www.itp.uni-hannover/~ zawischa/ITP/computecolour.html

The Colours of Thin Films

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The derivation of an expression for the reflectivity of a transparent film on a substrate is sketched. This can be used to compute the colours. For simplicity, only the case of perpendicular incidence of the light is considered. The substrate may be a metal or a dielectric.

Dielectric film on metal substrate

Assume that the surface of the substrate is the plane z = 0, and the *z*-axis is pointing into it. The substrate is covered by a transparent dielectric layer of thickness *D*.

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

$$\tilde{n} = n + \mathrm{i}\kappa \ . \tag{1}$$

The refractive index of the transparent layer is denoted by n_1 .

The electric field of the incident plane wave together with the reflected wave is assumed to oscillate in *x*-direction and is written as

$$E_x(z,t) = A_3 e^{i(kz-\omega t)} + A_4 e^{i(-kz-\omega t)}$$
⁽²⁾

where

$$k = \frac{2\pi}{\lambda} , \qquad (3)$$

 λ being the wavelength (in air or vacuum). A_3 and A_4 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

$$R = \left|\frac{A_4}{A_3}\right|^2 \,. \tag{4}$$

For the field in the dielectric layer we write

$$E_{x}(z,t) = A_{1}e^{i(n_{1}kz-\omega t)} + A_{2}e^{i(-n_{1}kz-\omega t)}$$
(5)

and, finally, that in the substrate is written as

$$E_x(z,t) = e^{i(\tilde{n}kz - \omega t)}$$
(6)

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

At the boundaries z = 0 and z = -D the electric field E_x and its partial derivative $\frac{\partial E_x}{\partial z}$ are continuous, which leads to the equations

$$A_1 + A_2 = 1 (7)$$

$$n_1 A_1 - n_1 A_2 = \tilde{n} \tag{8}$$

at z = 0 and

$$A_3 e^{-ikD} + A_4 e^{ikD} = A_1 e^{-ikn_1D} + A_2 e^{ikn_1D}$$
(9)

$$A_3 e^{-ikD} - A_4 e^{ikD} = n_1 A_1 e^{-ikn_1 D} - n_1 A_2 e^{ikn_1 D}$$
(10)

at z = -D. As in equation (4) only the ratio of A_4 over A_3 occurs, we could omit constant overall factors, but in view of later generalisations this is not done now. We thus get

$$2n_1A_1 = n_1 + \tilde{n} \tag{11}$$

$$2n_1A_2 = n_1 - \tilde{n} \tag{12}$$

and, re-defining $A_3 e^{-ikD} =: A'_3$ and $A_4 e^{ikD} =: A'_4$,

$$2n_1(A'_3 + A'_4) = (n_1 + \tilde{n})e^{-ikn_1D} + (n_1 - \tilde{n})e^{ikn_1D}$$
(13)

$$2n_1(A'_3 - A'_4) = n_1(n_1 + \tilde{n})e^{-ikn_1D} - n_1(n_1 - \tilde{n})e^{ikn_1D}$$
(14)

Solving these equations and separating real and imaginary parts, we obtain

$$4n_1A'_3 = (1+n)n_1\cos(kn_1D) + \kappa\sin(kn_1D) +i\left(n_1\kappa\cos(kn_1D) - (n_1^2+n)\sin(kn_1D)\right)$$
(15)

$$4n_1A'_4 = (1-n)n_1\cos(kn_1D) + \kappa\sin(kn_1D) +i\left(-n_1\kappa\cos(kn_1D) + (n_1^2 - n)\sin(kn_1D)\right)$$
(16)

and finally

$$R = \left[\left((1-n)n_1 \cos(kn_1D) + \kappa \sin(kn_1D) \right)^2 + \left(-n_1\kappa \cos(kn_1D) + (n_1^2 - n)\sin(kn_1D) \right)^2 \right] \\ \cdot \left[\left((1+n)n_1 \cos(kn_1D) + \kappa \sin(kn_1D) \right)^2 + \left(n_1\kappa \cos(kn_1D) - (n_1^2 + n)\sin(kn_1D) \right)^2 \right]^{-1}$$
(17)

In the limiting case D = 0 and also in the case $n_1 = 1$ one gets the reflectivity of the pure metal surface. Or, if n = 1 and $\kappa = 0$, the reflectance of a transparent film.

The incident light is supposed to have the spectral distribution $S(\lambda)$ of blackbody radiation of temperature T = 6504 K, which is similar to the standard daylight D65, approximating the overcast sky. From Planck's formula we have

$$S(\lambda) \propto [\lambda^5 (\exp(\frac{hc}{\lambda k_{\rm B}T} - 1)]^{-1}$$
 (18)

where *h* is Planck's constant, *c* the velocity of light, and k_B Boltzmann's constant.

Multiplying $S(\lambda)$ by the reflectivity R, the colour stimulus $\phi(D, \lambda)$ for a given thickness D of the film is obtained. The rest of the computation follows the lines described in detail here: www.itp.uni-hannover.de/~zawischa/ITP/soapfilmcalc.pdf



Figure 1: A transparent film on a titanium substrate. The scale gives the optical thickness, i.e. the thickness in nm $(10^{-9}m)$ multiplied by the film's refractive index.

The figures 1 and 2 show examples. The refraction index of the dielectric was $n_1 = 1.5$, while experimental data for n and κ have been used, taken from http://refractiveindex.info/.



Figure 2: A transparent film on a copper substrate. The scale gives the optical thickness, i.e. the thickness in nm $(10^{-9}m)$ multiplied by the film's refractive index.

Metal film on dielectric substrate

If in equations (13, 14), \tilde{n} is assumed to be real, i.e. $\kappa = 0$ and n_1 is replaced by $\tilde{n}_1 = n_1 + i\kappa_1$, they hold for a metal film on a dielectric substrate, or in case of n = 1 for a free metal film, and may be used to obtain transmission and reflection coefficients.

The outgoing wave now is taken to be

$$E_x(z,t) = e^{i(nkz - \omega t)}$$
(19)

and the transmission then is

$$T = \frac{1}{|A_3'|^2} \,. \tag{20}$$

For A'_3 we get

$$4A'_{3} = (\tilde{n}_{1} + n + 1 + \frac{n}{\tilde{n}_{1}})e^{-i\tilde{n}_{1}kD} - (\tilde{n}_{1} - n - 1 + \frac{n}{\tilde{n}_{1}})e^{i\tilde{n}_{1}kD}$$
(21)

which, after separating real and imaginary parts, yields

$$2A'_{3} = \cosh(\kappa_{1}kD) \left(\cos(n_{1}kD)(n+1) + \sin(n_{1}kD)(\kappa_{1} - \frac{n\kappa_{1}}{n_{1}^{2} + \kappa_{1}^{2}}) \right) + \sinh(\kappa_{1}kD) \cos(n_{1}kD)(n_{1} + \frac{nn_{1}}{n_{1}^{2} + \kappa_{1}^{2}}) + i \left[\sinh(\kappa_{1}kD) \left(\cos(n_{1}kD)(\kappa_{1} - \frac{n\kappa_{1}}{n_{1}^{2} + \kappa_{1}^{2}}) - \sin(n_{1}kD)(n+1) \right) - \cosh(\kappa_{1}kD) \sin(n_{1}kD)(n_{1} + \frac{nn_{1}}{n_{1}^{2} + \kappa_{1}^{2}}) \right]$$
(22)

Similarly A'_4 is obtained:

$$2A'_{4} = \cosh(\kappa_{1}kD) \left(\cos(n_{1}kD)(1-n) - \sin(n_{1}kD)(\kappa_{1} + \frac{n\kappa_{1}}{n_{1}^{2} + \kappa_{1}^{2}}) \right) + \sinh(\kappa_{1}kD) \cos(n_{1}kD)(-n_{1} + \frac{nn_{1}}{n_{1}^{2} + \kappa_{1}^{2}}) - i \left[\sinh(\kappa_{1}kD) \left(\cos(n_{1}kD)(\kappa_{1} + \frac{n\kappa_{1}}{n_{1}^{2} + \kappa_{1}^{2}}) + \sin(n_{1}kD)(1-n) \right) + \cosh(\kappa_{1}kD) \sin(n_{1}kD)(-n_{1} + \frac{nn_{1}}{n_{1}^{2} + \kappa_{1}^{2}}) \right]$$
(23)

which allows to compute the reflection coefficient

$$R = \frac{|A_4'|^2}{|A_3'|^2} \,. \tag{24}$$

Equations (20) and (24) have been used to obtain figure 3.



Figure 3: Transmission (red line) and remission (black line) of a gold foil. The remission of bulk gold is also shown (grey line). Experimental Data of n and κ from http://refractiveindex.info/