The Abdus Salam
International Centre for Theoretical Physics

United Nations
Educational, Scientific
and Cultural Organization

International Atomic
Energy Agency

Workshop on "Physics for Renewable Energy"
October 17 - 29, 2005

301/1679-15

"Optical Properties of Multilayer Systems by Computer Modeling"

E. Centurioni
CNR/IMM
AREA Science Park - Bologna
Italy

OPTICAL
Optical properties of multilayer systems by computer modeling

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ICTP, Trieste, Italy

Summary

- main features of the software "OPTICAL"
- multilayer systems overview
- theory for R and T calculation
- theory for internal light absorption calculation
- a short training

Main features of the software OPTICAL

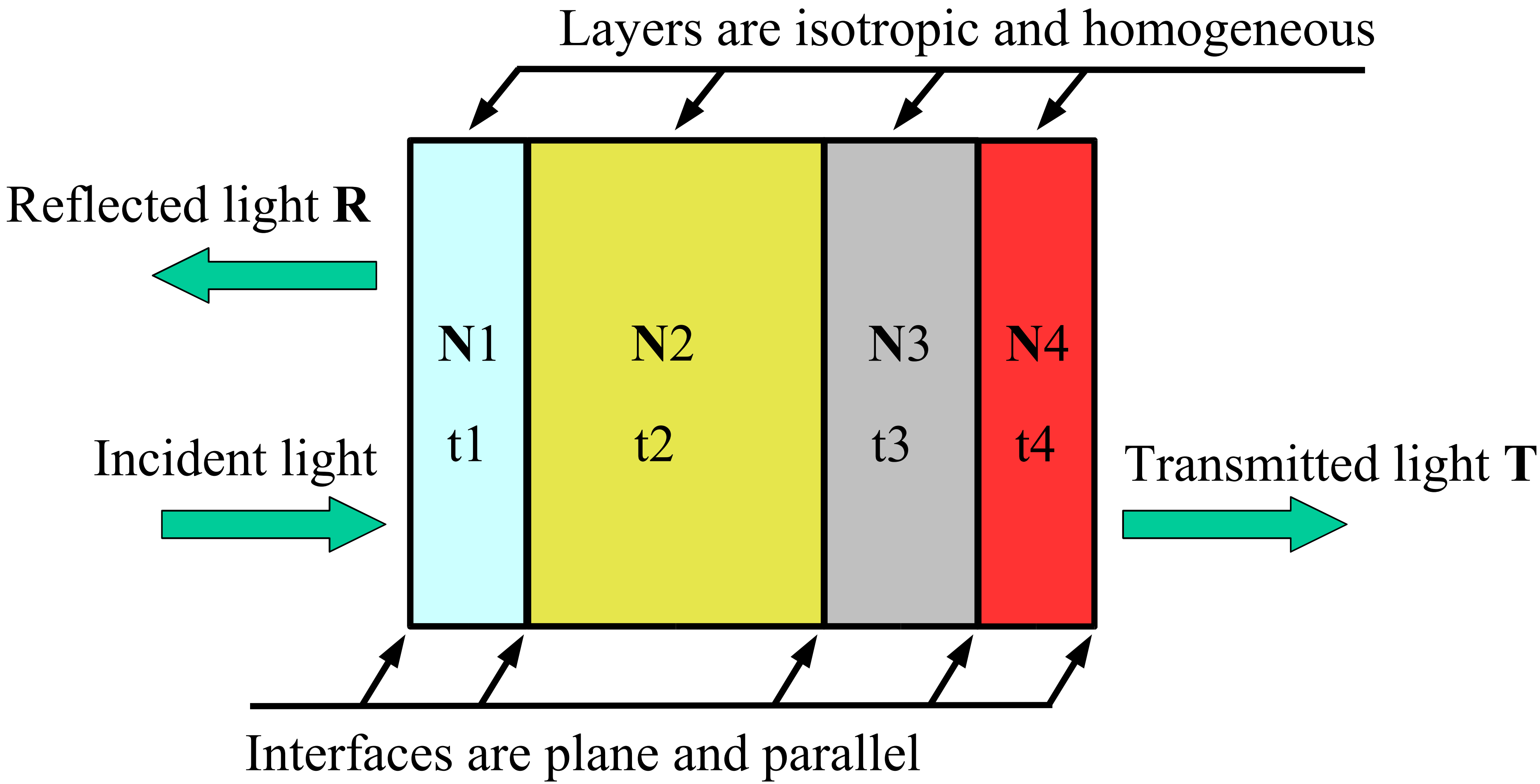
Is a cross-platform software released under the **GPL** license (**Open Source**): written using Python, wxWindows, wxPython and BoaConstructor

Can treat multilayers with any number of coherent and incoherent layer in any position and for any Incidence angle using a Generalized Scattering Matrix Method

Can compute total light Reflectance, Transmittance, internal Absorption and internal Energy Flux

EMA (Effective Medium Approximation) for mixed phase materials is integrated in the structure editor, many other function are present

Multilayer systems



T = 1 – R – A where **A** is the absorbed light

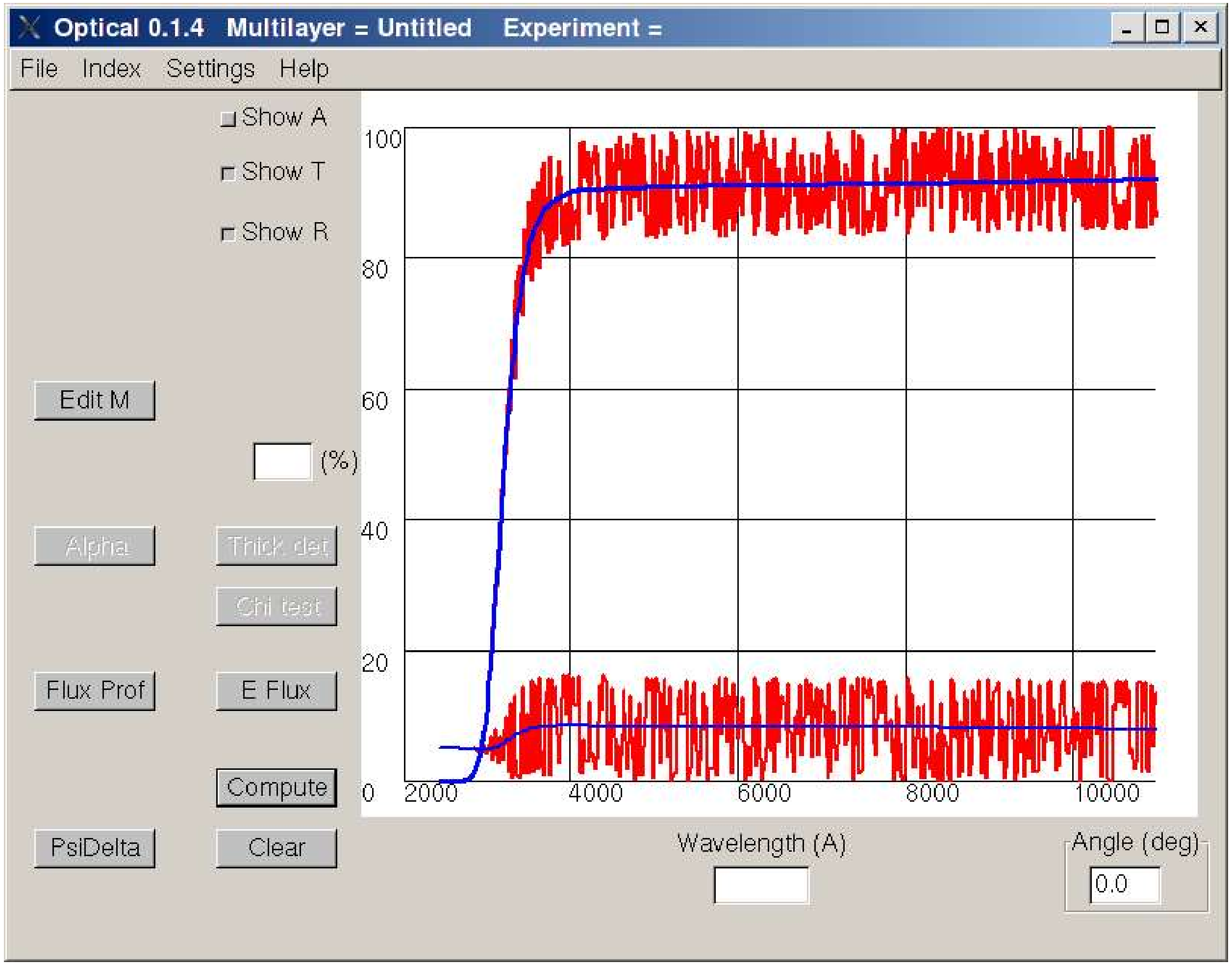
Coherent and incoherent behaviour of light

Usually to simulate experimental spectral measurements of a multilayer system it is necessary to treat some layers as coherent (internal interference taken into account), and some other as incoherent (internal interference ignored).

If the layer is very thick compared with the radiation wavelength and transparent, we should treat it as incoherent. If we don't we have multiple reflections leading to narrow oscillations in the calculated reflectance and transmittance spectra that are not present in the experimental data.

Interference-destroying causes are the limited resolution of the instrument, the non perfectly parallel interfaces of a layer and the limited light source coherence length

Coherent and incoherent behaviour of light



Computed Reflectance and Transmittance of 1 mm thick glass. Coherence (red) or incoherence (blue) has been used.

Basics of Transmittance and Reflectance calculation

Optical constants

Each layer is defined by its complex index of refraction N

$$N = n + ik$$

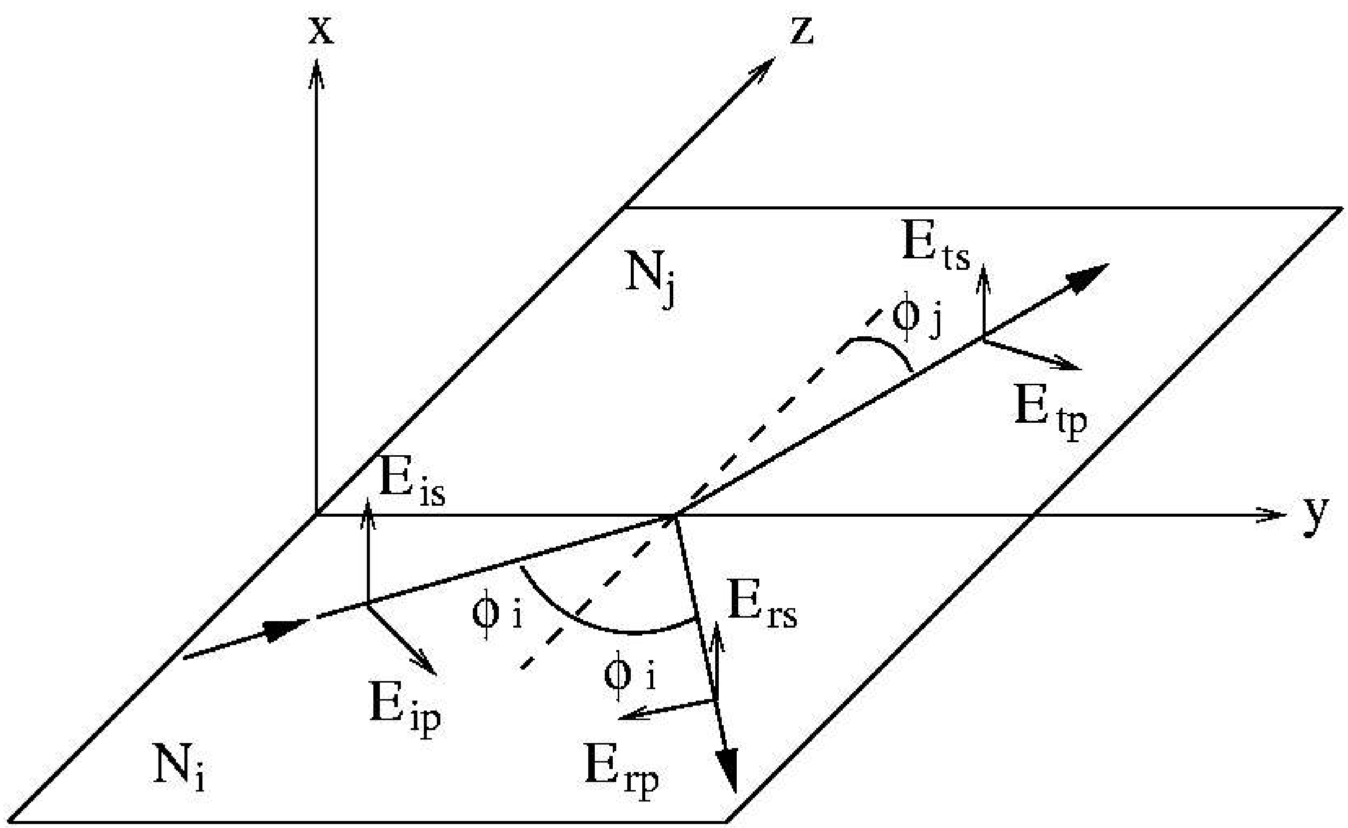
where k is the extinction coefficient related to the absorption coefficient α

$$\alpha = 4 \text{ pi } k / \lambda$$

where λ is the wavelength. The dielectric constant $\boldsymbol{\varepsilon}$ is directly related to N

$$\boldsymbol{\varepsilon} = N^2$$

Reflection and refraction of plane waves



Snell's law $N_i \sin \phi_i = N_J \sin \phi_J$

Complex angles !

The Fresnel coefficients

$$r_{ij,p} = \frac{E_{rp}}{E_{ip}} = \frac{N_j \cos\phi_i - N_i \cos\phi_j}{N_j \cos\phi_i + N_i \cos\phi_j}$$

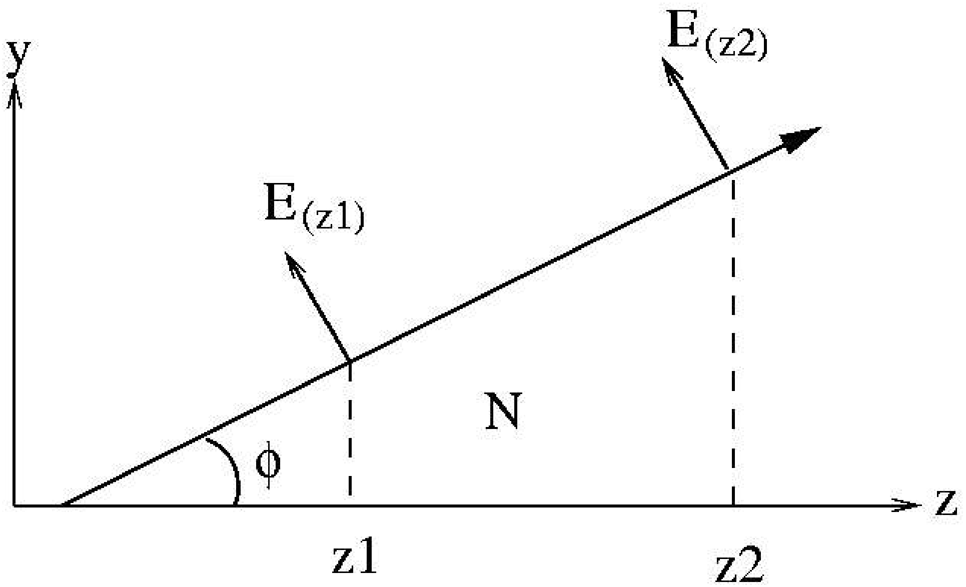
$$r_{ij,s} = \frac{E_{rs}}{E_{is}} = \frac{N_i \cos\phi_i - N_j \cos\phi_j}{N_i \cos\phi_i + N_j \cos\phi_j}$$

$$t_{ij,p} = \frac{E_{tp}}{E_{ip}} = \frac{2N_i \cos\phi_i}{N_j \cos\phi_i + N_i \cos\phi_j}$$

$$t_{ij,s} = \frac{E_{ts}}{E_{is}} = \frac{2N_i \cos\phi_i}{N_i \cos\phi_i + N_j \cos\phi_j}$$

Ratio of reflected and transmitted electric field components

Wave propagation

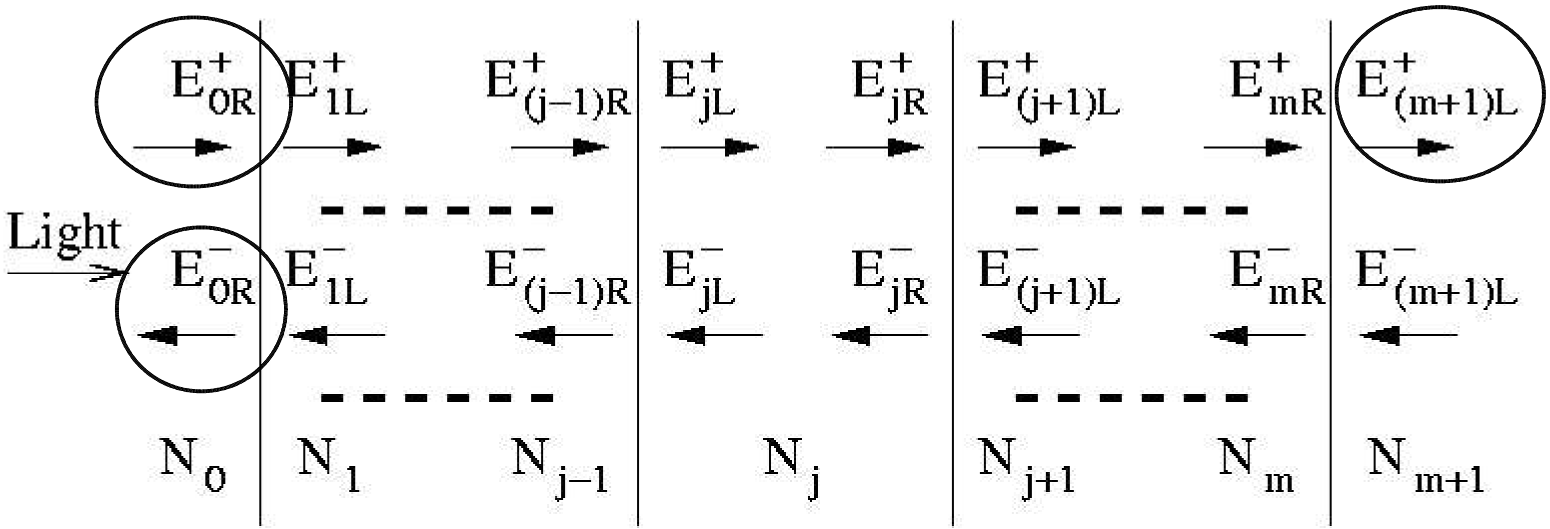


$E(z_2)=E(z_1) \exp (i \beta (z_2-z_1))$

$\beta (x) = (2 \pi x N \cos \phi) / \lambda$
(phase shift)

Wave propagation in a homogeneous medium

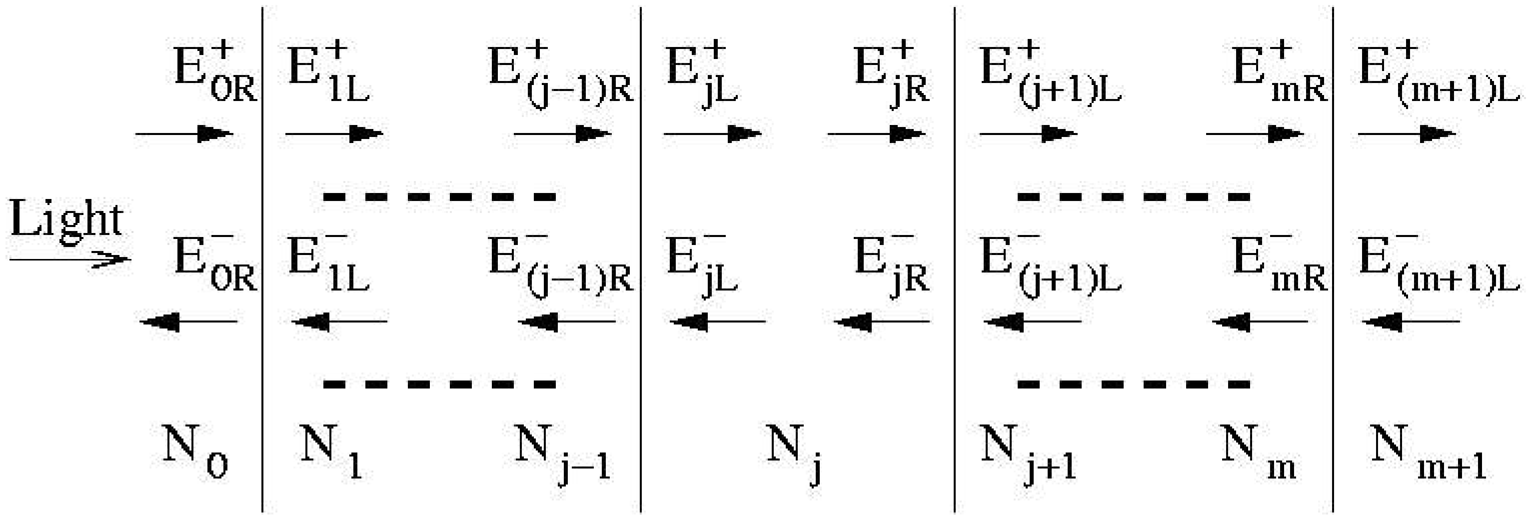
Multiple boundary problem



Using Snell's law, Fresnel coefficient and wave propagation equation the problem is analytically solvable (find solution for E). From the knowledge of the electric field R and T can be finally calculated.

Quite complicated !

The scattering-matrix formalism (coherent)



Light passing through this structure can be described with the scattering-matrix formalism, S is the 2x2 scattering-matrix

$$\begin{pmatrix} E_{0R}^{+} \\ E_{0R}^{-} \end{pmatrix} = \mathbf{S} \begin{pmatrix} E_{(m+1)L}^{+} \\ E_{(m+1)L}^{-} \end{pmatrix}$$

The scattering-matrix formalism (coherent)

$$\mathbf{S} = \mathbf{I}_{01}\mathbf{L}_1\mathbf{I}_{12}\ldots\mathbf{L}_m\mathbf{I}_{m(m+1)}$$

S is the 2x2 scattering matrix where I defines the wave propagation at the interfaces and L describes the wave propagation through the films

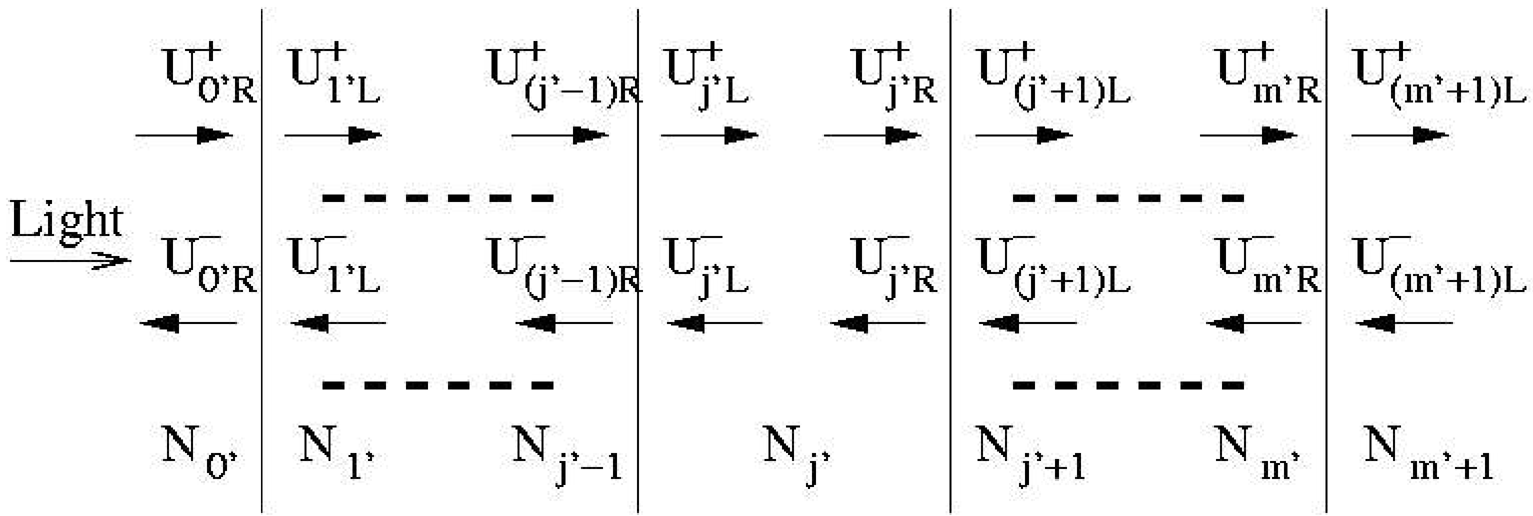
$$\mathbf{I}_{i,j} = \frac{1}{t_{ij}}\begin{pmatrix} 1 & r_{ij} \\ r_{ij} & 1 \end{pmatrix}$$

$$\mathbf{L}_j = \mathbf{L}(\beta_j) = \begin{pmatrix} \exp(-\imath\beta_j) & 0 \\ 0 & \exp(\imath\beta_j) \end{pmatrix}$$

I is associated to an interface

L is associated to a layer

The scattering-matrix formalism (incoherent)



Light passing through this structure can be described with the scattering-matrix formalism, S is the 2x2 scattering-matrix. $U = |E|^2$

$$\begin{pmatrix} U^+_{0'R} \\ U^-_{0'R} \end{pmatrix} = \bar{\mathbf{S}} \begin{pmatrix} U^+_{(m'+1)L} \\ U^-_{(m'+1)L} \end{pmatrix}$$

The scattering-matrix formalism (incoherent)

$$\bar{\mathbf{S}} = \bar{\mathbf{I}}_{0'1'}\bar{\mathbf{L}}_{1'}\bar{\mathbf{I}}_{1'2'}\ldots\bar{\mathbf{L}}_{m'}\bar{\mathbf{I}}_{m'(m'+1)}$$

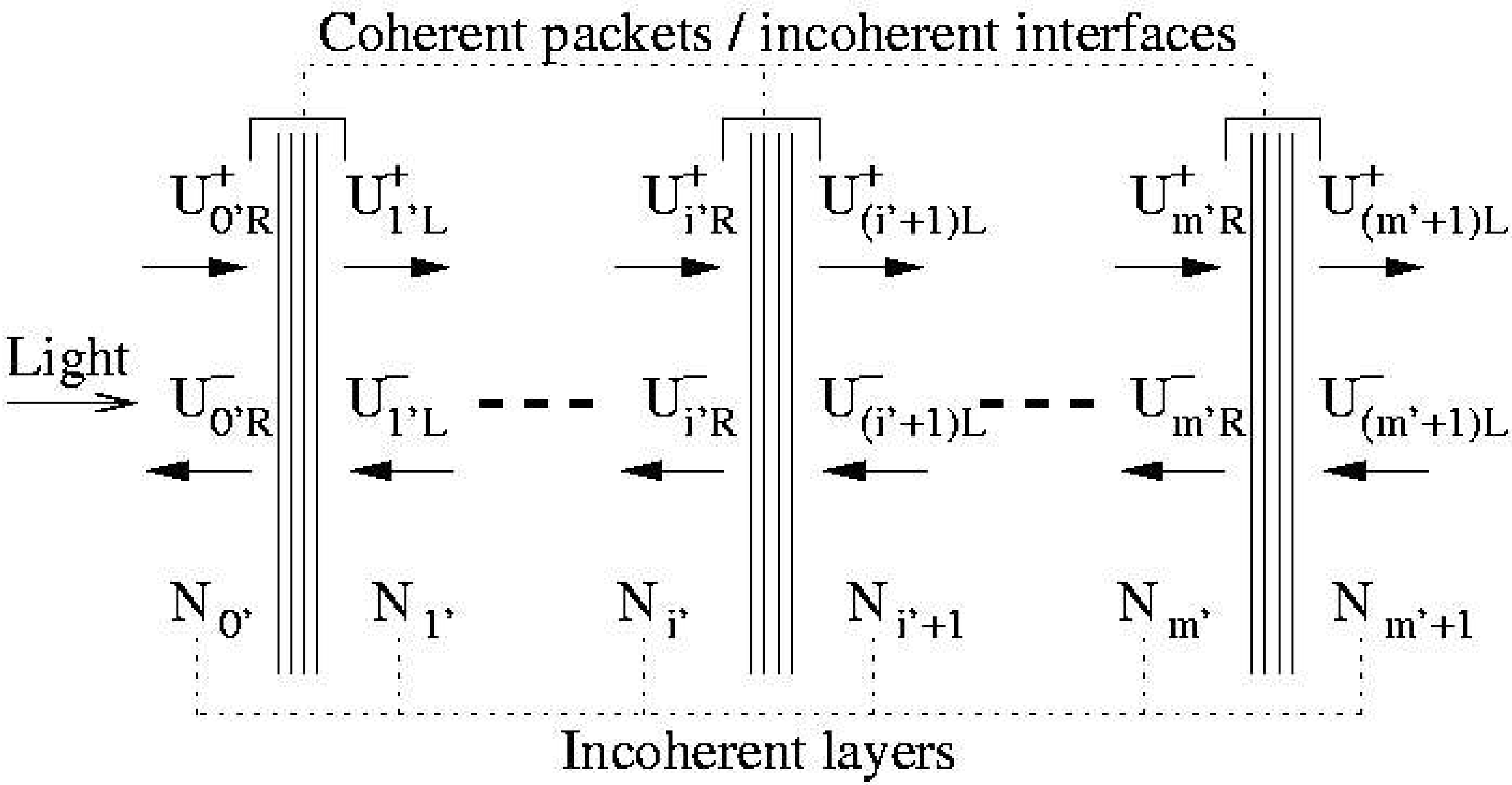
S is the 2x2 scattering matrix where I defines the wave propagation at the interfaces and L describes the wave propagation through the films

$$\bar{\mathbf{I}}_{j'(j'+1)} = \frac{1}{|t|^2}\begin{pmatrix} 1 & -|r'|^2 \\ |r|^2 & |tt'|^2 - |rr'|^2 \end{pmatrix} \quad \bar{\mathbf{L}}_{j'} = \bar{\mathbf{L}}(\beta_{j'}) = \begin{pmatrix} |\exp(-\imath\beta_{j'})|^2 & 0 \\ 0 & |\exp(\imath\beta_{j'})|^2 \end{pmatrix}$$

I is associated to an interface

L is associated to a layer

Mixed coherent and incoherent multilayer



$$\bar{\mathbf{I}}_{i'(i'+1)} = \begin{pmatrix} |S_{11}|^2 & -|S_{12}|^2 \\ |S_{21}|^2 & \frac{|\det \mathbf{S}|^2 - |S_{12}S_{21}|^2}{|S_{11}|^2} \end{pmatrix}$$

Energy flux

$$\Phi \sim U_s \, \mathrm{re}\,(N \cos \phi)$$

$$\Phi \sim U_p \, \mathrm{re}\,(N^* \cos \phi)$$

Light energy flux for a single wave moving in a homogeneous medium
The ambient medium on the light side must be transparent

$$\bar{r} = \frac{U^-_{0'R}}{U^+_{0'R}} = \frac{\bar{S}_{21}}{\bar{S}_{11}}$$

$$\bar{t} = \frac{U^+_{(m'+1)L}}{U^+_{0'R}} = \frac{1}{\bar{S}_{11}}$$

Transmission e reflection coefficients can be calculated from scattering matrix elements

Total Transmittance and Reflectance

$$T_s = \frac{\bar{t}_s Re\left(N_{m'+1}\cos\phi_{m'+1}\right)}{N_{0'}\cos\phi_{0'}}$$

$$T_p = \frac{\bar{t}_p Re\left(N^*_{m'+1}\cos\phi_{m'+1}\right)}{N_{0'}\cos\phi_{0'}}$$

Transmittance

$$R_s = r_s$$

$$R_p = r_p$$

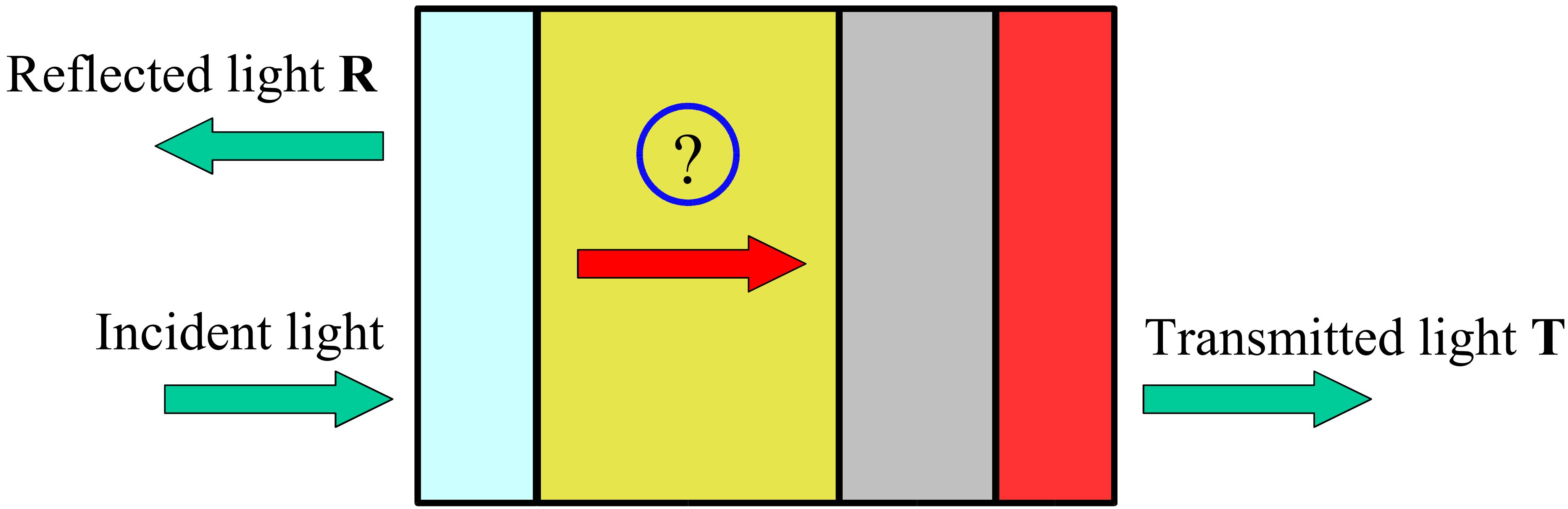
Reflectance

$$\mathbf{R = (R_p + R_s) / 2}$$

$$\mathbf{T = (T_p + T_s) / 2}$$

For unpolarized light

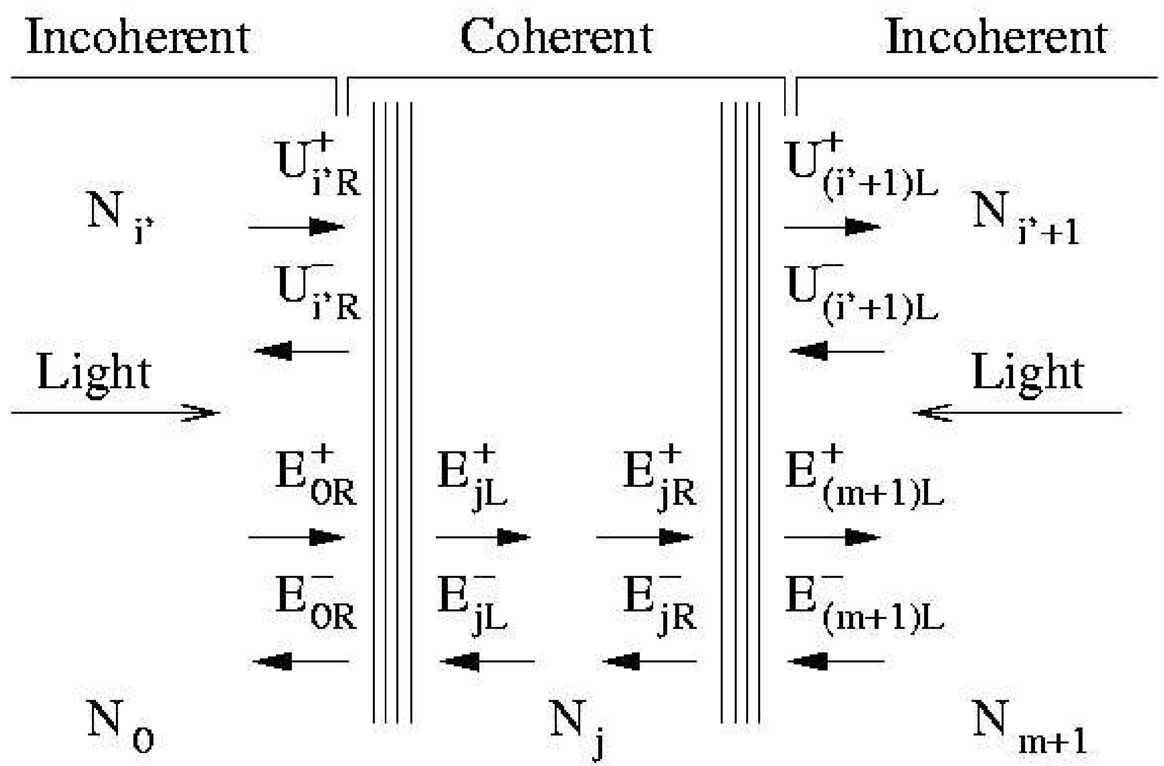
Light energy absorption inside the multilayer



$$A_{z_1 \leq z \leq z_2} = \int_{z_1}^{z_2} \alpha(z) I(z) dz$$ Light intensity approach

$$\mathbf{A_{z1<z<z2} = \Phi(z1) - \Phi(z2)}$$ Energy flux approach

Energy flux inside the multilayer



Incoherent layer: “single wave moving” equation can be used

Coherent layer: **Poynting vector**

The Poynting vector

$$\langle \mathbf{S} \rangle (z) = c \frac{Re\left(\mathbf{E}(z) \times (\mathbf{B}(z))^{*}\right)}{N_{0'} \cos \phi_{0'}}$$

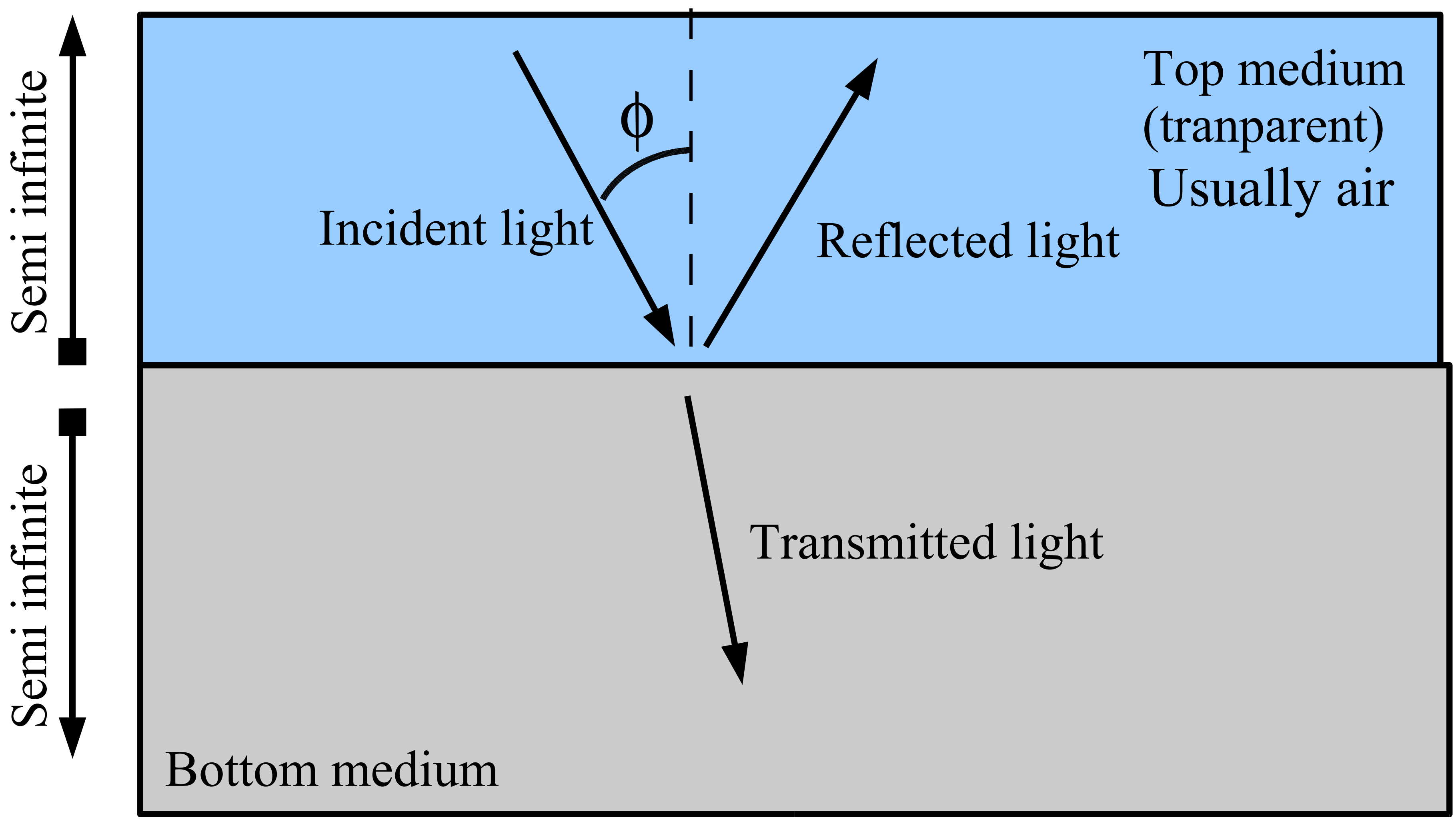
The normalized Poynting vector gives the energy flux along the direction of propagation.

Once the electric field profile is known the magnetic field B can be derived from Maxwell's equations, so it is possible to compute the energy flux using the complex Poynting vector

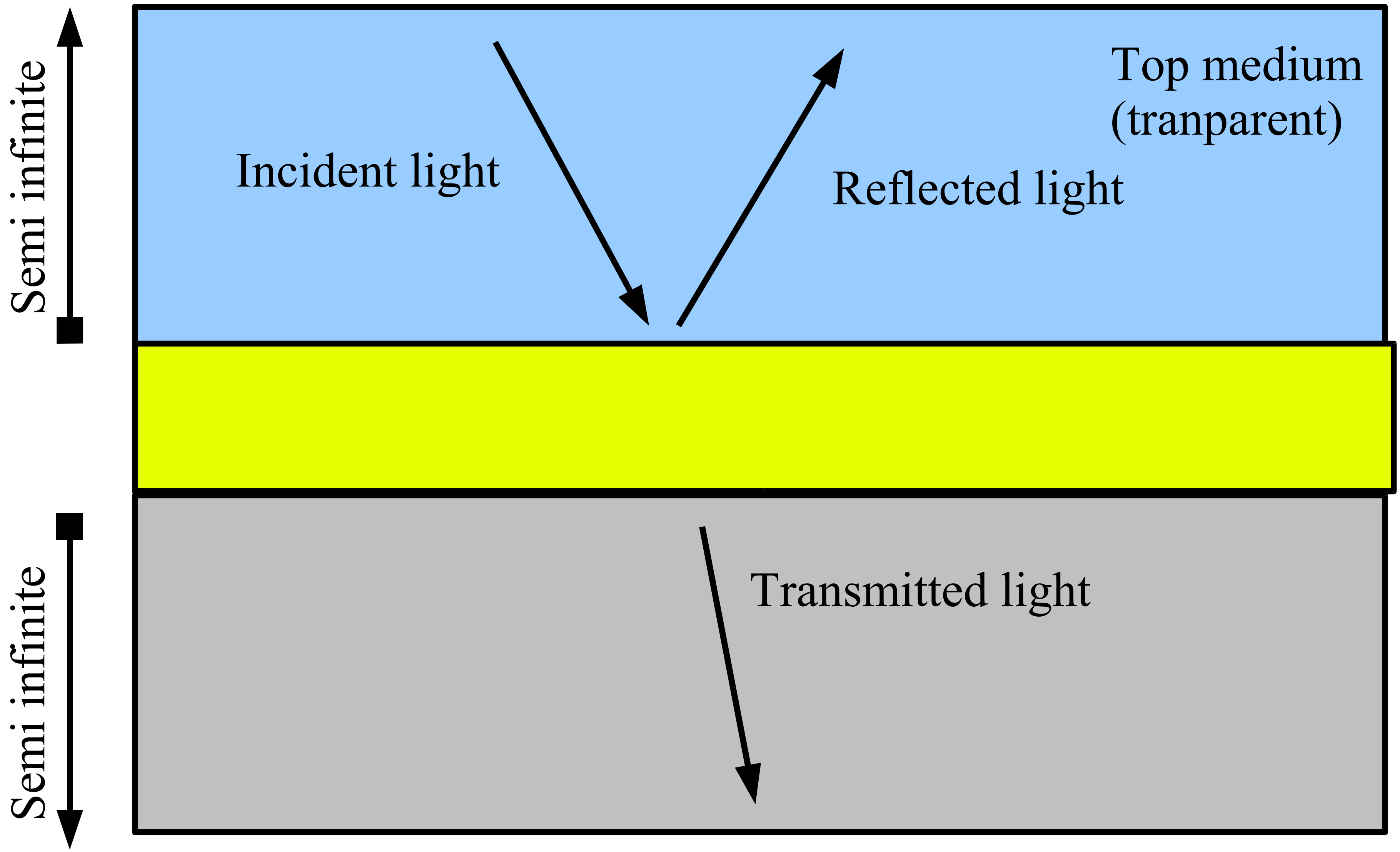
Electric field profile inside a coherent layer in a mixed coherent / incoherent multilayer can be calculated using a **full matrix formalism**

A short training on OPTICAL

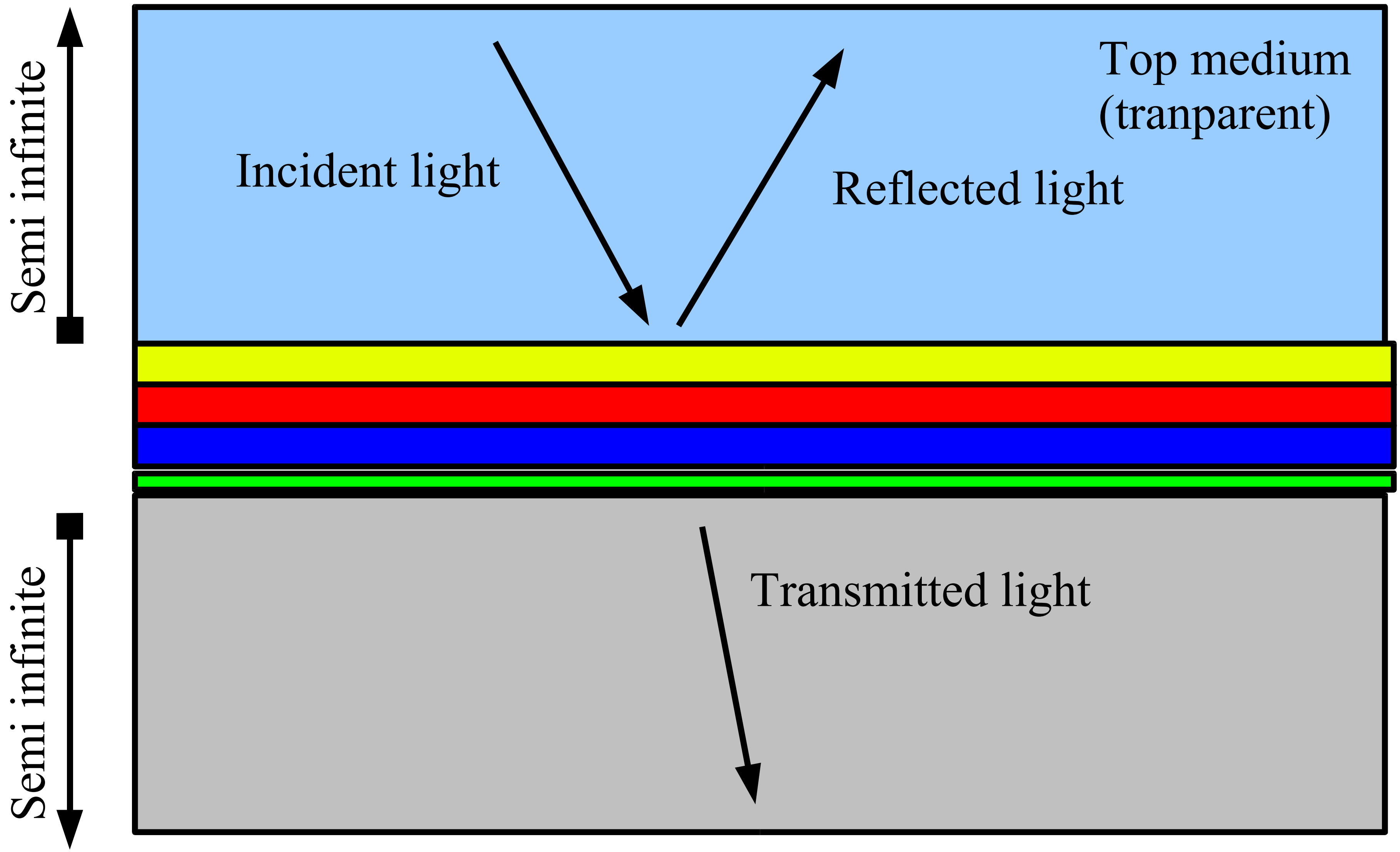
Example 1: simple interface



Example 2: single layer



Example 3: multilayer



Other examples

A simple mirror

Thin film solar cell analysis

Silicon solar cell, antireflecting coating

Thickness determination, alpha calculation

Interferential filter

Pseudo dielectric functions

Conclusion

Simulation of optical quantity like total transmittance (T), reflectance (R) and internal light absorption (A) are very useful in many fields like in optical coating design, solar cells optimization, thin film measurement systems, interferometric infrared absorber and emitter design, etc.

OTICAL can do these task. OPTICAL is an open source project, multi platform, and available for free under the GPL license.

References

Optical can be downloaded here www.bo.imm.cnr.it/~centurio/optical.html

E. Centurioni, "Generalized matrix method for calculation of internal light energy flux in mixed coherent and incoherent multilayer", Applied Optics, in press.