight1} = D_1n_1 / (D_1n_1 + D_2n_2)$
- θ or $\theta_{\text{start}}, \delta\theta, \theta_{\text{stop}}$, angle of incidence.

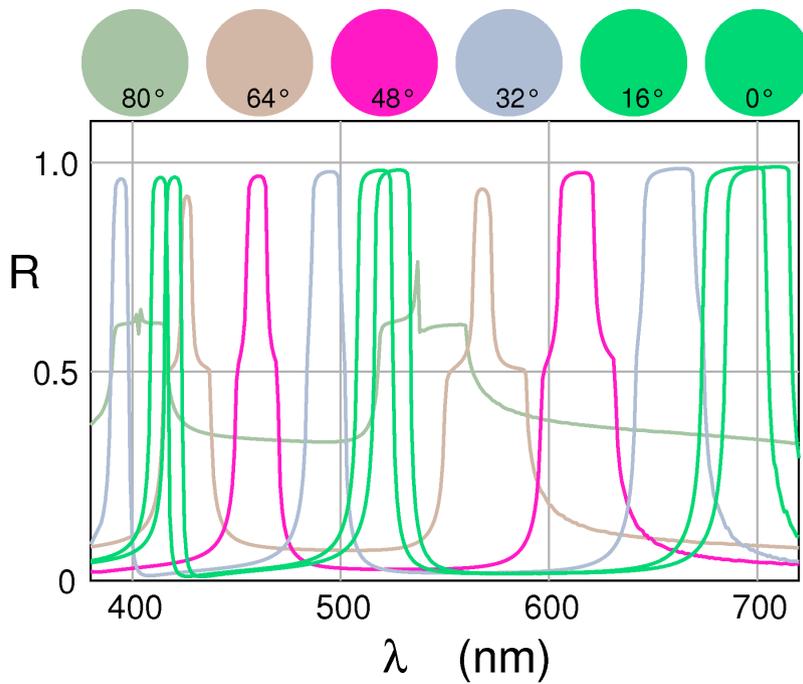


Figure 2: Reflection on a stack of 1024 double layers. Optical thickness of one double layer is 1050 nm, that of the first layer is 15% thereof. $n_1 = 1.3$, $\kappa_1 = 0.002$ and $n_2 = 1.6$, $\kappa_2 = 0$. The angles of incidence are given with the corresponding colours.

It is also possible to choose between unpolarized and polarized light:

- Case: 0 for unpolarized, 1 for s-, and 2 for p-polarization

If colours are to be computed, there are three logical variables which influence the output:

- AdobeRGB: for the sRGB standard, this has the value "false"
- Normabsolut: absolute normalization of brightness. For most practical purposes this is set to "false", then the possible maximum is chosen for the brightest colour.
- EqualBrightness: if true, it is attempted to render all colours with the same brightness. Normabsolut is ignored in this case.

In addition, the background colour and the colour of lettering and drawing may be chosen.

Though intended for stacks of layers, the program is versatile enough to treat also the simplest cases:

- a single surface. Choose $n_1 = n_0$, $\kappa_1 = \kappa_0$, $n_2 = 1$, $\kappa_2 = 0$, and $N = 0$.
- a single film. $n_0 = n_2 = 1$, $\kappa_0 = \kappa_2 = 0$, $\text{weight1} = 0.5$, $N = 0$.