Rigorous Coupled Wave Analysis (RCWA)

- Structure is composed of layers in which $\varepsilon(x,y,z) = \varepsilon(x,y)$

- Maxwell's equations are solved rigorously (up to truncation) in each layer, resulting in eigenmodes

- Continuity of fields at layer interfaces determines excitation strengths of modes, beginning with the incident field at the first interface

- Solution takes place in Fourier space, $\varepsilon(x,y)$ expressed in Fourier expansion → periodic in x and y direction; only finite number of harmonics used in numerics

See also:
Marcus Diem, “Beschreibung der optischen Eigenschaften nanostrukturierter Materialien mit Methoden der diffraktiven Optik“, Chapt. 2, http://digbib.ubka.uni-karlsruhe.de/volltexte/1000005852 (Text is in English!)
Rigorous Coupled Wave Analysis (RCWA)

Fourier composition in the layers, e.g.

\[ E_x = e^{i(k_{x,0}x + k_{y,0}y)} \sum_p \sum_q e^{i \left( \frac{2\pi}{\Lambda_x} px + \frac{2\pi}{\Lambda_y} qy \right)} \sum_m a_{x,m,p,q} \left( f_m e^{i\kappa_m z} + g_m e^{-i\kappa_m z} \right) \]

Plug into Maxwell’s equations \( \rightarrow \) Eigenvalue problem

RSOFT implementation of RCWA: DiffractMOD
RSoft: Simulation of Gratings and Metamaterials

Task 1
Simulate the transmission spectrum of a 1D binary dielectric grating with the RCWA method. What effects occur when the grating period becomes a multiple of the wavelength? Investigate the influence of the number of harmonics used in the computation.

Task 2
Simulate an asymmetric (blazed) grating. What happens in the diffraction orders?

Task 3
Simulate the spectrum of a subwavelength, metallic cut-wire metamaterial, see sketch.

Task 4
Write a MATLAB program which computes the effective parameters n, Z, ε, μ of the metamaterial layer on basis of the complex transmission and reflection coefficients obtained with RSoft.

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**Diagram:**
- **Ag** layer: 30 nm
- **Al₂O₃** layer: 40 nm, n=1.62
- **Ag** layer: 30 nm
- **SiO₂** layer: 30 nm, n=1.44
- **Air**
- **W = 300 nm**
- **P = 600 nm**
Parameter Retrieval

Generalized Fresnel Equations for normal incidence

\[ t = \frac{2}{(1 + z_r) \cos nk d - i(z_r z + z^{-1}) \sin nk d} \]

\[ r = \frac{t}{2} \left[ (1 - z_r) \cos nk d - i(z_r z - z^{-1}) \sin nk d \right] \]

\[ z_r = Z_i / Z_t \]

\[ z = Z / Z_i \]

\[ \rightarrow \text{Task: Invert these equations for n and Z} \]
Parameter Retrieval

Using Mathematica replaces overly tedious thinking

\[
\text{eqns = \{}
\begin{align*}
t &= \frac{2}{(1 + zr) \cos[n k d] - i (zr + 1/z) \sin[n k d])}, \\
r &= \frac{t}{2} ((1 - zr) \cos[n k d] - i (zr - 1/z) \sin[n k d])
\end{align*}
\}
\]

\[
\{t = \frac{2}{(1 + zr) \cos[d k n] - i \left( \frac{1}{z} + zr \right) \sin[d k n]} \}, \quad r = \frac{1}{2} t \left( (1 - zr) \cos[d k n] - i \left( \frac{1}{z} + zr \right) \sin[d k n] \right)
\]

\[
\text{sol = Solve[eqns, \{n, z\};}
\]

Solve::ifun: Inverse functions are being used by Solve, so some solutions may not be found; use Reduce for complete solution information.

\[
\text{sol2 = Simplify[sol];}
\]

\[
\text{Length[sol]}
\]

4

\[
\text{sol2[[1]]}
\]

\[
\text{\{Z \rightarrow \frac{\sqrt{1 - \frac{(1-r^2+\text{z}r)^2}{(1+\text{z}r)(1+\text{z}r+\text{z}r^2)}}}{-1 + 2 r - r^2 + t^2 z r^2} \}}
\]

\[
\text{ArcCos}\left[\frac{1-r^2+\text{z}r}{t (1+\text{z}r)(1+\text{z}r+\text{z}r^2)}\right]
\]

\[
\text{sol2[[2]]}
\]

\[
\text{\{Z \rightarrow \frac{\sqrt{1 - \frac{(1-r^2+\text{z}r)^2}{(1+\text{z}r)(1+\text{z}r+\text{z}r^2)}}}{-1 + 2 r - r^2 + t^2 z r^2} \}}
\]

\[
\text{ArcCos}\left[\frac{1-r^2+\text{z}r}{t (1+\text{z}r)(1+\text{z}r+\text{z}r^2)}\right]
\]

\[
\text{sol2[[3]]}
\]

\[
\text{\{Z \rightarrow \frac{\sqrt{1 - \frac{(1-r^2+\text{z}r)^2}{(1+\text{z}r)(1+\text{z}r+\text{z}r^2)}}}{-1 + 2 r - r^2 + t^2 z r^2} \}}
\]

\[
\text{ArcCos}\left[\frac{1-r^2+\text{z}r}{t (1+\text{z}r)(1+\text{z}r+\text{z}r^2)}\right]
\]

\[
\text{sol2[[4]]}
\]

\[
\text{\{Z \rightarrow \frac{\sqrt{1 - \frac{(1-r^2+\text{z}r)^2}{(1+\text{z}r)(1+\text{z}r+\text{z}r^2)}}}{-1 + 2 r - r^2 + t^2 z r^2} \}}
\]

\[
\text{ArcCos}\left[\frac{1-r^2+\text{z}r}{t (1+\text{z}r)(1+\text{z}r+\text{z}r^2)}\right]
\]
Parameter Retrieval

Careful: Use of inverse trigonometric functions

\[
\text{Re}(n) = \pm \text{Re} \left\{ \frac{1}{kd} \cos^{-1} \left[ \frac{1 - r^2 + z_r t^2}{t ((z_r - 1)r + 1 + z_r)} \right] \right\} + \frac{2\pi m}{kd}
\]

- Demand \( \text{Im}(n) > 0, \text{Re}(Z) > 0 \) (passive medium)
- Demand continuity in spectral behavior
- Eliminate ambiguity \( m \) at large \( \lambda/d \)
  (pick correct branch starting at large wavelengths)

\[ \rightarrow \text{Derive permittivity and permeability} \]

\[
\varepsilon = \frac{n}{z}, \quad \mu = nz
\]

See also:
Smith et al., PRB 66, 195104, (2002)
Smith et al., PRE 71 046617, (2005)
Menzel et al., PRB 77, 195328, (2008)
Parameter Retrieval

Retrieved quantities $\varepsilon$ and $\mu$ help in identifying the kind of resonance.
Amendment: Defining Cladding and Substrate in RSoft

Cladding and substrate are defined by the first and last layer in
Perform Simulation → Advanced… → Analyze Profile

There is no need to employ the Layer Table Editor.

Tight boundary definition is acceptable, but not recommended.
RSoft: Simulation of Gratings and Metamaterials

Task 5
Simulate the spectrum and retrieve the effective parameters for a dual-band magnetic resonator.

Fig. 1. A dual-band magnetic resonator: (a) Unit cell geometry. (b) Real part of its effective permeability for the designs with $p = 1200$ nm, $w_1 = 300$ nm, $t = 30$ nm, $d = 40$ nm, and $t_s = 20$ nm.

Kwon, Werner, Kildishev, Shalaev,
http://www.opticsinfobase.org/abstract.cfm?URI=oe-15-4-1647
Task 6
Modify the nanostructure to obtain a dual-band negative-index metamaterial. Explain its working principle by retrieving the effective parameters.