Electronic supplementary information: computation of reflectance spectra

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In this manuscript, reflectivities are calculated using the matrix methods for stratified systems [1–4]. These formulae have been implemented in a self-developed computer program [5]. For an overview, we here reproduce the essential equations needed for computation, without giving any derivations, following the treatment of Schubert [4].

Now, consider a stratisfied system, consisting of homogeneous layers, each with thickness d_j and complex permittivity $\epsilon_j = m_j^2$, where m_j is the complex refractive index of the respective layer. Light is incident on the stack through a medium of incidence with complex refractive index m_a under an angle ϕ, passes the stack, and exits through an exit medium with refractive index m_f.

For each wavelength, the complex amplitudes of the partial waves with s- and p-polarisations in the exit medium, C_s and C_p, are related to the corresponding amplitudes of the incident wave, A_s and A_p as well as the amplitudes of the reflected waves in the incident medium, B_s and B_p, through a transfer matrix $\hat{T}$,

$$\begin{pmatrix} A_s \\ B_s \\ A_p \\ B_p \end{pmatrix} = \hat{T} \begin{pmatrix} C_s \\ 0 \\ C_p \\ 0 \end{pmatrix} . \tag{1}$$

In each layer, a partial transfer matrix $\hat{T}_{i,p}$ connects the in-plane electric field components from the interface at the side of incidence to the field components at the interface on the exit side. Introducing incident $\hat{L}_a$ and exit matrix $\hat{L}_f$, $\hat{T}$ of a system with N layers is obtained as

$$\hat{T} = \hat{L}_a^{-1} \prod_{j=1}^{N} \hat{T}_{j,p}(-d_i) \hat{L}_f \, . \tag{2}$$

Here, we are considering isotropic layers only. A derivation for the general case can be found elsewhere [4]. With

$$q_j = \sqrt{m_j^2 - m_a^2 \sin^2(\phi)} \tag{3}$$

and a definition of the wave vector of the incoming wave in vacuum $k_0 = 2\pi/\lambda_0$ with the wavelength λ_0 of the incident light in vacuum, the partial transfer matrix $\hat{T}_{j,p}$ is obtained as

$$\hat{T}_{j,p} = \begin{pmatrix} \cos(k_0 d_j q_j) & 0 & 0 & i\frac{q_j}{\epsilon_j}\sin(k_0 d_j q_j) \\ 0 & \cos(k_0 d_j q_j) & -\frac{i}{q_j}\sin(k_0 d_j q_j) & 0 \\ 0 & -i q_j \sin(k_0 d_j q_j) & \cos(k_0 d_j q_j) & 0 \\ i\frac{\epsilon_j}{q_j}\sin(k_0 d_j q_j) & 0 & 0 & \cos(k_0 d_j q_j) \end{pmatrix} . \tag{4}$$

The incident matrix $\hat{L}_a^{-1}$ is given as

$$\hat{L}_a^{-1} = \frac{1}{2}\begin{pmatrix} 0 & 1 & -\left[m_a \cos(\phi)\right]^{-1} & 0 \\ 0 & 1 & \left[m_a \cos(\phi)\right]^{-1} & 0 \\ \cos(\phi)^{-1} & 0 & 0 & m_a^{-1} \\ -\cos(\phi)^{-1} & 0 & 0 & m_a^{-1} \end{pmatrix}. \tag{5}$$

The exit matrix $\hat{L}_f$ is

$$\hat{L}_f = \begin{pmatrix} 0 & 0 & \cos(\psi) & 0 \\ 1 & 0 & 0 & 0 \\ -n_f \cos(\psi) & 0 & 0 & 0 \\ 0 & 0 & n_f & 0 \end{pmatrix}, \tag{6}$$

where

$$\cos\psi = \sqrt{1 - \left[\frac{m_a}{m_f}\sin(\phi)\right]^2}. \tag{7}$$

After computation of the total transfer matrix using Eq. 2, the reflectivities can be computed from the matrix elements of $\hat{T}$. The reflectivity R_s of the system with s-polarisation is obtained as

$$R_s = \left|\frac{B_s}{A_s}\right|^2 = \left|\frac{T_{21}}{T_{11}}\right|^2, \tag{8}$$

while the reflectivity R_p for p-polarisation is

$$R_p = \left|\frac{B_p}{A_p}\right|^2 = \left|\frac{T_{43}}{T_{33}}\right|^2. \tag{9}$$

For computations of spectra, wavelength-dependent optical constants have been implemented and used [5].

It should be noted that the original formulation by Schubert contains minor errors, which have been corrected [6].

References

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