# PPML - RCWA

## (Periodically Patterned Multi Layer –

## Rigorous Coupled Wave Analysis)

# User manual

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Version 2.0 -- october 2019

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INCLUDED FOLDERS:

**`general`** -- utility functions (scattering matrix propagation, complex square root)

**`1d_tm`** -- functions for 1d patterned multilayers, TM polarization

**`1d`** -- functions for anisotropic 1d patterned multilayers

**`2d`** -- functions for 2d patterned multilayers (rectangular & L-shaped inclusions)

**`examples`** -- some examples

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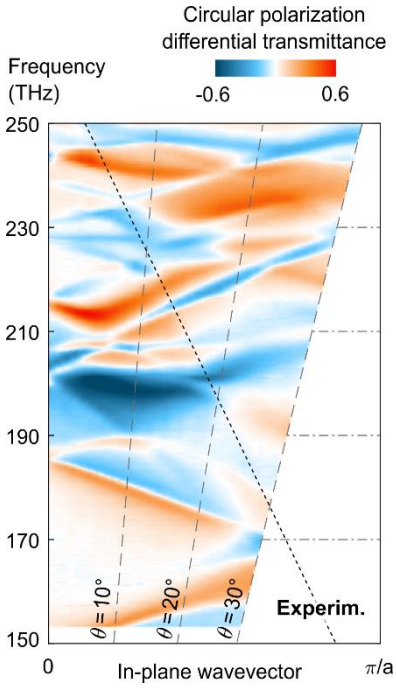
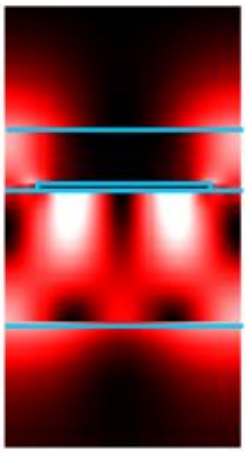



*Angularly-resolved circular polarization differential transmittance from a chiral dielectric metasurface (S. Zanotto et al., Nanophotonics (2019))*



*Intracavity field in a patterned membrane (S. Zanotto and A. Tredicucci, Scientific Reports 2016; 6: 24592)*

## *Contents of the* `1d-tm` *folder:*

**`RTA_1d_tm`** - calculates reflectance, transmittance, and layer-by-layer absorbance
**`SM_1d_tm`** – calculates the 2x2 scattering matrix
**`field_1d_tm`** – calculates some components of the E and S fields inside the structure

The "1d-tm" functions solve the periodically patterned multilayer problem in the 1-d geometry (fig. 1a). Only TM-polarization is considered, i.e., the H-field has the sole *y* component. This corresponds to *p*-polarized plane waves incident on a plane orthogonal to the 1d pattern (see fig. 1b). Their wavevector has modulus $k$ ($=k_0 \cdot \sqrt{\varepsilon_{sup}}$), being $k_0$ the vacuum wavevector and $\varepsilon_{sup}$ the superstrate permittivity; moreover, the incident wavevector has a projection $k_{par}$ along the $x$ axis.

The template structure comprises a superstrate, a substrate, and a number of internal layers. Super- and substrate are not patterned, while the internal layers can be. The unit cell geometry consists of a centered stripe of material B surrounded by material A. Super- and substrate have isotropic permittivity, while internal layers can have anisotropic permittivity of the form

$$\begin{pmatrix} \varepsilon_x & 0 & 0 \\ 0 & \varepsilon_y & 0 \\ 0 & 0 & \varepsilon_z \end{pmatrix} \quad ; \qquad \varepsilon_x = \varepsilon_y$$

Complex-valued permittivities are allowed. The method works well also for strongly negative epsilons (metals), but care has to be taken in choosing the convergence parameter (**`halfnpw`**, see below).

All the geometrical parameters are input as arguments of the function. See the comments below for the requirements specific to each function.

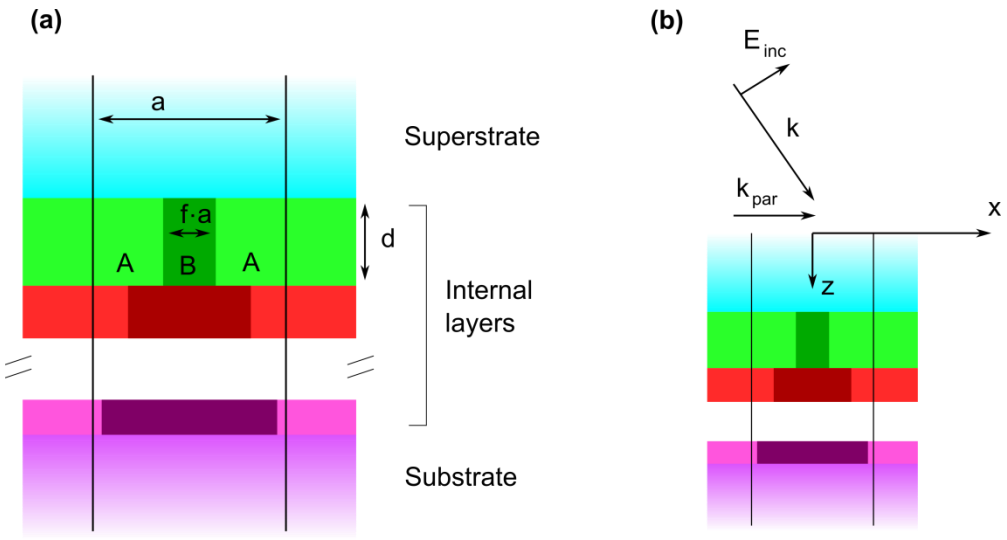



**Figure 1**

***INPUT VARIABLES***

Here follows a commented list of the input variables. This is the same for **`RTA_1d_tm`** and **`SM_1d_tm`**

| ***NAME*** | ***DESCRIPTION*** | ***TYPE*** |
|---|---|---|
| `a` | period | real > 0 |
| `L` | number of layers excluded superstrate and substrate | integer > 0 |
| `epssup, epssub` | super-and sub-strate permittivities | complex |
| `epsxA` | in-plane component of dielectric tensor for material A in the internal layers | 1x`L` complex |
| `epsxB` | idem, for material B | 1x`L` complex |
| `epszA, epszB` | idem, out-of-plane components | 1x`L` complex |
| `f` | duty cycle in the internal layers | 1x`L` real, each component in [0,1] |
| `d` | thicknesses of the layers, including super- and sub-strate | 1x`(L+2)` complex |
| `halfnpw` | half number of harmonic waves used in calculation [see below] | integer >= 0 |
| `k0` | wavevector in vacuum (= 2*pi/lambda0) | real > 0 |
| `kpar` | x-projection of the incident wavevector | real |

The function **`field_1d_tm`** also asks for two more inputs:

| ***NAME*** | ***DESCRIPTION*** | ***TYPE*** |
|---|---|---|
| nx | number of points along x for field display | integer > 0 |
| nz | number of points along z for field display, specified for each layer | 1x`(L+2)` integer > 0 |

***OUTPUT VARIABLES & NOTES TO EACH FUNCTION***

**`RTA_1d_tm`**

| ***NAME*** | ***DESCRIPTION*** | ***TYPE*** |
|---|---|---|
| `RR` | Reflectance<br>(total reflected flux/input flux) | real |
| `TT` | Transmittance<br>(total transmitted flux/input flux) | real |
| `AA` | Layer-by-layer absorbance<br>(power absorbed in the layer/input flux) | 1x`L` real |

Notes:

- `epssup` must be real (otherwise the incident waves are ill-defined)
  `epssub` can be either real or complex.
  In the first case, `TT` has the meaning of transmittance towards the far field.
  In the second case, `TT` has the meaning of absorbance in the substrate.
- Above diffraction thresholds, `RR` and `TT` contain also the contribution of diffracted beams.
- Thickness of superstrate and substrate do not influence the output of **`RTA_1d_tm`**. In this calculation, super- and substrate are at all effects semi-infinite.

**`SM_1d_tm`**

| ***NAME*** | ***DESCRIPTION*** | ***TYPE*** |
|---|---|---|
| `rl` | reflection coefficient from superstrate to superstrate ("left reflectance") | complex |
| `rr` | reflection coefficient from substrate to substrate ("right reflectance") | complex |
| `tlr` | transmission coefficient from superstrate to substrate ("left to right") | complex |
| `trl` | transmission coefficient from substrate to superstrate ("right to left") | complex |

Notes:

- The coefficients connect the amplitudes of the $H_y$ fields, calculated at the interface between superstrate and first layer, or substrate and last layer.
- Has been tested extensively only when superstrate and substrate have equal epsilon and thickness
- Why "left" and "right" and not "up" and "down"? …for historical reasons!

**field_1d_tm**

| *NAME* | *DESCRIPTION* | *TYPE* |
|---|---|---|
| x | vectors of x points where field is computed | 1x(nx) real |
| z | vectors of z points where field is computed | 1x[sum(nz)] real |
| Ex, Ez | E field x- and z-components , calculated on the x-y grid | (nx)x[sum(nz)] complex |
| Sz | Poynting vector z-component averaged over the unit cell, calculated on the z-grid | 1x[sum(nz)] complex |

Notes:

- epssup must be real (otherwise the incident waves are ill-defined)
- E fields are complex. The real, time-dependent fields are Re(E*exp(-i omega t)) [omega = c*k0]

**NOTES COMMON TO ALL FUNCTIONS**

- the lengths (a, d) and inverse lengths (k0, kpar) must be set in the same units (e.g. microns and inverse microns, respectively)

**The setting of halfnpw**

- As well known, the RCWA has a single convergence parameter which is the truncation order for the plane wave basis. Here, this is ruled by halfnpw, which is such that the complete basis is (-halfnpw, … 0, +halfnpw).
  Always pay attention that the selected value for halfnpw guarantees a satisfactory convergence for the problem under analysis.
- halfnpw = 0 sets the number of harmonic waves to 1, e.g. the scattering matrix reduces to the ordinary 2x2 formalism for unpatterned multilayers

## *Contents of the* `1d` *folder:*

**`epar_1d`** - calculates the vector containing the Fourier amplitudes of the electric field vector in-plane ("parallel") components

The "1d" functions solve the periodically patterned multilayer problem with 1-d pattern (fig. 2a). Plane waves are incident according to the scheme in fig. 2a. Their wavevector has modulus $k$ ($=k_0 \cdot \sqrt{\varepsilon_{sup}}$), being $k_0$ the vacuum wavevector and $\varepsilon_{sup}$ the superstrate permittivity; moreover, the incident wavevector has a projection $\boldsymbol{k_{par}}$ along on the x-y plane.

The template structure comprises a superstrate, a substrate, and a number of internal layers. Super- and substrate are not patterned, while the internal layers can be. The unit cell geometry consists of a centered stripe of material B surrounded by material A (fig. 1a). Super- and substrate have isotropic permittivity. In the internal layers, material A is isotropic, while material B has an anisotropic permittivity of the form

$$\begin{pmatrix} \varepsilon_{xx} & \varepsilon_{xy} & 0 \\ \varepsilon_{xy} & \varepsilon_{yy} & 0 \\ 0 & 0 & \varepsilon_z \end{pmatrix}$$

Complex-valued permittivities are allowed. The method works well also for strongly negative epsilons (metals), but care has to be taken in choosing the convergence parameter (**`halfnpw`**, see below).

All the geometrical parameters are input as arguments of the function. See the comments below for the requirements specific to each function.

***INPUT VARIABLES***

Here follows a commented list of the input variables for **`epar_1d`**

| ***NAME*** | ***DESCRIPTION*** | ***TYPE*** |
|---|---|---|
| `a` | period | real > 0 |
| `L` | number of layers excluded superstrate and substrate | integer > 0 |
| `epssup, epssub` | super-and sub-strate permittivities | complex |
| `epsA` | dielectric tensor for material A in the internal layers | 1x`L` complex |
| `epsxxB` | dielectric tensor xx-component for material B in the internal layers | 1x`L` complex |
| `epsxyB` | idem, xy-component | 1x`L` complex |
| `epsyyB` | idem, yy-component | 1x`L` complex |
| `epszB` | idem, z-component | 1x`L` complex |
| `f` | duty cycle in the internal layers | 1x`L` real, each component in [0,1] |

| | | |
|---|---|---|
| `d` | thicknesses of the layers, including super- and sub-strate | 1x`(L+2)` complex |
| `halfnpw` | half number of harmonic waves used in calculation [see below] | integer >= 0 |
| `k0` | wavevector in vacuum (= 2*pi/lambda0) | real > 0 |
| `kparx` | x-projection of the incident wavevector | real |
| `kpary` | y-projection of the incident wavevector | real |
| `pol` | polarization state of the incident light | `'s'` or `'p'` |

***OUTPUT VARIABLES & NOTES TO EACH FUNCTION***

**`epar_1d`**

| ***NAME*** | ***DESCRIPTION*** | ***TYPE*** |
|---|---|---|
| `epar` | Fourier amplitudes of the electric field vector in-plane components | complex, `2*(2*halfnpw+1)` |

Notes:

- `epssup` must be real (otherwise the incident waves are ill-defined)
- `epssub` can be complex or real. If it is real, and the periodicity is such that diffraction is allowed (i.e. the wavelength is shorter than the diffraction threshold), the meaning of `epar` is the following:

```
index         1,    ...,   h-1,            h,       h+1, ..., 2*h+1,
epar(index)   ..., ..., -Ey(D-1), -Ey(D0), -Ey(D+1), ...,    ...,


index         2*h+2, ..., 2*h+1+h-1, 2*h+1+h, 2*h+1+h+1, ..., 2*h+1+2*h+1,
epar(index)     ..., ...,    Ex(D-1),  Ex(D0),   Ex(D+1), ...,          ...,
```

where `h` is a shorthand for `halfnpw`. Here, `Ex` or `Ey` are the electric field *x*- and *y*- components of a diffracted wave. Please be careful since `Ey` have a minus sign. The diffracted order is identified by ... `D-1` , `D0` , `D+1` , ... , according to Fig. 2b.

For further details please refer to [1] .

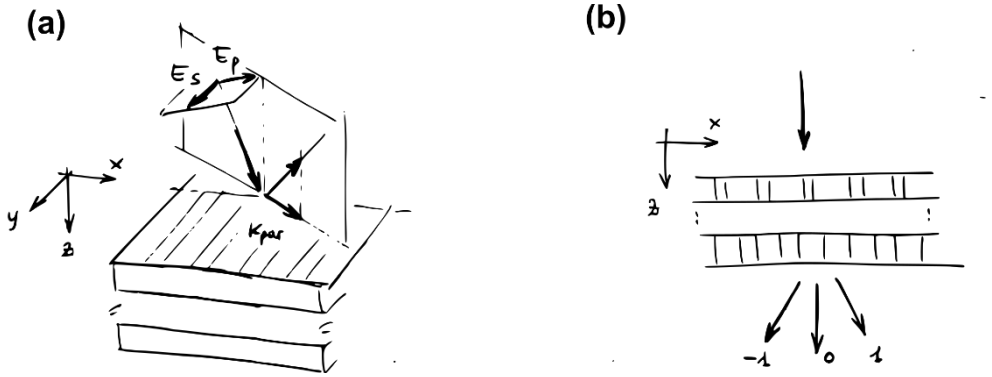



**Figure 2**

## *Contents of the* `2d` *folder:*

**`ZSM_2d_rect`** - calculates the zero-order scattering matrix for a layer stack comprising rectangle-shaped inclusions

**`ZSM_2d_Lshape`** – calculates the zero-order scattering matrix for a layer stack comprising L-shaped inclusions

The "2d" functions solve the periodically patterned multilayer problem in the 2-d geometry for two selected geometries (fig. 3 a-b), calculating the zero-order scattering matrix. The zero-order scattering matrix is defined as following:

$$\begin{pmatrix} S^-_{sup} \\ P^-_{sup} \\ S^-_{sub} \\ P^-_{sub} \end{pmatrix} = S \begin{pmatrix} S^+_{sup} \\ P^+_{sup} \\ S^+_{sub} \\ P^+_{sub} \end{pmatrix}$$

Polarizations are defined accordingly to fig. 4. Incident and reflected wavevectors have modulus $k_0 \cdot \varepsilon$, being $k_0$ the vacuum wavevector and $\varepsilon$ the permittivity of superstrate or substrate. The wavevector projection is $\boldsymbol{k}_{\mathrm{par}} = (k_{par,x}, k_{par,y})$

The unit cell geometry consists of an inclusion of material B within a region of material A. Unit cell is a square. All the layers have isotropic permittivity. Complex-valued permittivities are allowed. The method works well also for strongly negative epsilons (metals), but care has to be taken in choosing the convergence parameter (**`halfnpw`**, see below). This convergence property follows from the implementation of the factorization rules by L. Li (see the webpage for the reference), here implemented in terms of crossed mixed Fourier transforms.

All the geometrical parameters are input as arguments of the function. See the comments below for the requirements specific to each function.

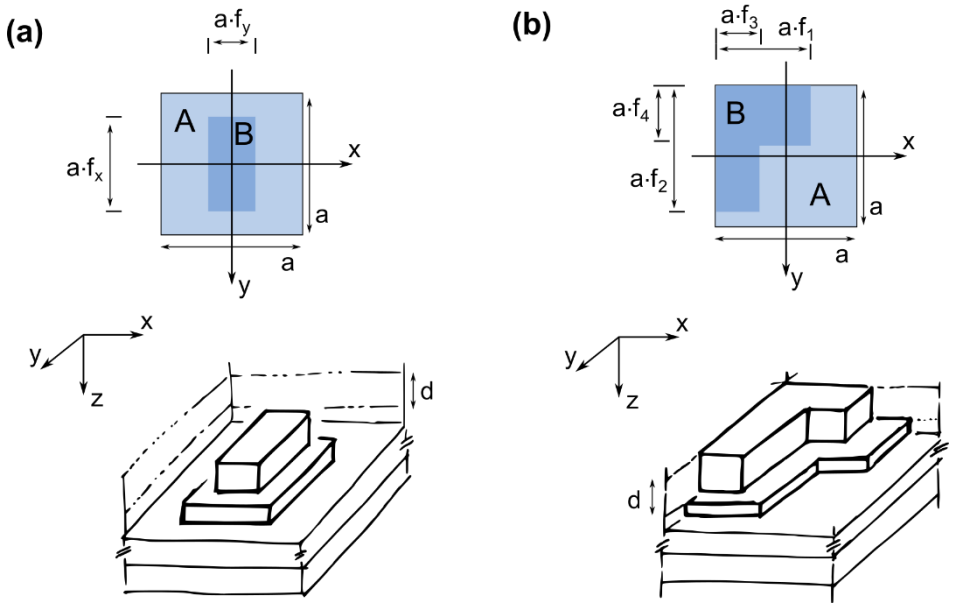



**Figure 3**

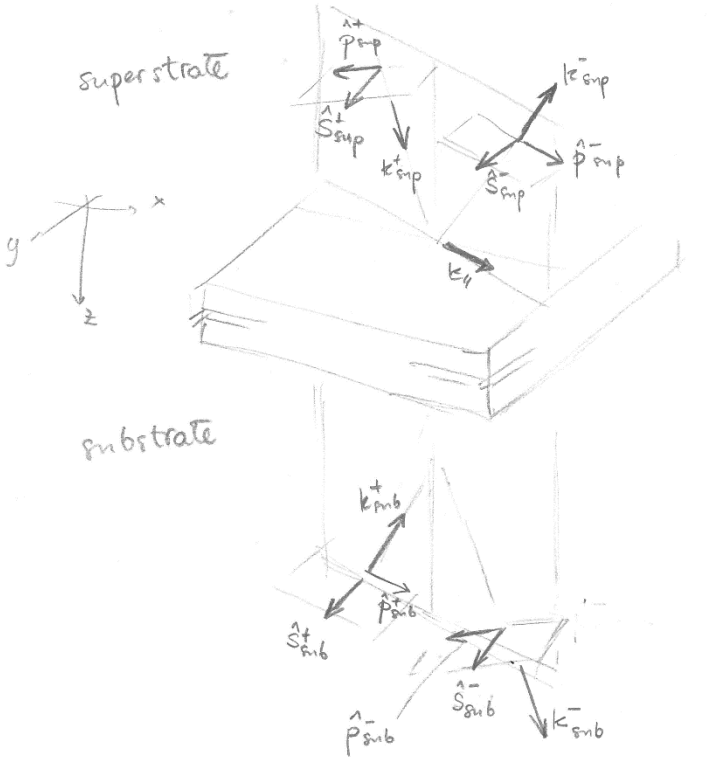



**Figure 4**

*WARNING! The convention for the polarization versors are different with respect to those for* epar_1d *(Fig. 2), and from those of* rxx_ *functions of previous versions.*

***INPUT VARIABLES***

Here follows a commented list of the input variables which are shared between **`ZSM_2d_rect`** and **`ZSM_2d_Lshape`**.

| ***NAME*** | ***DESCRIPTION*** | ***TYPE*** |
|---|---|---|
| `a` | period | real > 0 |
| `L` | number of layers excluded superstrate and substrate | integer > 0 |
| `epssup`, `epssub` | super-and sub-strate permittivities | real<br>complex |
| `epsA` | permittivity of material A in the internal layers | 1x`L` complex |
| `epsB` | permittivity of material B in the internal layers | 1x`L` complex |
| `d` | thicknesses of the layers,<br>including super- and sub-strate | 1x`(L+2)` real |
| `halfnpw` | truncation order [see below] | integer >= 0 |
| `k0` | wavevector in vacuum (= 2*pi/lambda0) | real > 0 |
| `kparx` | x-projection of the incident wavevector | real |

| | | |
|---|---|---|
| kpary | y-projection of the incident wavevector | real |

Here the input variables specific for **ZSM_2d_rect**

| *NAME* | *DESCRIPTION* | *TYPE* |
|---|---|---|
| fx | x-length of inclusion (relative to a) | real in [0,1] |
| fy | y-length of inclusion (relative to a) | real in [0,1] |

Here the input variables specific for **ZSM_2d_Lshape**

| *NAME* | *DESCRIPTION* | *TYPE* |
|---|---|---|
| f1 | see figure | real in [f3,1] |
| f2 | see figure | real in [f4,1] |
| f3 | see figure | real in [0,1] |
| f4 | see figure | real in [0,1] |

***OUTPUT VARIABLES & NOTES***

| *NAME* | *DESCRIPTION* | *TYPE* |
|---|---|---|
| S | zero-order scattering matrix | 4x4 complex |

Notes:

- Coefficients are determined assuming that the fields are evaluated at the interface between superstrate and first internal layer. In the case there are no internal layers (**L** = 0), the fields are evaluated at the interface between superstrate and substrate.

**NOTES COMMON TO ALL FUNCTIONS**

- the lengths (a, d) and inverse lengths (k0, kpar) must be set in the same units (e.g. microns and inverse microns, respectively)
- thickness of superstrate and substrate do not influence the result.
  The electromagnetic problem is solved de facto assuming semi-infinite super- and substrate boundary conditions.
  You find them in view of further development (field profile calculation).

**The setting of halfnpw**

- As well known, in two-dimensional RCWA a proper spatial harmonics basis must be chosen. Here we chose a square truncation scheme. This is ruled by halfnpw, which is such that the complete basis is built by the direct product of (-halfnpw, … 0, +halfnpw) partial harmonics along x- and y- directions.
  Always pay attention that the selected value for halfnpw guarantees a satisfactory convergence for the problem under analysis.
- halfnpw = 0 sets the number of harmonic waves to 1, e.g. the scattering matrix reduces to the ordinary 4x4 formalism for unpatterned multilayers.


## *Bibliography*

[1] D. Whittaker and I. Culshaw, Phys. Rev. B **60**, 2610 (1999).