Terms and Definition

Physical background

ReMagX solves the Maxwell-equations in matter

$$\nabla \times \vec{H} = \frac{\partial \vec{D}}{\partial t}$$
$$\nabla \times \vec{E} = \frac{-\partial \vec{B}}{\partial t}$$

with

$$\vec{D} = \varepsilon_0 \varepsilon_r \vec{E}$$
$$\vec{B} = \mu_0 \vec{H}$$

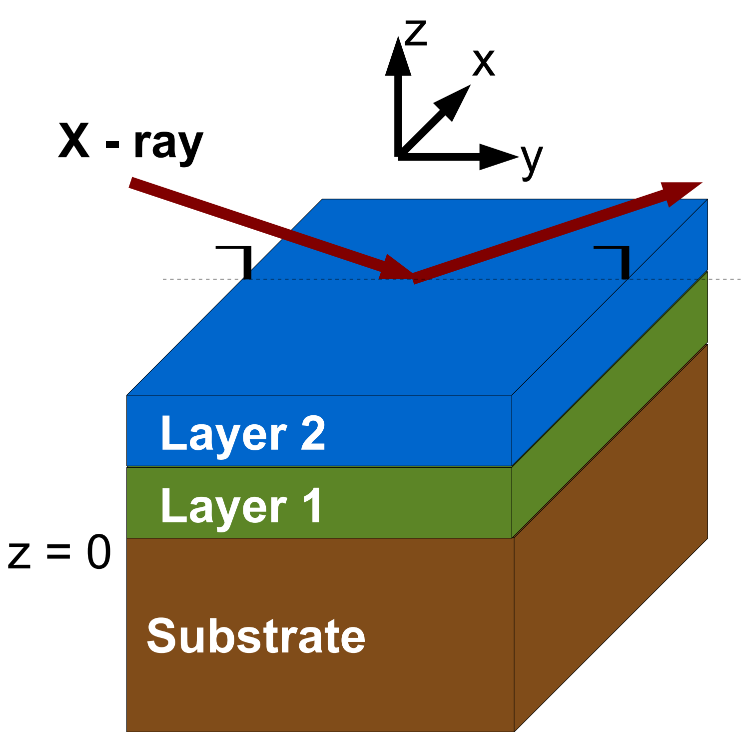
leading to the differential equation

$$\nabla^2 \vec{E} - \nabla \cdot (\nabla \cdot \vec{E}) = \frac{1}{c^2} \epsilon_r \frac{\partial^2 \vec{E}}{\partial t^2}$$

This equation is solved in case of infinitely extended thin films in x- and y-direction. The result of the simulation is the intensity of the scattered light (reflection and transmission) and the electric fields inside the film.

Coordinate system (layer system)

The thin film lies in the x-y-plane and are stacked along the z-direction. The coordinate z=0 is located at the interface between the substrate and layer 1.



Units / physical constants

Following units are used in the program

Variables	Unit	Description
ã	electron volt [eV]	Energy of incoming beam
nÌḾH́⌒Ǵi.·́.	dimensionless	Refractive index
⌒̣	dimensonless	Real part of the refractive index constant
.́.	dimensonless	Imaginary part of the refractive index
‴	g/cm^3	density of compound
‴$_m$	mol/cm^3	molar concentration of element
q_z	1 / Angstrom	z component of momentum transfer
t	Angstrom	Thickness of the film
N_A	Particles/mol	Avogadro constant
f=-r0(Z+f'+if")	meter	Scattering amplitude
r0	meter	Classical Electron radius
f1=Z+f'	dimensionless	Real part of scattering factor
f2=f"	dimensionless	Imaginary part of scattering factor

Incoming light

The incoming electromagnetic wave (only electric field) in vacuum is given as

$$\vec{E}(\vec{r},t)=\vec{E}_0 e^{i\vec{k}_{\text{in}}\cdot\vec{r}-i\omega t}$$

The wave vector $\vec{k}_{\text{in}}=k_0\begin{pmatrix}0\\ \cos\theta\\ \sin\theta\end{pmatrix}$ and the frequency ω are correlated with the speed of light by the dispersion relation $\omega=c k_o$. The frequency or wavelength of the light is defined as $E_0=\hbar\omega=\hbar c k_0$.

The scattering vector is defined as the difference of the wave vector before and after scattering.

$$\vec{q}=\vec{k}_{\text{in}}-\vec{k}_{out}=k_0\begin{pmatrix}0\\ \cos\theta\\ \sin\theta\end{pmatrix}-k_0\begin{pmatrix}0\\ \cos\theta\\ -\sin\theta\end{pmatrix}=\begin{pmatrix}0\\ 0\\ 2k_0\sin\theta\end{pmatrix}$$

Polarization

The polarization is given as a linear combination

$$\vec{E}_0 = \sigma \cdot \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} + \pi \cdot \begin{pmatrix} 0 \\ sin(\theta) \\ cos(\theta) \end{pmatrix}$$

···· and ✓ are complex numbers

Common polarizations

	····	✓	Normed ····	Normed ✓
linear ····	1	0	1	0
linear ✓	0	1	0	1
right circular	1	i	0.7071	0.7071i
left circular	1	-i	0.7071	-0.7071i

Dielectric Tensor

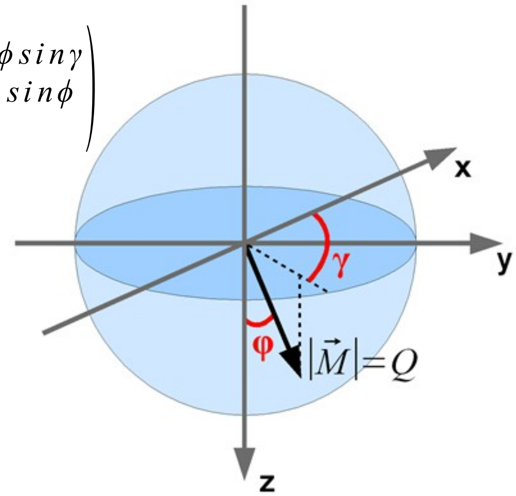
$$\vec{D} = \varepsilon_0 \cdot \varepsilon \cdot \vec{E} = \varepsilon_0 \cdot \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{yx} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{zx} & \epsilon_{zy} & \epsilon_{zz} \end{pmatrix} \cdot \vec{E}$$

special cases:

isotropic (cubic) $\epsilon = N^2 \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$ with the refractive index $N = 1 - \delta + i\beta$

tetragonal $\epsilon = \begin{pmatrix} \epsilon_{xx} & 0 & 0 \\ 0 & \epsilon_{xx} & 0 \\ 0 & 0 & \epsilon_{zz} \end{pmatrix}$

magnetization $\epsilon = N^2 \begin{pmatrix} 1 & iQ\cos\phi & -iQ\sin\phi\sin\gamma \\ -iQ\cos\phi & 1 & iQ\cos\gamma\sin\phi \\ iQ\sin\phi\sin\gamma & -iQ\cos\gamma\sin\phi & 1 \end{pmatrix}$



with the magneto-optic constant $Q = 2\delta_m - 2i\beta_m$

and the magnetization direction $\vec{M} = Q \cdot \begin{pmatrix} \cos\gamma\sin\phi \\ \sin\gamma\sin\phi \\ \cos\phi \end{pmatrix}$

Scattering Tensor

$$f = \begin{pmatrix} f_{xx} & f_{xy} & f_{xz} \\ f_{yx} & f_{yy} & f_{yz} \\ f_{zx} & f_{zy} & f_{zz} \end{pmatrix}$$

Isotropic scattering tensor (charge Thomson scattering)

$$f = -r_0 (Z + f' + i f'') \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = -r_0 (f_1 + i f_2) \cdot \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Magnetic scattering tensor

$$f = \begin{pmatrix} (f_1 + i f_2) & i f_m \cos\phi & -i f_m \sin\phi\sin\gamma \\ -i f_m \cos\phi & (f_1 + i f_2) & i f_m \cos\gamma\sin\phi \\ i f_m \sin\phi\sin\gamma & -i f_m \cos\gamma\sin\phi & (f_1 + i f_2) \end{pmatrix}$$

with the magnetic-scattering factor $f_m = f_{1m} + i f_{2m}$

Tetragonal scattering tensor

$$f = \begin{pmatrix} (f_1 + i f_2) & 0 & 0 \\ 0 & (f_1 + i f_2) & 0 \\ 0 & 0 & (f_{1m} + i f_{2m}) \end{pmatrix}$$

correlation between dielectric tensor and scattering tensor:

$$\varepsilon = 1 + \chi = 1 + \frac{4\pi}{k_0^2} N_A r_0 \sum_j \rho_{m,j} f_j$$

f_j: tensor of element j

$\rho_{m,j}$: molar concentration of element j