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INTERFERENCE, REFLECTANCE & TRANSMITTANCE FOR THIN FILMS

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How to measure the absorbance of FTIR peaks in presence of fringes (oscillating baseline)?

Represent FTIR absorption peak by a Gaussian : $A\exp\left(-\frac{(\nu-\nu_0)^2}{\sigma^2}\right)$,

where A is the amplitude, ν_0 the wavenumber of the peak position, and
σ is the the wavenumber shift for which the absorption falls by a factor $1/e$.
The Full Width Half Maximum is given by $FWHM = 2\sigma\sqrt{\ln 2}$
The area under the peak $= A\sigma\sqrt{\pi} \propto (A\sigma) \propto (A \times FWHM)$.

Suppose that the volume of 100% solid aSi is proportional to the area under
peak $\nu_0 = 2000$ cm^{-1} so that $V_{aSi} = S_{2000}(A\sigma)_{2000}$
where S_{2000} is the oscillator strength of the Si-H bond vibrations in the a-Si:H matrix.

Suppose that the volume of microvoids is given by $V_{void} = S_{2080}(A\sigma)_{2080}$
where S_{2080} is the oscillator strength of the Si-H bond vibrations in the internal voids.
(Dangerous, because 2080 cm^{-1} could be due to μc-Si:H. See Kroll thesis etc).

With these assumptions, define porosity as:

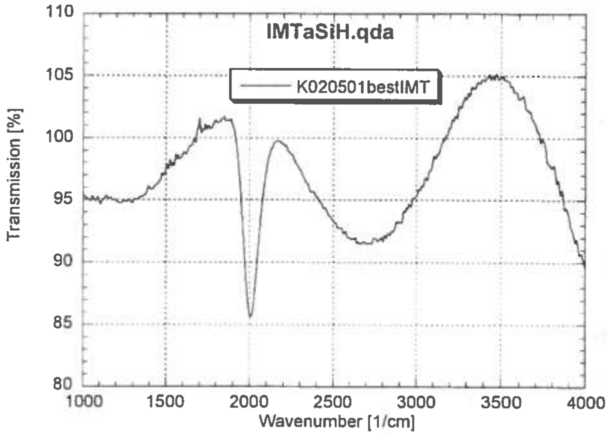
$$Porosity = \frac{\text{Vol. of microvoids}}{\text{Vol. of porous a-Si:H}} = \frac{\text{Vol. of microvoids}}{\text{Vol. of microvoids + Vol. of solid a-Si:H}}.$$

$$Porosity = \frac{1}{1+\frac{S_{2000}(A\sigma)_{2000}}{S_{2080}(A\sigma)_{2080}}}$$

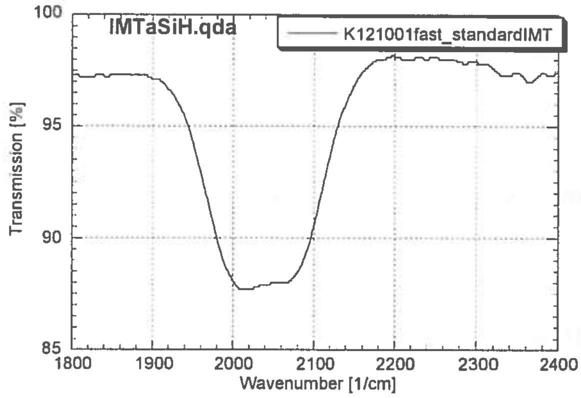
The unknown ratio $\frac{S_{2000}}{S_{2080}}$ could perhaps be estimated
by comparison with ellipsometric porosity.

NB The area under the peaks, even if baseline-corrected, does not give true absorption because the effective optical path in the absorbing substrate has changed.

Transmission aSiH on wafer / Transmission wafer



An example of peaks centred on 2000 and 2080 1/cm



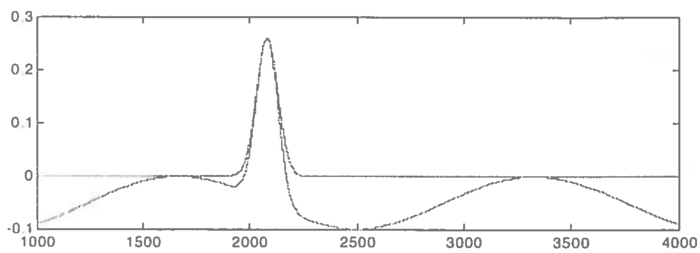
We need to understand the transmittance and absorbance for an absorbing film on an absorbing substrate

Where is the problem? Surely we just fit Gaussian curves and subtract a linear slope baseline.

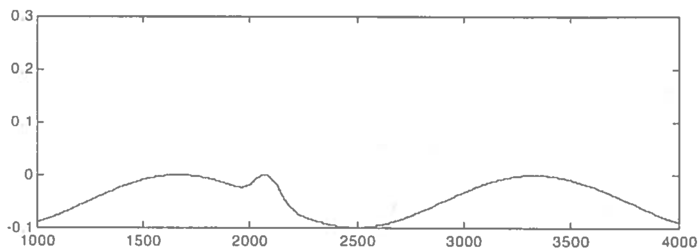
The basic problem is that *the baseline itself* will be changed at the peak positions, as explained below:
... the peak is there because there is absorption,
i.e. the peak is there because of a change in the refractive index of the film n+jk
i.e. the amplitude of the reflections in the substrate/film system will be changed by the change in n+jk
i.e. the absorbance of the *substrate and film* will be perturbed *at* the peak position
i.e. the baseline cannot be simply interpolated and subtracted from the peaks

green: model of an absorbance peak at 2080 1/cm.

red: simulated absorbance measurement of a 1µm a-Si:H film on a silicon substrate.



blue: demonstration of the change in baseline at the peak position.
The deviation of the baseline from the assumed, interpolated baseline gives an error in the peak area.



Basic revision of complex refractive index, starting from Maxwell's equations.
In contrast to most courses, we will NOT limit ourselves to transparent media (which have real refactive index).

$\nabla \times \underline{E} = -\frac{\partial B}{\partial t}$, for a plane-polarised (transverse) wave travelling along z axis: $\frac{\partial E_x}{\partial z} = -\mu \frac{\partial H_y}{\partial t}$, $(\mu = \mu_0 \mu_r)$ and

$\nabla \times \underline{H} = \underline{j} + \frac{\partial \underline{D}}{\partial t} = \sigma \underline{E} + \varepsilon \frac{\partial \underline{E}}{\partial t}$, for a plane-polarised wave along z: $-\frac{\partial H_y}{\partial z} = \varepsilon \frac{\partial E_x}{\partial t} + \sigma E_x$ $(\varepsilon = \varepsilon_0 \varepsilon_r)$.

Take a single Fourier component and try solutions of form $\exp\left[j\omega\left(\frac{nz}{c} - t\right)\right]$ for a wave travelling along +z,

where $\underline{n}$ is a complex refractive index. We now have:

$j\omega \frac{n}{c} E_x = j\omega\mu H_y$ and $-j\omega \frac{n}{c} H_y = (-j\omega\varepsilon + \sigma) E_x$ which are satisfied if $\underline{n}^2 = \mu_r \varepsilon_r + \frac{j\sigma\mu_r}{\omega\varepsilon_o}$.

Therefore $\underline{n = N + jK}$, where $N^2 - K^2 = \mu_r \varepsilon_r$ and $NK = \frac{\sigma\mu_r}{2\omega\varepsilon_o}$. (Note: if $\exp\left[j\omega\left(t - \frac{nz}{c}\right)\right]$, then $\underline{n} = N - jK$)

The intrinsic impedance of the medium is defined as $Z_0 = \frac{E_x}{H_y} = \frac{\mu c}{\underline{n}}$. (Note: free space impedance $= \mu_0 c = 376.7\Omega$)

(see Bleaney p235) Note: if we equivalently write $\nabla \times \underline{H} = \sigma \underline{E} + \varepsilon \frac{\partial \underline{E}}{\partial t} = \underline{\varepsilon} \frac{\partial \underline{E}}{\partial t}$, then $\underline{\varepsilon} = \underline{n}^2$

Basic revision of absorption index, absorption coefficient and absorbance.

From above, the electric field can be written as $\underline{E} = \underline{E_0} \exp\left[j\omega\left(\frac{nz}{c} - t\right)\right]$

$= \underline{E_0} \exp\left(-\frac{\omega K z}{c}\right) \exp\left[j\omega\left(\frac{Nz}{c} - t\right)\right] = \underline{E_0} \exp\left(-\frac{\omega K z}{c}\right) \exp\left[j(kz - \omega t)\right]$ (Note: if $\exp\left[j\omega\left(t - \frac{nz}{c}\right)\right]$, then $\underline{n} = N - jK$)

where $\frac{\omega N}{c} = \frac{\omega}{phase\ velocity} = k = \frac{2\pi}{\lambda}$ which is the wavenumber in the medium.

The wave intensity is proportional to the square of the amplitude (see below), therefore:

Intensity $= I(z) = I_0 \exp\left(-\frac{2\omega K z}{c}\right)$. Compare with the Lambert-Beer law: $I(z) = I_0 \exp(-\alpha z)$

Therefore, the <u>absorption coefficient</u> $\alpha = \underline{\left(\frac{2\omega K}{c}\right)}$.

$K = \mathrm{Im}(\underline{n})$, the imaginary part of the refractive index, is also called the <u>absorption index.</u>

The <u>absorbance</u> of a layer, thickness d, is defined as $\underline{\alpha d = \frac{2\omega K d}{c}}$.   (see Longhurst pp 493/4 & 503)

Basic revision of intensity and the Poynting vector.

Intensity I = Time-averaged value of instantaneous Poynting flux

$$I = \left\langle \underline{E}(\underline{r},t) \times \underline{H}(\underline{r},t) \right\rangle = \frac{1}{2}\mathrm{Re}\left(\underline{E}_0 \times \underline{H}_0^* \right)$$

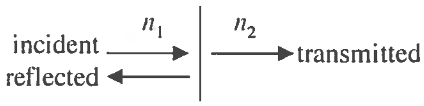
where $\underline{E}_0$ and $\underline{H}_0$ are complex amplitude vector functions of position (see Born & Wolf p33 for proof).

Using $\underline{Z}_0 = \frac{E_x}{H_y} = \frac{\mu c}{\underline{n}}$ from above, we obtain:

$$I = \frac{1}{2}\mathrm{Re}\left(\underline{E}_0 \times \underline{H}_0^* \right) = \frac{1}{2}\mathrm{Re}\left(\underline{E}_0 \cdot \frac{\underline{E}_0^*}{\underline{Z}_0^*} \right) = \frac{\left|\underline{E}_0\right|^2}{2}\mathrm{Re}\left(\frac{1}{\underline{Z}_0^*} \right)$$

$$\therefore \quad \underline{I = \frac{\left|\underline{E}_0\right|^2}{2c\mu_0}\mathrm{Re}(\underline{n}) = \frac{\left|\underline{E}_0\right|^2}{2c\mu_0} N} \quad \text{(assuming } \mu_r = 1\text{)}$$

Basic revision of Fresnel transmission & reflection coefficients; and transmittance and reflectance, at a single interface



For normal incidence (see, for example, Bleaney p244, Longhurst p522-3, Born & Wolf p630):

Complex amplitude reflection coefficient, $\underline{r}_{12} = \frac{E_0^{reflected}}{E_0^{incident}} = \left(\frac{\underline{n}_1 - \underline{n}_2}{\underline{n}_1 + \underline{n}_2} \right)$

Complex amplitude transmission coefficient, $\underline{t}_{12} = \frac{E_0^{transmitted}}{E_0^{incident}} = \left(\frac{2\underline{n}_1}{\underline{n}_1 + \underline{n}_2} \right)$

} Fresnel coeffts. are *true for every case.*

Reflectance, $R_{12} = \frac{\text{reflected power}}{\text{incident power}} = \frac{\left|E_0^{reflected}\right|^2 \mathrm{Re}(\underline{n}_1)}{\left|E_0^{incident}\right|^2 \mathrm{Re}(\underline{n}_1)} = \left|\underline{r}_{12}\right|^2 = \frac{(N_1 - N_2)^2 + (K_1 - K_2)^2}{(N_1 + N_2)^2 + (K_1 + K_2)^2}$

Transmittance, $T_{12} = \frac{\text{transmitted power}}{\text{incident power}} = \frac{\left|E_0^{transmitted}\right|^2 \mathrm{Re}(\underline{n}_2)}{\left|E_0^{incident}\right|^2 \mathrm{Re}(\underline{n}_1)} = \left|\underline{t}_{12}\right|^2 \frac{N_2}{N_1} = \frac{4\left(N_1^2 + K_1^2\right) N_2 / N_1}{(N_1 + N_2)^2 + (K_1 + K_2)^2}$

NOTE: There are no losses at the interface, BUT $R_{12} + T_{12} \neq 1$ UNLESS $K_1 = 0$!

REASON: Transmittance and reflectance are not uniquely defined in absorbing media! Salzberg, *Am.J.Phys.* **16** 444 (1948) & Macleod *"Thin-Film Optical Filters"* p42

MORAL: Use Fresnel coeffts. ONLY and, *at the end*, calculate transmittance & reflectance in transparent media.

DO NOT sum reflections of intensities in absorbing media!

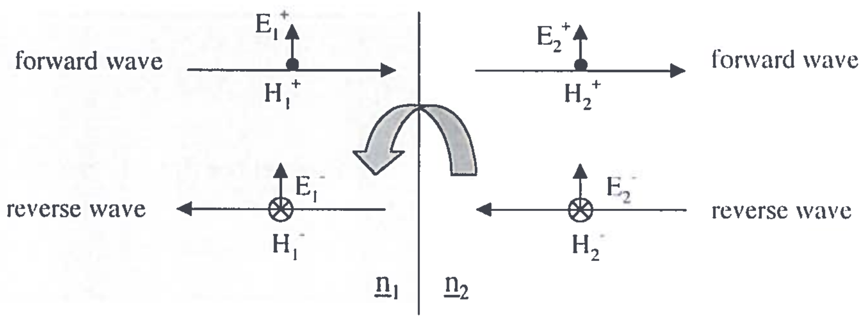
WARNING

We now consider a <u>general matrix treatment</u> for multi-layer structures.

But we will see that this general case gives the same result as the familiar '<u>infinite series of reflections</u>' calculation for a single layer on a substrate.

Do not panic.

Reflection and transmission of multilayer structures :- (A) The MATRIX technique.
following B. Harbecke, Appl. Phys. **B39** 165 (1986)



1) TRANSFORMATION OF E AMPLITUDE ACROSS AN INTERFACE

The fields represent the total, self - consistent amplitudes decomposed into forward and reverse travelling waves, they are not individual 'rays' or beams.

Continuity of tangential electric field at the interface: $E_1^+ + E_1^- = E_2^+ + E_2^-$

Continuity of magnetic field (using $H = E/Z_0 \propto E\underline{n}$): $\underline{n}_1 E_1^+ - \underline{n}_1 E_1^- = \underline{n}_2 E_2^+ - \underline{n}_2 E_2^-$ (NB H vectors are reversed)

Solve for E_1 in terms of E_2, and substitute t_{12} and r_{12} for combinations of the refractive indices:

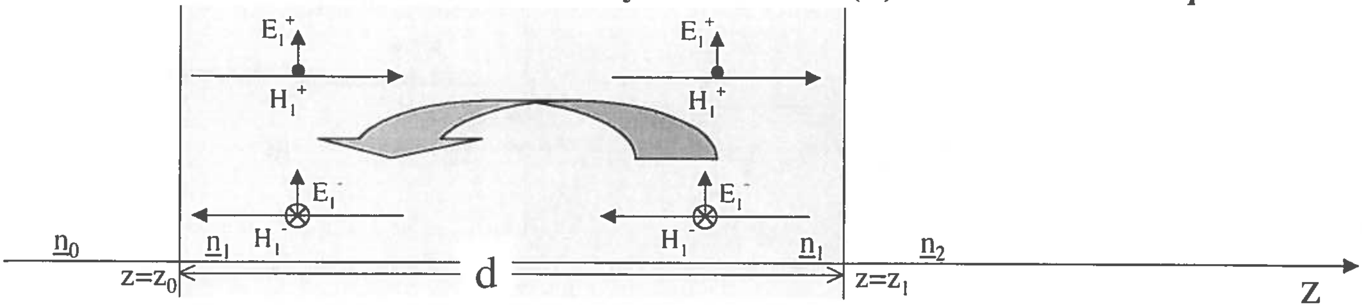
$E_1^+ = E_2^+ / t_{12} + r_{12} E_2^- / t_{12}$ and $E_1^- = r_{12} E_2^+ / t_{12} + E_2^- / t_{12}$

In matrix form:

$$\begin{bmatrix} E_1^+ \\ E_1^- \end{bmatrix} = \frac{1}{t_{12}} \begin{bmatrix} 1 & -r_{21} \\ r_{12} & 1 \end{bmatrix} \begin{bmatrix} E_2^+ \\ E_2^- \end{bmatrix}$$

which transforms E^+ and E^- across the interface from medium 2 back to medium 1.

Reflection and transmission of multilayer structures :- (A) The MATRIX technique.



2) TRANSFORMATION OF E AMPLITUDE THROUGH A SINGLE MEDIUM

For forward waves : $\underline{E}^+(z,t) = \underline{E}_0^+ \exp\left[j\omega\left(\frac{nz}{c} - t\right)\right]$, therefore :

$$\underline{E}^+(z_0,t) = \underline{E}_0^+ \exp\left[j\omega\left(\frac{nz_0}{c} - t\right)\right] = \underline{E}_0^+ \exp\left[-j\omega\frac{n(z_1 - z_0)}{c}\right]\exp\left[j\omega\left(\frac{nz_1}{c} - t\right)\right] = \exp\left(-\frac{j\omega nd}{c}\right)\underline{E}^+(z_1,t).$$

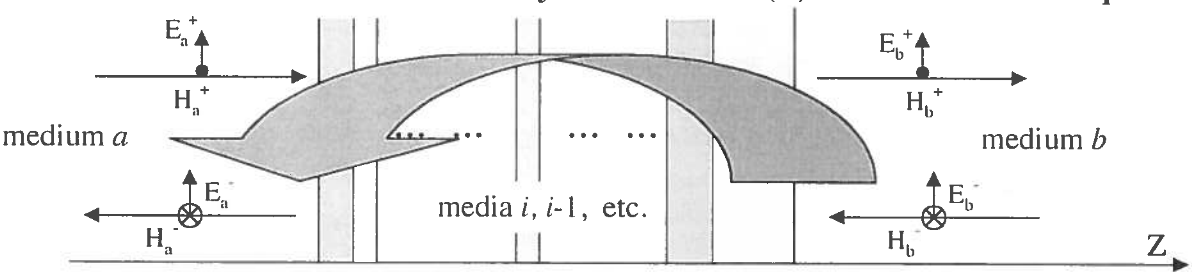
For reverse waves : $\underline{E}^-(z,t) = \underline{E}_0^- \exp\left[j\omega\left(-\frac{nz}{c} - t\right)\right]$, therefore :

$$\underline{E}^-(z_0,t) = \underline{E}_0^- \exp\left[j\omega\left(-\frac{nz_0}{c} - t\right)\right] = \underline{E}_0^- \exp\left[j\omega\frac{n(z_1 - z_0)}{c}\right]\exp\left[j\omega\left(-\frac{nz_1}{c} - t\right)\right] = \exp\left(\frac{j\omega nd}{c}\right)\underline{E}^-(z_1,t).$$

In matrix form, substituting complex phase factor $\varphi = \exp\left(\frac{j\omega nd}{c}\right)$:

$$\begin{bmatrix} E_1^+(z_0) \\ E_1^-(z_0) \end{bmatrix} = \begin{bmatrix} 1/\varphi & 0 \\ 0 & \varphi \end{bmatrix}\begin{bmatrix} E_1^+(z_1) \\ E_1^-(z_1) \end{bmatrix}$$ which transforms E^+ and E^- backwards across distance d in medium 1.

Reflection and transmission of multilayer structures :- (A) The MATRIX technique.



3) TRANSFORMATION OF E AMPLITUDE THROUGH A MULTI-LAYER

For transmission through any general system of m layers from a to b, there is no reverse wave in b:

$$\begin{bmatrix} E_a^+ \\ E_a^- \end{bmatrix} = [r_{a,1}, t_{a,1}][\varphi_1][r_{1,2}, t_{1,2}]\cdots[r_{i-1,i}, t_{i-1,i}][\varphi_i][r_{i,i+1}, t_{i,i+1}]\cdots[\varphi_m][r_{m,b}, t_{m,b}]\begin{bmatrix} E_b^+ \\ 0 \end{bmatrix} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}\begin{bmatrix} E_b^+ \\ 0 \end{bmatrix}.$$

Normalising by the incident amplitude E_a^+, we get : $\begin{bmatrix} 1 \\ r_{ab} \end{bmatrix} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}\begin{bmatrix} t_{ab} \\ 0 \end{bmatrix}$,

from which $M_{11} = 1/t_{ab}$ and $M_{21}/M_{11} = r_{ab}$.

Equivalently, going from b to a, we get : $\begin{bmatrix} 0 \\ t_{ba} \end{bmatrix} = \begin{bmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{bmatrix}\begin{bmatrix} r_{ba} \\ 1 \end{bmatrix}$,

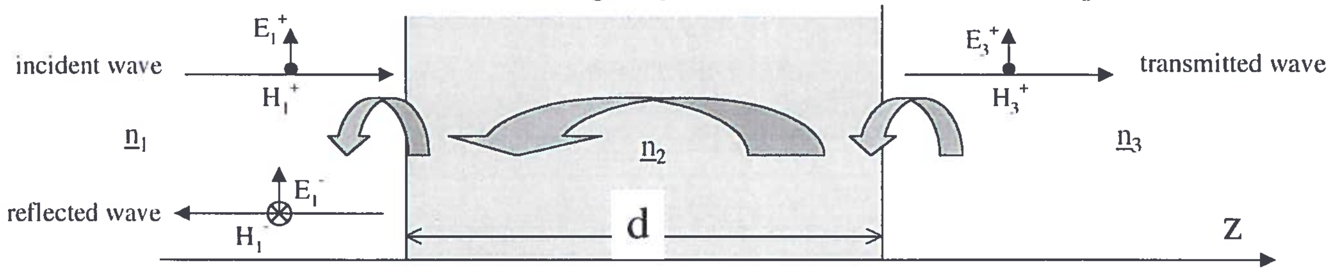
from which $M_{12}/M_{11} = -r_{ba}$ and $(M_{11}M_{22} - M_{12}M_{21})/M_{11} = t_{ba}$.

Now we know all the matrix elements in terms of reflection and transmission coefficients. Solve and substitute :

$$\begin{bmatrix} E_a^+ \\ E_a^- \end{bmatrix} = \frac{1}{t_{ab}}\begin{bmatrix} 1 & -r_{ba} \\ r_{ab} & (t_{ab}t_{ba} - r_{ab}r_{ba}) \end{bmatrix}\begin{bmatrix} E_b^+ \\ E_b^- \end{bmatrix}.$$ If front a & back b media are the same, then $\det(\underline{\underline{M}}) = 1$ & $t_{ab} = t_{ba}$;

but generally $r_{ab} \neq -r_{ba}$ (unless a and b are adjacent media (no layers!), for which $r_{ab} = -r_{ba}$ always).

Reflection and transmission of a single layer :- (A) The MATRIX technique.



4) TRANSFORMATION OF E AMPLITUDE BACKWARDS THROUGH A SINGLE LAYER

Now for a single layer, thickness d, index n_2, sandwiched between media of indices n_1 and n_3. From above :

$$\begin{bmatrix}1\\ r_{13}\end{bmatrix} = \frac{1}{t_{12}}\begin{bmatrix}1 & -r_{21}\\ r_{12} & 1\end{bmatrix}\begin{bmatrix}1/\varphi & 0\\ 0 & \varphi\end{bmatrix}\frac{1}{t_{23}}\begin{bmatrix}1 & -r_{32}\\ r_{23} & 1\end{bmatrix}\begin{bmatrix}t_{13}\\ 0\end{bmatrix}.$$

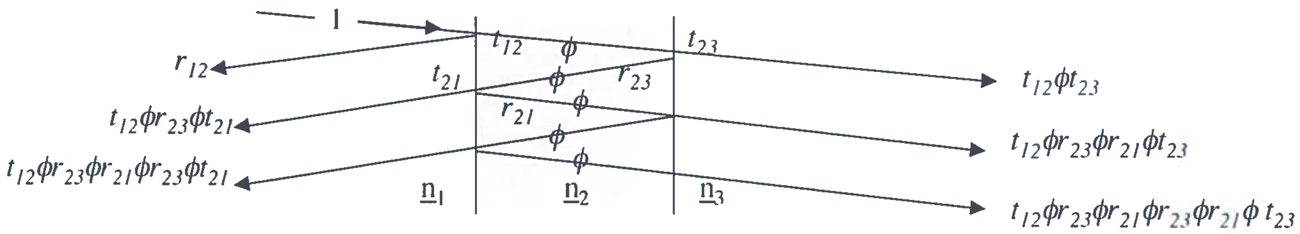
After straightforward multiplication we obtain :

Amplitude transmission coefficient, $t_{13} = \dfrac{t_{12}t_{23}\varphi}{1 - r_{21}r_{23}\varphi^2}$

Amplitude reflection coefficient, $r_{13} = r_{12} + \dfrac{t_{12}t_{21}r_{23}\varphi^2}{1 - r_{21}r_{23}\varphi^2}$

where complex phase factor $\varphi = \exp\left(\dfrac{j\omega nd}{c}\right)$.

Reflection and transmission of single layer :- (B) The INFINITE SERIES technique.



Amplitude transmission coefficient $t_{13} = t_{12}\varphi t_{23}\left\{1 + \left(r_{23}\varphi r_{21}\varphi\right) + \left(r_{23}\varphi r_{21}\varphi\right)^2 + \ldots\right\} = t_{12}\varphi t_{23}\sum_{p=0}^{\infty}\left(r_{23}r_{21}\varphi^2\right)^p$

$\therefore \underline{t_{13}} = \underline{\dfrac{t_{12}t_{23}\varphi}{1 - r_{21}r_{23}\varphi^2}}$ which is identical to the matrix method.

Note : $\varphi = \exp\left(\dfrac{j\omega nd}{c}\right)$ as before, used here to transform forwards.

Amplitude reflection coefficient $r_{13} = r_{12} + t_{12}\varphi r_{23}\varphi t_{21}\left\{1 + \left(r_{21}\varphi r_{23}\varphi\right) + \left(r_{21}\varphi r_{23}\varphi\right)^2 + \ldots\right\}$

$\therefore \underline{r_{13} = r_{12} + \dfrac{t_{12}t_{21}r_{23}\varphi^2}{1 - r_{21}r_{23}\varphi^2}}$ which is also identical to the matrix method.

CONCLUSION : Self - consistent result for matrix and infinite series methods but the 'infinite reflection' model is less elegant to generalise than the 'matrix method'.

PAUSE

Both methods give the same results for the ***amplitude*** coefficients of transmission & reflection.

Now we look at the ***intensities*** via the reflectance & transmittance, with
a) interference fringes, and
b) interference-free case
(Still for single layers only)

Reflectance and transmittance: a) interference fringes in a single, "coherent" absorbant layer.

From the p6 on Fresnel etc. (NB we assume the front and back layers are vacuum, $\underline{n}_1 = \underline{n}_3 = 1$):

Coherent Transmittance of the layer, $\left(T_{13}\right)_{\text{coh}} = \left|t_{13}\right|^2 \dfrac{\text{Re}(\underline{n}_3)}{\text{Re}(\underline{n}_1)} = \dfrac{t_{12}t_{23}\varphi}{1 - r_{21}r_{23}\varphi^2} \cdot \dfrac{t_{12}^* t_{23}^* \varphi^*}{1 - r_{21}^* r_{23}^* \left(\varphi^2\right)^*}$

$$= \frac{\left|t_{12}\right|^2 \left|t_{23}\right|^2 \exp(-\alpha d)}{1 + \left|r_{21}\right|^2 \left|r_{23}\right|^2 \exp(-2\alpha d) - 2\,\text{Re}\left[r_{21}r_{23}\varphi^2\right]}, \quad \text{since } \varphi^* \varphi = \exp\left(-2\omega K_2 d_2 / c\right) = \exp\left(-\alpha d_2\right).$$

To investigate the oscillatory term, we write $r_{21} = \left|r_{21}\right| \exp\left(j\delta_{r21}\right)$; also $\left|t_{12}\right|\left|t_{23}\right| = \left|t_{12}t_{23}\right|$:

$$\left(T_{13}\right)_{\text{coh}} = \frac{\left|t_{12}t_{23}\right|^2 \exp(-\alpha d)}{1 + \left|r_{21}r_{23}\right|^2 \exp(-2\alpha d) - 2\left|r_{21}r_{23}\right| \exp(-\alpha d) \cos\left(\theta + \delta_{r21} + \delta_{r23}\right)}, \quad \text{where } \theta = \frac{2\omega N_2 d_2}{c}.$$

This is the intensity of the transmitted light, with fringes, which would be observed with perfect resolution.

Similarly (*see pp18 - 19 for two treatments of complex amplitude reflection coefficient),

$$\left(R_{13}\right)_{\text{coh}} = \left|r_{13}\right|^2 = \left|r_{12}\right|^2 + \frac{\left|t_{12}t_{21}r_{23}\right|^2 \exp(-2\alpha d)}{1 + \left|r_{21}r_{23}\right|^2 \exp(-2\alpha d) - 2\left|r_{21}r_{23}\right| \exp(-\alpha d) \cos\left(\theta + \delta_{r21} + \delta_{r23}\right)} + 2\,\text{Re}\left[\frac{r_{12}^* t_{12} t_{21} r_{23} \varphi^2}{1 - r_{21}r_{23}\varphi^2}\right].$$

This is the intensity of the reflected light, with fringes, which would be observed with perfect resolution.

QUICK NOTE ON TAKING THE MAGNITUDE OF SUMS OF COMPLEX NUMBERS

The magnitude squared of $\left(\underline{a}+\underline{b}\right)$

$$= \left|\left(\underline{a}+\underline{b}\right)\right|^2$$
$$= \left(\underline{a}+\underline{b}\right)\left(\underline{a}+\underline{b}\right)^* = \left(\underline{a}+\underline{b}\right)\left(\underline{a}^*+\underline{b}^*\right)$$
$$= \left|\underline{a}\right|^2 + \left|\underline{b}\right|^2 + \underline{a}\cdot\underline{b}^* + \underline{a}^*\cdot\underline{b}$$
$$= \left|\underline{a}\right|^2 + \left|\underline{b}\right|^2 + \underline{a}\cdot\underline{b}^* + \left(\underline{a}\cdot\underline{b}^*\right)^*$$
$$= \left|\underline{a}\right|^2 + \left|\underline{b}\right|^2 + 2\,\mathrm{Re}\left[\underline{a}\cdot\underline{b}^*\right]$$

Write: $\underline{a} = \left|\underline{a}\right|\exp\left(j\delta_a\right)$

$$\therefore \left|\left(\underline{a}+\underline{b}\right)\right|^2 = \left|\underline{a}\right|^2 + \left|\underline{b}\right|^2 + 2\,\mathrm{Re}\left[\left|\underline{a}\right|\exp\left(j\delta_a\right)\left|\underline{b}\right|\exp\left(-j\delta_b\right)\right]$$
$$= \left|\underline{a}\right|^2 + \left|\underline{b}\right|^2 + 2\left|\underline{a}\right|\left|\underline{b}\right|\mathrm{Re}\left[\exp j\left(\delta_a-\delta_b\right)\right]$$
$$\therefore \left|\left(\underline{a}+\underline{b}\right)\right|^2 = \left|\underline{a}\right|^2 + \left|\underline{b}\right|^2 + 2\left|\underline{a}\right|\left|\underline{b}\right|\cos\left(\delta_a-\delta_b\right).$$

So $\left|\left(\underline{a}+\underline{b}\right)\right|^2$ is the same as $\left(a+b\right)^2 = a^2+b^2+2ab$ except for the factor $\cos\left(\delta_a-\delta_b\right)$ in the product.

Now consider what happens when the instrumental resolution is not high enough to resolve the fringes:

The intensities are convolved with a broad function; equivalent to taking the average over a fringe period. Note that this averaging conserves energy, since the convolved intensity is the power average of the fringes.

The result will be the interference-free intensity, due to a single "incoherent" layer.

NB We implicitly assume* that none of the refractive indices vary with wavenumber over a fringe period!

*this is OK for substrate fringes BUT not true if we average thin film fringes over Si, SiO_2, modes etc!

We will need the following 2 integrals:

$$1)\quad I1 = \frac{1}{2\pi}\int_{-\pi}^{\pi}\left(\frac{d\phi}{1+a^2\pm 2a\cos\phi}\right) = \left(\frac{1}{1-a^2}\right);\quad \left(\left|a\right|<1\right) \text{ or more generally:}$$

$$I1' = \frac{1}{2\pi}\int_{-\pi}^{\pi}\left(\frac{d\phi}{1\pm b\cos\phi}\right) = \frac{1}{\sqrt{\left(1-b^2\right)}};\quad \left(\left|b\right|<1\right)$$

$$2)\quad I2 = \frac{1}{2\pi}\int_{-\pi}^{\pi}\left(\frac{\exp\left(j\phi\right)d\phi}{1-\underline{A}\exp\left(j\phi\right)}\right) = \frac{1}{2\pi}\int_{-\pi}^{\pi}\left(\exp\left(j\phi\right)\left(1-\underline{A}\exp\left(j\phi\right)\right)^{-1}d\phi\right)$$

$$= \frac{1}{2\pi}\int_{-\pi}^{\pi}\left(\exp\left(j\phi\right)\left(1+\underline{A}\exp\left(j\phi\right)+\underline{A}^2\exp\left(2j\phi\right)+\ldots\right)d\phi\right)\ \left(\text{for } \left|\underline{A}\right|<1\right)$$
$$= 0$$

Reflectance and transmittance: b) interference-free intensities in a single, "incoherent" layer.

Taking the integral averages of the coherent intensities on p14, we directly obtain :

Incoherent Transmittance of the layer, $\left(T_{13}\right)_{incoh} = \left\langle |t_{13}|^2 \frac{\mathrm{Re}(\underline{n}_3)}{\mathrm{Re}(\underline{n}_1)} \right\rangle$; valid only for transparent media 1 and 3

$$\left(T_{13}\right)_{incoh} = \frac{|t_{12}t_{23}|^2 \exp(-\alpha d)}{1 - |r_{21}r_{23}|^2 \exp(-2\alpha d)},$$

where we have taken $\underline{n}_3 = N_3 = \underline{n}_1 = N_1$, for example, in vacuum.

same as Eq.(16) B. Harbecke, Appl. Phys. **B39** 165 (1986)

This is the intensity of the interference-free transmitted light, with low spectral resolution (or thick substrate).

Similarly, the Incoherent Reflectance of the layer is

$$\left(R_{13}\right)_{incoh} = \left\langle |r_{13}|^2 \frac{\mathrm{Re}(\underline{n}_1)}{\mathrm{Re}(\underline{n}_1)} \right\rangle = |r_{12}|^2 + \frac{|t_{12}t_{21}r_{23}|^2 \exp(-2\alpha d)}{1 - |r_{21}r_{23}|^2 \exp(-2\alpha d)},$$

valid only for transparent media 1 and 3

same as Eq.(17) B. Harbecke, Appl. Phys. **B39** 165 (1986)

This is the intensity of the interference-free reflected light, with low spectral resolution (or thick substrate).

NB notice we have not simply removed the oscillatory terms! The sign has also changed in the denominator!

*Simplification of complex amplitude reflection coefficient, in view of calculation of reflectance of a single layer :

NB All these expressions have been verified using *Testingr*13.*m*

Amplitude reflection coefficient, $r_{13} = r_{12} + \frac{t_{12}t_{21}r_{23}\varphi^2}{1 - r_{21}r_{23}\varphi^2}$ (rA)

$$r_{13} = \frac{r_{12}\left(1 - r_{21}r_{23}\varphi^2\right) + t_{12}t_{21}r_{23}\varphi^2}{1 - r_{21}r_{23}\varphi^2} = \frac{r_{12} + r_{23}\varphi^2\left(t_{12}t_{21} - r_{12}r_{21}\right)}{1 - r_{21}r_{23}\varphi^2} = \frac{r_{12} + r_{23}\varphi^2}{1 - r_{21}r_{23}\varphi^2} \quad \text{(rB)}$$

since $\left(t_{12}t_{21} - r_{12}r_{21}\right) = 1$ for ALL adjacent pairs of media, and where complex phase factor $\varphi = \exp\left(\frac{j\omega \underline{n} d}{c}\right)$.

(rA) and (rB) are two equivalent forms of complex amplitude reflection coefficient for a single layer.

The coherent reflectance can be calculated from both using $\left(R_{13}\right)_{coh} = |r_{13}|^2$. For (rA) :

$$\left(R_{13}\right)_{coh} = |r_{12}|^2 + \frac{|t_{12}t_{21}r_{23}|^2 \exp(-2\alpha d)}{1 + |r_{21}r_{23}|^2 \exp(-2\alpha d) - 2\,\mathrm{Re}\left(r_{21}r_{23}\varphi^2\right)} + 2\,\mathrm{Re}\left[\frac{r_{12}^{*}t_{12}t_{21}r_{23}\varphi^2}{1 - r_{21}r_{23}\varphi^2}\right] \quad \text{(RcohA) as on p14.}$$

For (rB) :

$$\left(R_{13}\right)_{coh} = \frac{|r_{12}|^2 + |r_{23}|^2 \exp(-2\alpha d) + 2\,\mathrm{Re}\left(r_{12}^{*}r_{23}\varphi^2\right)}{1 + |r_{21}r_{23}|^2 \exp(-2\alpha d) - 2\,\mathrm{Re}\left(r_{21}r_{23}\varphi^2\right)}.$$

(RcohB) - the best for coherent reflectance calculations

(RcohA) and (RcohB) give identical results. PTO for incoherent reflectance

The incoherent reflectance can be directly calculated only from (RcohA) :

$$\left(R_{13}\right)_{\text{incoh}} = \left|r_{12}\right|^2 + \frac{\left|t_{12}t_{21}r_{23}\right|^2 \exp(-2\alpha d)}{1-\left|r_{21}r_{23}\right|^2 \exp(-2\alpha d)} \quad \text{(RincohA) as on p16.}$$

and this can be written :

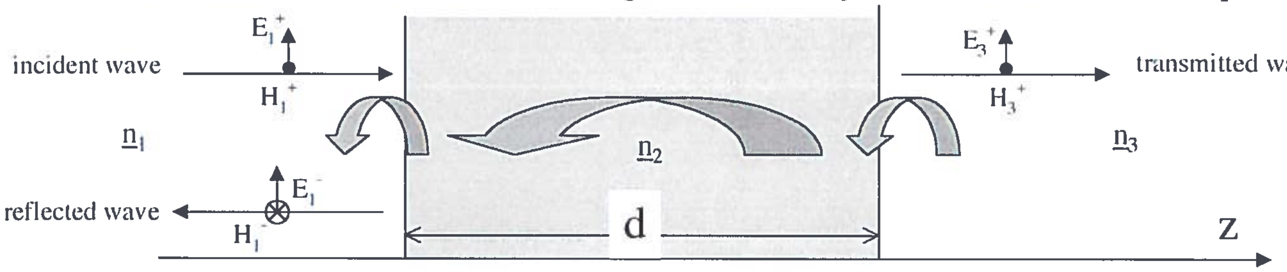
$$\left(R_{13}\right)_{\text{incoh}} = \frac{\left|r_{12}\right|^2\left(1-\left|r_{21}r_{23}\right|^2 \exp(-2\alpha d)\right) + \left|t_{12}t_{21}r_{23}\right|^2 \exp(-2\alpha d)}{1-\left|r_{21}r_{23}\right|^2 \exp(-2\alpha d)}$$

finally

$$\left(R_{13}\right)_{\text{incoh}} = \frac{\left|r_{12}\right|^2 + \left|r_{23}\right|^2 \exp(-2\alpha d)\left[\left|t_{12}t_{21}\right|^2 - \left|r_{12}r_{21}\right|^2\right]}{1-\left|r_{21}r_{23}\right|^2 \exp(-2\alpha d)}$$ (RincohA)'-best for incoherent reflectance calculations

Note that $\left(t_{12}t_{21} - r_{12}r_{21}\right) = 1$, whereas $\left(\left|t_{12}t_{21}\right|^2 - \left|r_{12}r_{21}\right|^2\right)$ is nothing special.

Reflectance and transmittance of a single incoherent layer :- The MATRIX technique.



TRANSFORMATION OF INTENSITY BACKWARDS THROUGH A SINGLE INCOHERENT LAYER

For a single layer, thickness d, index n_2, sandwiched between media of indices n_1 and n_3. From Harbecke :

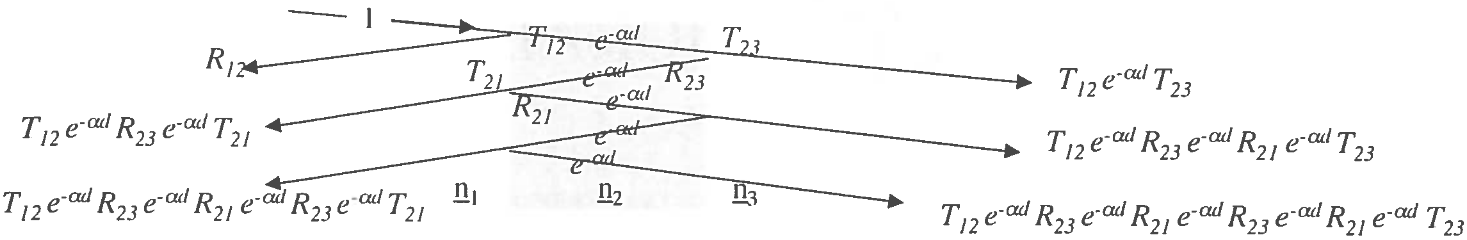
$$\begin{bmatrix} 1 \\ \left(R_{13}\right)_{\text{incoh}} \end{bmatrix} = \frac{1}{T_{12}}\begin{bmatrix} 1 & -R_{21} \\ R_{12} & T_{12}T_{21}-R_{12}R_{21} \end{bmatrix}\begin{bmatrix} 1/X & 0 \\ 0 & X \end{bmatrix}\frac{1}{T_{23}}\begin{bmatrix} 1 & -R_{32} \\ R_{23} & T_{23}T_{32}-R_{23}R_{32} \end{bmatrix}\begin{bmatrix} \left(T_{13}\right)_{\text{incoh}} \\ 0 \end{bmatrix}. \quad \text{where } X = e^{-\alpha d}.$$

After straightforward multiplication we obtain :

$$\left.\begin{cases} \text{Incoherent transmittance, } \left(T_{13}\right)_{\text{incoh}} = \dfrac{T_{12}T_{23}X}{1-R_{21}R_{23}X^2} \\ \text{Incoherent reflectance, } \left(R_{13}\right)_{\text{incoh}} = \dfrac{R_{12}+R_{23}X^2\left(T_{12}T_{21}-R_{12}R_{21}\right)}{1-R_{21}R_{23}X^2} \end{cases}\right\} \text{same as previous results}$$

I guess that here, Harbecke means T as $|t|^2$ etc. because the intensities are not uniquely defined in absorbing media...

Reflectance and transmittance of single layer :- The INFINITE SERIES revisited for intensities



Incoherent Transmittance $\left(T_{13}\right)_{\text{incoh}} = T_{12}e^{-\alpha d}T_{23}\left\{1+\left(R_{23}e^{-\alpha d}R_{21}e^{-\alpha d}\right)+\left(R_{23}e^{-\alpha d}R_{21}e^{-\alpha d}\right)^2+\ldots\right\}$

$$= T_{12}e^{-\alpha d}T_{23}\sum_{p=0}^{\infty}\left(R_{23}R_{21}e^{-2\alpha d}\right)^p = \frac{T_{12}T_{23}e^{-\alpha d}}{1-R_{21}R_{23}e^{-2\alpha d}}.$$

Incoherent Reflectance $\left(R_{13}\right)_{\text{incoh}} = R_{12} + T_{12}e^{-\alpha d}R_{23}e^{-\alpha d}T_{21}\left\{1+\left(R_{21}e^{-\alpha d}R_{23}e^{-\alpha d}\right)+\left(R_{21}e^{-\alpha d}R_{23}e^{-\alpha d}\right)^2+\ldots\right\}$

$$\therefore \left(R_{13}\right)_{\text{incoh}} = R_{12} + \frac{T_{12}T_{21}R_{23}e^{-2\alpha d}}{1-R_{21}R_{23}e^{-2\alpha d}}.$$

If $R_{12}\to\left|r_{12}\right|^2$, $T_{12}\to\left|t_{12}\right|^2$ and $\varphi = e^{-\alpha d}$ we get the previous incoherent transmittance and reflectance directly!

$R_{12}=\left|r_{12}\right|^2$ is valid for reflectance, BUT $T_{12}=\left|t_{12}\right|^2$ is NOT the transmittance, since $T_{12}=\left|t_{12}\right|^2 N_2/N_1 \neq \left|t_{12}\right|^2$

$\therefore$ We are NOT adding an ∞ series of intensities (undefined if absorbing!), we are adding an ∞ series of $\left|\text{amp}\right|^2$.

The intensity *seems* to work because $T_{12}T_{23}=\left|t_{12}\right|^2\dfrac{N_2}{N_1}\cdot\left|t_{23}\right|^2\dfrac{N_3}{N_2}=\left|t_{12}\right|^2\left|t_{23}\right|^2\dfrac{N_3}{N_1}=\left|t_{12}\right|^2\left|t_{23}\right|^2$ in this case.

Transmittance of a single absorbant layer surrounded by non-identical media.

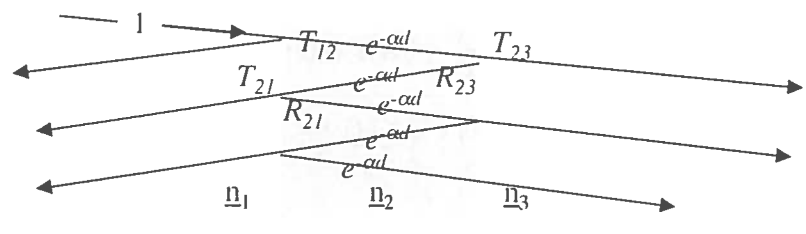
From the pages on single layer transmission, we stated that the front and back layers are vacuum, $\underline{n}_1=\underline{n}_3=1$.
IF the front and back media are different, then (valid only for transparent media 1 and 3):

$$\text{Coherent Transmittance, } \left(T_{13}\right)_{\text{coh}} = \left|t_{13}\right|^2\frac{\mathrm{Re}\left(\underline{n}_3\right)}{\mathrm{Re}\left(\underline{n}_1\right)} = \left\{\frac{\left|t_{12}\right|^2\left|t_{23}\right|^2\exp\left(-\alpha d\right)}{1+\left|r_{21}\right|^2\left|r_{23}\right|^2\exp\left(-2\alpha d\right)-2\,\mathrm{Re}\left[r_{21}r_{23}\varphi^2\right]}\right\}\frac{\mathrm{Re}\left(\underline{n}_3\right)}{\mathrm{Re}\left(\underline{n}_1\right)}, \text{ and}$$

$$\text{Incoherent Transmittance, } \left(T_{13}\right)_{\text{incoh}} = \left\{\frac{\left|t_{12}t_{23}\right|^2\exp\left(-\alpha d\right)}{1-\left|r_{21}r_{23}\right|^2\exp\left(-2\alpha d\right)}\right\}\frac{\mathrm{Re}\left(\underline{n}_3\right)}{\mathrm{Re}\left(\underline{n}_1\right)} = \left\langle\left|t_{13}\right|^2\frac{\mathrm{Re}\left(\underline{n}_3\right)}{\mathrm{Re}\left(\underline{n}_1\right)}\right\rangle.$$

Therefore, the Incoherent and Coherent transmittances are the same even if the media are different on each side of the layer.

NB We have taken the media to be infinite on each side : this is as if the substrate were infinitely thick, and the power measurements were made INSIDE the infinite substrate material, which is physically unlike the Bruker.



MORAL

Don't sum intensities in *absorbing* media => Don't use transmittance nor reflectance in *absorbing* media

Always use Fresnel coefficients and calculate transmittance and reflectance in vacuum at the front and back, since then

$$T_{ab} = \left|t_{ab}\right|^2, \quad R_{ab} = \left|r_{ab}\right|^2$$

A simple example: Interference-free transmittance of a clean silicon wafer.

Transmittance = Transmitted intensity/Incident intensity, measured using e.g. the Bruker.
For a gas, $T_{gas}(\nu) = I(\nu)/I_0(\nu) = \exp(-k_{gas}(\nu)d)$; Absorbance $A_{gas} = -\ln(T(\nu)) = k_{gas}(\nu)d$.
- see internal note INT 190/97.

BUT THIS IS NOT CORRECT FOR A WAFER BECAUSE OF REFLECTIONS. Instead we use:

$$\left(T_{13}\right)_{\text{incoh}} = \frac{I_{wafer}}{I_{no\ wafer}} = \frac{\left|t_{12}t_{23}\right|^2 \exp(-\alpha d)}{1-\left|r_{21}r_{23}\right|^2 \exp(-2\alpha d)},$$

where we have taken $\underline{n}_3 = N_3 = \underline{n}_1 = N_1 = 1$, e.g., in vacuum.

This is the interference-free transmittance for low spectral resolution, for example 8 cm^{-1} with a 200 μm wafer.
For the wafer: $\underline{n}_2 = N_{Si}(\nu) + jK_{Si}(\nu) \approx 3.42$ for the wavenumber range ν = 400 - 3000 cm^{-1} because $K << N$ (see next page).

Calculate the Fresnel coefficients: $t_{12} = \dfrac{2\underline{n}_1}{\underline{n}_1 + \underline{n}_2} = \dfrac{2\cdot 1}{1+3.42} = 0.45$, similarly $t_{23} = 1.55$, $r_{21} = r_{23} = 0.55$

Also, $\alpha = 2\omega K_{Si}(\nu)/c = 2\cdot 2\pi \cdot K_{Si}(\nu)/\lambda = 2\cdot 2\pi\cdot 100\nu\left[\text{cm}^{-1}\right]K_{Si}(\nu) = 400\pi K_{Si}(\nu)\cdot\nu\left[\text{cm}^{-1}\right]$,
where $K_{Si}(\nu)$ is taken from data tables.

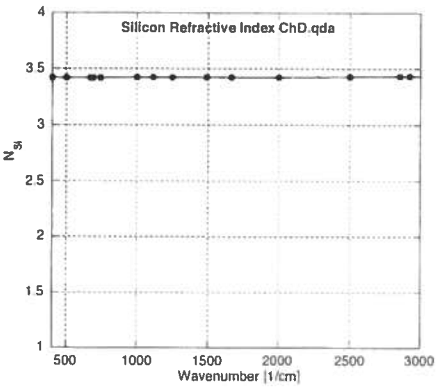
continued...

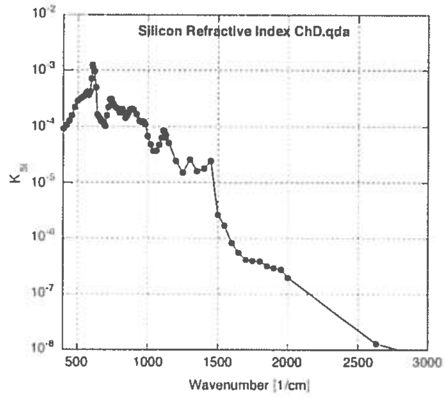
$\therefore$ Interference - free transmission of a Si wafer, $\left(T_{13}\right)_{\text{incoh}} = \dfrac{\left|0.45 \cdot 1.55\right|^2 \exp\left(-400\pi K_{Si}(\nu) \cdot \nu \left[\text{cm}^{-1}\right] \cdot d\right)}{1 - \left|0.55 \cdot 0.55\right|^2 \exp\left(-2 \cdot 400\pi K_{Si}(\nu) \cdot \nu \left[\text{cm}^{-1}\right] \cdot d\right)}$.

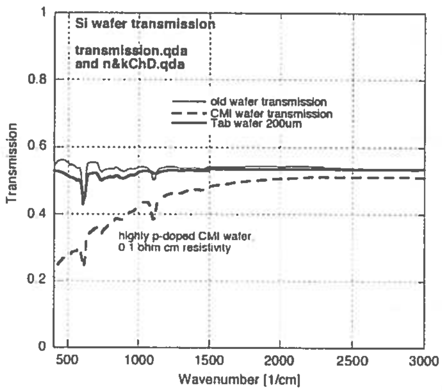
In the absence of absorption peaks $K_{Si}(\nu) = 0$, and $\left(T_{13}\right)_{\text{incoh}} = \dfrac{\left|0.45 \cdot 1.55\right|^2}{1 - \left|0.55 \cdot 0.55\right|^2} = 0.54$

Good agreement between model and measurement, using literature values for N_{Si} and K_{Si}.
Note $K_{\text{Si}} << N_{\text{Si}}$ as assumed above.

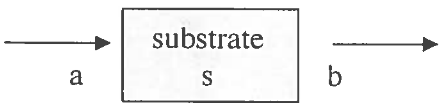
NB To eliminate the absorption due to doping, use intrinsic silicon or high resistivity n-doped wafers (holes have lower mobility than electrons to infrared excitation)







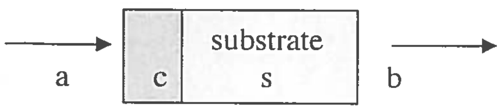
Up to now, we considered only single absorbing layers



$$\left(T_{ab}\right)_{\text{incoh}} = \frac{\left|t_{as} t_{sb}\right|^2 \exp\left(-\alpha_s d_s\right)}{1 - \left|r_{sa} r_{sb}\right|^2 \exp\left(-2\alpha_s d_s\right)}$$

for a single thick substrate.

Now add an absorbing film on one side:



$$\left(T_{ab}\right)_{\text{film/incoh}} = \frac{\left|t'_{as} t_{sb}\right|^2 \exp\left(-\alpha_s d_s\right)}{1 - \left|r'_{sa} r_{sb}\right|^2 \exp\left(-2\alpha_s d_s\right)}$$

for a film on a thick substrate.

We will also use the matrix transform to add extra layers, but for one extra layer we can also proceed as follows:
Replace the Fresnel magnitudes $\left|t_{as}\right|^2$ and $\left|r_{sa}\right|^2$ in the above by the effective magnitudes:

$\left|t'_{as}\right|^2$ = p14 for coherent layer, p17 for incoherent layer $(a \equiv 1, c \equiv 2, s \equiv 3)$ (respecting the layer sequence),

$\left|r'_{sa}\right|^2$ = p14 for coherent layer, p17 for incoherent layer $(s \equiv 1, c \equiv 2, a \equiv 3)$ (note the reversal of the subscripts)

These are the modified Fresnel coefficients due to the thin layer c between media a and s.
Coherent magnitudes result in interference fringes due to a (thin) coherent layer.

Wait a minute: does a thin native oxide change the wafer transmission?

(because the interface refractive indices are changed)

Without oxide, $t_{as} = \dfrac{2\underline{n}_a}{\underline{n}_a + \underline{n}_s}$

With oxide, $t'_{as} = \dfrac{t_{ac} t_{cs} \varphi_c}{1 - r_{ca} r_{cs} \varphi_c^2} = \dfrac{\dfrac{2\underline{n}_a}{\underline{n}_a + \underline{n}_c} \cdot \dfrac{2\underline{n}_c}{\underline{n}_c + \underline{n}_s} \cdot \varphi_c}{1 - \dfrac{\underline{n}_c - \underline{n}_a}{\underline{n}_c + \underline{n}_a} \cdot \dfrac{\underline{n}_c - \underline{n}_s}{\underline{n}_c + \underline{n}_s} \cdot \varphi_c^2}$

$$\varphi_c = \exp\left(\frac{j\omega \underline{n}_c d_c}{c}\right) \approx \exp\left(\frac{j2\pi N_{SiO_2} d_c}{\lambda}\right) \approx \exp\left(j2\pi \cdot 1.41 \cdot 30 \cdot 10^{-9} \cdot 2 \cdot 10^{5}\right) \approx \exp(0.05j) \approx 0.99 + 0.05j$$

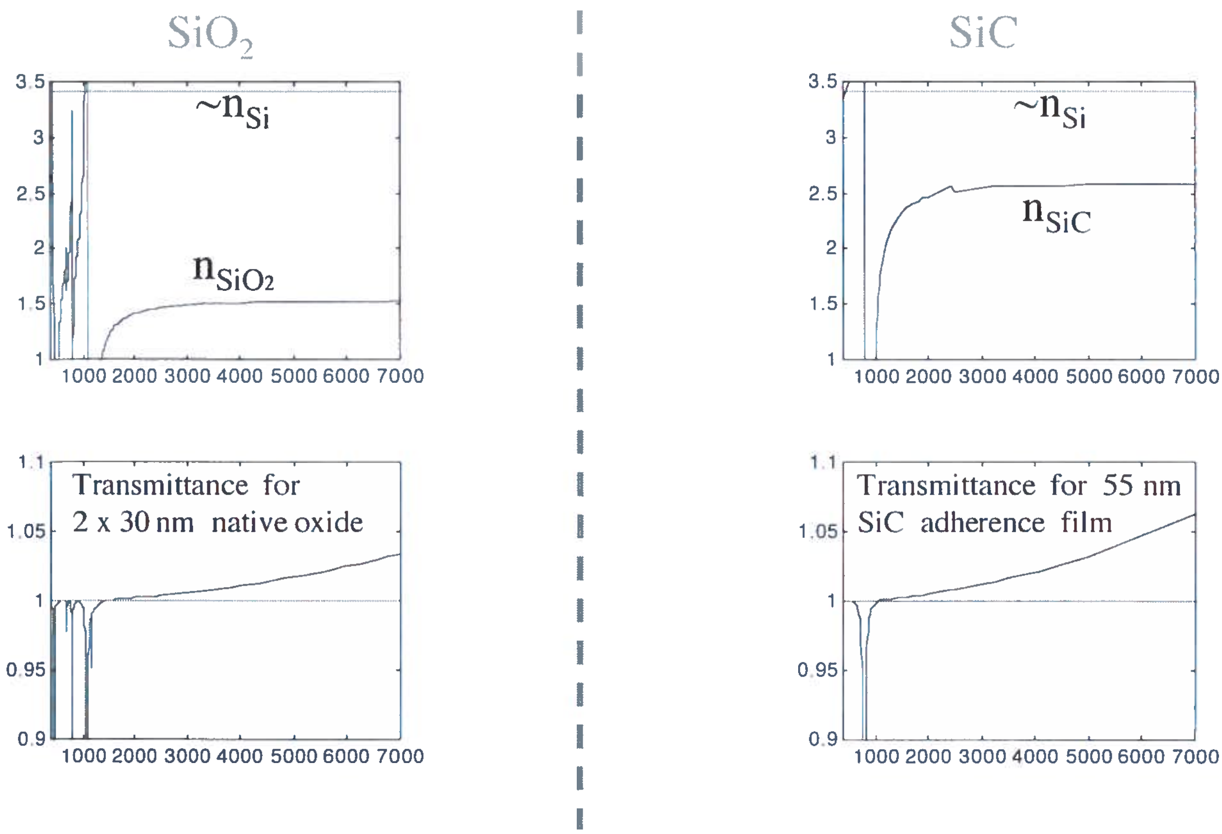
for 30 nm oxide (index 1.41) at 2000 cm^{-1}.

In the limit of thin oxide, $\varphi_c \approx 1$, and simplification shows that :
$t'_{as} = t_{as}$ and also $r'_{sa} = r_{sa}$, $\therefore \left(T_{ab}\right)_{incoh}$ is unchanged.

$\left(T_{ab}\right)_{incoh}$ changes in fact by $\approx 1\%$ at 2000 cm^{-1} for a single native oxide of 30 nm. (*see Taboxidewafer.m*)

We can ignore thin native oxide for accuracy of few per cent.

Expect only weak effects (no fringes) for the thin films on the wafer before a-Si:H deposition.



What have other authors done for film - substrate transmittance?

So far, I have found no analytic expressions for an absorbing coherent film on an absorbing incoherent substrate: everybody considers incoherent films on incoherent substrates (which is wrong since fringes are observed!) and guesses the baseline which leads to errors. Let's calculate an incoherent film on an incoherent substrate and compare different authors: See *Tincoh_SiH.m*

$$\left(T_{ab}\right)_{\text{film/incoh}} = \frac{\left|t'_{as}\, t_{sb}\right|^2 e^{-\alpha_s d_s}}{1-\left|r'_{sa}\, r_{sb}\right|^2 e^{-2\alpha_s d_s}}$$

for a film on side a of a thick (incoherent) substrate, as on p25.

this is Eq.(1) in N. Maley & I. Szafranek. MRS Proc.**192** 663 (1990) - he assumes a transparent substrate.

We use the <u>incoherent</u> magnitudes (see pp17, 19) : is this permissible?

$$\left|t'_{as}\right|^2 = \frac{\left|t_{ac}t_{cs}\right|^2 e^{-\alpha_c d_c}}{1-\left|r_{ca}r_{cs}\right|^2 e^{-2\alpha_c d_c}},$$

respecting the sequence $\left(a \equiv 1, c \equiv 2, s \equiv 3\right)$,

$$\left|r'_{sa}\right|^2 = \frac{\left|r_{sc}\right|^2 + \left|r_{ca}\right|^2 e^{-2\alpha_c d_c}\left[\left|t_{sc}t_{cs}\right|^2 - \left|r_{sc}r_{cs}\right|^2\right]}{1-\left|r_{ca}r_{cs}\right|^2 e^{-2\alpha_c d_c}}$$

$\left(s \equiv 1, c \equiv 2, a \equiv 3\right)$ (note the reversal of the subscripts).

$$\left(T_{ab}\right)_{\text{incoh/incoh}} = \frac{\left|t_{ac}t_{cs}t_{sb}\right|^2 e^{-\alpha_s d_s} e^{-\alpha_c d_c}}{1-\left|r_{ca}r_{cs}\right|^2 e^{-2\alpha_c d_c} - \left|r_{sb}\right|^2 e^{-2\alpha_s d_s}\left\{\left|r_{sc}\right|^2 + \left|r_{ca}\right|^2 e^{-2\alpha_c d_c}\left[\left|t_{sc}t_{cs}\right|^2 - \left|r_{sc}r_{cs}\right|^2\right]\right\}},$$

with $\theta_{ac} = \left|t_{ac}\right|^2$ etc.:

$$\left(T_{ab}\right)_{\text{incoh/incoh}} = \frac{\theta_{ac}\theta_{cs}\theta_{sb}e^{-\alpha_s d_s}e^{-\alpha_c d_c}}{1-\Gamma_{ca}\Gamma_{cs}e^{-2\alpha_c d_c} - \Gamma_{sb}e^{-2\alpha_s d_s}\left\{\Gamma_{sc} + \Gamma_{ca}e^{-2\alpha_c d_c}\left[\theta_{sc}\theta_{cs} - \Gamma_{sc}\Gamma_{cs}\right]\right\}},$$

NB where θ is NOT transmittance, but (magnitude transmission coefft.)^2, although Γ is identical to reflectance.

For later comparison with the coherent film transmission, we write $X_c = e^{-\alpha_c d_c}$ and $X_s = e^{-\alpha_s d_s}$

$$\left(T_{ab}\right)_{\text{incoh/incoh}} = \frac{\theta_{ac}\theta_{cs}\theta_{sb}X_s X_c}{1-\Gamma_{ca}\Gamma_{cs}X_c^2 - \Gamma_{sb}X_s^2\left\{\Gamma_{sc} + \Gamma_{ca}X_c^2\left[\theta_{sc}\theta_{cs} - \Gamma_{sc}\Gamma_{cs}\right]\right\}},$$

collect coefficients of X_c :

$$= \frac{\theta_{ac}\theta_{cs}\theta_{sb}X_s X_c}{\left(1-\Gamma_{sb}\Gamma_{sc}X_s^2\right) - X_c^2\Gamma_{ca}\left\{\Gamma_{cs} + \Gamma_{sb}X_s^2\left[\theta_{sc}\theta_{cs} - \Gamma_{sc}\Gamma_{cs}\right]\right\}}$$

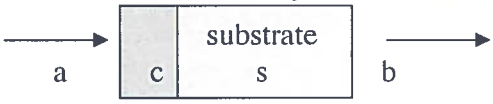
$$\therefore \left(T_{ab}\right)_{\text{incoh/incoh}} = \frac{AX_c}{B - D' X_c^2}$$

$$\left\{\begin{aligned} &\text{where } A = \theta_{ac}\theta_{cs}\theta_{sb}X_s, \\ &B = \left(1-\Gamma_{sb}\Gamma_{sc}X_s^2\right), \\ &D' = \Gamma_{ca}\left\{\Gamma_{cs} + \Gamma_{sb}X_s^2\left[\theta_{sc}\theta_{cs} - \Gamma_{sc}\Gamma_{cs}\right]\right\} \end{aligned}\right\}$$

Two, thick (incoherent) layers

(?! We will see that $\left\langle T_{\text{coh/incoh}}\right\rangle \neq T_{\text{incoh/incoh}}$ except in special cases.)

Transmittance of a double incoherent layer :- The MATRIX technique.



is this permissible?

For adjacent incoherent layers, thickness d_c and d_s, sandwiched between media a and b. From Harbecke :

$$\begin{bmatrix} 1 \\ (R_{ab})_{\text{incoh/incoh}} \end{bmatrix} = \frac{1}{\theta_{ac}}\begin{bmatrix} 1 & -\Gamma_{ca} \\ \Gamma_{ac} & \theta_{ac}\theta_{ca}-\Gamma_{ac}\Gamma_{ca} \end{bmatrix}\begin{bmatrix} 1/X_c & 0 \\ 0 & X_c \end{bmatrix}\frac{1}{\theta_{cs}}\begin{bmatrix} 1 & -\Gamma_{sc} \\ \Gamma_{cs} & \theta_{cs}\theta_{sc}-\Gamma_{cs}\Gamma_{sc} \end{bmatrix}\cdots$$

$$\cdots\begin{bmatrix} 1/X_s & 0 \\ 0 & X_s \end{bmatrix}\frac{1}{\theta_{sb}}\begin{bmatrix} 1 & -\Gamma_{bs} \\ \Gamma_{sb} & \theta_{sb}\theta_{bs}-\Gamma_{sb}\Gamma_{bs} \end{bmatrix}\begin{bmatrix} (T_{ab})_{\text{incoh/incoh}} \\ 0 \end{bmatrix}, \quad \text{where } X_c = e^{-\alpha_c d_c}, \quad X_s = e^{-\alpha_s d_s}.$$

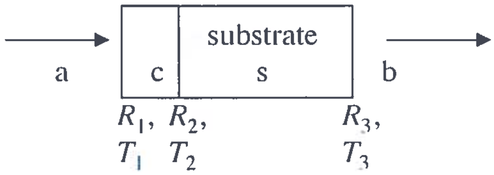
$$\begin{bmatrix} 1 \\ (R_{ab}) \end{bmatrix} = \frac{1}{\theta_{ac}\theta_{cs}\theta_{sb}X_cX_s}\begin{bmatrix} 1 & -\Gamma_{ca} \\ \Gamma_{ac} & \text{you} \end{bmatrix}\begin{bmatrix} 1 & -\Gamma_{sc} \\ \Gamma_{cs}X_c^2 & (\theta_{cs}\theta_{sc}-\Gamma_{cs}\Gamma_{sc})X_c^2 \end{bmatrix}\begin{bmatrix} 1 & -\Gamma_{bs} \\ \Gamma_{sb}X_s^2 & \text{sideways} \end{bmatrix}\begin{bmatrix} (T_{ab}) \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 \\ (R_{ab}) \end{bmatrix} = \frac{1}{\theta_{ac}\theta_{cs}\theta_{sb}X_cX_s}\begin{bmatrix} (1-\Gamma_{ca}\Gamma_{cs}X_c^2) & -\Gamma_{sc}-\Gamma_{ca}(\theta_{cs}\theta_{sc}-\Gamma_{cs}\Gamma_{sc})X_c^2 \\ \text{with} & \text{a} \end{bmatrix}\begin{bmatrix} 1 & \text{bargepole} \\ \Gamma_{sb}X_s^2 & \text{gently} \end{bmatrix}\begin{bmatrix} (T_{ab}) \\ 0 \end{bmatrix}$$

$$\begin{bmatrix} 1 \\ (R_{ab}) \end{bmatrix} = \frac{1}{\theta_{ac}\theta_{cs}\theta_{sb}X_cX_s}\begin{bmatrix} (1-\Gamma_{ca}\Gamma_{cs}X_c^2)-\Gamma_{sb}X_s^2\left(\Gamma_{sc}+\Gamma_{ca}(\theta_{cs}\theta_{sc}-\Gamma_{cs}\Gamma_{sc})X_c^2\right) & \text{you} \\ \text{thank} & \text{madam} \end{bmatrix}\begin{bmatrix} (T_{ab}) \\ 0 \end{bmatrix}$$

$$\therefore (T_{ab})_{\text{incoh/incoh}} = \frac{\theta_{ac}\theta_{cs}\theta_{sb}X_sX_c}{(1-\Gamma_{ca}\Gamma_{cs}X_c^2)-\Gamma_{sb}X_s^2\left(\Gamma_{sc}+\Gamma_{ca}X_c^2(\theta_{cs}\theta_{sc}-\Gamma_{cs}\Gamma_{sc})\right)}, \quad \text{same as top of previous page.}$$

To compare with other authors, we adapt (degrade) our notation from p28/9:



For these authors' notation, $R_1 = R_{ac} = R_{ca}$, $R_2 = R_{cs} = R_{sc}$, $R_3 = R_{sb} = R_{bs}$ which is true generally, also the reflectances $R = \Gamma$.

Authors also substitute the (mag.)^2 product $\theta_{ac}\theta_{cs}\theta_{sb}$ by a transmittance product $T_1T_2T_3$ where I suppose that $T_1T_2T_3$ is intended to equal the transmittance product $T_{ac}T_{cs}T_{sb}$, although $T_{ac} = |t_{ac}|^2 \dfrac{\text{Re}(\underline{n}_c)}{\text{Re}(\underline{n}_a)} \neq T_{ca} = |t_{ca}|^2 \dfrac{\text{Re}(\underline{n}_a)}{\text{Re}(\underline{n}_c)}$,

therefore it is lax to represent a transmittance with a single subscript.

However, the product $T_1T_2T_3$ is fortunately correct because $T_{ac}T_{cs}T_{sb} = |t_{ac}|^2\dfrac{\text{Re}(\underline{n}_c)}{\text{Re}(\underline{n}_a)}|t_{cs}|^2\dfrac{\text{Re}(\underline{n}_s)}{\text{Re}(\underline{n}_c)}|t_{sb}|^2\dfrac{\text{Re}(\underline{n}_b)}{\text{Re}(\underline{n}_s)}$

$= |t_{ac}|^2|t_{cs}|^2|t_{sb}|^2\dfrac{\text{Re}(\underline{n}_b)}{\text{Re}(\underline{n}_a)} = \theta_{ac}\theta_{cs}\theta_{sb}$ because we take a and b to be vacuum. $\therefore$ we can admit that $T_1T_2T_3 = \theta_{ac}\theta_{cs}\theta_{sb}$.

Furthermore, $\theta_{bs}\theta_{sc}\theta_{ca} = \theta_{ac}\theta_{cs}\theta_{sb}$ as can be seen by expanding the θ's and using $|\underline{n}_a|^2 = |\underline{n}_b|^2$, i.e. symmetric.

They also replace $\theta_{sc}\theta_{cs}$ by $T_2^2 = T_{sc}T_{cs}$ if we give them the benefit of the doubt, and

$T_{sc}T_{cs} = |t_{sc}|^2\dfrac{\text{Re}(\underline{n}_c)}{\text{Re}(\underline{n}_s)}|t_{cs}|^2\dfrac{\text{Re}(\underline{n}_s)}{\text{Re}(\underline{n}_c)} = |t_{sc}|^2|t_{cs}|^2 = \theta_{sc}\theta_{cs}$, $\therefore$ we can also admit that $T_2^2 = \theta_{sc}\theta_{cs}$.

Note that the final transmittance is symmetric, i.e. $\left(T_{ab}\right)_{\text{incoh/incoh}} = \left(T_{ba}\right)_{\text{incoh/incoh}}$ as required generally :

$$\left(T_{ab}\right)_{\text{incoh/incoh}} = \frac{T_1 T_2 T_3 e^{-\alpha_s d_s} e^{-\alpha_c d_c}}{1 - R_1 R_2 e^{-2\alpha_c d_c} - R_3 e^{-2\alpha_s d_s}\left\{R_2 + R_1 e^{-2\alpha_c d_c}\left[T_2^2 - R_2^2\right]\right\}}.$$ This expression is exact.

fractional error~10^{-4}

However, it is only possible to obtain their following expressions if we now substitute $T_2^2 = \left(1 - R_2\right)^2$

Check validity of this substitution : $T_2^2 = \theta_{sc}\theta_{cs} = \dfrac{16\left(N_s^2 + K_s^2\right)\left(N_c^2 + K_c^2\right)}{\left|\underline{n}_s + \underline{n}_c\right|^4}$ whereas

$\left(1 - R_2\right)^2 = \dfrac{16\left(N_s N_c + K_s K_c\right)^2}{\left|\underline{n}_s + \underline{n}_c\right|^4}$. $\therefore T_2^2 = \left(1 - R_2\right)^2$ only if K_s & $K_c = 0$, or $K_s N_c = K_c N_s$ (Heaviside condition?)

Substituting nevertheless : $$\left(T_{ab}\right)_{\text{incoh/incoh}} \overset{1st}{\approx} \frac{T_1 T_2 T_3 e^{-\alpha_s d_s} e^{-\alpha_c d_c}}{1 - R_1 R_2 e^{-2\alpha_c d_c} - R_3 e^{-2\alpha_s d_s}\left\{R_2 + R_1 e^{-2\alpha_c d_c}\left[1 - 2R_2\right]\right\}}$$

Writing $x_1 = e^{-\alpha_c d_c}$ and $x_2 = e^{-\alpha_s d_s}$ and collecting terms, we get :

$$\left(T_{ab}\right)_{\text{incoh/incoh}} \overset{1st}{\approx} \frac{T_1 T_2 T_3 x_1 x_2}{\left(1 - R_2 R_3 x_2^2\right) - x_1^2\left\{R_1 R_2 + R_1 R_3 x_2^2 - 2R_1 R_2 R_3 x_2^2\right\}},$$ same as D. Franz thesis III.36. Ref. Keradec.

Quadratic solution for the film medium transmission $x_1 = e^{-\alpha_c d_c}$:

$$x_1 = \left\{P + \sqrt{P^2 + 2QT_{ab}\left(1 - R_2 R_3 x_2^2\right)}\right\} \Big/ Q; \quad P = -T_1 T_2 T_3 x_2; \quad Q = 2T_{ab}\left(R_1 R_2 + R_1 R_3 x_2^2 - 2R_1 R_2 R_3 x_2^2\right)$$

If we approximate the substrate by a transparent dielectric $\left(x_2 = 1\right)$, we get :

$$\left(T_{ab}\right)_{\text{incoh/incoh}} \overset{2nd}{\approx} \frac{T_1 T_2 T_3 e^{-\alpha d}}{\left(1 - R_2 R_3\right) - e^{-2\alpha d}\left\{R_1 R_2 + R_1 R_3 - 2R_1 R_2 R_3\right\}},$$

and further substitute $T_n = \left(1 - R_n\right)$ for $n = 1,2,3$ (which is WRONG for absorbing media!), we get :

$$\left(T_{ab}\right)_{\text{incoh/incoh}} \overset{3rd}{\approx} \frac{\left(1 - R_1\right)\left(1 - R_2\right)\left(1 - R_3\right)e^{-\alpha d}}{1 - R_2 R_3 - \left\{R_1 R_2 + R_1 R_3 - 2R_1 R_2 R_3\right\}e^{-2\alpha d}},$$ same as N. Maley Eq.(2).

This equation is also used by G. Connell* & A. Lewis, Phys.Stat.Solidi B60 291 (1973) and E. Freeman & W. Paul, Phys.Rev. B18 4288 (1978). (*Tsu et al, Phys.Rev. 172 779 (1968) is wrong).

The 'classic' method is due to M. Brodsky, M. Cardona & J. Cuomo (BCC) Phys.Rev.B16, 3556 (1977), and they *further* assume that $\underline{n}_s = \underline{n}_c$ so that $R_1 = R_3$ and $R_2 = 0$; then :

$$\left(T_{ab}\right)_{\text{incoh/incoh}} \overset{4th}{\approx} \frac{4T_0^2 e^{-\alpha d}}{\left(1 + T_0\right)^2 - \left(1 - T_0\right)^2 e^{-2\alpha d}},$$ same as BCC, Maley Eq.(3), Langford (Solar Cells **27** 373 (1989) and Ulli.

where $T_0 = \left(\dfrac{1 - R_1}{1 + R_1}\right)$ is the non-absorbing baseline transmission.

Conclusion : we can reproduce all the expressions used in the literature for two incoherent layers
In any case, these authors IGNORE the fringe baseline!
Errors in eliminating the oscillating baseline 'by eye' can be serious!
Therefore we will return to consider coherent film on incoherent substrate.

NOW THE $50'000 QUESTION:

What is the transmittance of a **thin** absorbing film on a thick absorbing substrate?

$$(T_{ab})_{\text{incoh}} = \frac{|t_{as}t_{sb}|^2 e^{-\alpha_s d_s}}{1-|r_{sa}r_{sb}|^2 e^{-2\alpha_s d_s}}$$ for a clean thick (incoherent) substrate.

$$(T_{ab})_{\text{film/incoh}} = \frac{|t'_{as}t_{sb}|^2 e^{-\alpha_s d_s}}{1-|r'_{sa}r_{sb}|^2 e^{-2\alpha_s d_s}}$$ for a general film on side a of a thick (incoherent) substrate,

where (see pp14, 21): $|t'_{as}|^2 = \dfrac{|t_{ac}t_{cs}|^2 e^{-\alpha_c d_c}}{\left|1-r_{ca}r_{cs}\varphi_c^2\right|^2}$, for a <u>coherent</u> film on side a. ...Eq.(1)

and $r'_{sa} = r_{sc} + \dfrac{t_{sc}t_{cs}r_{ca}\varphi_c^2}{1-r_{cs}r_{ca}\varphi_c^2} = \dfrac{r_{sc}+r_{ca}\varphi_c^2}{1-r_{cs}r_{ca}\varphi_c^2}$ (since $t_{sc}t_{cs}-r_{sc}r_{cs} \equiv 1$) for a <u>coherent</u> film on side a.

We have used the COHERENT amplitude expressions for a THIN film (p18)

$$\therefore |r'_{sa}|^2 = \frac{|r_{sc}|^2 + |r_{ca}|^2 e^{-2\alpha_c d_c} + 2e^{-\alpha_c d_c}\,\mathrm{Re}\left[r_{sc}^* r_{ca} e^{j4\pi\nu N_c d_c}\right]}{\left|1-r_{ca}r_{cs}\varphi_c^2\right|^2}$$ (wavenumber ν in 1/m here) ...Eq.(2)

Denominator $\left|1-r_{ca}r_{cs}\varphi_c^2\right|^2 = 1+|r_{cs}|^2|r_{ca}|^2 e^{-2\alpha_c d_c} - 2e^{-\alpha_c d_c}\,\mathrm{Re}\left[r_{cs}r_{ca}e^{j4\pi\nu N_c d_c}\right]$ ...Eq.(3)

... no-one said this would be easy... *NB All this has been checked in Tmodel.m*

Substituting into $(T_{ab})_{\text{film/incoh}}$ for $|t'_{as}|^2$ and $|r'_{sa}|^2$ to obtain $(T_{ab})_{\text{coh/incoh}}$

$$= \frac{|t_{ac}t_{cs}t_{sb}|^2 e^{-\alpha_c d_c} e^{-\alpha_s d_s}}{1+|r_{cs}|^2|r_{ca}|^2 e^{-2\alpha_c d_c} - 2e^{-\alpha_c d_c}\,\mathrm{Re}\left[r_{cs}r_{ca}e^{j4\pi\nu N_c d_c}\right] - |r_{sb}|^2 e^{-2\alpha_s d_s}\left\{|r_{sc}|^2 + |r_{ca}|^2 e^{-2\alpha_c d_c} + 2e^{-\alpha_c d_c}\,\mathrm{Re}\left[r_{sc}^* r_{ca}e^{j4\pi\nu N_c d_c}\right]\right\}}$$

For simplification, write: $|t_{ac}|^2 = \theta_{ac}$, (which is NOT the transmittance), $|r_{ca}|^2 = \Gamma_{ac}$, etc. and $X_c = e^{-\alpha_c d_c}$ etc.:

$$(T_{ab})_{\text{coh/incoh}} = \frac{\theta_{ac}\theta_{cs}\theta_{sb}X_c X_s}{1+\Gamma_{cs}\Gamma_{ca}X_c^2 - 2X_c\,\mathrm{Re}\left[r_{cs}r_{ca}e^{j4\pi\nu N_c d_c}\right] - \Gamma_{sb}X_s^2\left\{\Gamma_{sc}+\Gamma_{ca}X_c^2 + 2X_c\,\mathrm{Re}\left[r_{sc}^* r_{ca}e^{j4\pi\nu N_c d_c}\right]\right\}}$$

$$(T_{ab})_{\text{coh/incoh}} = \frac{\theta_{ac}\theta_{cs}\theta_{sb}X_c X_s}{\left(1-\Gamma_{sb}\Gamma_{sc}X_s^2\right) + X_c^2\Gamma_{ca}\left(\Gamma_{cs}-\Gamma_{sb}X_s^2\right) - 2X_c\,\mathrm{Re}\left[r_{ca}e^{j4\pi\nu N_c d_c}\left(r_{cs}+r_{sc}^*\Gamma_{sb}X_s^2\right)\right]}.$$

<u>This can be written as</u>

$$(T_{ab})_{\text{coh/incoh}} = \frac{AX_c}{B+DX_c^2-CX_c}$$ where $X_c = e^{-\alpha_c d_c}$ and

$A = \theta_{ac}\theta_{cs}\theta_{sb}X_s$, $B = \left(1-\Gamma_{sb}\Gamma_{sc}X_s^2\right)$, $C = 2\,\mathrm{Re}\left[r_{ca}e^{j4\pi\nu N_c d_c}\left(r_{cs}+r_{sc}^*\Gamma_{sb}X_s^2\right)\right]$, $D = \Gamma_{ca}\left(\Gamma_{cs}-\Gamma_{sb}X_s^2\right)$,

which explicitly shows the dependence on the transmission of the film medium, $X_c = e^{-\alpha_c d_c}$.

NB A quadratic soln. of the coherent transmittance for X_c (by analogy with incoh. case) is possible but impractical.

If we temporarily make the approximation of a transparent substrate, $\underline{n}_s = s, \quad X_s = 1$;
and write the film refractive index as $\underline{n}_c = n + jk$ we obtain the result of R. Swanepoel,
J. Phys. E: Sci. Instrum. 16 1215 (1983), App. (A1) $\left(k \to -k \quad \because \underline{n}_c = n - jk \text{ for Swanepoel}\right)$:

$$\left(T_{ab}\right)_{\text{coh/incoh}} \overset{K_s=0}{\approx} \frac{A_S X_c}{B + DX_c^2 - CX_c} \quad \text{where } X_c = e^{-\alpha_c d_c} \text{ and } \varphi = 4\pi n d/\lambda;$$

$$A_S = 16s\left(n^2 + k^2\right); \quad B_{\text{Swanepoel}} = \left[(n+1)^2 + k^2\right]\left[(n+1)\left(n + s^2\right) + k^2\right];$$

$$D_S = \left[(n-1)^2 + k^2\right]\left[(n-1)\left(n - s^2\right) + k^2\right];$$

$$C_S = 2\cos\varphi\left[\left(n^2 - 1 + k^2\right)\left(n^2 - s^2 + k^2\right) - 2k^2\left(s^2 + 1\right)\right] + 2k\sin\varphi\left[2\left(n^2 - s^2 + k^2\right) + \left(n^2 - 1 + k^2\right)\left(s^2 + 1\right)\right];$$

$$\text{and } \left[A_S, B_S, C_S, D_S\right] = \left[A, B, C, D\right] \times 4s \Big/ \left\{\left[(n+1)^2 + k^2\right]\left[(n+s)^2 + k^2\right](1+s)^2\right\}.$$

Now we go back to the exact expression, to calculate the coherent film transmission:

$$\text{For the } \underline{\text{clean}} \text{ thick (incoherent) substrate reference: } \left(T_{ab}\right)_{\text{ref}} = \frac{\left|t_{as} t_{sb}\right|^2 e^{-\alpha_s d_s}}{1 - \left|r_{sa} r_{sb}\right|^2 e^{-2\alpha_s d_s}} = \frac{\theta_{as}\theta_{sb}X_s}{1 - \Gamma_{sa}\Gamma_{sb}X_s^2}.$$

$$T_{\text{coh/incoh}} = \frac{\left(T_{ab}\right)_{\text{coh/incoh}}}{\left(T_{ab}\right)_{\text{ref}}} = \frac{X_c\theta_{ac}\theta_{cs}\left(1 - \Gamma_{sa}\Gamma_{sb}X_s^2\right)/\left(\theta_{as}\right)}{\left(1 - \Gamma_{sb}\Gamma_{sc}X_s^2\right) + X_c^2\Gamma_{ca}\left(\Gamma_{cs} - \Gamma_{sb}X_s^2\right) - 2X_c\,\text{Re}\left[r_{ca}e^{j4\pi\nu N_c d_c}\left(r_{cs} + r_{sc}^*\Gamma_{sb}X_s^2\right)\right]},$$

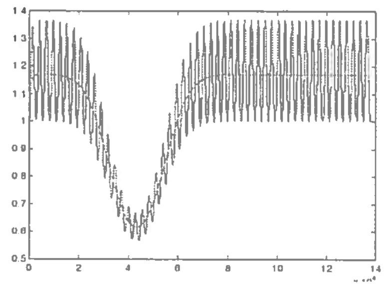
Comparison of incoherent (p29) and coherent (p34) expressions for transmission.
The expressions are almost equivalent as shown using *Tmodel.m*;
it should be possible to prove the equivalence analytically (see integral averages) BUT THEY AREN'T!

$$\left(T_{ab}\right)_{\text{incoh/incoh}} = \frac{AX_c}{B - D'X_c^2}, \text{ where } A = \theta_{ac}\theta_{cs}\theta_{sb}X_s, \; B = \left(1 - \Gamma_{sb}\Gamma_{sc}X_s^2\right), \; D' = \Gamma_{ca}\left\{\Gamma_{cs} + \Gamma_{sb}X_s^2\left[\theta_{sc}\theta_{cs} - \Gamma_{sc}\Gamma_{cs}\right]\right\},$$

$$\left(T_{ab}\right)_{\text{coh/incoh}} = \frac{AX_c}{B + DX_c^2 - CX_c} \text{ where } D = \Gamma_{ca}\left(\Gamma_{cs} - \Gamma_{sb}X_s^2\right), \text{ and } C = 2\,\text{Re}\left[r_{ca}e^{j4\pi\nu N_c d_c}\left(r_{cs} + r_{sc}^*\Gamma_{sb}X_s^2\right)\right].$$

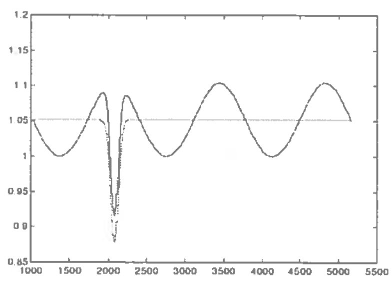
$\left(T_{ab}\right)_{\text{incoh/incoh}}$ is green

$\left(T_{ab}\right)_{\text{coh/incoh}}$ is blue



These are the thin film fringes; the substrate fringes have been averaged out for all cases (by the incoherent substrate).

If width of absorption peak >> fringe width, then incoherent expression is sufficient, because the incoherent expression averages over the fringe period.



If width of absorption peak < fringe width, then incoherent expression is likely to be inaccurate because the averaging assumes that N, K are constant over a fringe period (see * on p16).

Use the integral averages shown by Swanepoel *J.Phys.E : Sci.Instrum.* 16 p1215 (1983);
These are identical to the averages I1 and I'1 shown on p16 earlier, but Swanepoel notation is more relevant now (φ here includes the phase angle of complex C):

$$\text{Interference-free Transmission} = \langle T_{\text{coh}} \rangle = \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{Ax\, d\varphi}{\left(B+Dx^2\right)-|C|x\cos\varphi} = \frac{Ax}{\sqrt{\left(B+Dx^2-|C|x\right)\left(B+Dx^2+|C|x\right)}}.$$

The envelope of fringe maxima is $T_{\text{maxima}} = \dfrac{Ax}{\left(B+Dx^2\right)-|C|x}$;

The envelope of fringe minima is $T_{\text{minima}} = \dfrac{Ax}{\left(B+Dx^2\right)+|C|x}$ and so:

Interference-free transmission $\langle T_{\text{coh}} \rangle = \sqrt{T_{\text{maxima}} \cdot T_{\text{minima}}}$ = geometric mean of coherent transmission extrema.

NOTE THAT IF $|C|^2 = 4BD$, then

Interference-free transmission $\langle T_{\text{coh}} \rangle = \dfrac{Ax}{\sqrt{\left(B-Dx^2\right)^2}} = \dfrac{Ax}{B-Dx^2}$ which is the result for T_{incoh} of single layers.

BUT IF $|C|^2 \neq 4BD$, which is generally the case for double layers, then $\langle T_{\text{coh}} \rangle \neq T_{\text{incoh}}$!
HOW TO INTERPRET THIS ??

We need to know the magnitude, $|C|$ where $C = 2\,\text{Re}\left[r_{ca}e^{j4\pi\nu N_c d_c}\left(r_{cs} + r_{sc}^{*}\Gamma_{sb}X_s^2\right)\right]$.
Re-write as $C = \text{Re}\left[e^{j4\pi\nu N_c d_c}|C|e^{j\delta}\right]$, where $\arg(C) = \left(4\pi\nu N_c d_c + \delta\right)$ and $C = |C|\cos\left(4\pi\nu N_c d_c + \delta\right)$
and $|C| = \left|2r_{ca}\left(r_{cs} + r_{sc}^{*}\Gamma_{sb}X_s^2\right)\right|$. Therefore:

$$|C|^2 = 4\Gamma_{ca}\left(r_{cs} + r_{sc}^{*}\Gamma_{sb}X_s^2\right)\left(r_{cs}^{*} + r_{sc}\Gamma_{sb}X_s^2\right) = 4\Gamma_{ca}\left(\Gamma_{cs} + \Gamma_{sc}\Gamma_{sb}^2X_s^4 + \Gamma_{sb}X_s^2\left(r_{sc}^{*}r_{cs}^{*} + r_{sc}r_{cs}\right)\right).$$

Using the identity $\left(r_{sc}^{*}r_{cs}^{*} + r_{sc}r_{cs}\right) \equiv \left(\theta_{sc}\theta_{cs} - \Gamma_{sc}\Gamma_{cs} - 1\right)$ (which is not obvious and tedious to prove), we get:

$$\underline{|C|^2 = 4\Gamma_{ca}\left(\Gamma_{cs} + \Gamma_{sc}\Gamma_{sb}^2X_s^4 - \Gamma_{sb}X_s^2\left(\Gamma_{sc}\Gamma_{cs} + 1 - \theta_{sc}\theta_{cs}\right)\right)}.$$ (checked OK in Tmodel_aSiH.m)

Let's check the error term between <(Tab)$_{coh/incoh}$> and (Tab)$_{incoh/incoh}$

$\langle (T_{ab})_{\text{coh/incoh}} \rangle$ could be simplified if the denominator were a perfect square.

This requires $|C|^2 = 4BD$. We already have $|C|^2 = 4\Gamma_{ca}\left(\Gamma_{cs} + \Gamma_{sc}\Gamma_{sb}^2 X_s^4 - \Gamma_{sb}X_s^2\left(\Gamma_{sc}\Gamma_{cs} + 1 - \theta_{sc}\theta_{cs}\right)\right)$.

$$4BD = 4\left(1 - \Gamma_{sb}\Gamma_{sc}X_s^2\right)\Gamma_{ca}\left(\Gamma_{cs} - \Gamma_{sb}X_s^2\right) = 4\Gamma_{ca}\left(\Gamma_{cs} + \Gamma_{sc}\Gamma_{sb}^2 X_s^4 - \Gamma_{sb}X_s^2\left(\Gamma_{sc}\Gamma_{cs} + 1\right)\right)$$

$\therefore\ |C|^2 = 4BD + 4\Gamma_{ca}\Gamma_{sb}X_s^2\theta_{sc}\theta_{cs}$, so the "error" term is $4\Gamma_{ca}\Gamma_{sb}X_s^2\theta_{sc}\theta_{cs}$. What is the physical origin of it?

NOTE the error term can be removed in three trivial cases:

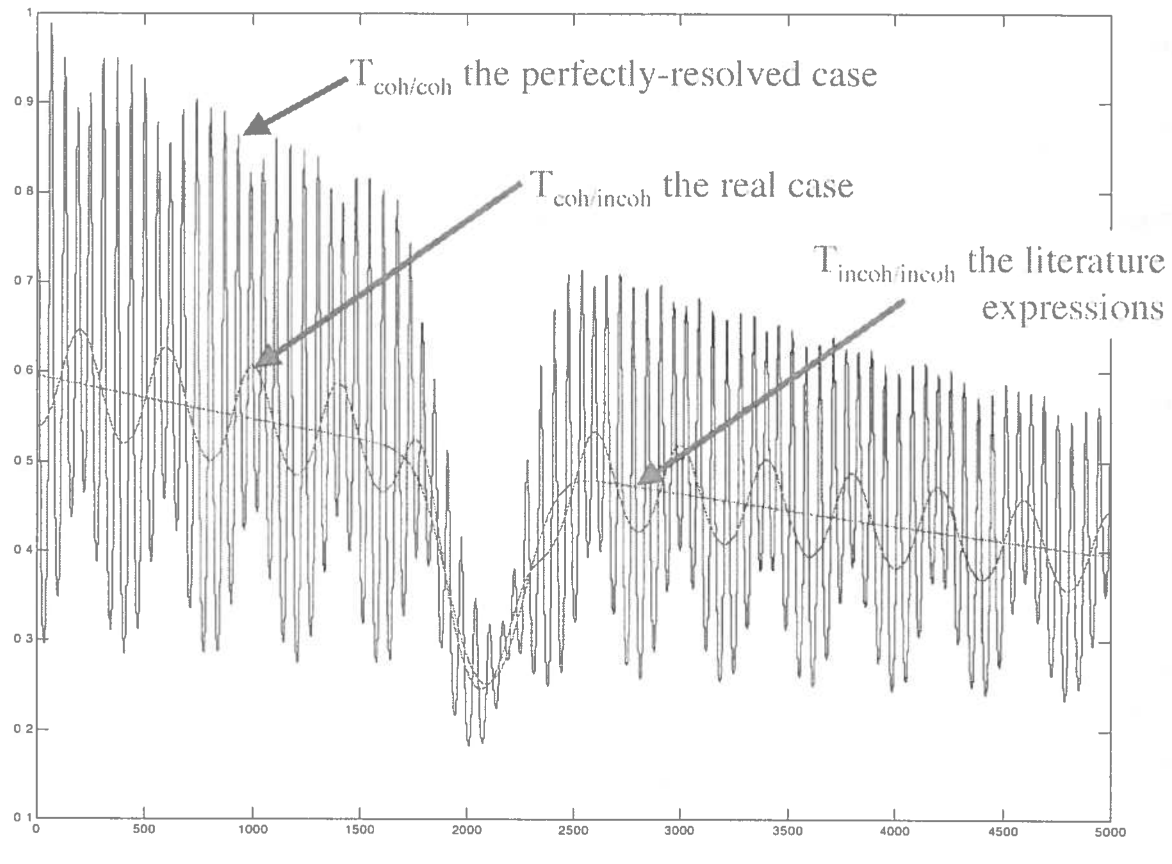
A) If $\underline{n}_s = \underline{n}_b$ then $\Gamma_{sb} = 0 \Rightarrow \langle (T_{ab})_{\text{coh/incoh}} \rangle = (T_{ab})_{\text{incoh/incoh}} = \dfrac{\theta_{ac}\theta_{cb}X_c}{1 - \Gamma_{ca}\Gamma_{cb}X_c^2}$ as for a single incoherent layer c;

B) If $\underline{n}_c = \underline{n}_a$ then $\Gamma_{ca} = 0 \Rightarrow \langle (T_{ab})_{\text{coh/incoh}} \rangle = (T_{ab})_{\text{incoh/incoh}} = \dfrac{\theta_{as}\theta_{sa}X_s}{1 - \Gamma_{sa}\Gamma_{sb}X_s^2}$ as for a single incoherent layer s;

C) If $\underline{n}_c = \underline{n}_s$ then $\Gamma_{cs} = \Gamma_{sc} = 0;\ \ \theta_{sc} = \theta_{cs} = 1\ \ \therefore B = 1,\ \ |C|^2 = 0$ and

$\langle (T_{ab})_{\text{coh/incoh}} \rangle = (T_{ab})_{\text{incoh/incoh}} = \dfrac{\theta_{ac}\theta_{sb}X_sX_c}{1 - \Gamma_{ca}\Gamma_{sb}X_s^2X_c^2}$ as for a single incoherent layer made up of c,s.

Graphic demonstration of T$_{incoh/incoh}$, T$_{coh/incoh}$, T$_{coh/coh}$ for an artificial case



Try to understand the error between coh/incoh and incoh/incoh layers using coh/coh layers.

AIM : First, calculate the full fringe structure for a coherent film on a coherent substrate, then check if :

$\langle\langle T_{\text{coh/coh}}\rangle\rangle \overset{?}{=} \langle T_{\text{coh/incoh}}\rangle \overset{?}{=} T_{\text{incoh/incoh}}$. Reverting to transmission complex amplitude :

$t_{ab} = \dfrac{t'_{as} t_{sb}\varphi_s}{1 - r'_{sa} r_{sb}\varphi_s^2}$ for a general film on side a of a coherent substrate,

where (see p33) : $t'_{as} = \dfrac{t_{ac}t_{cs}\varphi_c}{1 - r_{ca}r_{cs}\varphi_c^2}$, and $r'_{sa} = \dfrac{r_{sc} + r_{ca}\varphi_c^2}{1 - r_{cs}r_{ca}\varphi_c^2}$ for a coherent film on side a.

$\therefore t_{ab} = \dfrac{t_{ac}t_{cs}t_{sb}\varphi_c\varphi_s}{1 - r_{ca}r_{cs}\varphi_c^2 - r_{sc}r_{sb}\varphi_s^2 - r_{ca}r_{sb}\varphi_c^2\varphi_s^2}$ which is symmetric in s and c. Could have started with s and c inversed.

If we wish to average only over fringes of a thick substrate, first write :

$t_{ab} = \dfrac{t_{ac}t_{cs}t_{sb}\varphi_c\varphi_s}{\left(1 - r_{ca}r_{cs}\varphi_c^2\right) - \left(r_{sc} + r_{ca}\varphi_c^2\right) r_{sb}\varphi_s^2}$ for a thick film, write : $t_{ab} = \dfrac{t_{ac}t_{cs}t_{sb}\varphi_c\varphi_s}{\left(1 - r_{sc}r_{sb}\varphi_s^2\right) - \left(r_{cs} + r_{sb}\varphi_s^2\right) r_{ca}\varphi_c^2}$.

Continue to average only over fringes of a thick substrate (but exactly same for a thick film). Take transmittance :

$$T_{\text{coh/coh}} = \frac{\theta_{ac}\theta_{cs}\theta_{sb}X_c X_s}{\left|1 - r_{ca}r_{cs}\varphi_c^2\right|^2 - \left|r_{sc} + r_{ca}\varphi_c^2\right|^2 \Gamma_{sb} X_s^2 - 2\left|1 - r_{ca}r_{cs}\varphi_c^2\right|\left|r_{sc} + r_{ca}\varphi_c^2\right|\left|r_{sb}\right| X_s \cos(2\varphi_s + \delta\ldots)}$$

which is in the form $\dfrac{AX_s}{B + DX_s^2 - C\cos(2\varphi_s + \delta\ldots)}$ where $C^2 = 4BD$ as for the square of any expression

which averages over the substrate fringes to give :

$$\langle T_{ab}\rangle_{\text{coh/coh}} = \frac{AX_s}{B - DX_s^2} = \frac{\theta_{ac}\theta_{cs}\theta_{sb}X_c X_s}{\left|1 - r_{ca}r_{cs}\varphi_c^2\right|^2 - \left|r_{sc} + r_{ca}\varphi_c^2\right|^2 \Gamma_{sb} X_s^2} = \langle T_{ab}\rangle_{\text{coh/incoh}}$$

i.e. averaging the coh/coh transmittance over one set of fringes gives the coh/incoh result.

Do we have the right to average over φ_s without simultaneously averaging over φ_c ?

The best thing, to calculate $\langle T_{ab}\rangle_{\text{incoh/incoh}}$ would be to average simultaneously over φ_c and φ_s (since both are $\propto \nu$)
i.e. find $\langle\langle T_{ab}\rangle\rangle_{\text{coh/coh}}$ and compare with expressions for $\langle T_{ab}\rangle_{\text{incoh/incoh}}$.

IF the directly - obtained expression for incoherent/incoherent transmittance is wrong, does this mean that the Harbecke method for ADJACENT incoherent substrates is wrong? Why?
Is it because reflections at an interface can never be truly interference- free? Then the energy transmitted in presence of interference really will be different from the incoherent/incoherent case, and so the averages also!
(We cannot justify that the transmittance is different when the layers are incoherent compared with just low resolution!)

It looks as if we cannot use $\langle T_{ab}\rangle_{\text{incoh/incoh}}$ as a short - cut calculation for interference- free transmittance!
...unless the approximation is tolerably good for that particular situation.

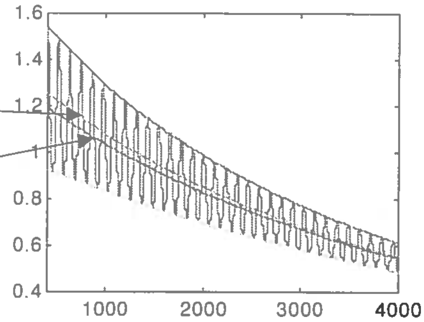
Compare results for (incoh/incoh), (coh/incoh), (coh/coh) and (geom. mean)
see *Tcohcoh.m*

An extreme case:

$\left\langle \left(T_{ab}\right)_{\text{incoh/incoh}} \right\rangle = 0.8451$

$\left\langle \left(T_{ab}\right)_{\text{coh/coh}} \right\rangle = \left\langle \left(T_{ab}\right)_{\text{coh/incoh}} \right\rangle = \left\langle \left(T_{ab}\right)_{\text{geom.mean}} \right\rangle = 0.8197$

3% error only in incoh/incoh for extreme case



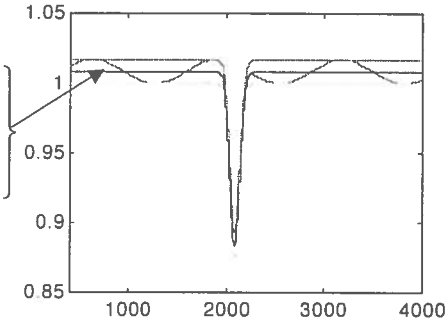
$n_{film}=2.916$;
$k_{film}=0.01$;
$d_{film}=15\mu m$;
$n_{substrate}=18$;
$k_{substrate}=0$;
$d_{substrate}=200\mu m$;

A 'normal' case:

$\left\langle \left(T_{ab}\right)_{\text{incoh/incoh}} \right\rangle = 1.0042$

$\left\langle \left(T_{ab}\right)_{\text{coh/coh}} \right\rangle = \left\langle \left(T_{ab}\right)_{\text{coh/incoh}} \right\rangle = \left\langle \left(T_{ab}\right)_{\text{geom.mean}} \right\rangle = 1.0044$

negligible error for usual case of a - Si : H on Si (similar n)



$n_{film}=3.35$;
k_{film}=gaussian;
$d_{film}=1.17\mu m$;
$n_{substrate}=3.42$;
$k_{substrate}=0$;
$d_{substrate}=200\mu m$;

NB Only <(incoh/incoh)> is different, whereas
<(coh/incoh)>, <(coh/coh)> and <(geom. mean)> all give the same result

RAPID DEMONSTRATION OF INCOHERENCE & COHERENCE

Suppose that a set of electric field complex amplitudes $\underline{E}_n = \underline{A}_n e^{j\varphi_n}$ are superposed at a point in space.
The total amplitude is $\underline{A} = \sum_n \underline{E}_n$

The total time-averaged intensity $I = \langle \underline{A}\underline{A}^* \rangle = \left\langle \left(\sum_n \underline{E}_n\right)\left(\sum_n \underline{E}_n^*\right) \right\rangle = \left(\sum_n |\underline{E}_n|^2\right) + \left\langle \left(\sum_{n\neq m} \underline{E}_n \underline{E}_m^*\right) \right\rangle$

$$= \left(\sum_n A_n^2\right) + \left\langle \left(\sum_{n\neq m} \underline{A}_n \underline{A}_m^* e^{j(\varphi_n-\varphi_m)}\right) \right\rangle = \left(\sum_n A_n^2\right) + \left\langle \left(\sum_{n>m} \underline{A}_n \underline{A}_m^* \cos(\varphi_n-\varphi_m)\right) \right\rangle = \left(\sum_n A_n^2\right) + \left(\sum_{n>m} \underline{A}_n \underline{A}_m^* \overline{\cos(\varphi_n-\varphi_m)}\right)$$

$\therefore I = \left(\sum_n A_n^2\right)$ INCOHERENT INTENSITY if phases are random, because $\overline{\cos(\varphi_n-\varphi_m)} = 0$; or

$I = \left(\sum_n A_n^2\right) + \left(\sum_{n>m} \underline{A}_n \underline{A}_m^* \overline{\cos(\varphi_n-\varphi_m)}\right)$ for COHERENT INTENSITY where the phase relations are fixed.

EXAMPLE: Suppose $\underline{A} = \sum_n \underline{E}_n = T + RTe^{-j\varphi} + R^2Te^{-2j\varphi} + \ldots + R^nTe^{-nj\varphi} + \ldots$

INCOHERENT: The phases φ are random, so

$$I = \sum_{n=0}^{\infty} T^2R^{2n} = \frac{T^2}{1-R^2};$$

COHERENT: The phases φ are constant, so

$$I = \left(\sum_{n=0}^{\infty} TR^n e^{-nj\varphi}\right)\left(\sum_{n=0}^{\infty} TR^n e^{-nj\varphi}\right)^* = \left(\frac{T}{1-R^{-j\varphi}}\right)\left(\frac{T}{1-R^{j\varphi}}\right) = \frac{T^2}{1+R^2-2R\cos\varphi}$$

Incoherent / incoherent paradox solution...?

Thermal photon coherence length is order of cm (Longhurst p160), therefore transmittance and reflectance are always coherent for sub-mm substrates and films!

Therefore, coh/incoh and incoh/incoh are false supposition: the "incoherence" is an artefact of observation (poor resolution).

The observation should be represented by averaging over reality which is coh/coh, and NOT by supposing single or adjacent films with no phase relation!

Remember: we want the film medium absorbance $= \alpha_c d_c$

By definition, the measured film absorbance $A_{\text{meas}} \equiv -\ln\left(T_{\text{film}}\right) \equiv \ln\left(T_{\text{coh/incoh}} / T_{\text{ref}}\right)$.

But the required true film absorbance $= \alpha_c d_c$.

Using the coherent/incoherent expression :

$$A_{\text{meas}} = -\ln\left[\frac{AX_c / T_{\text{ref}}}{B + DX_c^2 - CX_c}\right] \quad \text{where} \quad X_c = \exp\left(-\alpha_c d_c\right) \text{ as always,}$$

A, B, C, D using the previous definitions, and $T_{\text{ref}} = \theta_{as}\theta_{sb}X_s / \left(1 - \Gamma_{sa}\Gamma_{sb}X_s^2\right) = 0.5387$ for transparent silicon.

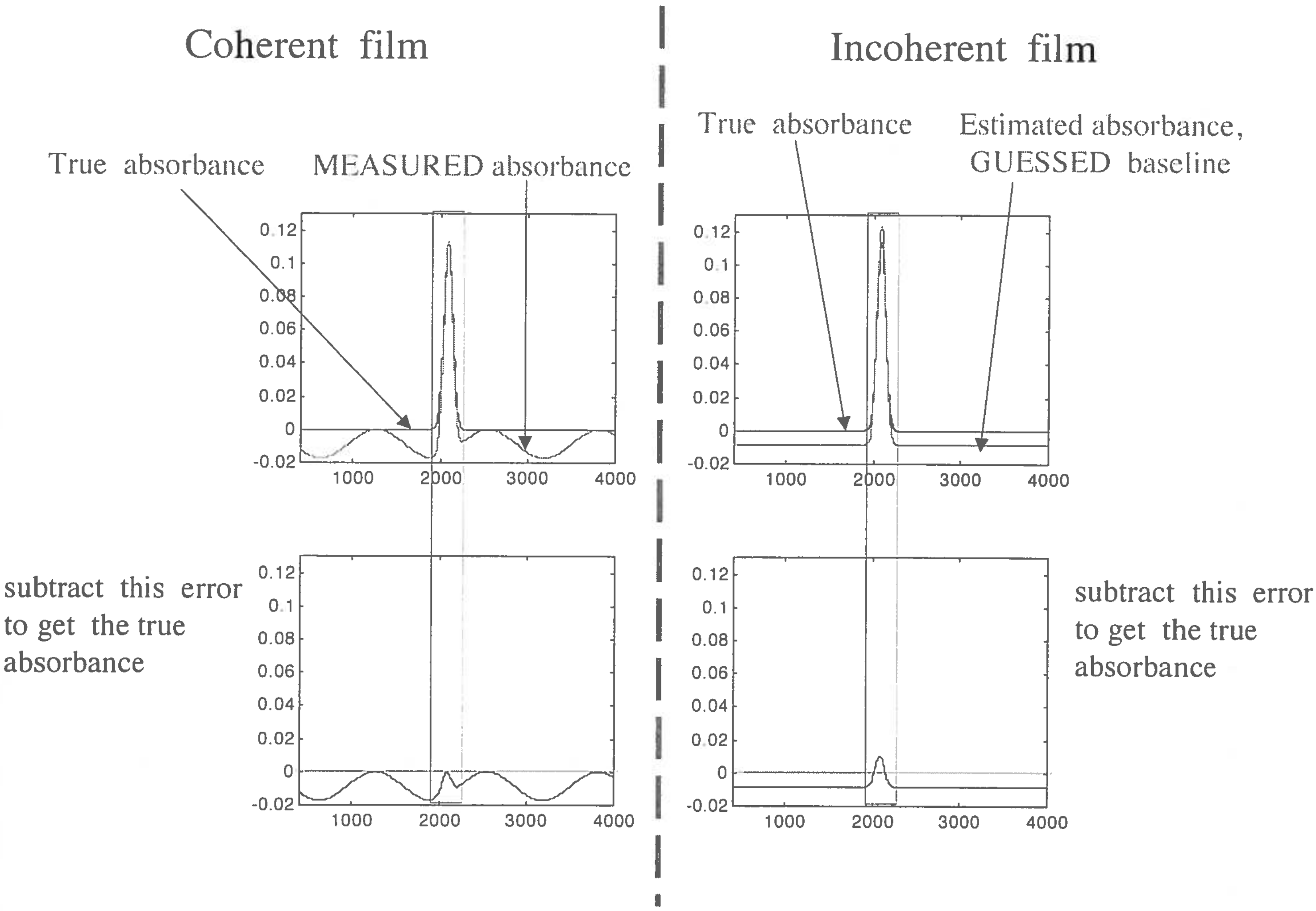
$$A_{\text{meas}} = \alpha_c d_c - \ln\left[\frac{A / T_{\text{ref}}}{B + DX_c^2 - CX_c}\right] \quad \text{... still exact, using } \alpha_c d_c = -\ln X_c.$$

Note that $A_{\text{meas}} \neq \alpha_c d_c$! In principle, area under the peak is not the true film absorbance.

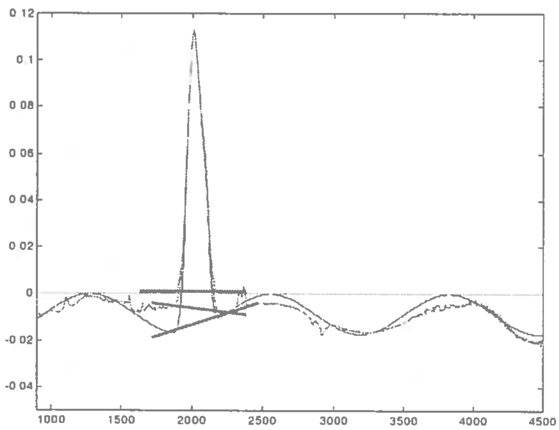
If we use the incoh/incoh expression for the film absorbance $A_{\text{meas}} \equiv -\ln\left(T_{\text{film}}\right) \equiv \ln\left(T_{\text{incoh/incoh}} / T_{\text{ref}}\right)$.

$$A_{\text{meas}} = -\ln\left[\frac{AX_c / T_{\text{ref}}}{B - D' X_c^2}\right] = \alpha_c d_c - \ln\left[\frac{A / T_{\text{ref}}}{B - D' X_c^2}\right].$$

Note that $A_{\text{meas}} \neq \alpha_c d_c$! The area under the peak is never the true film absorbance.



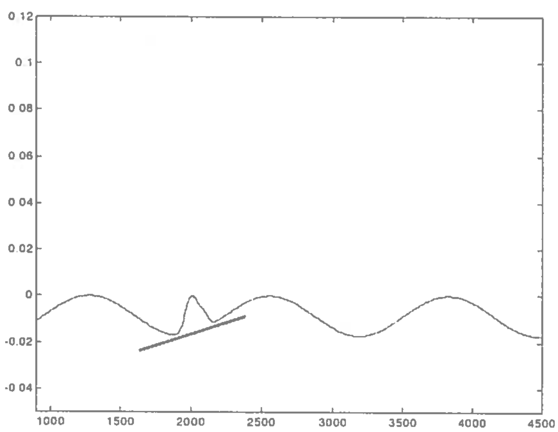
A practical example of a-Si:H film on a clean Si wafer



Green: measured absorbance = -ln(Tmeasured/Tsubstrate)

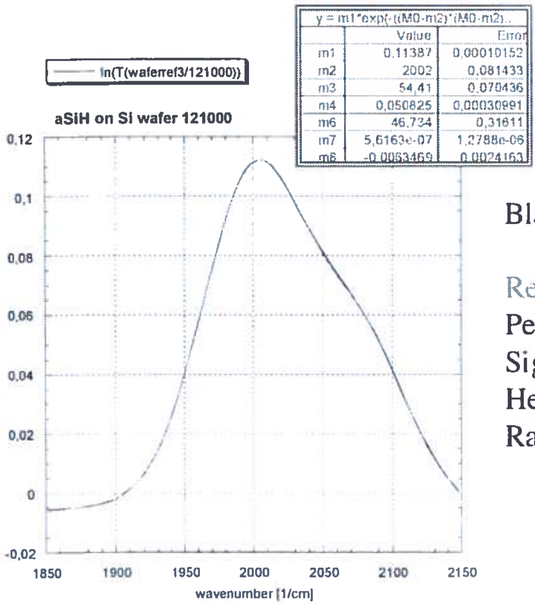
Blue: fitted curve for coherent expression using Matlab
FITTING PROCEDURE :
i) Fit N_c=3.35 for the correct fringe amplitude
ii) Fit film thickness d=1.17 µm for correct fringe period
(phase seems to be automatically OK)
iii) Choose peak position, width and height to fit peak (PTO)

Red: The true value of the fitted absorbance:
area = Σ[sqrt(pi).sigma.height]



This is the correct baseline from the model fit.
Note that it is incorrect to interpolate the "transparent" region oscillation because the baseline itself is affected by the absorbance of the film!

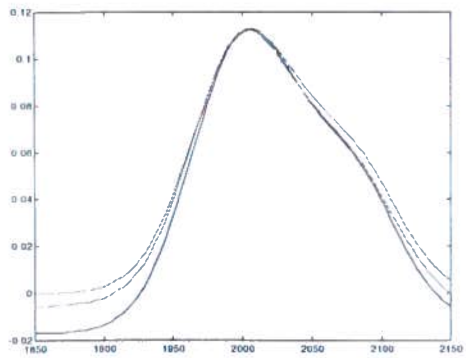
If the baseline is interpolated, the 'bump' is the overestimated error in the absorbance.
Predict overestimate by 13% due to baseline effect alone.



CONCLUSION: Directly estimated absorbance is incorrect
BUT: Ratio of absorbances is OK, so *porosity is valid.*

Black: measured absorbance = -ln(Tmeasured/Tsubstrate)

Red: directly fitted Gaussian curves (on a sloping baseline)
Peak positions: 2002 and 2080 1/cm
Sigma: 54.4 and 46.7 1/cm
Heights: 0.114 and 0.051;
Ratio = 2.24 used for porosity estimation

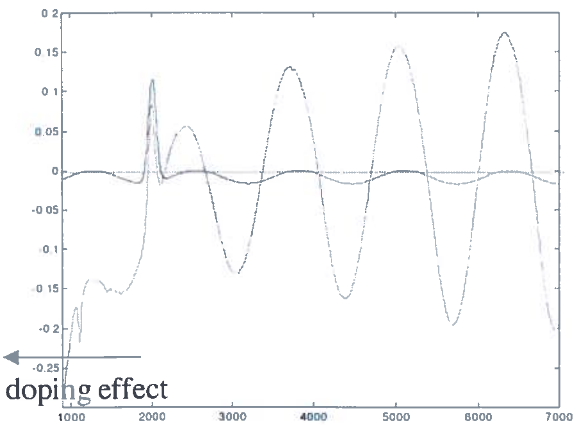


Green: measured absorbance = -ln(Tmeasured/Tsubstrate)

Blue: fitted curve for coherent expression:
Peak positions: 2002 and 2080 1/cm
Sigma: 54.4 and 46.7 1/cm
'True' heights: 0.1089 and 0.0505; smaller (by 5%) than the direct fit.
(Note: measurement distortion artificially reduced the error this time)
Ratio = 2.24 which is correct for porosity estimation.

Red: The true value of the fitted absorbance;
total area = Σ[sqrt(pi).sigma.height]

How to interpret recent measurements?



Blue curve: previous fit to absorbance for a-Si:H on Si wafer

Green curve: measured aborbance for a-Si:H on Si:C on Si wafer
Note that the fringe amplitude is much larger, because the refractive indices are not so similar?

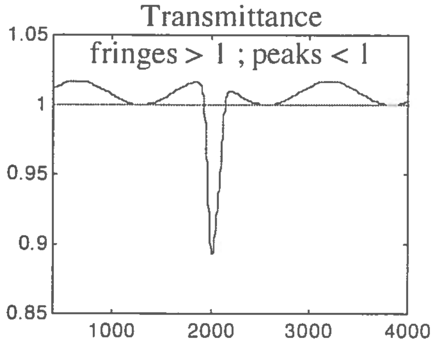
This requires a full matrix treatment...? But thin SiC layer should not have such a strong effect?

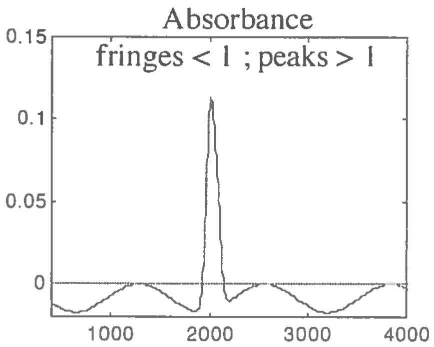
Maybe a problem with strongly-absorbing doped wafer reference?

For a single a-Si:H layer, it is difficult to understand transmission fringes < 1 and absorbance fringes > 1, because we don't expect a-Si:H to be more dense than Si wafer (unless SiO_2 and SiC layers influence?)

OK

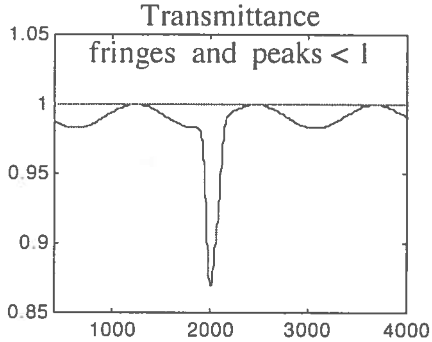
$n_{film} = 3.35 < n_{Si} = 3.42$

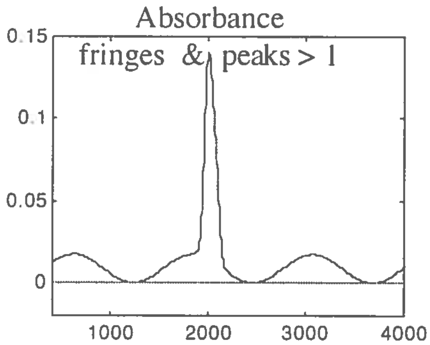




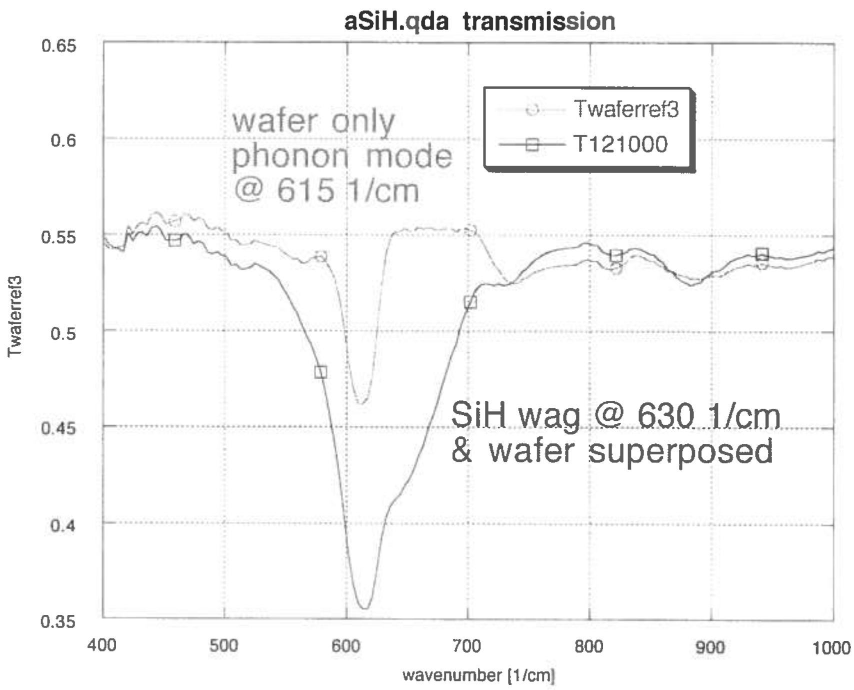
NOT OK??

$n_{film} = 3.49 > n_{Si} = 3.42$

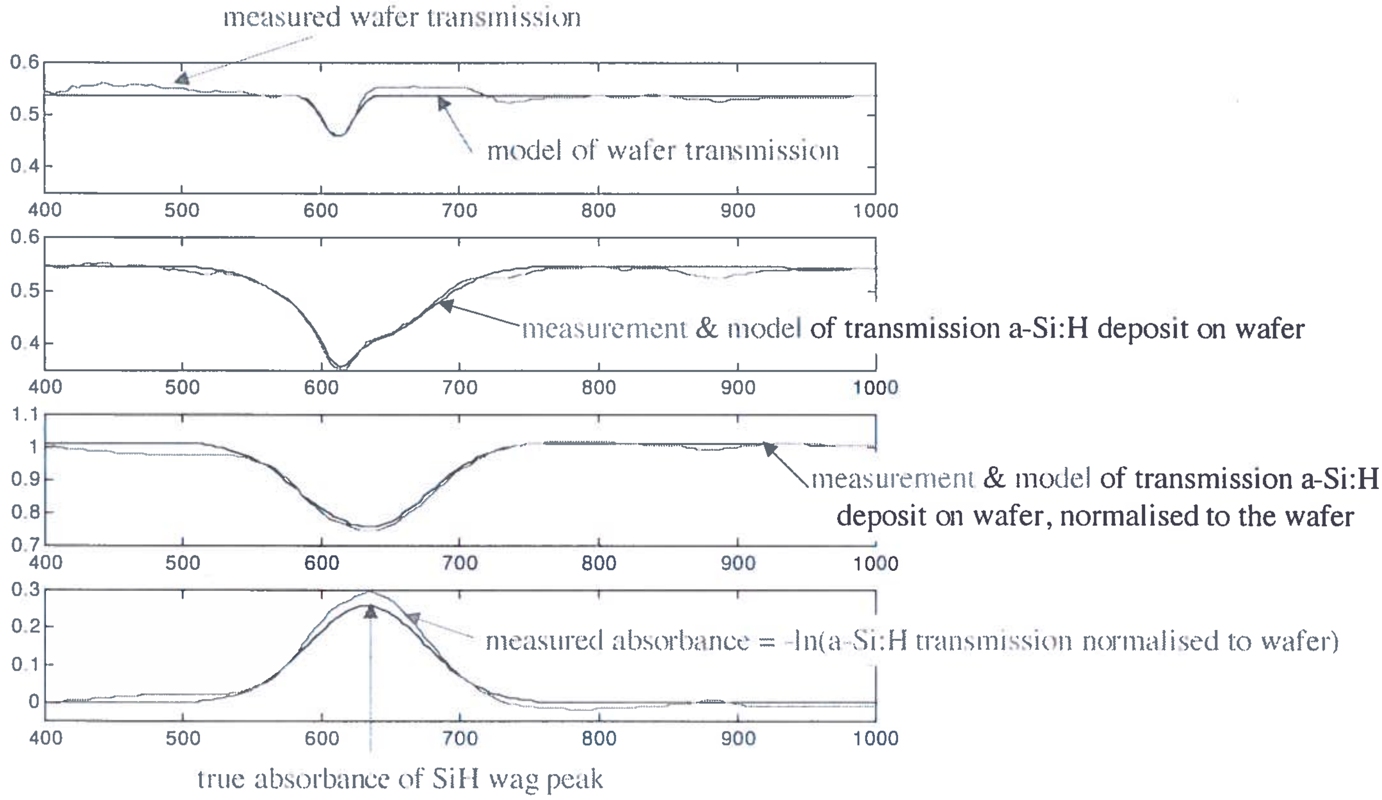




Estimation of hydrogen density from Si-H wag peak @ 630 cm^{-1} complicated by partial superposition with c-Si phonon mode @ 615 cm^{-1}



Estimation of absorbance of Si-H wag peak @ 630 cm^{-1}



H concentration = constant x (integrated absorbance of Si-H wag peak)

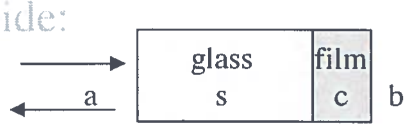
Was the Fredometer analysis correct? Check:

$$(R_{ab})_{\text{ref}} = |r_{as}|^2 + \frac{|t_{as}t_{sa}r_{sb}|^2 \exp(-2\alpha_s d_s)}{1 - |r_{sa}r_{sb}|^2 \exp(-2\alpha_s d_s)}$$ for a single thick substrate.

For transparent glass index s : $|r_{as}|^2 = |r_{sa}|^2 = |r_{sb}|^2 = \left(\frac{s-1}{s+1}\right)^2 = R$. For glass, $s \approx 1.5$; $R \approx 4\%$ (one side only).

$$|t_{as}|^2 |t_{sa}|^2 = \frac{4}{(1+s)^2} \cdot \frac{4s^2}{(1+s)^2} = (1-R)^2 \text{ (all transparent)}. \quad \therefore (R_{ab})_{\text{ref}} = R + \frac{(1-R)^2 R}{1-R^2} = \frac{2R}{(1+R)} \approx 7.7\% \text{ (both sides)}.$$

Now add an absorbing layer on the opposite side:



Now $|r_{sb}|^2 \to \left|\frac{r_{sc} + r_{cb}\varphi^2}{1 - r_{cs}r_{cb}\varphi^2}\right|^2 = R_{gf}$, say, where $r_{sc} = \frac{s - n_c}{s + n_c} = -r_{cs}$; $r_{cb} = \frac{n_c - 1}{n_c + 1}$; $\varphi = \exp(j2\pi d n_c/\lambda)$

$$\therefore (R_{ab})_{\text{signal}} = R + \frac{(1-R)^2 R_{gf}}{1 - RR_{gf}} = \frac{R + R_{gf} - 2RR_{gf}}{1 - RR_{gf}}.$$

... the analysis of Fredometer in *Fringe7.m* is correct because

i) glass is transparent, ii) reflectance is measured, & iii) absorbing film on the opposite side

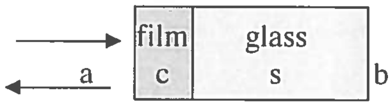
Note that there are three principal configurations for single, coherent, absorbing films on thick, incoherent, absorbing substrates:

1) TRANSMISSION. This has been treated above for the example of infrared measurements.

2) REFLECTION FROM THE SUBSTRATE SIDE. This is the case of the Fredometer described on the previous page.

3) REFLECTION FROM THE FILM SIDE. This is the case of spectrophotometer reflectance measurements directly onto the film (viz. G. Benvenuti); rapidly described below:

$$(R_{ab})_{\text{ref}} = |r_{as}|^2 + \frac{|t_{as}t_{sa}r_{sb}|^2 \exp(-2\alpha_s d_s)}{1-|r_{sa}r_{sb}|^2 \exp(-2\alpha_s d_s)}$$ for a single thick substrate.



But now there are FOUR coefficients which are changed by the absorbing film:

$$r_{as} \rightarrow r'_{as} = r_{af} + \frac{t_{af}t_{fa}\varphi^2}{1-r_{fa}r_{fs}\varphi^2}; \quad r_{sa} \rightarrow r'_{sa} = r_{sf} + \frac{t_{sf}t_{fs}\varphi^2}{1-r_{fa}r_{fs}\varphi^2};$$ (and their simpler versions)

$$t_{as} \rightarrow t'_{as} = \frac{t_{af}t_{fs}\varphi}{1-r_{fa}r_{fs}\varphi^2}; \quad t_{sa} \rightarrow t'_{sa} = \frac{t_{sf}t_{fa}\varphi}{1-r_{fa}r_{fs}\varphi^2}.$$ At least they all have the same denominator!

Note that if the substrate is thick and strongly absorbing, then $\exp(-2\alpha_s d_s) << 1$ and

$$(R_{ab})_{\text{signal}} \approx |r'_{as}|^2.$$

CONCLUSIONS

Found a fitting routine for analysis of absorbing coherent film on an absorbing incoherent substrate.
(use for porosity and H-content estimation)

Literature expressions for incoherent film on incoherent substrate are invalid if the absorption peak is narrower than the fringe period.

There seems to be a basic physical error in assuming adjacent incoherent films-and-substrates...?

The Fredometer analysis is correct, for three separate reasons.

Infrared fringe measurements should show $T>1$ and negative absorbance, before analysis is feasible.
(take care to use same substrate reference).