Thin-film optics

Theory and measurements

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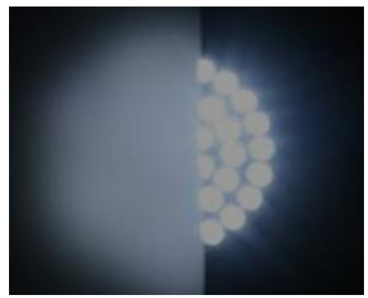
Theory

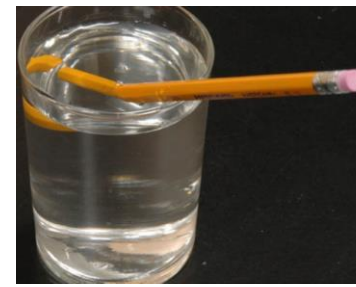
Optical phenomena

Specular

Scattering/diffusion

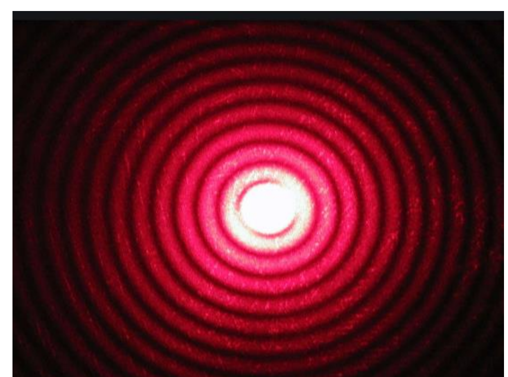


Refraction



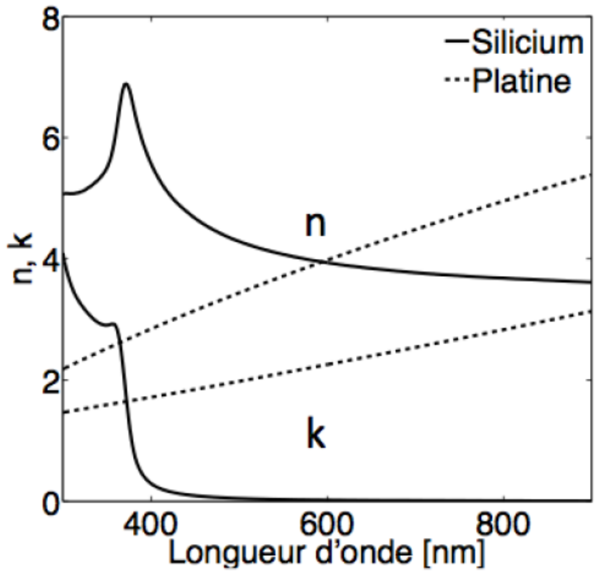
Interferences

Diffraction



Each material is optically defined by a refractive index

The refractive index indicates how the material behave

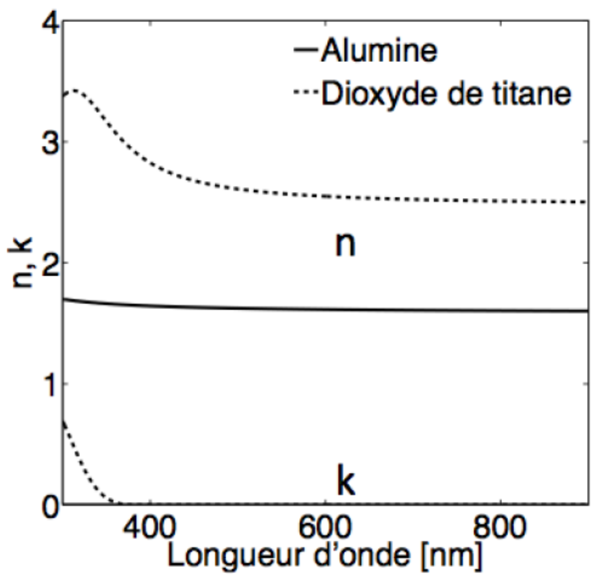


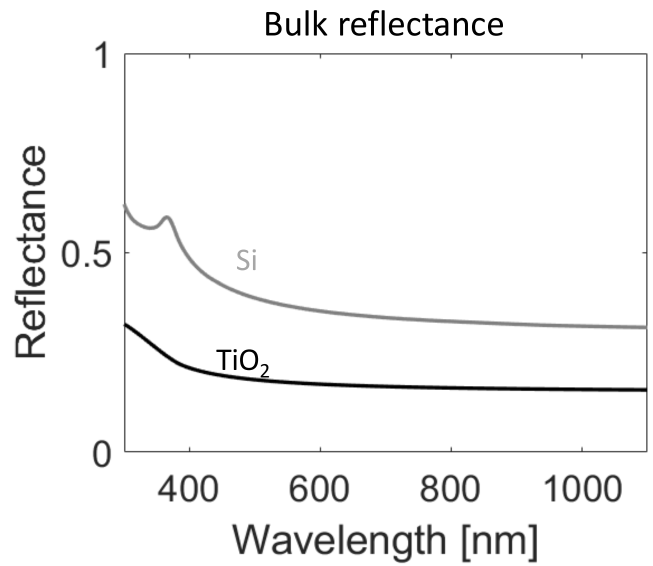
$$\tilde{n} \triangleq n + ik$$

Index

Extinction coefficient

$$n_i = \frac{C}{v_i}$$



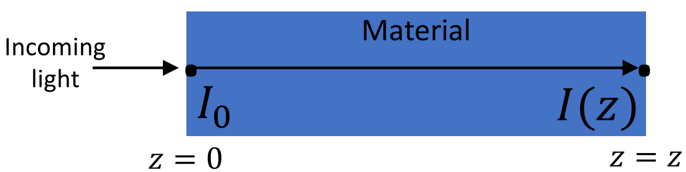


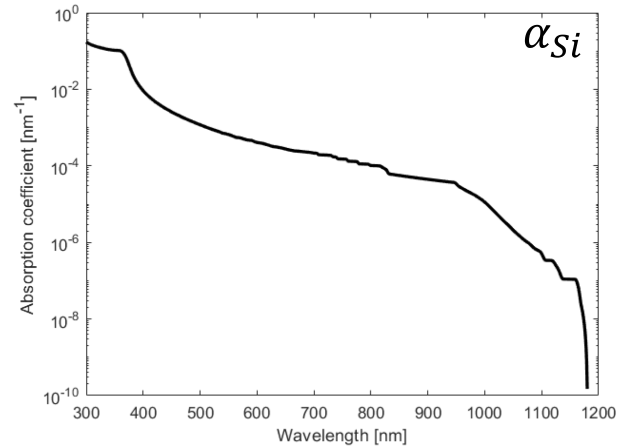
The imaginary part describes how a system dissipates energy

Absorption coefficient

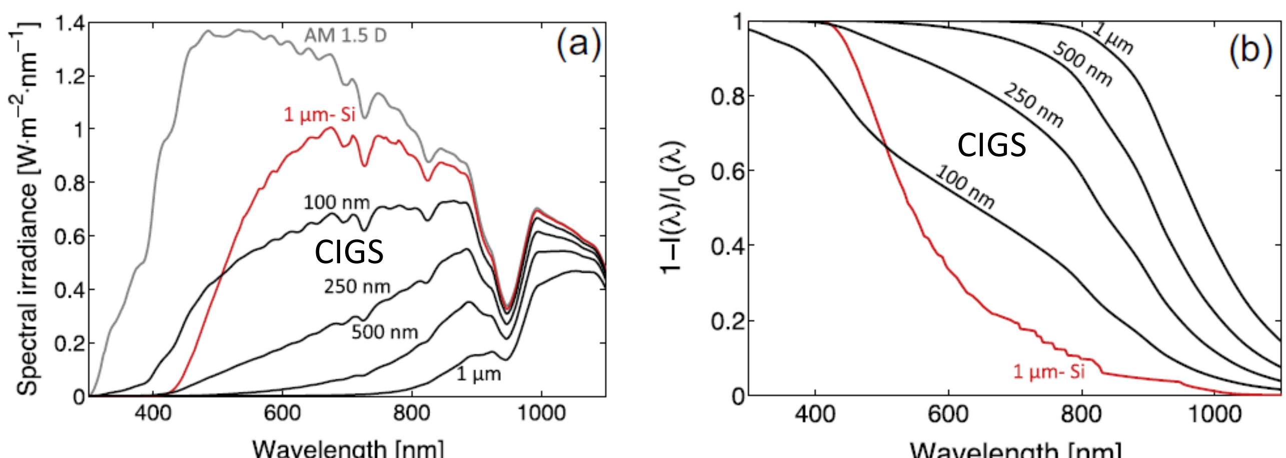
$n + ik$

Lambert-Beer's law: $$\frac{I(z)}{I_0} = e^{-\alpha z} = e^{-\frac{4\pi k}{\lambda} z}$$





We can easily compute how fast the light is absorbed in a material:



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n and k are linked by Kramers-Kronïg relation

Because of the causality condition

Relation between the complex refractive index and the complex dielectric function

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$$

$$\tilde{\varepsilon} = \tilde{n}^2$$

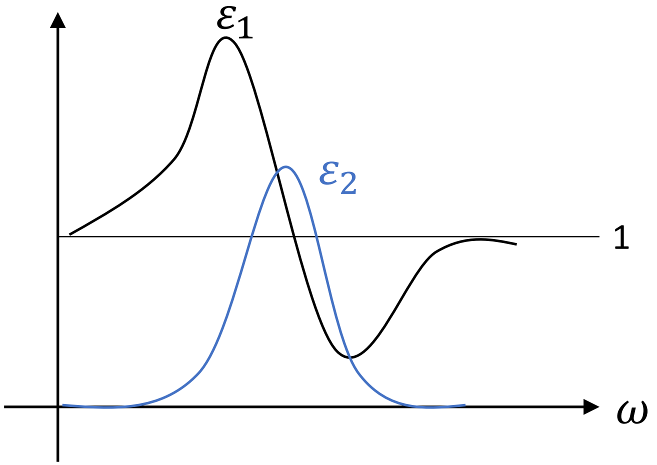
$$n = \frac{1}{\sqrt{2}}\left(\varepsilon_1 + (\varepsilon_1^2 + \varepsilon_2^2)^{1/2}\right)^{1/2}$$

$$k = \frac{1}{\sqrt{2}}\left(-\varepsilon_1 + (\varepsilon_1^2 + \varepsilon_2^2)^{1/2}\right)^{1/2}$$

Kramers-Konïg transformation (KK transformation)

$$\varepsilon_1(\omega') - 1 = \frac{2}{\pi} P \int_0^\infty \frac{\varepsilon_2(\omega)\omega}{\omega^2 - \omega'^2} d\omega$$

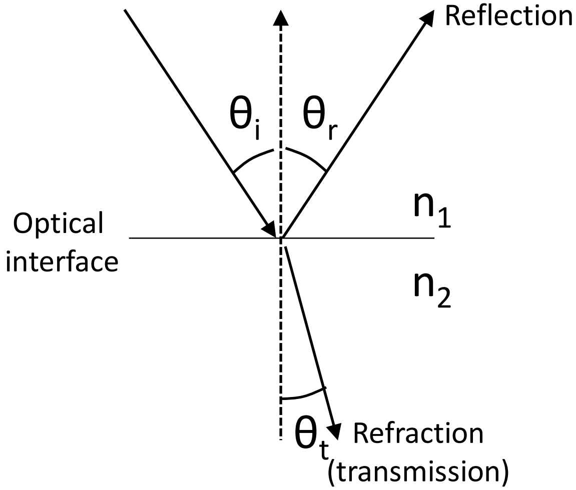
$$\varepsilon_2(\omega') = -\frac{2\omega'}{\pi} P \int_0^\infty \frac{\varepsilon_1(\omega)}{\omega^2 - \omega'^2} d\omega$$



Of the upmost important for ellispometry and (n,k) fitting!

Snell's law and Fresnel coefficients

Refraction, reflection, transmission in a specular way



Fresnel reflection and transmission coefficients

$$r = \frac{E_r}{E_i} \qquad t = \frac{E_t}{E_i}$$

$$r = \frac{n_1 - n_2}{n_1 + n_2} \qquad t = \frac{2n_1}{n_1 + n_2}$$

Specular reflection: $\theta_i = \theta_r$

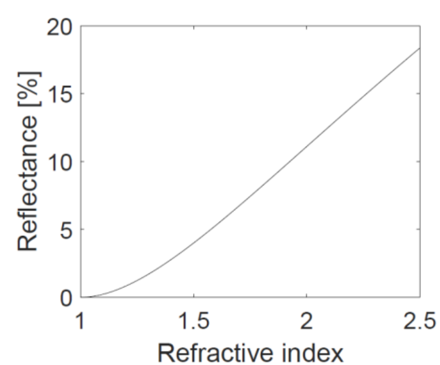
Snell's law: $n_1 \sin\theta_1 = n_2 \sin\theta_2$

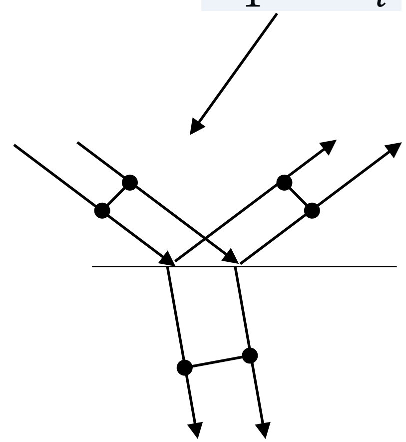
$$n_i = \frac{C}{v_i}$$

The intensity is proportional to the square of the amplitude

$$R = |r|^2 \qquad T = \frac{n_2}{n_1}\frac{\cos\theta_t}{\cos\theta_i}|t|^2$$

Refractive index contrast increases the reflectivity:

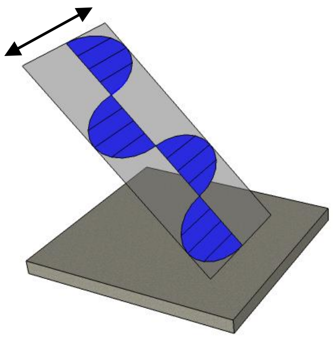


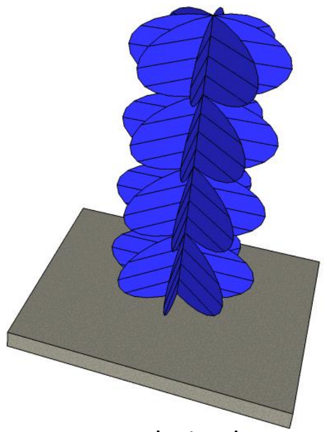


Polarization

Do I have to pay attention to?

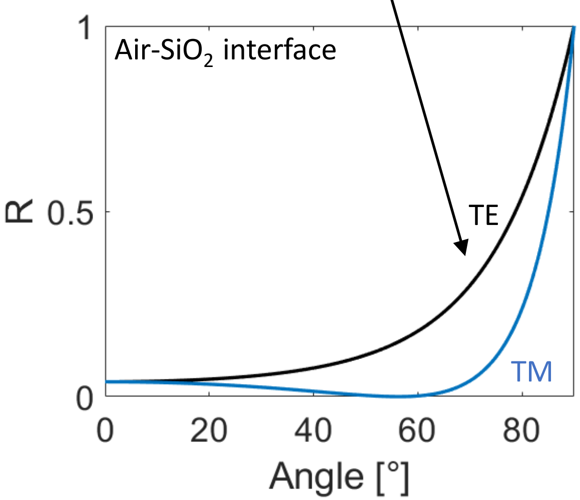
Most of the time, we don't care about the polarization. Standard measurement: unpolarized light, at 0° angle …



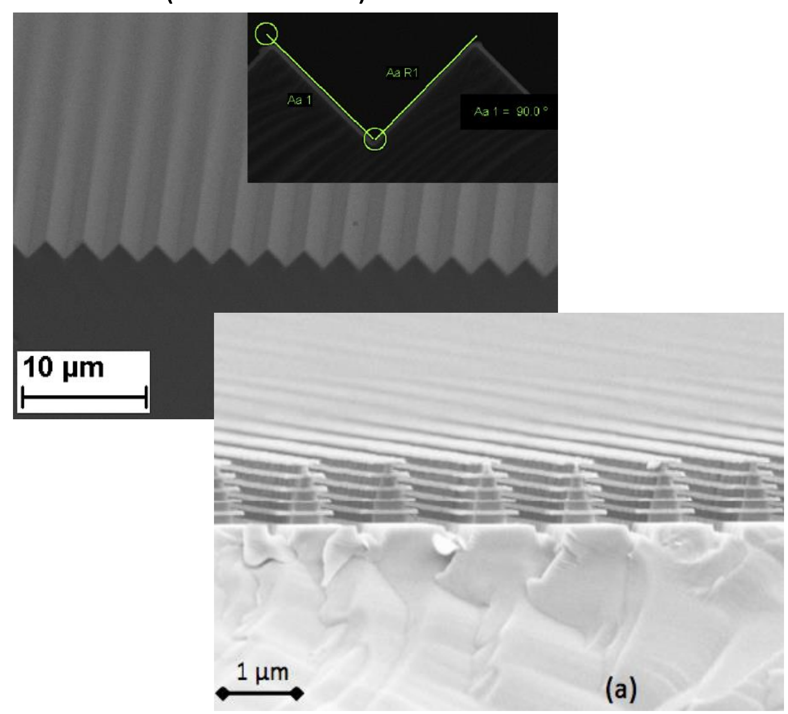


Transverse electric (TE)

Unpolarized



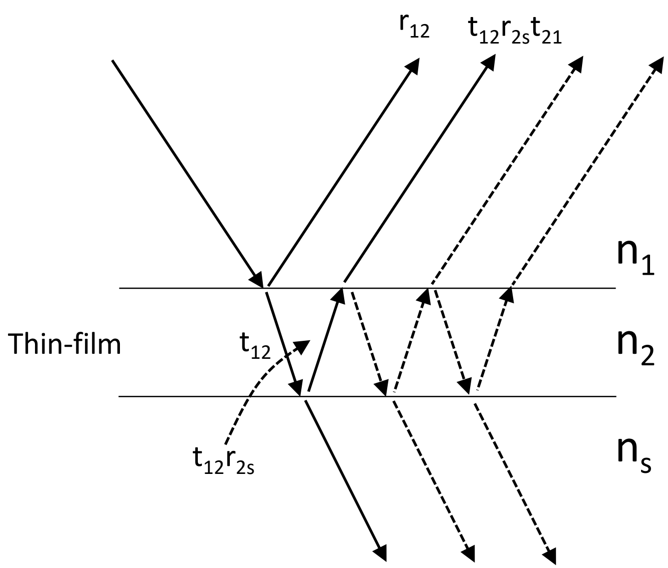
… Unless your device has an oriented optical micro/nano structure (and size ≈ λ)



Thin-film optics

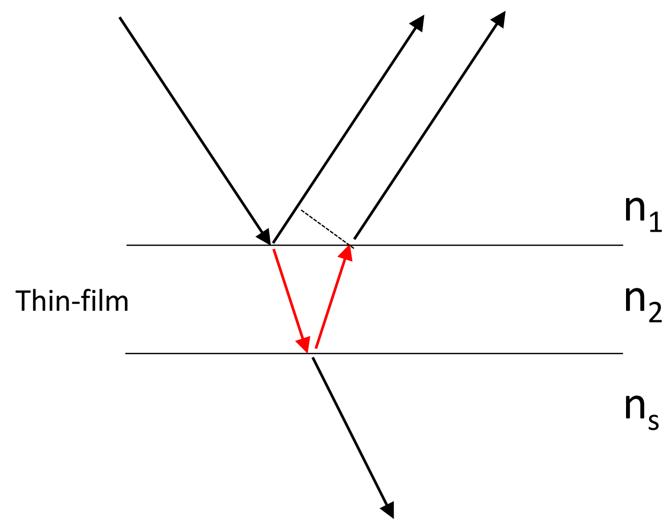
Ray-tracing and interferences

Multiple beams



Amplitude-related

Interferences between beams



Phase-related

$$\Delta x = 2n_t L \cos\theta_t \qquad \Phi = \frac{2\pi}{\lambda}\Delta x = \frac{4\pi}{\lambda} n_t L \cos\theta_t$$

Destructive or constructive interferences: If $\phi = (2m-1)\pi$ then $L = \dfrac{\lambda}{4n_t}$

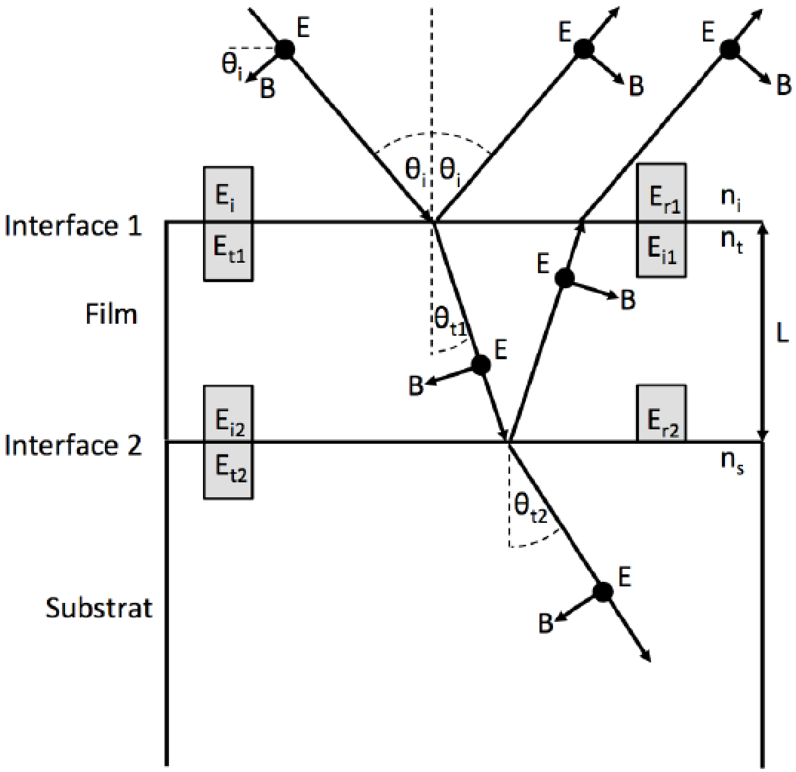
$m = [1, \dots, m]$

Quarter-wave film!

Transfer matrix method (TMM)

Can solve any thin-film stack system

Limit conditions on fields require that tangential components must be continuous through the interface



$$E_1 = E_i + E_{r1} = E_{t1} + E_{i1}$$
$$E_2 = E_{i2} + E_{r2} = E_{t2}$$
$$B_1 = B_i\cos(\theta_i) - B_{r1}\cos(\theta_i) = B_{t1}\cos(\theta_{t1}) - B_{i1}\cos(\theta_{t1})$$
$$B_2 = B_{i2}\cos(\theta_{t1}) - B_{r2}\cos(\theta_{t1}) = B_{t2}\cos(\theta_{t2})$$

$$\begin{pmatrix} E_1 \\ B_1 \end{pmatrix} = \begin{pmatrix} \cos(\phi) & \frac{i\sin(\phi)}{\gamma_t} \\ i\gamma_t\sin(\phi) & \cos(\phi) \end{pmatrix} \begin{pmatrix} E_2 \\ B_2 \end{pmatrix} \qquad \gamma_t = \frac{\widetilde{n}_t}{c}\cdot\cos^m(\theta_{t1}) \qquad \phi = \frac{2\pi}{\lambda}\widetilde{n}_t L\cos(\theta_{t1})$$

$$\mathfrak{M} = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}$$

The matrix only depends on material properties and on thickness

$$\begin{pmatrix} E_1 \\ B_1 \end{pmatrix} = \mathfrak{M}_1 \begin{pmatrix} E_2 \\ B_2 \end{pmatrix}$$
$$\begin{pmatrix} E_2 \\ B_2 \end{pmatrix} = \mathfrak{M}_2 \begin{pmatrix} E_3 \\ B_3 \end{pmatrix}$$
$$\vdots$$
$$\begin{pmatrix} E_1 \\ B_1 \end{pmatrix} = \mathfrak{M}_1\mathfrak{M}_2\mathfrak{M}_3\cdots\mathfrak{M}_n \begin{pmatrix} E_n \\ B_n \end{pmatrix} = \mathfrak{M}\begin{pmatrix} E_n \\ B_n \end{pmatrix}$$

$$r = \frac{\gamma_i m_{11} + \gamma_i\gamma_s m_{12} - m_{21} - \gamma_s m_{22}}{\gamma_i m_{11} + \gamma_i\gamma_s m_{12} + m_{21} + \gamma_s m_{22}} \qquad \gamma_i = \frac{\widetilde{n}_i}{c}\cdot\cos^m(\theta_i)$$

$$t = \frac{2\gamma_i}{\gamma_i m_{11} + \gamma_i\gamma_s m_{12} + m_{21} + \gamma_s m_{22}} \qquad \gamma_s = \frac{\widetilde{n}_s}{c}\cdot\cos^m(\theta_{t2})$$

c=speed of light

$$R = |r|^2$$

$$T = \frac{n_2\cos\theta_t}{n_1\cos\theta_i}|t|^2$$

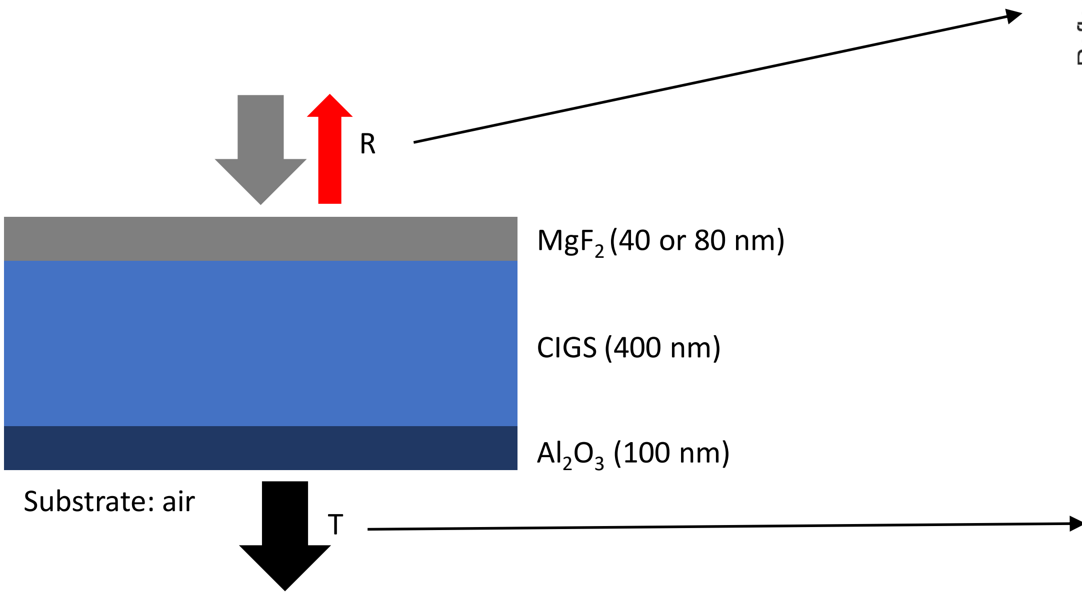
$$A = 1 - R - T$$

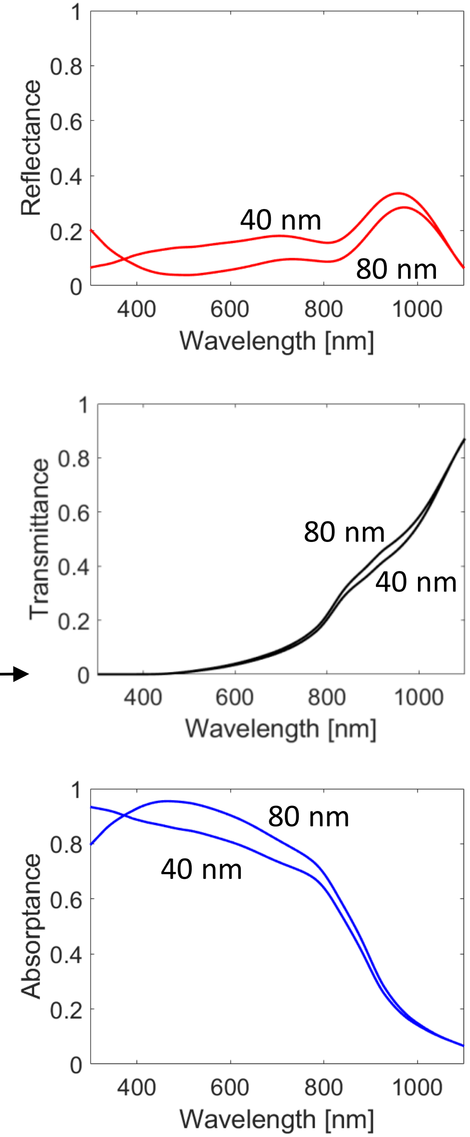
Transfer matrix method (TMM)

Output: R, T and A of any stack system

Where can I find (n,k) dispersion?

- -https://refractiveindex.info/
- -On the computer of an ellipsometer
- -Papers
- -Fitting

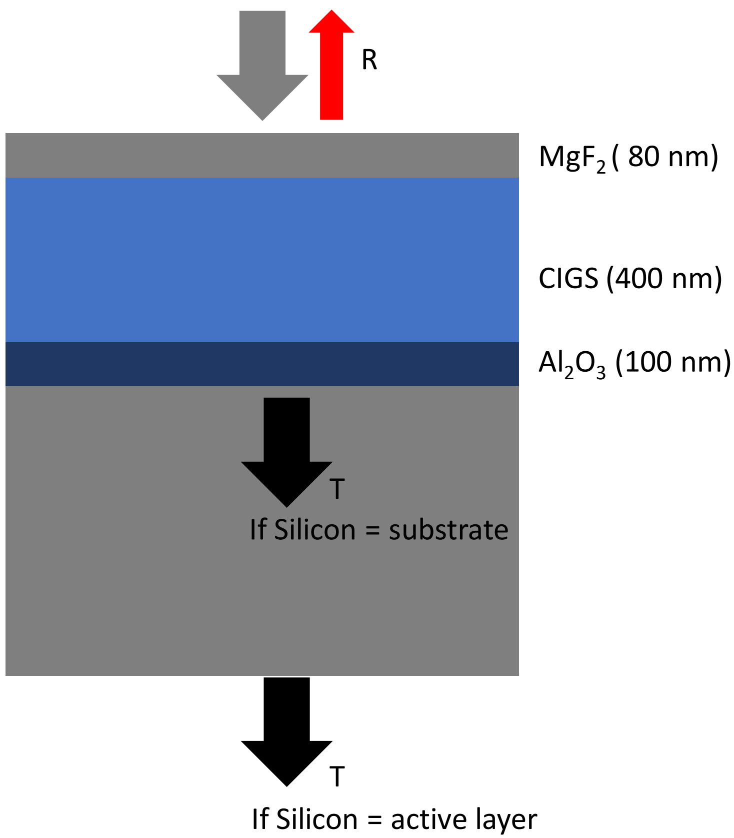


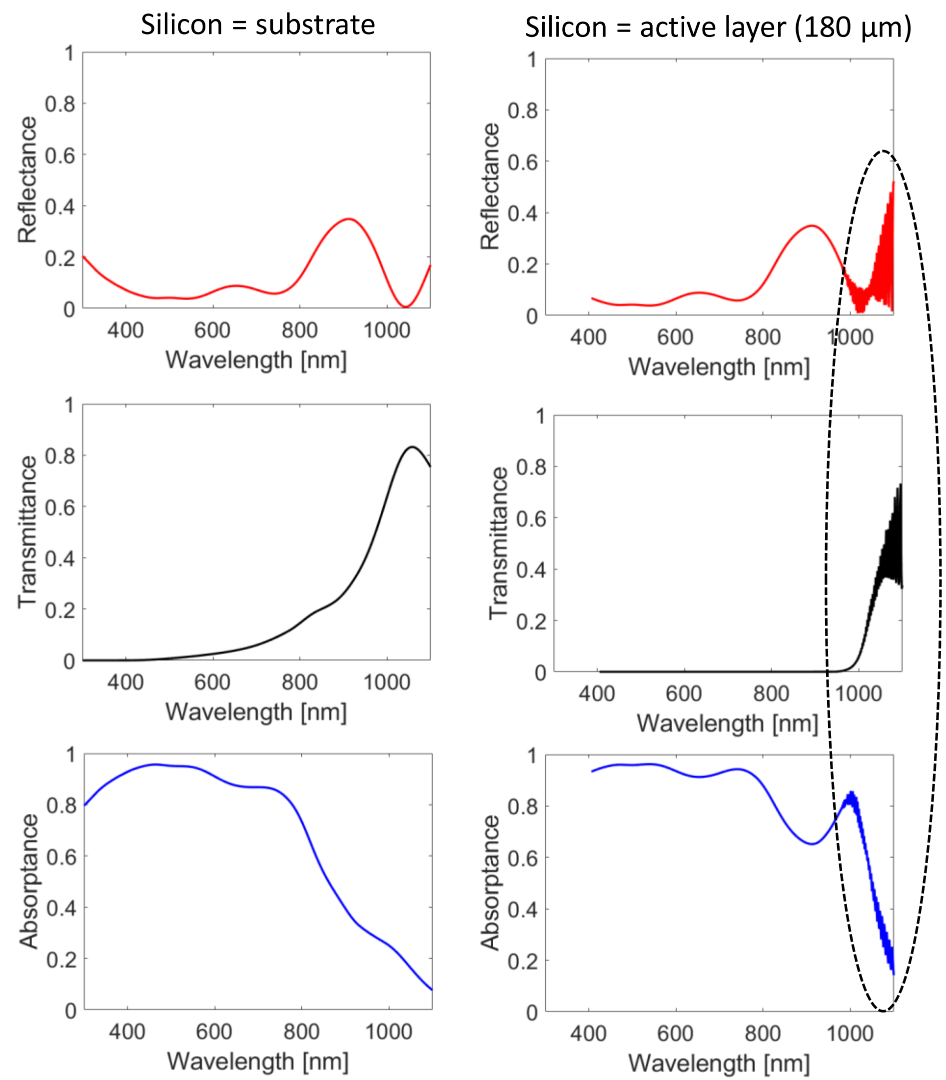


Transfer matrix method (TMM)

Limitation – coherent substrate

TMM assumes an infinite substrate, but in reality, the substrate also has a thickness

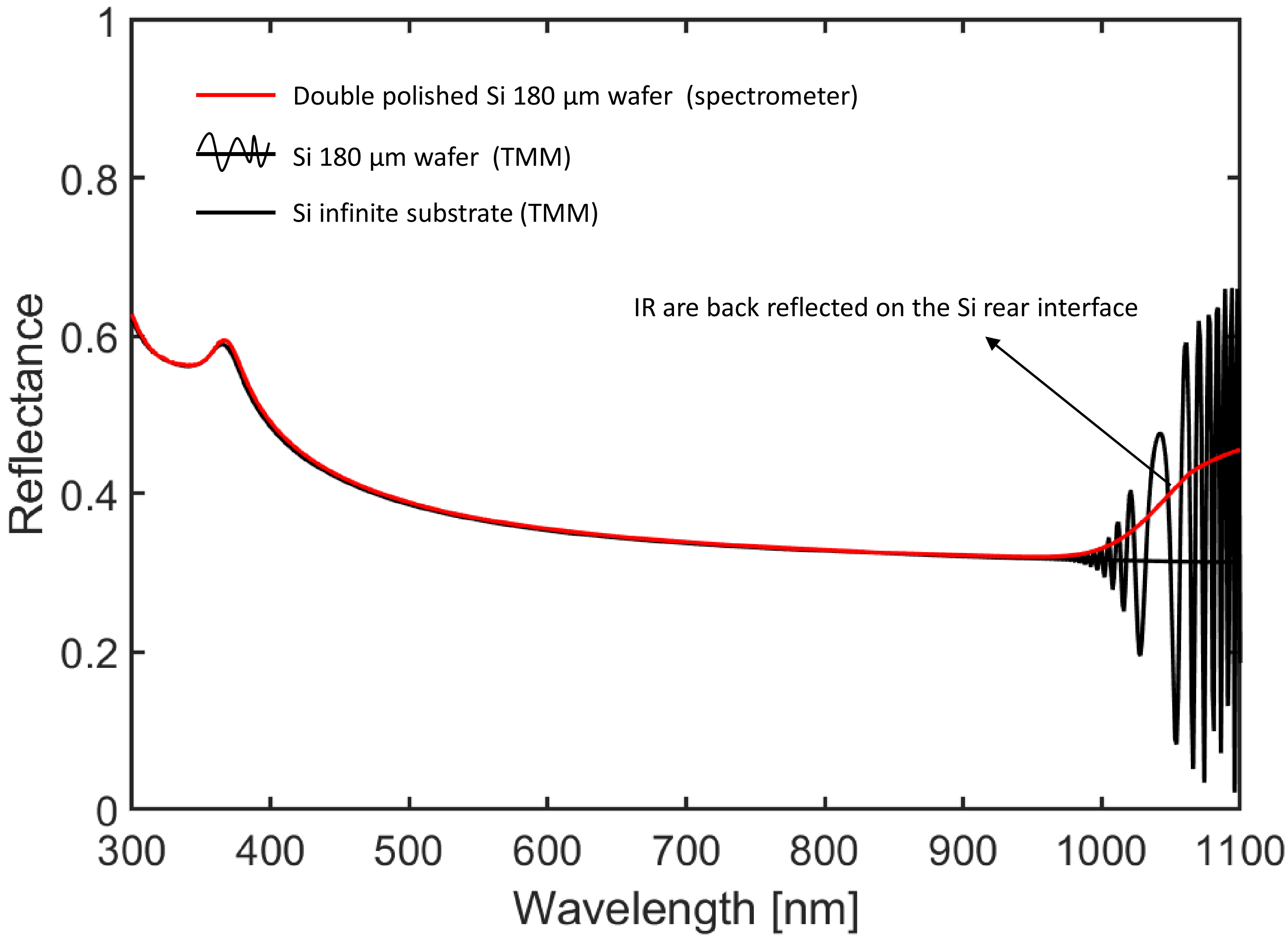




Transfer matrix method (TMM)

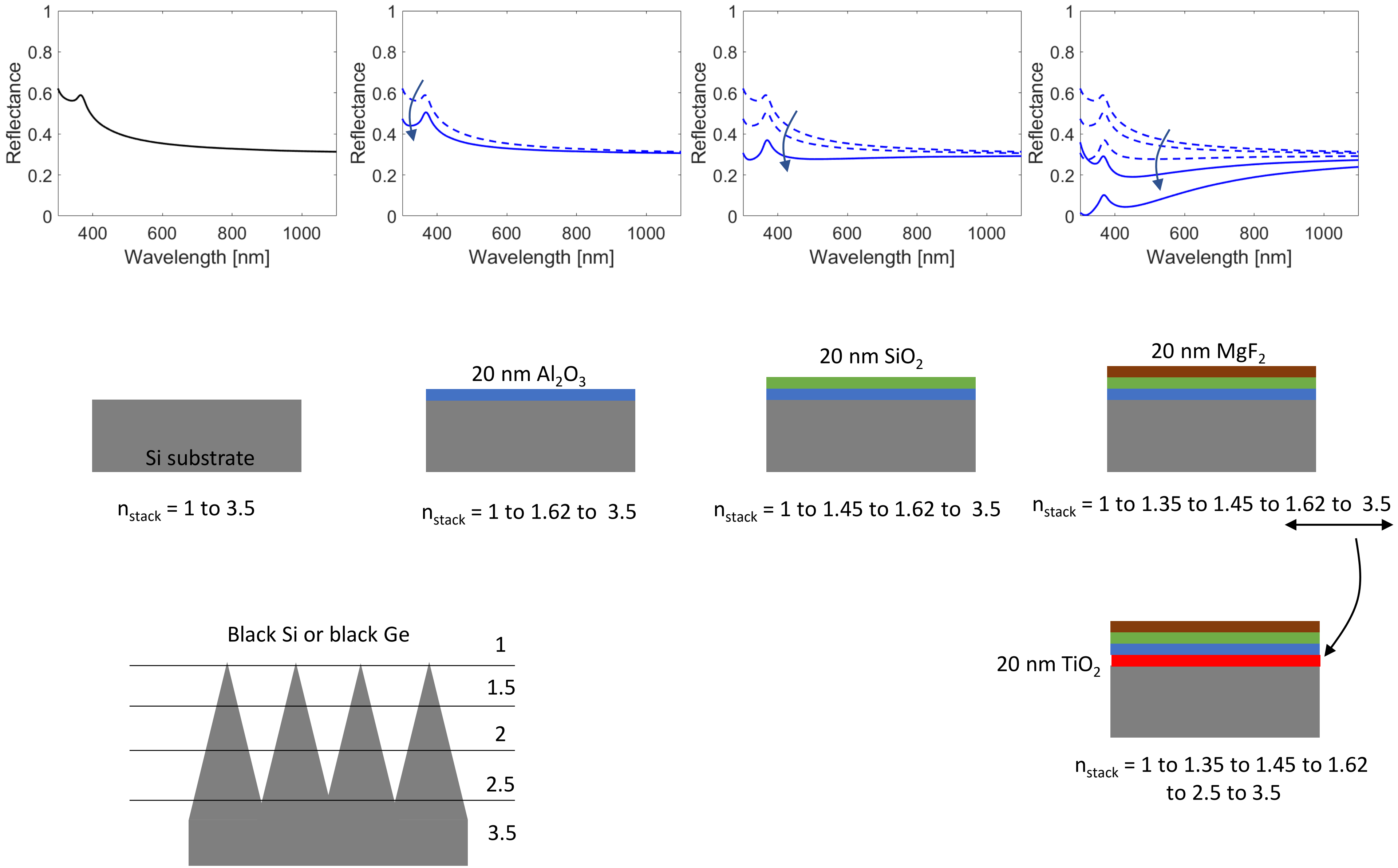
Limitation – coherent substrate

Thick materials need to be processed as uncoherent layers !!



Transfer matrix method (TMM)

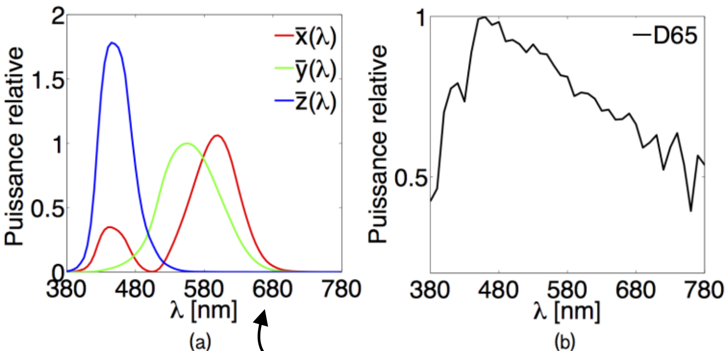
Decreasing R by smoothing optical interfaces



Transfer matrix method (TMM)

CIE xyY 1931 Diagrams

Given the reponse of eyes to light, color can be simulated



$$x_{CIE} = \frac{X}{X+Y+Z}$$

$$y_{CIE} = \frac{Y}{X+Y+Z}$$

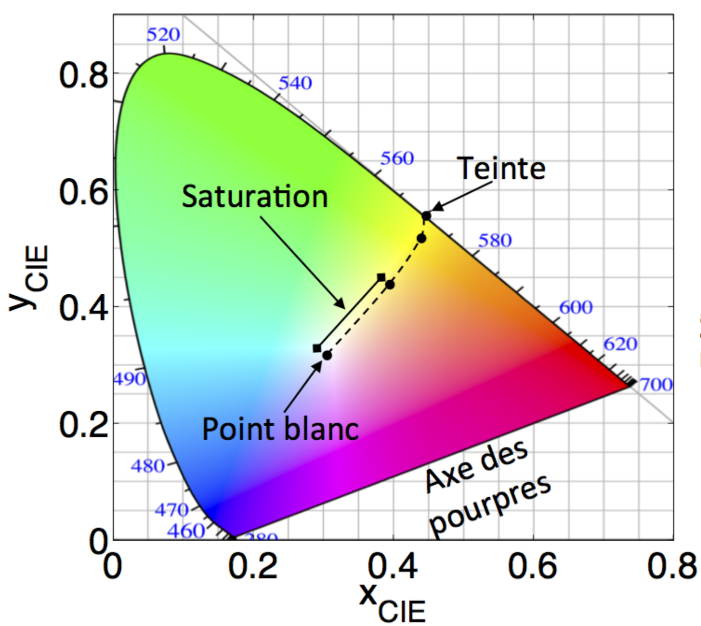
Your spectrum

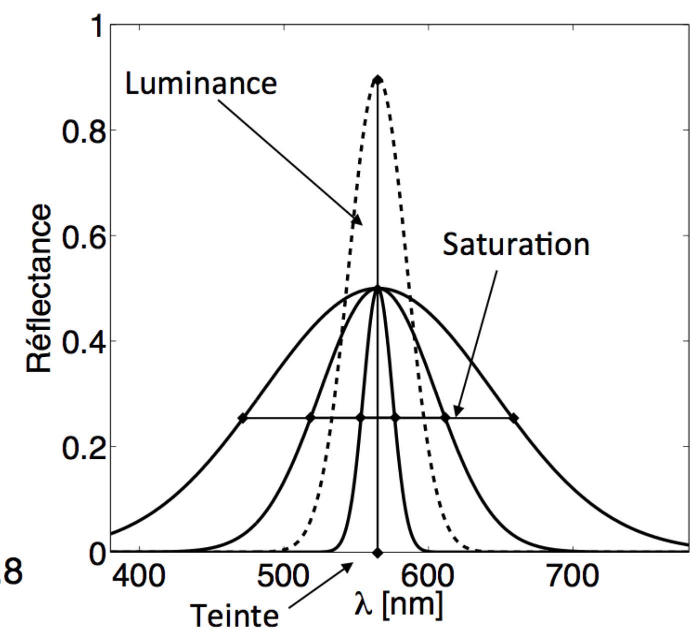
$$X = k \cdot \int \bar{x}(\lambda) S(\lambda) I(\lambda) d\lambda$$

$$Y = k \cdot \int \bar{y}(\lambda) S(\lambda) I(\lambda) d\lambda$$

$$Z = k \cdot \int \bar{z}(\lambda) S(\lambda) I(\lambda) d\lambda$$

$$k = \frac{100}{\int I(\lambda) \bar{y} d\lambda}$$





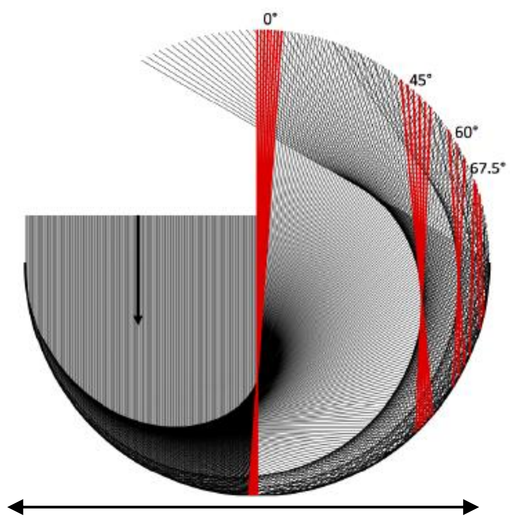
Finite Difference – Time Domain (FDTD) for 3D complex structures

Lumerical solution

Lumerical is part of ANSYS now

Multi-scale simulations

Ray-tracing + TMM



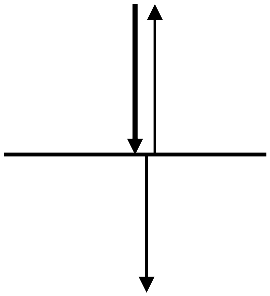
Much larger than the wavelength

Measurements

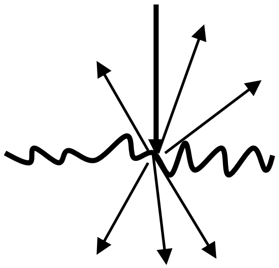
Specular or hemispherical reflectance

Depending on your device…

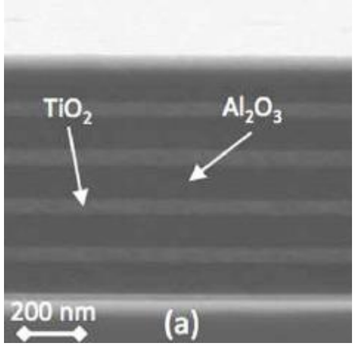
Specular measurements
Flat interfaces/thin-films

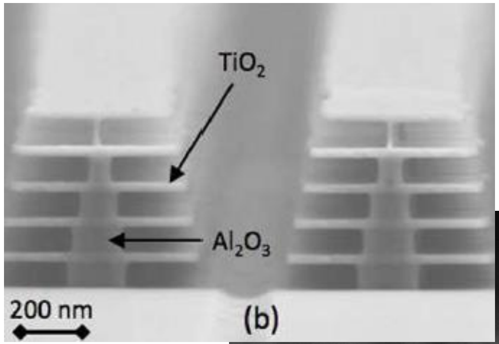


Hemispherical measurements
Anything else

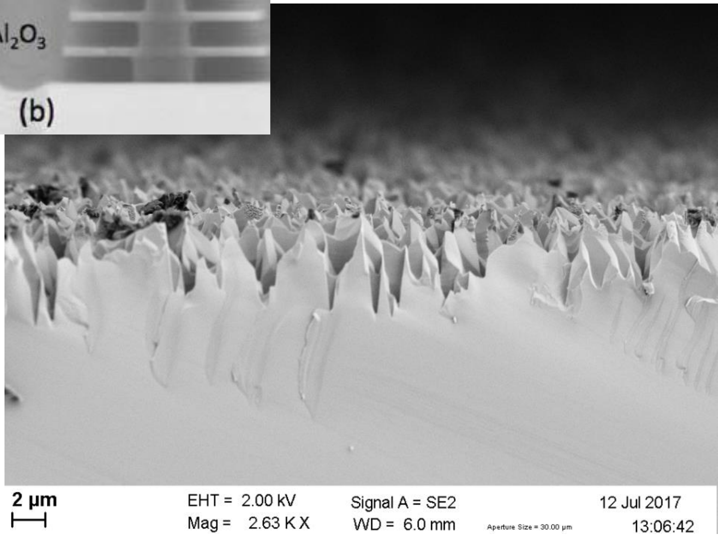


As long as roughness is low!





Roughness increases scattering



Specular

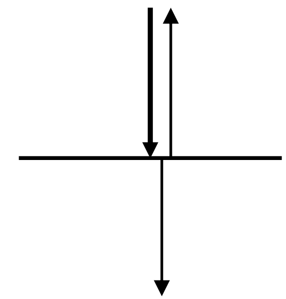
What you need

Best option is a full-in-one spectrophotometer

Can measure the absolute values of R and T (and thus A)

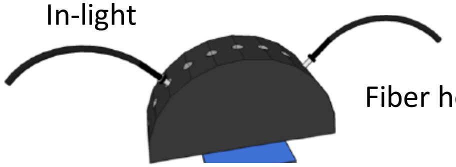
We have one in IMAP!

Specular measurements
Flat interfaces/thin-films



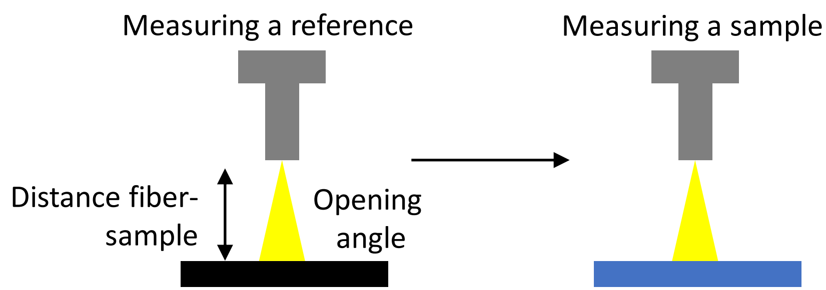
Pros: easy to use, gives **absolute** R and T
Cons: Samples need to be large. Light beam is about 1 cm height and a few mm wide, samples should be about 2-3 cm wide to fit the holding system. Can't be moved.

Or optical fibers + light source + spectrophotometer + reference



All those stuffs are available somewhere in cleanroom (ask me or Roseline)

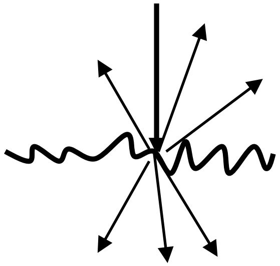
Pros: moveable, can measure very small samples
Cons: available light sources are limited in range, same for the spectro, **no absolute** R and T



Hemispherical

What you need

All-in-one integrating sphere

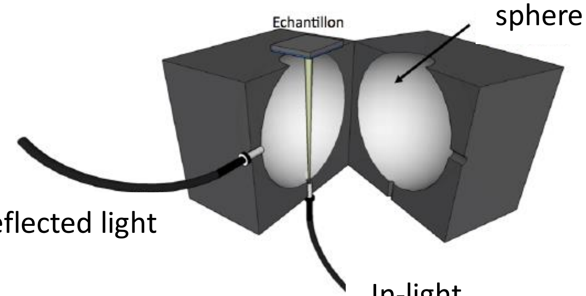


Can't measure the **absolute** R and T

They have one at UNamur (Perkin-Elmer)

Pro: nice, you will know how much light your sample scatters
Cons: large sample**,** **Can't** measure the **absolute** R and T

Or optical fibers + powerfull light source + spectrophotometer + reference + integrating sphere



All those stuffs are available somewhere in cleanroom

Pro: moveable, small sample
Cons: need a very powerfull lamp and an expensive reference. **Can't** measure the **absolute** R and T

If specular spectrum ≈ hemispherical spectrum: then there is no scattering

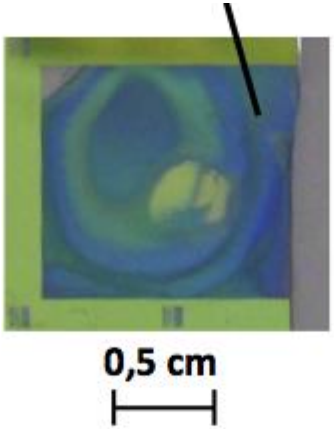
General comments about the measurements

Keep in mind that

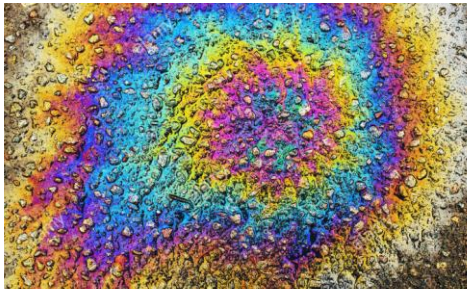
If you use optical fibers: they must be transparent in the optical range you are looking for. Do not bend them! Do not move them after you measured the reference.

There are special optical fibers for UV as well as for IR

If the color of your sample is not homogenous, do not expect to have reliable/reproducible measurements

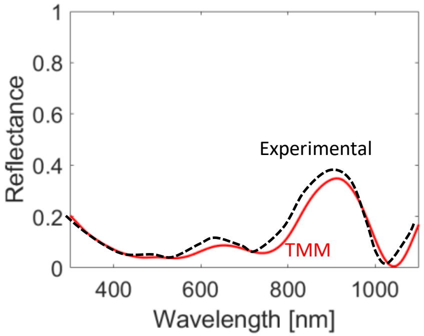


Color shift means inhomogenous material or thickness, optical phenomena are very sensitive!



$$\lambda = 4n * Thickness$$

Don't be too rude with your measurement/simulation:



Ellipsometry

Fitting the thickness or (n,k)

Ellipsometry helps you to fit either (n,k) or the thickness of one or more thin-films

If you don't know both, you must be careful when doing ellipsometry: thickness and (n,k) are somehow linked together $L = \frac{\lambda}{4n_t}$

It is a very sensitive technique (1 nm)

If you want to fit (n,k) experimentally, you must know the thickness

Ellipsometer uses mathematical dispersion model to fit your data. But…which model do I have to use?

Basic model: **Cauchy** model $\longrightarrow$ Doesn't take into account the **KK consistency**. Easily leads to unphysical results

Model for absorbing materials: **Lorentz** model or **Drude** model, **Tauc-Lorentz** model and more….

Or, you can fit your R and T spectrum by modifying (n,k) with TMM but you can also get unrealistic solution or multiple solution

Unfortunately, there is no easy method to fit (n,k)..