A Onelab model for the parametric study of mono-dimensional diffraction gratings

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Abstract

This document aims at presenting both theoretical and practical aspects of the grating_2D Onelab model (available at http://onelab.info/wiki/Diffraction_grating). This model applies to so-called mono-dimensional grating, i.e. structures having one direction of invariance. Various geometries and materials can be handled or easily added. The two classical polarization cases, denoted here $E^\parallel$ and $H^\parallel$, are addressed. The output consists in a full energy balance of the problem computed from the field maps. This model is based on free the GNU softwares Gmsh [1], GetDP [2] and their interface Onelab.

1 Intro

This document aims at presenting both theoretical and practical aspects regarding the grating_2D Onelab model, mainly for educational purposes. This model applies to so-called mono-dimensional grating, i.e. structures having one direction of invariance. Various geometries and materials can be handled or easily added. The two classical polarization cases, denoted here $E^\parallel$ and $H^\parallel$, are addressed. The output consists in a full energy balance of the problem computed from the field maps. For more detailed information and associated bibliography, the curious reader is invited refer to [3].

2 Theoretical model

2.1 Set up of the problem and notations

We denote by $\mathbf{x}$, $\mathbf{y}$ and $\mathbf{z}$, the unit vectors of the axes of an orthogonal co-ordinate system $Oxyz$. Time-harmonic regime is assumed; consequently, the electric and magnetic fields are represented by the complex vector fields $\mathbf{E}$ and $\mathbf{H}$, with a time dependance chosen in $\exp(+i\omega t)$.

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Figure 1: Example of grating structure covered by the present Onelab model.
Besides, in this model, we assume that the tensor fields of relative permittivity \( \varepsilon \) and relative permeability \( \mu \) can be written as follows:

\[
\varepsilon = \begin{pmatrix}
\varepsilon_{xx} & \varepsilon_a & 0 \\
\varepsilon_a & \varepsilon_{yy} & 0 \\
0 & 0 & \varepsilon_{zz}
\end{pmatrix}
\quad \text{and} \quad
\mu = \begin{pmatrix}
\mu_{xx} & \mu_a & 0 \\
\mu_a & \mu_{yy} & 0 \\
0 & 0 & \mu_{zz}
\end{pmatrix},
\]

(1)

where \( \varepsilon_{xx}, \varepsilon_a, \ldots, \mu_{zz} \) are possibly complex valued functions of the two variables \( x \) and \( y \) and where \( \bar{\varepsilon}_a \) (resp. \( \bar{\mu}_a \)) represents the conjugate complex of \( \varepsilon_a \) (resp. \( \mu_a \)). These kinds of materials are said to be \( z \)-anisotropic. It is of importance to note that with such tensor fields, lossy materials can be studied (the lossless materials correspond to tensors with real diagonal terms represented by Hermitian matrices) and that the problem is invariant along the \( z \)-axis but the tensor fields can vary continuously (gradient index gratings) or discontinuously (step index gratings). We define the wavenumber \( k_0 := \omega/c \).

The gratings that we are dealing with are made of three regions (See Fig. [I]).

- **The superstrate** \( y > y_g \) which is supposed to be homogeneous, isotropic and lossless and characterized solely by its real valued relative permittivity \( \varepsilon^+ \) and its relative permeability \( \mu^+ \). We denote \( k^+ := k_0 \sqrt{\varepsilon^+ \mu^+} \).

- **The substrate** \( y < 0 \) is supposed to be homogeneous and isotropic and therefore characterized by its relative permittivity \( \varepsilon^- \) and its relative permeability \( \mu^- \). We denote \( k^- := k_0 \sqrt{\varepsilon^- \mu^-} \).

- **The groove region** \( 0 < y < y_g \) is heterogeneous and \( z \)-anisotropic. It is characterized by the two tensor fields \( \bar{\varepsilon}_g(x, y) \) and \( \bar{\mu}_g(x, y) \). It is worth noting that the method presented in this paper does work irrespective of whether the tensor fields are piecewise constant. The grating periodicity along \( x \)-axis will be denoted \( d \).

This grating is illuminated by an incident plane wave of wave vector \( k^+_i = \alpha x - \beta^+ y = k^+ (\sin \theta_0 x - \cos \theta_0 y) \), whose electric field (\( E^\parallel \) polarization case) (resp. magnetic field (\( H^\parallel \))) is linearly polarized along the \( z \)-axis:

\[
E^0_e = A^0_e \exp(-i k_i^+ \cdot r) z \quad (\text{resp. } H^0_m = A^0_m \exp(-i k_i^+ \cdot r) z),
\]

(2)

where \( A^0_e \) (resp. \( A^0_m \)) is an arbitrary complex number. The magnetic (resp. electric) field derived from \( E^0_e \) (resp. \( H^0_m \)) is denoted \( H^0_e \) (resp. \( E^0_m \)) and the electromagnetic field associated with the incident field is therefore denoted \( (E^0, H^0) \) which is equal to \( (E^0_e, H^0_e) \) (resp. \( (E^0_m, H^0_m) \)).

The problem of diffraction that we address in this paper is therefore to find Maxwell’s equation solutions in harmonic regime i.e. the unique solution \((E, H)\) of:

\[
\begin{align*}
\text{curl } E &= -i \omega \mu_0 \mu H \\
\text{curl } H &= +i \omega \varepsilon_0 \varepsilon E
\end{align*}
\]

(3a) (3b)

such that the diffracted field satisfies an Outgoing Waves Condition (O.W.C. [5]) and where \( E \) and \( H \) are quasi-periodic functions with respect to the \( x \) co-ordinate.
2.2 Appropriate diffracted field formulation

2.2.1 Decoupling of fields and $z$–anisotropy

We assume that $\hat{\delta}(x,y)$ is a $z$–anisotropic tensor field ($\delta_{xz} = \delta_{yz} = \delta_{zx} = \delta_{zy} = 0$). Moreover, the left upper matrix extracted from $\hat{\delta}$ is denoted $\tilde{\delta}$, namely:

$$\tilde{\delta} = \begin{pmatrix} \delta_{xx} & \tilde{\delta}_{a} \\ \tilde{\delta}_{a} & \delta_{yy} \end{pmatrix}.$$  

(4)

For $z$–anisotropic materials, with non-conical incidence, the problem of diffraction can be split into two fundamental cases ($H^\parallel$ case and $E^\parallel$ case). This property results from the following equality which can be easily derived:

$$-\text{rot}\left(\hat{\delta}^{-1}\text{rot}\left(u\mathbf{z}\right)\right) = \text{div}\left(\tilde{\delta}^T/\det(\tilde{\delta})\nabla u\right)\mathbf{z},$$

(5)

where $u$ is a function which does not depend on the $z$ variable. From the previous equality, it appears that the non-conical problem of diffraction amounts to looking for an electric (resp. magnetic) field which is polarized along the $z$–axis; $E = e(x,y)\mathbf{z}$ (resp. $H = h(x,y)\mathbf{z}$). The functions $e$ and $h$ are therefore solutions of similar differential equations:

$$\mathcal{L}_2^\xi\chi(u) := \text{div}\left(\xi\nabla u\right) + k_0^2\chi u = 0$$

(6)

with

$$u = e, \quad \xi = \hat{\mu}^T/\det(\hat{\mu}), \quad \chi = \varepsilon_{zz},$$

(7)

in the $E^\parallel$ case and

$$u = h, \quad \xi = \hat{\varepsilon}^T/\det(\hat{\varepsilon}), \quad \chi = \mu_{zz}.$$  

(8)

in the $H^\parallel$ case.

2.2.2 Reducing the diffraction problem to a radiation problem with localized sources

In its initial form, the problem of diffraction summed up by Eq. (6) is not well suited to the Finite Element Method. We propose to split the unknown function $u$ into a sum of two functions $u_1$ and $u_2^d$, the first term being known as a closed form and the latter being a solution of a radiation problem whose sources are localized within the obstacles. This is, in essence, a diffracted field formulation extended to the case where the substrate and superstrate are made of different materials.

We have assumed that outside the groove region (cf. Fig. 1), the tensor field $\xi$ and the function $\chi$ are constant and equal respectively to $\xi^-$ and $\chi^-$ in the substrate ($y < 0$) and equal respectively to $\xi^+$ and $\chi^+$ in the superstrate ($y > y_g$). Besides, for the sake of clarity, the superstrate is supposed to be made of an isotropic and lossless material and is therefore solely defined by its relative permittivity $\varepsilon^+$ and its relative permeability $\mu^+$, which leads to:

$$\xi^+ = \frac{1}{\mu^+}\text{Id}_2 \quad \text{and} \quad \chi^+ = \varepsilon^+ \quad \text{in } H^\parallel \text{ case}.$$  

(9)
\( \xi^+ = \frac{1}{\varepsilon^+} \text{Id}_2 \) and \( \chi^+ = \mu^+ \) in \( E^\parallel \) case,

where \( \text{Id}_2 \) is the \( 2 \times 2 \) identity matrix. With such notations, \( \xi \) and \( \chi \) are therefore defined as follows:

\[
\xi(x, y) := \begin{cases} 
\xi^+ & \text{for } y > y_g \\
\xi^g(x, y) & \text{for } y_g > y > 0 \\
\xi^- & \text{for } y < 0
\end{cases}
, \quad \chi(x, y) := \begin{cases} 
\chi^+ & \text{for } y > y_g \\
\chi^g(x, y) & \text{for } y_g > y > 0 \\
\chi^- & \text{for } y < 0
\end{cases}.
\]

(11)

It is now apropos to introduce an auxiliary tensor field \( \xi_{\parallel 1} \) and an auxiliary function \( \chi_{1} \):

\[
\xi_{\parallel 1}(x, y) := \begin{cases} 
\xi^+ & \text{for } y > 0 \\
\xi^- & \text{for } y < 0
\end{cases}, \quad \chi_{1}(x, y) := \begin{cases} 
\chi^+ & \text{for } y > 0 \\
\chi^- & \text{for } y < 0
\end{cases}.
\]

(12)

these quantities corresponding, of course, to a simple plane interface. Besides, we introduce the constant tensor field \( \xi_{\parallel 0} \) which is equal to \( \xi^+ \) everywhere and a constant scalar field \( \chi_{0} \) which is equal to \( \chi^+ \) everywhere. Finally, we denote \( u_{0} \) the function which equals the incident field \( u_{\text{inc}} \) in the superstrate and vanishes elsewhere:

\[
u_{0}(x, y) := \begin{cases} 
u_{\text{inc}} & \text{for } y > y_g \\
0 & \text{for } y < y_g
\end{cases}.
\]

(13)

We are now in a position to reformulate the diffraction problem of interest. The function \( u \) is the unique solution of

\[
\mathcal{L}_{\xi, \chi}(u) = 0 \quad \text{such that } u_{d} := u - u_{0} \text{ satisfies an O.W.C.}
\]

(14)

In order to reduce this problem of diffraction to a radiation problem, an intermediate function is necessary. This function, called \( u_{1} \), is defined as the unique solution of the equation:

\[
\mathcal{L}_{\xi_{\parallel 1}, \chi_{1}}(u_{1}) = 0 \quad \text{such that } u_{d_{1}} := u_{1} - u_{0} \text{ satisfies an O.W.C.}
\]

(15)

The function \( u_{1} \) corresponds thus to an annex problem associated to a simple interface and can be solved in closed form and from now on is considered as a known function. As written above, we need the function \( u_{d_{2}} \) which is simply defined as the difference between \( u \) and \( u_{1} \):

\[
u_{2} := u - u_{1} = u_{d} - u_{d_{1}}.
\]

(16)

The presence of the superscript \( d \) is, of course, not irrelevant: As the difference of two diffracted fields, the O.W.C. of \( u_{2} \) is guaranteed (which is of prime importance when dealing with PML cf. 2.2.4). As a result, the Eq. (14) becomes:

\[
\mathcal{L}_{\xi, \chi}(u_{2}) = -\mathcal{L}_{\xi_{\parallel 1}, \chi_{1}}(u_{1})
\]

(17)

where the right hand member is a scalar function which may be interpreted as a known source term \( \mathcal{S}_{1}(x, y) \) and the support of this source is localized only within the groove region. To prove it, all we have to do is to use Eq. (15):

\[
\mathcal{S}_{1} := \mathcal{L}_{\xi, \chi}(u_{1}) = \mathcal{L}_{\xi_{\parallel 1}, \chi_{1}}(u_{1}) = \mathcal{L}_{\xi_{\parallel 1}, \chi_{1}}(u_{1}) = \mathcal{L}_{\xi_{\parallel 1}, \chi_{1}}(u_{1}) = 0.
\]

(18)
Now, let us point out that the tensor fields $\xi$ and $\xi_1$ are identical outside the groove region and the same holds for $\chi$ and $\chi_1$. The support of $\mathcal{S}_1$ is thus localized within the groove region as expected. It remains to compute more explicitly the source term $\mathcal{S}_1$. Making use of the linearity of the operator $L$ and the equality $u_1 = u_1^d + u_0$, the source term can be split into two terms:

$$\mathcal{S}_1 = \mathcal{S}_1^0 + \mathcal{S}_1^d,$$

where

$$\mathcal{S}_1^0 = L_{\xi, \xi_1, \chi, \chi_1}(u_0)$$

and

$$\mathcal{S}_1^d = L_{\xi, \xi_1, \chi, \chi_1}(u_1^d).$$

Now, since $u_0$ is nothing but a plane wave $u_0 = -\exp(ik_0^+ \cdot r)$ (with $k_0^+ = \alpha x - \beta^+ y$), it is sufficient to give $\nabla u_0 = -i k_0^+ u_0$ for the weak formulation associated with Eq. (17):

$$\mathcal{S}_1^0 = \left\{-i \text{div} \left((\xi - \xi_1) k_0^+ \exp(-i k_0^+ \cdot r) + k_0^2 (\chi - \chi_1) \exp(-i k_0^+ \cdot r)\right)\right\}.$$  

The same holds for the term associated with the diffracted field ($u_1^d = \rho \exp(-i k_1^+ \cdot r)$, with $(k_1^+ = \alpha x + \beta^+ y)$):

$$\mathcal{S}_1^d = \rho \left\{-i \text{div} \left((\xi - \xi_1) k_1^+ \exp(-i k_1^+ \cdot r) + k_1^2 (\chi - \chi_1) \exp(-i k_1^+ \cdot r)\right)\right\},$$

where $\rho$ is nothing but the complex reflection coefficient associated with the simple interface:

$$\rho = \frac{p^+ - p^-}{p^+ + p^-} \text{ with } p^\pm = \left\{ \begin{array}{ll} \beta^\pm \text{ in the } E^\parallel \text{ case} \\ \frac{\beta^\pm}{\varepsilon^\parallel} \text{ in the } H^\parallel \text{ case} \end{array} \right\}.$$  

### 2.2.3 Quasi-periodicity and weak formulation

The weak formulation follows the classical lines and is based on the construction of a weighted residual of Eq. (6), which is multiplied by the complex conjugate of a weight function $u'$ and integrated by part to obtain:

$$\mathcal{R}_{\xi, \chi}(u, u') = \int_\Omega -(\xi \nabla u) \cdot \nabla u' + k_0^2 \chi u \nabla u' d\Omega + \int_{\partial \Omega} u \left(\xi \nabla u\right) \cdot \mathbf{n} dS$$  

The solution $u$ of the weak formulation can therefore be defined as the element of the space $L^2(\text{curl}, d, k)$ of quasi-periodic functions (i.e. such that $u(x, y) = u_\#(x, y) e^{ikx}$ with $u_\#(x, y) = u_\#(x + d, y)$, a $d$-periodic function) of $L^2(\text{curl})$ on $\Omega$ such that:

$$\mathcal{R}_{\xi, \chi}(u, u') = 0 \quad \forall u' \in L^2(\text{curl}, d, k).$$

As for the boundary term introduced by the integration by part, it can be classically set to zero by imposing Dirichlet conditions on a part of the boundary (the value of $u$ is imposed and the weight function $u'$ can be chosen equal to zero on this part of the boundary) or by imposing homogeneous Neumann conditions $(\xi \nabla u) \cdot \mathbf{n} = 0$ on another part of the boundary (and $u$ is therefore an unknown to be determined on the boundary). A third possibility are the so-called
quasi-periodicity conditions of particular importance in the modeling of gratings. Denote by \( \Gamma_l \) and \( \Gamma_r \) the lines parallel to the \( y \)-axis delimiting a cell of the grating respectively from its left and right neighbor cell. Considering that both \( u \) and \( u' \) are in \( L^2(\text{curl}, d, k) \), the boundary term for \( \Gamma_l \cup \Gamma_r \) is

\[
\int_{\Gamma_l \cup \Gamma_r} \overline{u'} \left( \xi \nabla u \right) \cdot n \, dS = \int_{\Gamma_l \cup \Gamma_r} \overline{u'} e^{-ikx} \left( \xi \nabla (u e^{+ikx}) \right) \cdot n \, dS = \int_{\Gamma_l \cup \Gamma_r} \overline{u'} \left( \xi (\nabla u + iku) \right) \cdot n \, dS = 0
\]

because the integrand \( \overline{u'} \left( \xi (\nabla u + iku) \right) \cdot n \) is periodic along \( x \) and the normal \( n \) has opposite directions on \( \Gamma_l \) and \( \Gamma_r \) so that the contributions of these two boundaries have the same absolute value with opposite signs. The contribution of the boundary terms vanishes therefore naturally in the case of quasi-periodicity.

The finite element method is based on this weak formulation and both the solution and the weight functions are classically chosen in a discrete space made of linear or quadratic Lagrange elements, i.e. piecewise first or second order two variable polynomial interpolation built on a triangular mesh of the domain \( \Omega \) (cf. Fig. 1b). Dirichlet and Neumann conditions may be used to truncate the PML domain in a region where the field (transformed by the PML) is negligible. The quasi-periodic boundary conditions are imposed by considering the \( u \) as unknown on \( \Gamma_l \) (in a way similar to the homogeneous Neumann condition case) while, on \( \Gamma_r \), \( u \) is forced equal to the value of the corresponding point on \( \Gamma_l \) (i.e. shifted by a quantity \( -d \) along \( x \)) up to the factor \( e^{i\alpha d} \).

### 2.2.4 Perfectly Matched Layers

The main drawback encountered in electromagnetism when tackling theory of gratings through the finite element method is the non-decreasing behaviour of the propagating modes in superstrate and substrate (if they are made of lossless materials): The PML has been introduced by [4] in order to get round this obstacle. Standard constant profile PMLs are implemented in the present model.

### 2.2.5 Post-processing: Diffraction efficiencies calculation

The rough result of the FEM calculation is the total complex field solution of Eq. (6) at each point of the bounded domain. We deduce from \( u^d \) (cf Eq. (14)) the diffraction efficiencies with the following method. The superscripts \( ^+ \) (resp. \( ^- \)) correspond to quantities defined in the superstrate (resp. substrate) as previously.

On the one hand, since \( u^d \) is quasi-periodic along the \( x \)-axis, it can be expanded as a Rayleigh expansion (see for instance [5]):

\[
\text{for } y < 0 \text{ and } y > y_g, \quad u^d(x, y) = \sum_{n \in \mathbb{Z}} u_n^d(y) e^{i\alpha_n x},
\]

where

\[
u_n^d(y) = \frac{1}{d} \int_{-d/2}^{d/2} u^d(x, y) e^{-i\alpha_n x} \, dx \quad \text{with} \quad \alpha_n = \alpha + \frac{2\pi}{d} n.
\]
On the other hand, introducing Eq. (27) into Eq. (6) leads to the Rayleigh coefficients:

\[
\begin{cases}
    u_n^d(y) = \begin{cases}
    s_n e^{+i\beta_n^+ y} + r_n e^{-i\beta_n^+ y} & \text{for } y > y_g \\
    u_n e^{-i\beta_n^- y} + t_n e^{+i\beta_n^- y} & \text{for } y < 0
    \end{cases} \\
    \text{with } \beta_n^{\pm 2} = k^{\pm 2} - \alpha_n^2
\end{cases}
\]  

(29)

For a temporal dependance in \( e^{+i\omega t} \), the O.W.C. imposes \( s_n = u_n = 0 \). Combining Eq. (28) and Eq. (29) at a fixed \( y_0 \) altitude leads to:

\[
\begin{cases}
    r_n = \frac{1}{d} \int_{-d/2}^{d/2} u^d(x, y_0) e^{-i(\alpha_n x - \beta_n^+ y_0)} \, dx & \text{for } y_0 > y_g \\
    t_n = \frac{1}{d} \int_{-d/2}^{d/2} u^d(x, y_0) e^{-i(\alpha_n x + \beta_n^- y_0)} \, dx & \text{for } y_0 < 0
\end{cases}
\]

(30)

We extract these two coefficients by numerical integration along \( x \) from a cut of the previously calculated field map at altitudes \( y_0 = -h_{\text{sub}} \) in the substrate and \( y_0 = y_g + h_{\text{sup}} \) in the superstrate. From this we immediately deduce the reflected and transmitted diffracted efficiencies of propagative orders \( (T_n, R_n) \) defined by:

\[
\begin{cases}
    R_n := r_n \frac{\beta_n^+}{\beta^n} & \text{for } y_0 > y_g \\
    T_n := t_n \frac{\beta^n}{\beta^-} \frac{\gamma^+}{\gamma^-} & \text{for } y_0 < 0
\end{cases}
\]

(31)

with \( \gamma^\pm = \begin{cases} 1 \text{ in the } E_\parallel \text{ case} \\
\varepsilon^\pm \text{ in the } H_\parallel \text{ case}
\end{cases} \)

3 Onelab model description

In this section, the parameters of the Onelab model are briefly commented in their order of appearance in the gmsh’s left panel.

3.1 Geometry

3.1.1 Grating period

- **value** grating period [nm] Important parameter of the grating indeed!

3.1.2 Stack thicknesses

The following parameters can take any positive float value.

- **value** substrate thickness [nm] sets \( h_{\text{sub}} \), given in nanometers. Quantitative results do not depend on this parameter.

- **value** deposit layer thickness [nm] sets \( h_{\text{dep}} \), given in nanometers.

- **value** cover layer thickness [nm] sets \( h_{\text{cov}} \), given in nanometers
• **value [superstrate thickness [nm]]** sets \( h_{\text{sup}} \), given in nanometers. Quantitative results do not depend on this parameter.

Note that \( h_{\text{emb}} \) is set by the diffractive element dimensions detailed hereafter.

### 3.1.3 Diffractive element dimensions

In order to illustrate the various grating or photonic crystal slabs covered by this model, let us start from the lamellar grating situation shown in Fig. 4:

- **✓ glue rod to substrate?** having the element relying directly on the substrate changes the topology, it needs to be specified. The checking/unchecking of this box is illustrated in Figs. 2(a-b) and (d-e).

- **▼ menu rod section shape** Choose between elliptical or trapezoidal rod section. See Figs. 2(e-f).

- **value number of rods [-]** Integer value setting the number of rods to consider along \( y \) axis spaced by \( d_y \) (see below). See Figs. 2(h-i).

- **value bottom rod width [nm]** In case of a trapezoidal rod, this value sets the bottom width Figs. 2(c). In case of an elliptical rod, this value has no effect. See Figs. 2(b-c).

- **value top rod width [nm]** In case of a trapezoidal rod, this value sets the top width Figs. 2(c). In case of an elliptical rod, this value sets its diameter \((2r_x)\). See Figs. 2(c-d).

- **value rod thickness [nm]** In case of a trapezoidal rod, this value sets the thickness (dimension along \( y \)). In case of an elliptical rod, this value sets its diameter \((2r_y)\).

- **value embedding layer thickness or “period” along \( y \) if number of rods \( >1 \), [nm]** If the number of rods is set to 1, this value sets \( h_{\text{emb}} \). In case of several rods, this value sets their periodic spacing along \( y \) \((d_y)\). See Figs. 2(i).

- **value rotate rod [deg]** Rotates the rod around himself (axis formed by its barycenter, the \( Oz \) direction). See Figs. 2(g-h).

- **value chirp angle?** In case of several rods, the rotation angle of the next rod along increasing values of \( y \) is increased by the value described in the previous item. See Figs. 2(i-j).

- **value chirp size factor [%]**

- **✓ chirp size?** In case of several rods, the size of the next rod along increasing values of \( y \) is scaled of the value given in the previous item. See Figs. 2(j-k).
Figure 2: (a) Initial configuration described in Fig. 4. (b) Unchecking glue rod to substrate. (c) Decreasing value of bottom rod width [nm]. (d) Decreasing value of top rod width [nm]. (e) Checking back glue rod to substrate. (f) Choosing elliptical section in rod section shape menu. (g) Decreasing value of embedding layer thickness or... (h) Increasing value of rotate rod [deg]. (i) Increasing value of number of rods [-]. (j) Checking chirp angle? (k) Checking chirp size? and decreasing chirp size factor [%].

3.2 Materials

3.2.1 Dispersive materials

For each constitutive layer, a choice of materials is proposed. The file `grating_2D_materials.pro` contains frequency dispersion tables for some selected materials. Relative permittivity values are linearly interpolated using these tables. The available materials are currently:

- **Air**: freespace
- **SiO2**: silicon dioxide
- **Ag (palik)**: silver, values from [6]
- **Al (palik)**: aluminium, values from [6]
- **Au (johnson)**: gold, values from [7]
- **Nb2O5**: niobium pentoxide, values from [8]
• **ZnSe**: zinc selenide, values from [8]
• **MgF2**: magnesium fluoride, values from [8]
• **TiO2**: titanium dioxide, values from [8]
• **PMMA**: methyl polymethacrylate, values from [8]
• **Si**: silicon, values from [6]
• **ITO**: indium tin oxide, values from [8]
• **Cu (palik)**: copper, values from [6]
• **custom 1**: custom dispersion free material, see next section
• **custom 2**: custom dispersion free material, see next section
• **custom 3**: custom dispersion free material, see next section

It is quite easy to add another material, please follow the instructions given in comments at the beginning of `grating_2D_materials.pro`.

### 3.2.2 Custom non-dispersive materials

Another possibility is to set a material permittivity to **custom 1**, **custom 2**, or **custom 3** in which case the real and imaginary parts of the complex relative permittivity will be set to the one manually specified in this section. Beware that due to the $+i\omega t$ time dependance, passive (lossy) materials have a negative imaginary relative permittivity. Finally, the so called permittivity of the rods (and the rods only) can be $z$-anisotropic, *i.e.* of the form given in Eq. (1).

- **Enable anisotropy for rods?** If checked, the permittivity of the rods (and the rods only) will be $z$-anisotropic with values given below. Checking this will override material rods above.
  - **value** $\epsilon_{xx}$ re sets $\Re\{\epsilon_{xx}\}$
  - **value** $\epsilon_{xx}$ im sets $\Im\{\epsilon_{xx}\}$
  - **value** $\epsilon_{yy}$ re sets $\Re\{\epsilon_{yy}\}$
  - **value** $\epsilon_{yy}$ im sets $\Im\{\epsilon_{yy}\}$
  - **value** $\epsilon_{zz}$ re sets $\Re\{\epsilon_{zz}\}$
Note that so-called z-anisotropy means for the relative permittivity tensor that $\varepsilon_{xz} = \varepsilon_{yz} = \varepsilon_{zx} = \varepsilon_{zy} = 0$ and that $\varepsilon_{yx} = \varepsilon_{xy}$. A full anisotropy (or tensor) would require to tackle the conical incidence trough a 2D vector formulation.

### 3.3 Incident plane wave
- **value wavelength [nm]** sets the operating freespace wavelength $\lambda_0$ of the incident plane wave.
- **value incident plane wave angle [deg]** sets the angle of incidence $\theta_i$ of the incident plane wave.
- **▼ menu polarization case** allows to choose between the $H\parallel$ and $E\parallel$ polarization cases (see Eq. (2)).
- **value number of post-processed diffraction orders** sets the number of diffraction orders to post-process (e.g. if set to 2, five Fourier coefficients will be computed corresponding to diffraction orders $-2,-1,0,+1,+2$)

### 3.4 Mesh size and PMLs parameters
- **value top PML size [nm]** sets the top PML thickness. Typically, it should not be set to a value smaller than $\lambda_0/2$. Typically, setting it to a value larger than $3\lambda_0$ is pointless. Typically, $\lambda_0$ is a good value.
- **value bottom PML size [nm]** sets the bottom PML thickness. Typically, it should to a value smaller than $\lambda_0/2$. Typically, setting it to a value larger than $3\lambda_0$ is pointless. Typically, $\lambda_0$ is a good value.
- **value nb of mesh elements per wavelength [-]** sets the average number of triangles used to discretize one freespace wavelength (mesh refinement). Typically, setting it to 30 offers 4 or 5 significant digits over energy related quantities. Typically, setting it to 1 leads to very wrong results... 
- **Custom Mesh parameters**: When dealing with metals and/or very small objects, it is sometimes necessary to locally refine the mesh in the affected subdomain, which can be prescribed in this section. For instance, Figs. 3 shows a local refinement of the rods. In Fig. 3(a), the mesh is very coarse, its typical size is $\lambda_0/6$ everywhere. The mesh size within the rods in Fig. 3(b) is 3 times smaller ($\lambda_0/(6 \times 3)$).
3.5 Post plot options

- **✓** Plot solution on multiple periods. If checked, the field \((E_z(x, y))\) in \(E\parallel\) polarization case, \((H_z(x, y))\) in \(H\parallel\) polarization case) is post-processed over 9 grating periods cells, as shown in Fig. 4. The field in a neighboring cell is indeed nothing but the field in the reference cell up to a phase shift \(e^{\pm i\alpha}\).

4 Energy balance post-processing in python

The provided file `grating_2D_postplot.py` gives a possible representation of energy related quantities. If only a single OneLab run was made, it provides bar plot of non-null absorption, reflection and transmission. If a parametric OneLab run was made, e.g. a spectrum, it provides a plot of non-null absorption, reflection and transmission.

5 Examples

In this section, various example of the literature are retrieved.

5.1 General recommendations.

The OneLab model internal files, `grating_2D.geo` and `grating_2D.pro`, both call a configuration file named `grating_2D_data.geo` setting all the parameters displayed in the gmsh left panel. Thus in order to load directly one of the provided configurations, just rename `grating_2D_data_someconfig.geo` to `grating_2D_data.geo` (and `grating_2D_data.geo` to `grating_2D_data_old.geo`). Then, open `grating_2D.pro` with gmsh. It is advised to clean the working directory between two different study. To do so, remove at least the output directory `run_results` and the mesh file `grating_2d.msh` need to be deleted. Rarely, the Bloch boundary condition fails and getdp will complain not finding twin nodes on the two boundaries. Just change the mesh parameter a little and ... remesh. Finally, if you are not satisfied with the numerical precision, try to refine the mesh and/or increase the size of the PMLs.
5.2 Lamellar grating example.

The example `grating_2D_data_LamellarGrating.geo` reproduces some of the results found in lower half of Table n°2 in [9].

![Lamellar grating example](image)

Figure 4: Lamellar grating example. The bar plot shows the output of `grating_2D_postplot.py`.

At least three significant digits are obtained.

5.3 Anisotropic grating

The example `grating_2D_data_AnisotropicGrating.geo` illustrates the numerical results in [3]. Figure 5 shows the field map $\Re\{E_z\}$ in $V/m$ for an angle of incidence $\theta^i = -20^\circ$. There is no anisotropic behavior here since $E_z$ only "sees" $\varepsilon_{zz}$. Figure 6 shows the field map $\Re\{H_z\}$ in $A/m$ for an angle of incidence $\theta^i = 0^\circ$. The lack of symmetry due to the anisotropy of the scatterer is clearly visible here.
Figure 5: $H^\parallel$ case. See Fig. 5b and 6th line of Tab. 2 in reference [3].
5.4 Photonic crystal slab example.

This example grating_2D_data_PhotonicCrystalSlab.geo illustrates some of the results found in [10] (see Fig. 2, page 68). In this example, the band structure of a 2D photonic crystal is given in the two polarization cases. The $E_{\parallel}$ case features a full photonic bandgap. As a consequence, a sufficiently thick slice of this infinite crystal is expected to exhibit good reflecting properties for an incident plane wave with frequency within the bandgap. The photonic crystal is made of circular rods of diameter $0.4a$ with relative permittivity $\varepsilon_r = 8.9$ arranged in a square lattice with lattice constant $a$, with background relative permittivity $\varepsilon_r = 1$. The $E_{\parallel}$ gap is found to be roughly in the normalized frequency $\omega a/2\pi c$ range $[0.3, 0.43]$. In other words, setting in the period $d$ to 150 nm should place the bandgap in the wavelength range $[440, 660]$ nm. The gap is total so the reflexion on a slab with a few lattices should lead to high reflexion for any angle of incidence.

As depicted in Fig. 7(a), for an angle of incidence $\theta^i = 30^\circ$, a very high reflexion coefficient is obtained for $N_{\text{rods}} = 5$ only. The python program grating_2D_postplot.py produces the figure in Fig. 7(b).
Figure 7: Photonic crystal slab example.

Finally, one wonders the slab thickness necessary to witness a high reflectivity (i.e. how many periods in y do we need to see the gap?). A possible parametric study is possible by simply:

- unchecking “looping over” $\lambda_0$, setting it to $\lambda_0 = 500$ nm,
- checking “looping over” $N_{\text{rods}}$, setting looping parameters to $1:10:1$.

Figure 8 shows in log scale the transmission coefficient decaying exponentially with photonic crystal slab thickness. This is expected given the evanescent nature of the field inside photonic crystal slab.
5.5 Resonant grating

The example `grating_2D_data_ResonantGrating.geo` illustrates the behavior of resonant grating that can be used to obtain a very sharp spectral response as detailed in Ref. [11].

5.5.1 Spectral response

The spectral response of such a grating is depicted in Fig. 9.
5.5.2 Angular response

From the very same model up to a few preliminary clicks, one can obtain the angular response of the filter by:

- unchecking “looping over” $\lambda_0$, setting it to $\lambda_0 = 1550.05$ nm: $1550.05$ nm
- checking “looping over” $\theta_i$: $6$ incident plane wave angle [deg]
- setting the looping parameters for $\theta_i$ from $5.85^\circ$ to $6.0^\circ$ by $0.0025^\circ$ steps using the button and filling $5.85:6:0.0025$

The angular response of this grating is depicted in Fig. 10.
5.6 Plasmonic grating

The example in grating_2D.data.geo has no concrete purpose but demonstrating that the model handles exotic so-called plasmonic configurations. The detailed energy balance associated to this weird silver structure in Fig. 11 shows an equilibrated repartition of the energy occurring inside losses in each rod, reflexion and transmission in both specular and non-specular diffraction efficiencies. It still looks OK!
6 Conclusion

This model is a general tool for the study of so-called mono-dimensional grating. Various geometries and materials can be handled or easily added. For instance, it can be easily adapted to nano-structured solar cells. The two classical polarization cases, denoted here $E^{∥}$ and $H^{∥}$, are addressed. The output consists in a full energy balance of the problem computed from the field maps.

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