Mueller matrix approach to the propagation of light in stratified anisotropic media

F. Ferrieu*[,1], E. Garcia-Caurel[2], M. Stchakovsky[3]
STMicroelectronics, France, [2] LPICM-Ecole polytechnique, France, [3] Horiba Jobin Yvon, France
frederic.ferrieu@cea.fr, **enric.garcia-caurel@polytechnique.edu,

•Propagation of light in anisotropic material suscites a growing interest of new synthesized materials for nanotechnologies. For a large number of anisotropic substrates or thin films, weak birefringence can be measured by new polarimeters.

• The experimentalist has then to deal with a large number of acquired data such as with these 4x4 Mueller matrix.

•The aim is to revise the existing formalism detailed in several publications and to give an overall view in order to build a general computational algorithm to calculate the Mueller matrix and the Jones matrix of a given sample.

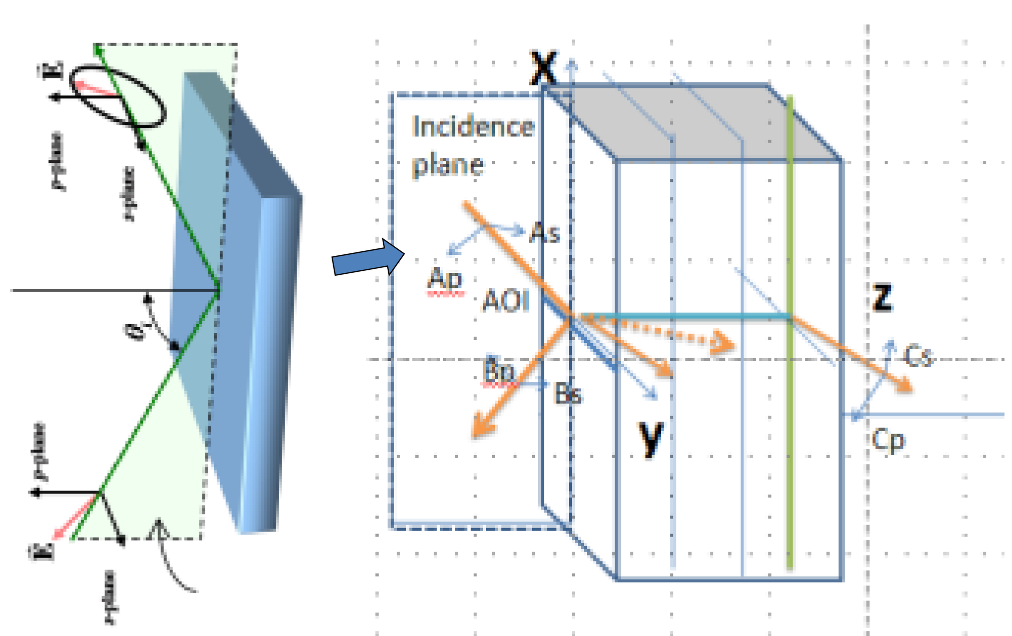
•The explicit equations given hereafter can be applied for both transmitted and reflected light propagating into anisotropic multilayered media. They can be implemented with the aid of commercial linear algebra libraries.

Propagation of light: Maxwell Equations

*The propagation of light through a general linear and non-magnetic anisotropic medium can described using **Maxwell equations** written in their wave form:*

$$curl\,\vec{H} = j\omega\vec{D}$$
$$-curl\,\vec{E} = j\omega\vec{B}$$

$$\frac{\partial\Psi(z)}{\partial z} = -j\omega\Delta\Psi(z)$$
$$\Psi = [E_x, E_y, H_x, H_y]^T$$
$$k_0 = \omega / c$$



$$\Psi(z+d_i) = \exp\{ik_0\Delta d_i\}\Psi)z) = T_{pi} * \Psi(z)$$

$$\begin{bmatrix} A_s \\ B_s \\ A_p \\ B_p \end{bmatrix} = T \begin{bmatrix} C_s \\ D_s \\ C_p \\ D_p \end{bmatrix} = \begin{bmatrix} T_{11} & T_{12} & T_{13} & T_{14} \\ T_{21} & T_{22} & T_{23} & T_{24} \\ T_{31} & T_{32} & T_{33} & T_{34} \\ T_{41} & T_{42} & T_{43} & T_{44} \end{bmatrix} \begin{bmatrix} C_s \\ 0 \\ C_p \\ 0 \end{bmatrix}$$

Multilayer case (thickness d_i)

$$T = L^{-1}_a \prod_{i=1}^{n} T_{pi}(-d_i) L_f$$

$$L_a, L_f$$

Transition matrices respectively between **air and film** and **film with substrate**

Euler angles

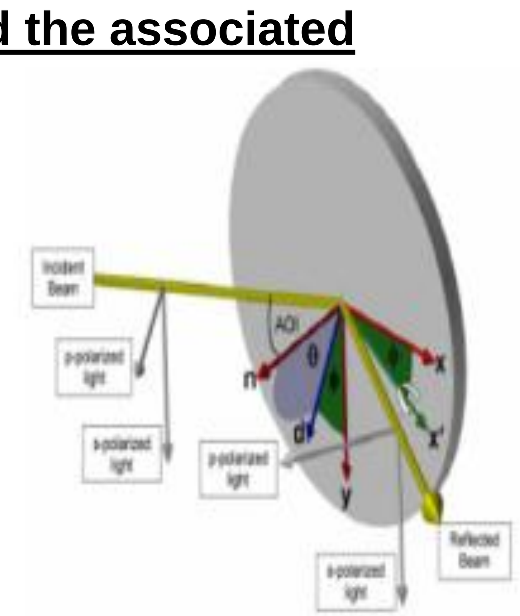
In general the coordinate system of the laboratory and the main coordinate system of the anisotropic media are not the same.

They can be related by a rotation transformation. A common way of writing a rotation transformation is to use the **Euler matrices and the associated Euler angles (θ,Ψ,Φ).**

$$\varepsilon = \begin{bmatrix} \varepsilon_x = \varepsilon_\perp & 0 & 0 \\ 0 & \varepsilon_y = \varepsilon_\perp & 0 \\ 0 & 0 & \varepsilon_z = \varepsilon_{//} \end{bmatrix} \Rightarrow \{\varepsilon_{ij}\} = \begin{bmatrix} \varepsilon_{11} & \varepsilon_{12} & \varepsilon_{13} \\ \varepsilon_{21} & \varepsilon_{22} & \varepsilon_{23} \\ \varepsilon_{31} & \varepsilon_{32} & \varepsilon_{33} \end{bmatrix}$$

Main frame of the medium — Laboratory frame

$$\{\varepsilon_{ij}\} = A(\varphi,\psi,\theta)\,\varepsilon\,A^{-1}(\varphi,\psi,\theta)$$



Construction of the Δ Matrix :

Following the ***curl*** operator in Maxwell equations for E and H the Δ matrix depends on the dielectric tensor and the component k_x of the wave propagation vector k_0,

$$\Delta = \begin{bmatrix} -k_x\frac{\varepsilon_{31}}{\varepsilon_{33}} & -k_x\frac{\varepsilon_{32}}{\varepsilon_{33}} & 0 & 1-\frac{k_x^2}{\varepsilon_{33}} \\ 0 & 0 & -1 & 0 \\ \varepsilon_{23}-\varepsilon_{13}\frac{\varepsilon_{31}}{\varepsilon_{33}} & k_x^2-\varepsilon_{22}+\varepsilon_{23}\frac{\varepsilon_{32}}{\varepsilon_{33}} & 0 & k_x\frac{\varepsilon_{23}}{\varepsilon_{33}} \\ \varepsilon_{11}-\varepsilon_{13}\frac{\varepsilon_{31}}{\varepsilon_{33}} & \varepsilon_{12}-\varepsilon_{13}\frac{\varepsilon_{32}}{\varepsilon_{33}} & 0 & -k_x\frac{\varepsilon_{13}}{\varepsilon_{33}} \end{bmatrix} \qquad k_x = n_a \sin\Phi_a$$

Evaluation of $\exp(ik_0\Delta d_i)$

The **exponential** matrix applying the **Cayley Hamilton thorem.**

$$T_p = \exp ik\ \Delta d = \beta_0 I + \beta_1\Delta + \beta_2\Delta^2 + \beta_3\Delta^3 \qquad \exp\{ik_q q_k d\} \equiv \sum_{j=0}^{3}\beta_j q_k^j \quad k=1,\dots 4$$

$$\beta_0 = \sum_{i=1}^{4} q_j q_k q_l \frac{f_i}{q_{ij}q_{ik}q_{il}} \qquad \beta_2 = -\sum_{i=1}^{4}(q_j+q_k+q_l)\frac{f_i}{q_{ij}q_{ik}q_{il}}$$

$$\beta_1 = \sum_{i=1}^{4}(q_j q_k + q_j q_l + q_k q_l)\frac{f_i}{q_{ij}q_{ik}q_{il}} \qquad \beta_3 = \sum_{i=1}^{4}\frac{f_i}{q_{ij}q_{ik}q_{il}}$$

$$e^{iq_i k_0 d} = M\{\beta_0, \beta_1, \beta_2, \beta_3\}^T$$

The exponential of the Δ matrix is a function of the eigenvalues of the same Δ matrix.

The value of the eigenvalues β_i can be also found using commercially available software to solve the corresponding system of linear equations.

Evaluation of Transition matrices air/film L_a, L_f

The continuity of tangential components imposes the relation between, **E**, and **H**.

The projection of the fields on both, s and p components yield:

$$L_a\Psi_a = \Psi_{inc}(z=0) + \Psi_{ref}(z=0) \quad \begin{cases} \Psi_{inc} = [A_p\cos\Phi_a, A_s, -n_a A_s\cos\Phi_a, n_a A_p] \\ \Psi_{ref} = [-B_p\cos\Phi_a, B_s, n_a B_s\cos\Phi_a, n_a B_p] \end{cases}$$

$$\{L_{ij}\}^{-1} = \begin{bmatrix} 0 & 1 & -1/n_a Cos\,\Phi_a & 0 \\ 0 & 1 & 1/n_a Cos\,\Phi_a & 0 \\ 1 & 0 & 0 & 1/n_a \\ -1 & 0 & 0 & 1/n_a \end{bmatrix}$$

Φa AOI (Angle of Incidence)
n_a=ambient index n_a=1

Transition matrices film/anisotropic substrate L_f

Ψ_f is a linear combination of the eigenvectors Ξ of Δ

$$\Psi_f = \sum_{i=1}^{4} c_i\,\Xi_i(q_i) \quad \{L_{fjk}\} = \Xi_{jk}, L_{fj(k+1)} = 0 \quad j=1..4\ k=1,3 \qquad Ré\{q_i\} > 0$$

For a biaxial system eignevectors are easily obtained
Such as with axis aligned. To the laboratory frame one gets thus for the c_i:

$$\{c_i\} = \{0, -n_y\cos\Phi_y, 0, n_x\} \qquad (L_{fjk}) = \begin{bmatrix} \Xi_{11}=q_{21} & 0 & \Xi_{13}=q_{31} & 0 \\ \Xi_{21}=q_{22} & 0 & \Xi_{23}=q_{32} & 0 \\ \Xi_{31}=q_{23} & 0 & \Xi_{33}=q_{33} & 0 \\ \Xi_{41}=q_{24} & 0 & \Xi_{43}=q_{34} & 0 \end{bmatrix}$$

Calculation of Mueller matrices

The T_{ij} elements correspond to the general transfer matrix= matrix product of each layer thickness d_i

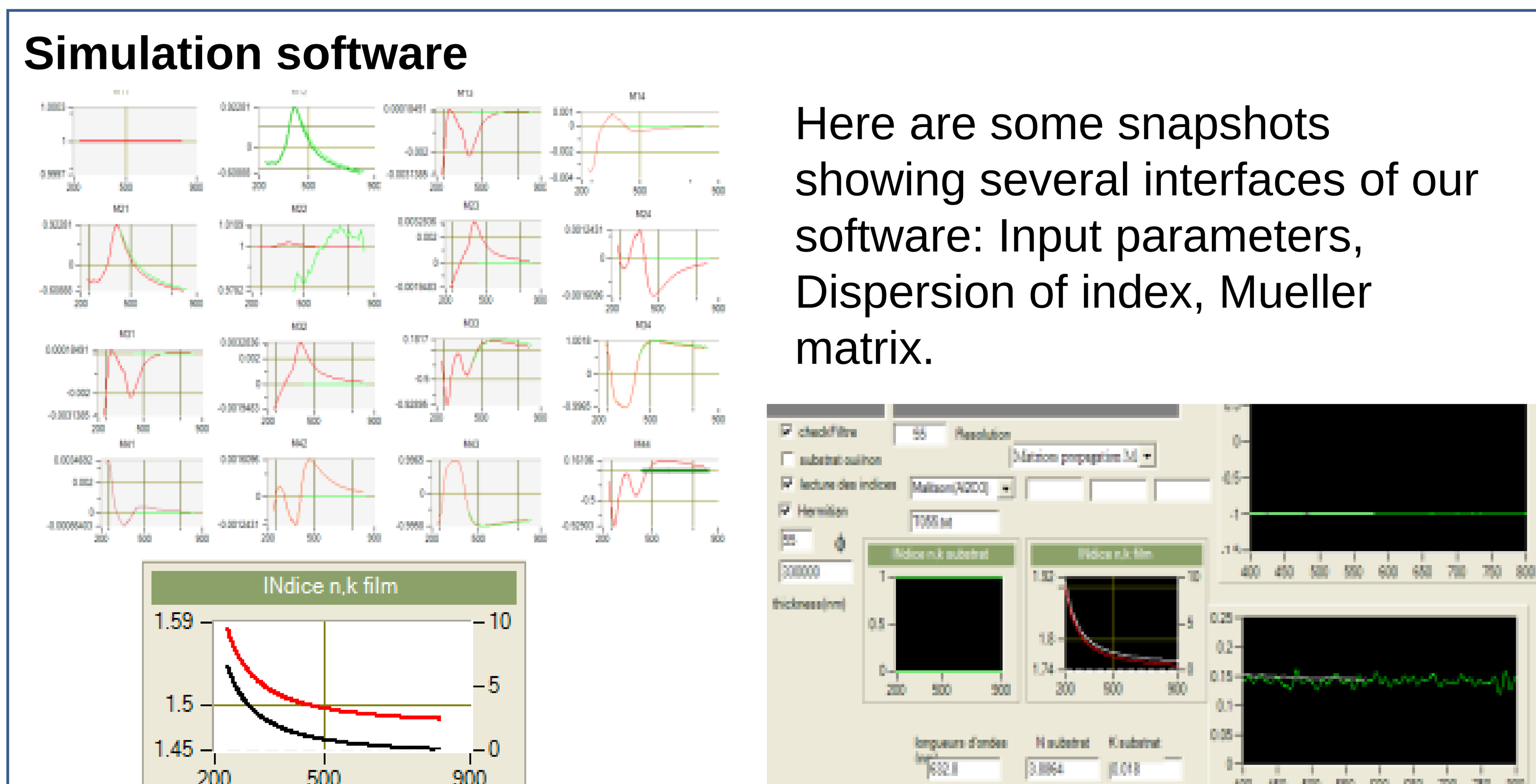
The four elements of the Jones matrix are calculated through he Kronecker product with matrices A and A^{-1} (*P. Yeh*)

$$J \equiv \begin{bmatrix} r_{pp} & r_{ps} \\ r_{sp} & r_{ss} \end{bmatrix} \qquad M \equiv A\left(J \otimes J^*\right)A^{-1} \qquad A \equiv \begin{bmatrix} 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & -1 \\ 0 & 1 & 1 & 0 \\ 0 & -j & j & 0 \end{bmatrix}$$

$$r_{ps} = \left(\frac{B_s}{A_p}\right)_{A_s=0} = \frac{T_{11}T_{23}-T_{21}T_{13}}{T_{11}T_{33}-T_{13}T_{31}} \qquad r_{ss} = \left(\frac{B_s}{A_s}\right)_{A_p=0} = \frac{T_{21}T_{33}-T_{23}T_{31}}{T_{11}T_{33}-T_{13}T_{31}}$$

$$r_{pp} = \left(\frac{B_p}{A_p}\right)_{A_s=0} = \frac{T_{11}T_{43}-T_{41}T_{13}}{T_{11}T_{33}-T_{13}T_{31}} \qquad r_{sp} = \left(\frac{B_p}{A_s}\right)_{A_p=0} = \frac{T_{41}T_{33}-T_{43}T_{31}}{T_{11}T_{33}-T_{13}T_{31}}$$

Simulation software



Here are some snapshots showing several interfaces of our software: Input parameters, Dispersion of index, Mueller matrix.