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The Colours of Thin Films and Stacked Layers

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The derivation of an expression for the reflectivity of transparent films or stacks of thansparent 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 stacks of layers with alternating index of refraction, and next also absorbing layers are considered, in the most important case of perpendicular incidence of the light and finally in the general case of oblique incidence.

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

$$E_x(z,t) = A_\mathrm{r}(z)\mathrm{e}^{-\mathrm{i}\omega t} + A_\mathrm{l}(z)\mathrm{e}^{-\mathrm{i}\omega t} = A_\mathrm{r}(0)\mathrm{e}^{\mathrm{i}(kz-\omega t)} + A_\mathrm{l}(0)\mathrm{e}^{\mathrm{i}(-kz-\omega t)} \tag{1}$$

where

$$k = \frac{2\pi}{\lambda}\,, \tag{2}$$

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.

We are looking for the reflectivity which is given by

$$R = \left| \frac{A_\mathrm{l}}{A_\mathrm{r}} \right|^2 . \tag{3}$$

For the field in the dielectric layer we write

$$E_x(z,t) = A'_\mathrm{r} \mathrm{e}^{\mathrm{i}(nkz-\omega t)} + A'_\mathrm{l} \mathrm{e}^{\mathrm{i}(-nkz-\omega t)} \tag{4}$$

and, finally, the outgoing wave to the right is

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

where the amplitude is arbtrarily 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 $\frac{\partial E_x}{\partial z}$:

$$\begin{aligned} A'_\mathrm{r}(0) + A'_\mathrm{l}(0) &= 1 \\ nA'_\mathrm{r}(0) - nA'_\mathrm{l}(0) &= 1 \end{aligned} \tag{6}$$

at $z = 0$ and

$$A_\mathrm{r}(-D) + A_\mathrm{l}(-D) = A'_\mathrm{r}(0)\mathrm{e}^{-\mathrm{i}knD} + A'_\mathrm{l}(0)\mathrm{e}^{\mathrm{i}knD} \tag{7}$$

$$A_\mathrm{r}(-D) - A_\mathrm{l}(-D) = nA'_\mathrm{r}\mathrm{e}^{-\mathrm{i}knD} - nA'_\mathrm{l}\mathrm{e}^{\mathrm{i}knD} \tag{8}$$

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

$$A'_\mathrm{r}(0) \propto n+1 \tag{9}$$

$$A'_\mathrm{l}(0) \propto n-1 \tag{10}$$

and

$$A_{\mathrm{r}}(-D) + A_{\mathrm{l}}(-D) \propto A'_{\mathrm{r}}(0)\mathrm{e}^{-\mathrm{i}knD} + A'_{\mathrm{l}}(0)\mathrm{e}^{\mathrm{i}knD} \tag{11}$$

$$A_{\mathrm{r}}(-D) - A_{\mathrm{l}}(-D) \propto nA'_{\mathrm{r}}(0)\mathrm{e}^{-\mathrm{i}knD} - nA'_{\mathrm{l}}(0)\mathrm{e}^{\mathrm{i}knD} \tag{12}$$

Solving these equations we obtain

$$\begin{aligned} A_{\mathrm{r}}(-D) &\propto 2\cos(nkD) - \mathrm{i}(n+n^{-1})\sin(nkD) \\ A_{\mathrm{l}}(-D) &\propto -\mathrm{i}(n-n^{-1})\sin(nkD) \end{aligned} \tag{13}$$

and

$$R = \left|\frac{A_{\mathrm{l}}(-D)}{A_{\mathrm{r}}(-D)}\right|^2 = \frac{(n-n^{-1})^2\sin^2(nkD)}{4+(n-n^{-1})^2\sin^2(nkD)} \tag{14}$$

for the reflectivity.

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 and thickness D_1. The layers are numbered consecutively in the order they are deposited.

An electromagnetic plane wave propagates and θ is the angle between the z axis and its wave vector $\vec{k}$ in the vacuum, where $k = |\vec{k}| = \frac{2\pi}{\lambda}$, λ being the wavelength.

We choose the coordinate system such that the plane of incidence is the x–z–plane. Thus the wave vector, which for the incident wave in vacuum (or air) is $\vec{k} = (k_x, 0, k_z)$, is in the layer with number j

$$\vec{k}_j = (k_x, 0, n_j k\cos(\theta_j)) \tag{15}$$

and for the reflected wave it is

$$\vec{k}'_j = (k_x, 0, -n_j k\cos(\theta_j)) \tag{16}$$

where

$$n_j \sin(\theta_j) = \sin(\theta) \tag{17}$$

We write for the two polarisations in the layer with index j

$$\vec{E}_{j,s}(\vec{r},t) = S_r \vec{\mathrm{e}}_y \mathrm{e}^{\mathrm{i}(\vec{k}_j\cdot\vec{r}-\omega t)} + S_l \vec{\mathrm{e}}_y \mathrm{e}^{\mathrm{i}(\vec{k}'_j\cdot\vec{r}-\omega t)} \tag{18}$$

$$\vec{E}_{j,p}(\vec{r},t) = P_r \vec{\mathrm{e}}_y \times \frac{\vec{k}_j}{k_j} \mathrm{e}^{\mathrm{i}(\vec{k}_j\cdot\vec{r}-\omega t)} + P_l \vec{\mathrm{e}}_y \times \frac{\vec{k}'_j}{k_j} \mathrm{e}^{\mathrm{i}(\vec{k}'_j\cdot\vec{r}-\omega t)} \tag{19}$$

As the factor $\mathrm{e}^{-\mathrm{i}\omega t}$ is the same in all terms, it is omitted in the following.

From Maxwell's equations it follows that at boundaries the tangential components of the electric field and of the magnetic field are continuous. This leads to the boundary conditions depending on the polarisation of the waves; $\vec{E}_s$ is perpendicular to the plane of incidence and $\vec{E}_p$ is parallel to it. Denoting the z-coordinate of the boundary between layer i and layer j by z_b, the boundary conditions are

$$\begin{aligned}
E_s^{(i)}(z_\mathrm{b}) &= E_s^{(j)}(z_\mathrm{b}) && (20)\\
\frac{\partial}{\partial z}E_s^{(i)}(z_\mathrm{b}) &= \frac{\partial}{\partial z}E_s^{(j)}(z_\mathrm{b}) && (21)\\
\cos(\theta_i)E_p^{(i)}(z_\mathrm{b}) &= \cos(\theta_j)E_p^{(j)}(z_\mathrm{b}) && (22)\\
\frac{1}{\cos(\theta_i)}\frac{\partial}{\partial z}E_p^{(i)}(z_\mathrm{b}) &= \frac{1}{\cos(\theta_j)}\frac{\partial}{\partial z}E_p^{(j)}(z_\mathrm{b})\,. && (23)
\end{aligned}$$

The s-polarisation

From equations (20, 21) we see that the quantities

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

are continuous across the boundaries. Knowing their values at $z = 0$, then from equation (18) we can get the values at $z = -D_1$.

$$\begin{aligned} F(0) &= S_\mathrm{r} + S_\mathrm{l} && (25)\\ G(0) &= \mathrm{i}n_1 \cos(\theta_1)(S_\mathrm{r} - S_\mathrm{l}) \\ F(-D_1) &= S_\mathrm{r}\mathrm{e}^{-\mathrm{i}n_1 k \cos(\theta_1) D_1} + S_\mathrm{l}\mathrm{e}^{\mathrm{i}n_1 k \cos(\theta_1) D_1} && (26)\\ G(-D_1) &= \mathrm{i}n_1 \cos(\theta_1)(S_\mathrm{r}\mathrm{e}^{-\mathrm{i}n_1 k \cos(\theta_1) D_1} - S_\mathrm{l}\mathrm{e}^{\mathrm{i}n_1 k \cos(\theta_1) D_1}) && (27) \end{aligned}$$

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

$$\begin{aligned} S_\mathrm{r} &= \frac{1}{2}(F(0) + \frac{G(0)}{\mathrm{i}n_1 \cos(\theta_1)}) && (28)\\ S_\mathrm{l} &= \frac{1}{2}(F(0) - \frac{G(0)}{\mathrm{i}n_1 \cos(\theta_1)}) && (29) \end{aligned}$$

we arrive at the following matrix equation:

$$\begin{pmatrix} F(-D_1) \\ G(-D_1) \end{pmatrix} = M_{1,s} \begin{pmatrix} F(0) \\ G(0) \end{pmatrix} \tag{30}$$

with

$$M_{1,s} = \begin{pmatrix} \cos(n_1 k \cos(\theta_1) D_1) & -\frac{1}{n_1 \cos(\theta_1)} \sin(n_1 k \cos(\theta_1) D_1) \\ n_1 \cos(\theta_1) \sin(n_1 k \cos(\theta_1) D_1) & \cos(n_1 k \cos(\theta_1) D_1) \end{pmatrix} \tag{31}$$

The matrix is the transfer matrix which gives the name to the method. If there is a second layer with n_2, D_2, the combined matrix is $M_2 M_1$, and so on. On top of the uppermost layer, there is air or vacuum, and

$$\begin{aligned} S_\mathrm{r}(z) &= \frac{1}{2}F(z) + \frac{1}{2\mathrm{i}\cos(\theta)}G(z) \\ S_\mathrm{l}(z) &= \frac{1}{2}F(z) - \frac{1}{2\mathrm{i}\cos(\theta)}G(z) \end{aligned} \tag{32}$$

In the substrate, there is only an outgoing amplitude S_r which may arbitrarily chosen and is given the value 1.

The reflection coefficient is given by

$$R_s(\theta) = \left| \frac{S_\mathrm{l}(z)}{S_\mathrm{r}(z)} \right|^2 \tag{33}$$

and the transmission is $1 - R_s(\theta)$, as there is no absorption.

The p-polarisation

Equations (22, 23) show that now the quantities

$$\begin{aligned} F(z) &:= \cos(\theta_1)E_p(z) = \cos(\theta_1)(P_\mathrm{r}(z) + P_\mathrm{l}(z)) \quad \text{and} \\ G(z) &:= \frac{1}{k\cos(\theta_1)}\frac{\partial}{\partial z}E_p(z) = \mathrm{i}n_1(P_\mathrm{r}(z) - P_\mathrm{l}(z)) \end{aligned} \tag{34}$$

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

$$\begin{pmatrix} F(-D_1) \\ G(-D_1) \end{pmatrix} = M_{1,p} \begin{pmatrix} F(0) \\ G(0) \end{pmatrix} \tag{35}$$

with

$$M_{1,p} = \begin{pmatrix} \cos(n_1 k\cos(\theta_1)D_1) & -\frac{\cos(\theta_1)}{n_1}\sin(n_1 k\cos(\theta_1)D_1) \\ \frac{n_1}{\cos(\theta_1)}\sin(n_1 k\cos(\theta_1)D_1) & \cos(n_1 k\cos(\theta_1)D_1) \end{pmatrix} \tag{36}$$

The amplitudes are recovered by

$$\begin{aligned} P_{\mathrm{r}}(z) &= \frac{1}{2\cos(\theta)}F(z) - \frac{\mathrm{i}}{2}G(z) \\ P_{\mathrm{l}}(z) &= \frac{1}{2\cos(\theta)}F(z) + \frac{\mathrm{i}}{2}G(z) \end{aligned} \tag{37}$$

The reflection coefficient is given by

$$R_p(\theta) = \left| \frac{P_{\mathrm{l}}(z)}{P_{\mathrm{r}}(z)} \right|^2 \tag{38}$$

and the transmission is $1 - R_p(\theta)$.

Unpolarised light

In this case, we have

$$R(\theta) = \frac{1}{2}\left(R_s(\theta) + R_p(\theta)\right) . \tag{39}$$

Including Absorption

The geometry is assumed to be the same as before; now only the most important case of normal incidence is treated, i.e. $\theta = 0$.

We denote by n_0 the refractive index of the substrate, by κ_0 its extinction coefficient. Both quantities may be combined to the complex index of refraction

$$\tilde{n}_0 = n_0 + \mathrm{i}\kappa_0 . \tag{40}$$

The refractive index of the first transparent layer is denoted by $\tilde{n}_1$. By admitting a complex value, we can also deal with absorbing layers.

The electric field of the incident plane wave in the vacuum together with the reflected wave is given by equations (1, 2).

For the field in the first layer we write

$$E_x(z) = A_1 \mathrm{e}^{\mathrm{i}\tilde{n}_1 kz} + A_2 \mathrm{e}^{-\mathrm{i}\tilde{n}_1 kz} \tag{41}$$

and that in the substrate is written as

$$E_x(z) = \mathrm{e}^{\mathrm{i}\tilde{n}_0 kz} \tag{42}$$

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

At the boundaries between different layers the electric field E_x and its partial derivative $\frac{\partial E_x}{\partial z}$ are continuous, therefore F and G are defined as before in eq. (24):

$$F(z) := E_s(z) \quad \text{and} \quad G(z) := \frac{1}{k}\frac{\partial}{\partial z}E_s(z) \tag{43}$$

and we have now

$$\begin{aligned} F(0) &= A_\mathrm{r} + A_\mathrm{l} && (44) \\ G(0) &= \mathrm{i}\tilde{n}_1(A_\mathrm{r} - A_\mathrm{l}) \\ F(-D_1) &= A_\mathrm{r}\mathrm{e}^{-\mathrm{i}\tilde{n}_1 kD_1} + A_\mathrm{l}\mathrm{e}^{\mathrm{i}\tilde{n}_1 kD_1} && (45) \\ G(-D_1) &= \mathrm{i}\tilde{n}_1(A_\mathrm{r}\mathrm{e}^{-\mathrm{i}\tilde{n}_1 kD_1} - A_\mathrm{l}\mathrm{e}^{\mathrm{i}\tilde{n}_1 kD_1}) && (46) \end{aligned}$$

Expressing A_r and A_l through $F(0)$ and $G(0)$

$$\begin{aligned} A_\mathrm{r} &= \frac{1}{2}(F(0) + \frac{G(0)}{\mathrm{i}\tilde{n}_1}) && (47) \\ A_\mathrm{l} &= \frac{1}{2}(F(0) - \frac{G(0)}{\mathrm{i}\tilde{n}_1}) && (48) \end{aligned}$$

we arrive at the matrix equation:

$$\begin{pmatrix} F(-D_1) \\ G(-D_1) \end{pmatrix} = M_1 \begin{pmatrix} F(0) \\ G(0) \end{pmatrix} \tag{49}$$

with

$$M^{(1)} = \begin{pmatrix} \cos(\tilde{n}_1 kD_1) & -\frac{1}{\tilde{n}_1}\sin(\tilde{n}_1 kD_1) \\ \tilde{n}_1 \sin(\tilde{n}_1 kD_1) & \cos(\tilde{n}_1 kD_1) \end{pmatrix} \tag{50}$$

The matrix looks simpler than those obtained before, but it is not, because it is no longer real. If there is a second layer with n_2, D_2, there is a similar matrix M_2, and so on. On top of the uppermost layer, there is air or vacuum, and

$$\begin{aligned} A_\mathrm{r}(z) &= \frac{1}{2}F(z) + \frac{1}{2\mathrm{i}}G(z) \\ A_\mathrm{l}(z) &= \frac{1}{2}F(z) - \frac{1}{2\mathrm{i}}G(z) \end{aligned} \tag{51}$$

In the substrate, there is only an outgoing amplitude S_r which may arbitrarily chosen and is given the value 1.

The reflection coefficient is given by

$$R_s(\theta) = \left| \frac{S_\mathrm{l}(z)}{S_\mathrm{r}(z)} \right|^2 \tag{52}$$

While it is not difficult to implement the above equations using complex algebra, if the aim is a PostScript figure, real and imaginary parts must be separated, as complex numbers are not defined in PostScript. We therefore rewrite eq. (50) as

$$M^{(1)} = \begin{pmatrix} \frac{1}{2}(\mathrm{e}^{\mathrm{i}\tilde{n}_1 kD_1} + \mathrm{e}^{-\mathrm{i}\tilde{n}_1 kD_1}) & -\frac{1}{2\mathrm{i}\tilde{n}_1}(\mathrm{e}^{\mathrm{i}\tilde{n}_1 kD_1} - \mathrm{e}^{-\mathrm{i}\tilde{n}_1 kD_1}) \\ \frac{\tilde{n}_1}{2\mathrm{i}}(\mathrm{e}^{\mathrm{i}\tilde{n}_1 kD_1} - \mathrm{e}^{-\mathrm{i}\tilde{n}_1 kD_1}) & \frac{1}{2}(\mathrm{e}^{\mathrm{i}\tilde{n}_1 kD_1} + \mathrm{e}^{-\mathrm{i}\tilde{n}_1 kD_1}) \end{pmatrix} \tag{53}$$

$$\begin{aligned} M^{(1)}_{1,1} = M^{(1)}_{2,2} &= \frac{1}{2}\Big(\mathrm{e}^{-\kappa_1 kD_1}(\cos(n_1 kD_1) + \mathrm{i}\sin(n_1 kD_1)) \\ &\quad + \mathrm{e}^{\kappa_1 kD_1}(\cos(n_1 kD_1) - \mathrm{i}\sin(n_1 kD_1))\Big) \end{aligned} \tag{54}$$

$$M_{1,2}^{(1)} = \frac{\mathrm{i}n_1 + \kappa_1}{2(n_1^2 + \kappa_1^2)} \Big(\mathrm{e}^{-\kappa_1 k D_1} (\cos(n_1 k D_1) + \mathrm{i} \sin(n_1 k D_1)) - \mathrm{e}^{\kappa_1 k D_1} (\cos(n_1 k D_1) - \mathrm{i} \sin(n_1 k D_1)) \Big) \tag{55}$$

$$M_{2,1}^{(1)} = \frac{-\mathrm{i}n_1 + \kappa_1}{2} \Big(\mathrm{e}^{-\kappa_1 k D_1} (\cos(n_1 k D_1) + \mathrm{i} \sin(n_1 k D_1)) - \mathrm{e}^{\kappa_1 k D_1} (\cos(n_1 k D_1) - \mathrm{i} \sin(n_1 k D_1)) \Big) \tag{56}$$

We now write

$$M^{(1)} = M^{(1,\mathrm{re})} + \mathrm{i} M^{(1,\mathrm{im})} \tag{57}$$

and have

$$M_{1,1}^{(1,\mathrm{re})} = M_{2,2}^{(1,\mathrm{re})} = \cos(n_1 k D_1) \cosh(\kappa_1 k D_1)$$

$$M_{1,1}^{(1,\mathrm{im})} = M_{2,2}^{(1,\mathrm{im})} = -\sin(n_1 k D_1) \sinh(\kappa_1 k D_1)$$

$$\begin{aligned} M_{1,2}^{(1,\mathrm{re})} &= -\frac{\kappa_1}{n_1^2 + \kappa_1^2} \cos(n_1 k D_1) \sinh(\kappa_1 k D_1) \\ &\quad - \frac{n_1}{n_1^2 + \kappa_1^2} \sin(n_1 k D_1) \cosh(\kappa_1 k D_1) \end{aligned}$$

$$\begin{aligned} M_{1,2}^{(1,\mathrm{im})} &= -\frac{n_1}{n_1^2 + \kappa_1^2} \cos(n_1 k D_1) \sinh(\kappa_1 k D_1) \\ &\quad + \frac{\kappa_1}{n_1^2 + \kappa_1^2} \sin(n_1 k D_1) \cosh(\kappa_1 k D_1) \end{aligned}$$

$$\begin{aligned} M_{2,1}^{(1,\mathrm{re})} &= -\kappa_1 \cos(n_1 k D_1) \sinh(\kappa_1 k D_1) \\ &\quad + n_1 \sin(n_1 k D_1) \cosh(\kappa_1 k D_1) \end{aligned}$$

$$M_{2,1}^{(1,\mathrm{im})} = n_1 \cos(n_1 k D_1) \sinh(\kappa_1 k D_1) + \kappa_1 \sin(n_1 k D_1) \cosh(\kappa_1 k D_1) \tag{58}$$