PPML - RCWA

(Periodically Patterned Multi Layer –

Rigorous Coupled Wave Analysis)

User manual

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Version 3.0 – feb 2022

WARNING! PPML 3.0 is a major release, that includes conducting interfaces between the layers. The software interface of all the functions is changed with respect to previous versions. Compatibility is however fully guaranteed. Look at the end of this Manual for details.

INCLUDED FOLDERS:

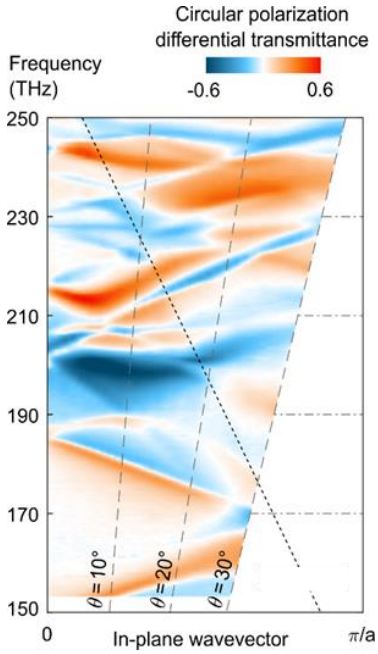
`general` ---------- utility functions (scattering matrix propagation, complex square root)

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

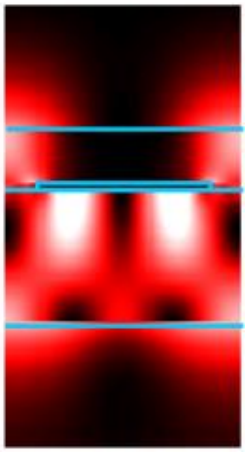
`1d` ---------- functions for anisotropic 1d patterned multilayers

`2d_rect; 2d_Lshape` ---- functions for 2d patterned multilayers (rectangular & L-shaped inclusions)

`examples` ---------- some examples



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 ε_{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). The layers are separated by zero-thickness, two-dimensional conducting interfaces, whose 2d-conductivity can be specified as a complex number. Notice that setting the conductivity to zero is equivalent to assuming the direct contact between the dielectric materials of adjacent layers.

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

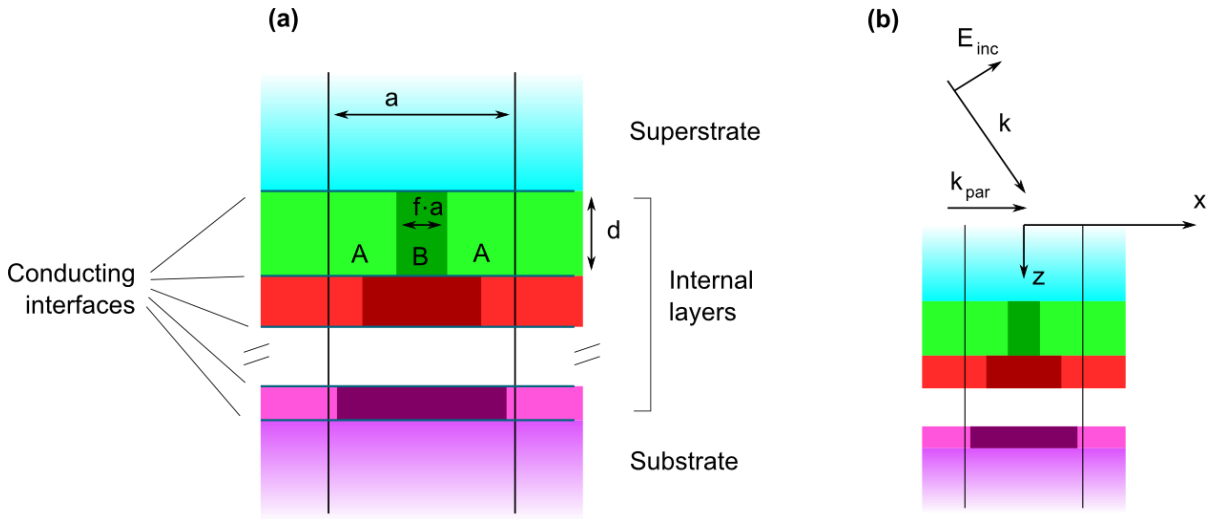


Figure 1

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
`sigma`	conductivity of the interfaces	1x`(L+1)` 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 (total reflected flux/input flux)	real
`TT`	Transmittance (total transmitted flux/input flux)	real
`AA`	Layer-by-layer absorbance (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.
- Layer-by-layer absorbance includes also the energy absorbed by some conducting surfaces. Specifically, `AA(l)` is the absorbance of internal layer number `l` plus the absorbance of the interface that separates layer `l` from layer `l+1`. (Here, `l=1` is the first internal layer).

`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 (for instance microns and inverse microns, or meters and inverse meters)
- the units of sigma must be inverse Ohms.

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 ε_{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). The layers are separated by zero-thickness, two-dimensional conducting interfaces, whose 2d-conductivity can be specified as a complex number (see also Fig. 1a). Notice that setting the conductivity to zero is equivalent to assuming the direct contact between the dielectric materials of adjacent layers.

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`	permittivity of 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

sigma	conductivity of the interfaces	1x(L+1) complex
f	duty cycle in the internal layers	1xL 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] .

- the lengths (a, d) and inverse lengths (k0, kpar) must be set in the same units (for instance microns and inverse microns, or meters and inverse meters)
- the units of sigma must be inverse Ohms.

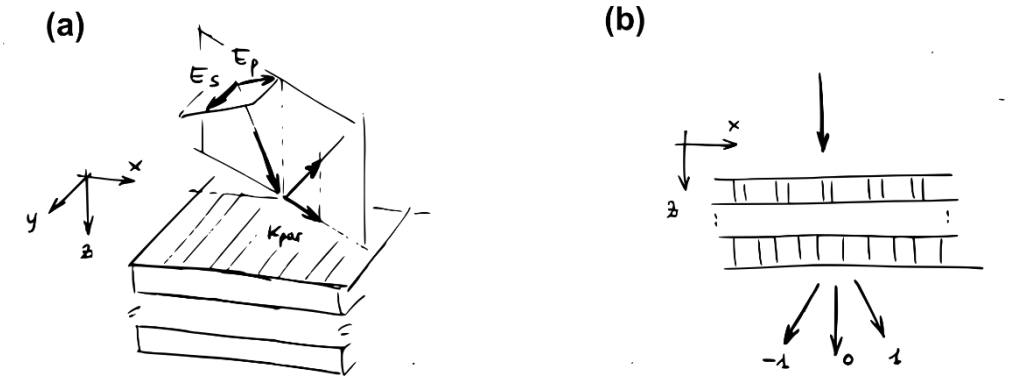


Figure 2

Contents of the `2d_` *folders:*

`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 scattering matrix for the zero-order diffracted waves. The zero-order scattering matrix **S** is defined as following:

$$\begin{pmatrix} s^-_{\mathrm{sup}} \\ p^-_{\mathrm{sup}} \\ s^-_{\mathrm{sub}} \\ p^-_{\mathrm{sub}} \end{pmatrix} = \mathbf{S} \begin{pmatrix} s^+_{\mathrm{sup}} \\ p^+_{\mathrm{sup}} \\ s^+_{\mathrm{sub}} \\ p^+_{\mathrm{sub}} \end{pmatrix}$$

Polarizations are defined according to fig. 4. Incident and reflected wavevectors have modulus $k_0 \cdot \varepsilon$, being k_0 the vacuum wavevector and ε 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. For **`ZSM_2d_rect`** the unit cell is a rectangle; for **`ZSM_2d_Lshape`** the 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. The layers are separated by zero-thickness, two-dimensional conducting interfaces, whose 2d-conductivity can be specified as a complex number (see also Fig. 1a). Notice that setting the conductivity to zero is equivalent to assuming the direct contact between the dielectric materials of adjacent layers.

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

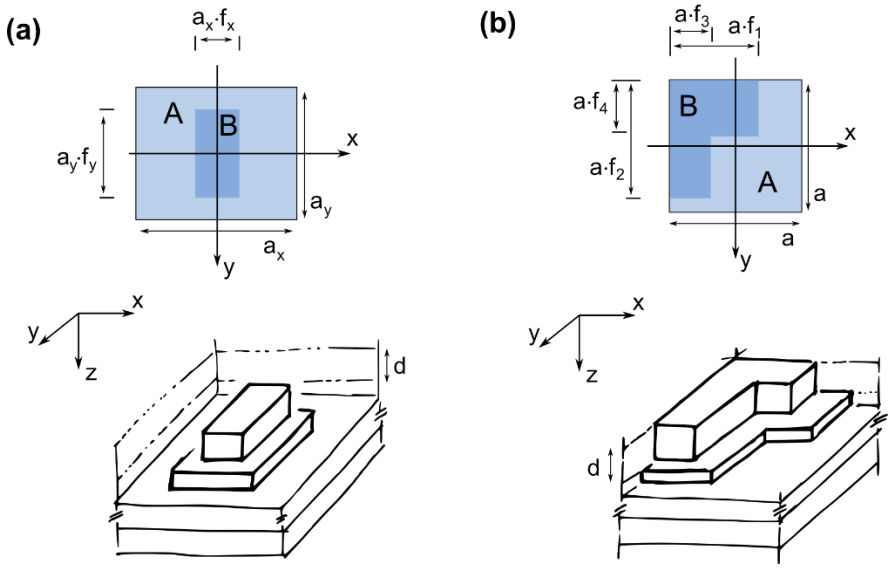


Figure 3

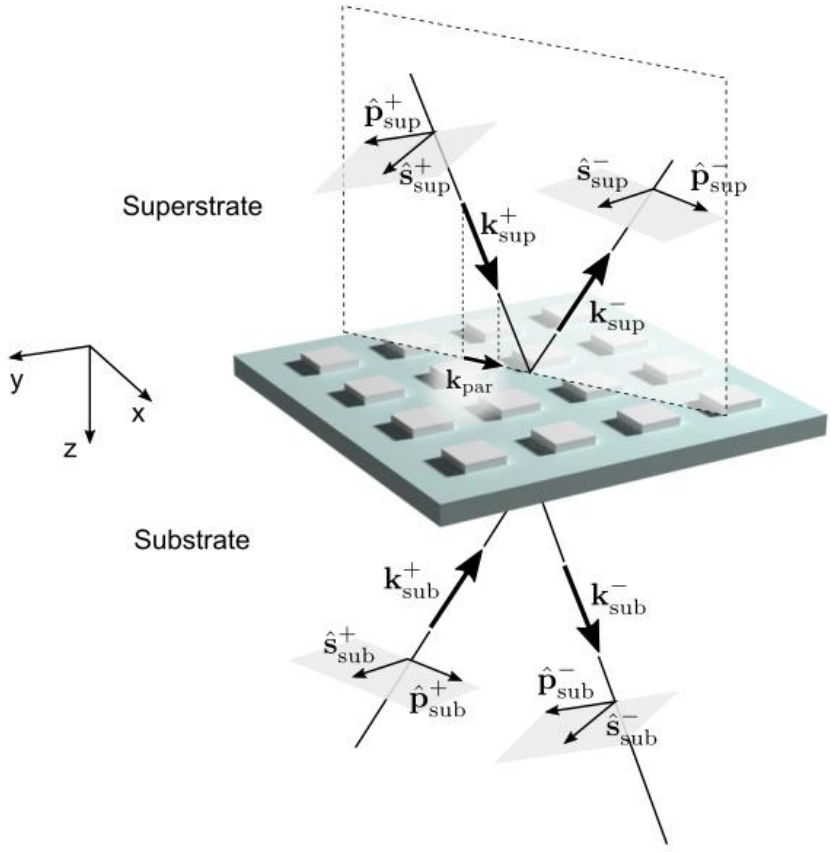


Figure 4

WARNING! The convention for the polarization versors are different with respect to those for epar_1d *(Fig. 2), and from those of* rxx_ *functions found in PPML versions older than 2.0.*

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***
`L`	number of layers excluded superstrate and substrate	integer > 0
`epssup, epssub`	super-and sub-strate permittivities	real 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
`sigma`	conductivity of the interfaces	1x (`L+1`) complex
`d`	thicknesses of the layers, 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***
`ax`	x-period	real > 0
`ay`	y-period	real > 0
`fx`	x-length of inclusion (relative to `ax`)	real in [0,1]
`fy`	y-length of inclusion (relative to `ay`)	real in [0,1]

Here the input variables specific for **`ZSM_2d_Lshape`**

NAME	***DESCRIPTION***	***TYPE***
`a`	period	real > 0
`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, ax, ay, d`) and inverse lengths (`k0, kparx, kpary`) must be set in the same units (for instance microns and inverse microns, or meters and inverse meters)
- the units of `sigma` must be inverse Ohms.
- 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.

Note on the compatibility between PPML 3.0 and older versions:

All the calculations possible in older versions of PPML can be done in PPML 3.0 with a very simple setting. Since a conducting interface with zero conductivity can always be included anywhere without affecting the electromagnetic response, one can adapt the old codes by simply setting `sigma = zeros(L+1)`, where `L` is the number of internal layers.

Bibliography

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