Supplemental equations

Calculation of spectral optical constants using combined ellipsometric and reflectance methods for smooth and rough bulk samples

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Equations S.1: n and k from ellipsometric measurements

When n_i is purely real, the spectra of the optical constants n and k are calculated analytically in the ellipsometric method with

$$\tilde{n} = n + jk = A\sqrt{B + jC} \tag{S.1a}$$

$$n = A\sqrt{\left(\sqrt{B^2 + C^2} + B\right)/2} \tag{S.1b}$$

$$k = A\sqrt{\left(\sqrt{B^2 + C^2} - B\right)/2} \tag{S.1c}$$

$$A = n_i \sin\theta_i \tag{S.1d}$$

$$B = X^2 + Y^2 - Z^2 \tag{S.1e}$$

$$C = -2\,Y\,Z \tag{S.1f}$$

$$X = 1 \tag{S.1g}$$

$$Y = \frac{\tan\theta_i\left(1 - \tan^2\Psi_{p/s\,\mathrm{meas}}\right)}{1 + \tan^2\Psi_{p/s\,\mathrm{meas}} + 2\tan\Psi_{p/s\,\mathrm{meas}}\cos\Delta_{p/s\,\mathrm{meas}}} \tag{S.1h}$$

$$Z = \frac{2\,\tan\theta_i\,\tan\Psi_{p/s\,\mathrm{meas}}\,\sin\Delta_{p/s\,\mathrm{meas}}}{1 + \tan^2\Psi_{p/s\,\mathrm{meas}} + 2\tan\Psi_{p/s\,\mathrm{meas}}\cos\Delta_{p/s\,\mathrm{meas}}} \tag{S.1i}$$

Equations S.2: $R_{s\,\mathrm{sim}}$ and $R_{p\,\mathrm{sim}}$

For the perfectly flat and smooth surface of a bulk, homogeneous, and isotropic sample (r_s and r_p described with Eqs. 6 and 8 from the main paper), and when n_i is purely real, the reflectance simulations $R_{s\,\mathrm{sim}}$ and $R_{p\,\mathrm{sim}}$ are calculated with

$$r_s = |r_s|\,e^{j\Delta_s} = \frac{\alpha_s - \sqrt{\beta_s + j\gamma_s}}{\alpha_s + \sqrt{\beta_s + j\gamma_s}} \tag{S.2a}$$

$$r_p = |r_p|\,e^{j\Delta_p} = \frac{\alpha_p + j\gamma_p - \sqrt{\beta_s + j\gamma_s}}{\alpha_p + j\gamma_p + \sqrt{\beta_s + j\gamma_s}} \tag{S.2b}$$

$$R_{s\,\mathrm{sim}} = |r_s|^2 = \frac{\alpha_s^2 + \sqrt{\beta_s^2 + \gamma_s^2} - \alpha_s\delta_1}{\alpha_s^2 + \sqrt{\beta_s^2 + \gamma_s^2} + \alpha_s\delta_1} \tag{S.2c}$$

$$R_{p\,\mathrm{sim}} = |r_p|^2 = \frac{\alpha_p^2 + \gamma_p^2 + \sqrt{\beta_s^2 + \gamma_s^2} - (\alpha_p\delta_1 + \gamma_p\delta_2)}{\alpha_p^2 + \gamma_p^2 + \sqrt{\beta_s^2 + \gamma_s^2} + (\alpha_p\delta_1 + \gamma_p\delta_2)} \tag{S.2d}$$

$$\alpha_s = n_i\cos\theta_i \tag{S.2e}$$

$$\alpha_p = (n^2 - k^2)\cos\theta_i/n_i \tag{S.2f}$$

$$\beta_s = n^2 - k^2 - n_i^2\sin^2\theta_i \tag{S.2g}$$

$$\gamma_s = 2\,n\,k \tag{S.2h}$$

$$\gamma_p = 2\,n\,k\cos\theta_i/n_i \tag{S.2i}$$

$$\delta_1 = \sqrt{2\left(\sqrt{\beta_s^2 + \gamma_s^2} + \beta_s\right)} \tag{S.2j}$$

$$\delta_2 = \sqrt{2\left(\sqrt{\beta_s^2+\gamma_s^2}-\beta_s\right)} \tag{S.2k}$$

where n and k are calculated using Eqs. S.1.

Equations S.3: n' and k' from reflectance measurement

When n_i is purely real, the adjusted spectra of the optical constants n' and k' can be calculated analytically in the single-angle reflectance method with

$$\tilde{n}' = n' + jk' = A_s\sqrt{B_s + jC_s} \tag{S.3a}$$

$$n' = A_s\sqrt{\left(\sqrt{B_s^2+C_s^2}+B_s\right)/2} \tag{S.3b}$$

$$k' = A_s\sqrt{\left(\sqrt{B_s^2+C_s^2}-B_s\right)/2} \tag{S.3c}$$

$$A_s = n_i \tag{S.3d}$$

$$B_s = X_s^2 + Y_s^2 - Z_s^2 \tag{S.3e}$$

$$C_s = -2\,Y_s Z_s \tag{S.3f}$$

$$X_s = \sin\theta_i \tag{S.3g}$$

$$Y_s = \frac{\cos\theta_i\,(1-R_s')}{1+R_s'+2\sqrt{R_s'}\cos\Delta_s} \tag{S.3h}$$

$$Z_s = \frac{2\,\cos\theta_i\,\sqrt{R_s'}\,\sin\Delta_s}{1+R_s'+2\sqrt{R_s'}\cos\Delta_s} \tag{S.3i}$$

Equation S.4: Δ_s from n and k

Assuming a purely real value for n_i and using the nomenclature defined in Eqs. S.2, Δ_s can be calculated analytically from n and k with

$$\Delta_s = \arctan\left(\frac{-\alpha_s\delta_2}{\alpha_s^2-\sqrt{\beta_s^2+\gamma_s^2}}\right) \tag{S.4}$$

Equations S.5: $\Psi_{p/s}$ and $\Delta_{p/s}$ from n' and k'

Assuming a purely real value for n_i, adjusted simulations of $\Psi_{p/s}$ and $\Delta_{p/s}$ can be calculated analytically from n' and k' with

$$\tan\Psi_{p/s}\,e^{j\Delta_{p/s}} = \frac{\alpha-\sqrt{\beta+j\gamma}}{\alpha+\sqrt{\beta+j\gamma}} \tag{S.5a}$$

$$\tan\Psi_{p/s} = \left[\frac{\alpha^2+\sqrt{\beta^2+\gamma^2}\;-\;\alpha\sqrt{2\left(\sqrt{\beta^2+\gamma^2}+\beta\right)}}{\alpha^2+\sqrt{\beta^2+\gamma^2}\;+\;\alpha\sqrt{2\left(\sqrt{\beta^2+\gamma^2}+\beta\right)}}\right]^{\frac{1}{2}} \tag{S.5b}$$

$$\Delta_{p/s} = \arctan\left\{\frac{-\alpha\sqrt{2\left(\sqrt{\beta^2+\gamma^2}-\beta\right)}}{\alpha^2-\sqrt{\beta^2+\gamma^2}}\right\} \tag{S.5c}$$

$$\alpha = n_i\sin\theta_i\tan\theta_i \tag{S.5d}$$

$$\beta = (n')^2-(k')^2-n_i^2\sin^2\theta_i \tag{S.5e}$$

$$\gamma = 2\,n'\,k' \tag{S.5f}$$