A Tutorial: Computing QNMs for a Silver Grating in Air

1. Introduction

In this document, we present how, with **QNMEig,** computing QNMs for a 1D Ag grating. Since we provide all details about implementing **QNMEig** with COMSOL Multiphysics in the document''*QNMEig_Sphere.pdf*'', we do not repeat here the steps that are already documented in ''*QNMEig_Sphere.pdf*'' and we only give the essential details. This document should be read in conjugation with the COMSOL model sheet ***''QNMEig_1Dgrating.mph''.*** This tutorial has been established in relation with Ref. [1].

2. Model Definition

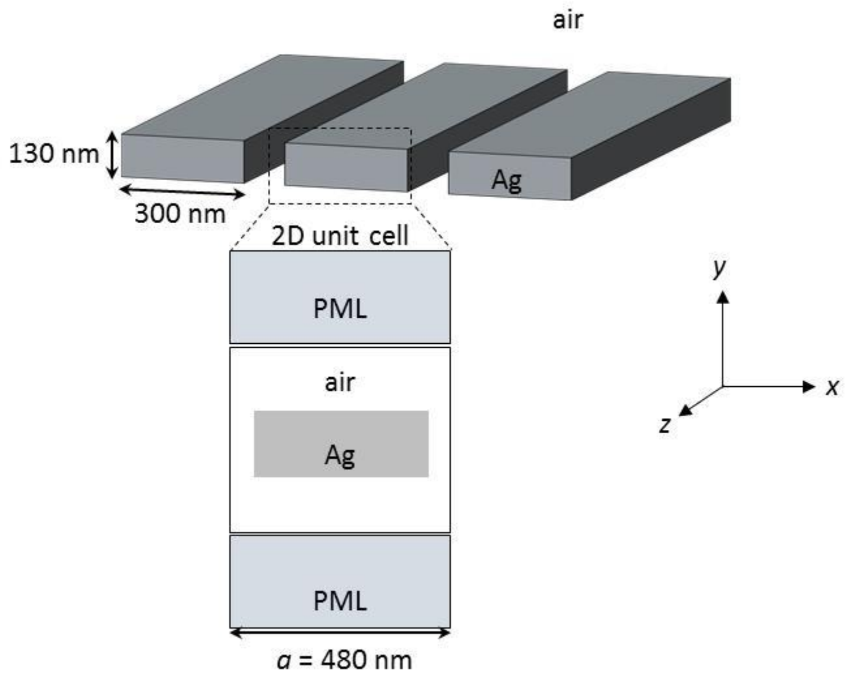


Figure 1. Geometry of a 1D Ag grating surrounded by air.

1 Ag has permittivity

$$\varepsilon_{\mathrm{Ag}} = \varepsilon_{\infty,\mathrm{Ag}}[1 - \frac{\omega_{p,\mathrm{Ag}}^2}{\omega^2 - \omega_{0,\mathrm{Ag}}^2 + i\omega\gamma_{\mathrm{Ag}}}] , \quad (1)$$

with $\varepsilon_{\infty,\mathrm{Ag}} = 1$, $\omega_{p,\mathrm{Ag}} = 1.35\mathrm{e}16\ [\mathrm{rad/s}]$ corresponding to $\lambda_{p,\mathrm{Ag}} = 138$ nm in vacuum, $\gamma_{\mathrm{Ag}} = 0.0023\omega_{p,\mathrm{Ag}}$, and $\omega_{0,\mathrm{Ag}} = 0$.

2 We compute TM-polarized Bloch modes, with electric fields only having *x, y* components that are in the same plane as the 2D unit cell in Fig. 1. The magnetic field is parallel to the slits. Owing to the periodicity in the *x* direction, see Fig. 1, the electric fields of the Bloch modes take the form

$$\widetilde{\boldsymbol{E}}_{k_b}(\boldsymbol{r}) = \widetilde{\boldsymbol{u}}_{k_b}(\boldsymbol{r})\mathrm{e}^{-jk_b x}, \tag{2}$$

where $k_b \in [-\pi/a, \pi/a]$ is called the Bloch wavenumber, and it is a free parameter input by the user; $\widetilde{\boldsymbol{u}}_{k_b}(\boldsymbol{r})$ is a periodical function satisfying $\widetilde{\boldsymbol{u}}_{k_b}(\boldsymbol{r}) = \widetilde{\boldsymbol{u}}_{k_b}(\boldsymbol{r} + a)$, where a is the grating periodicity.

3. Modelling Instructions

Open **COMSOL Multiphysics**. From its **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **2D**.

2 We choose two physics modules: 1/ **Radio Frequency**->**Electromagnetic Waves**, **Frequency Domain (emw)**; 2/ **Mathematics**->**PDE Interfaces**, **Weak Form PDE**, with dependent variables named ***P1x***, ***P1y***, defined by

$$\boldsymbol{P1} = -\frac{\omega_{p,\mathrm{Ag}}^2}{\omega^2 - \omega_{0,\mathrm{Ag}}^2 + i\omega\gamma_{\mathrm{Ag}}}\boldsymbol{E}, \tag{3}$$

in the Ag domain.

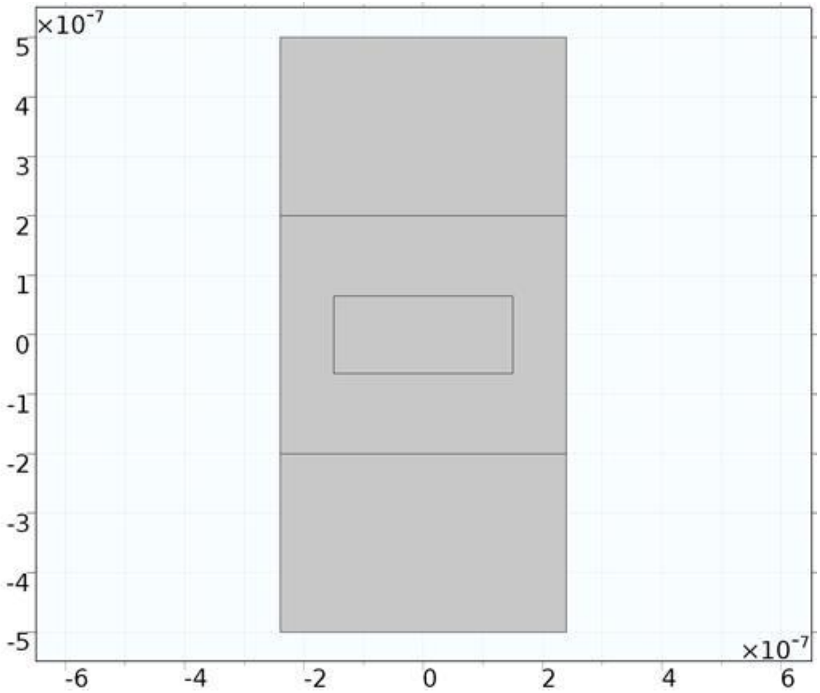
3 We choose the **Eigenfrequency** study.

DEFINITIONS

All global parameters with their descriptions can be found in the COMSOL model sheet "*QNMEig_1Dgrating.mph*". Here, we only emphasize important parameter, k_b, the Bloch wavenumber, which is defined in Eq. (1) and is chosen to have a value *0.2*pi/a* (*a* denotes the grating periodicity) in the "*QNMEig_1Dgrating.mph*". This parameter is later used when imposing the periodic boundary condition for the grating.

GEOMETRY

The geometry of the built 2D unit cell is given below.



MATERIALS

We set relative permittivity of Ag with its non-dispersive permittivity, $\varepsilon_{\infty,\mathrm{Ag}}$.

DEFINITIONS (Local)

In the **Model Builder Window->Component 1->Definition**, we define/add the following things:

1 PMLs, chosen to be *Cartesian-type* PMLs.

2 Two sets of variables, {***DP1x, DP1y***} that relate with {***P1x***, ***P1y*** } defined in the Ag domain

DP1x=epsilon0_const*(emw.epsilonrxx*P1x+emw.epsilonrxy*P1y),

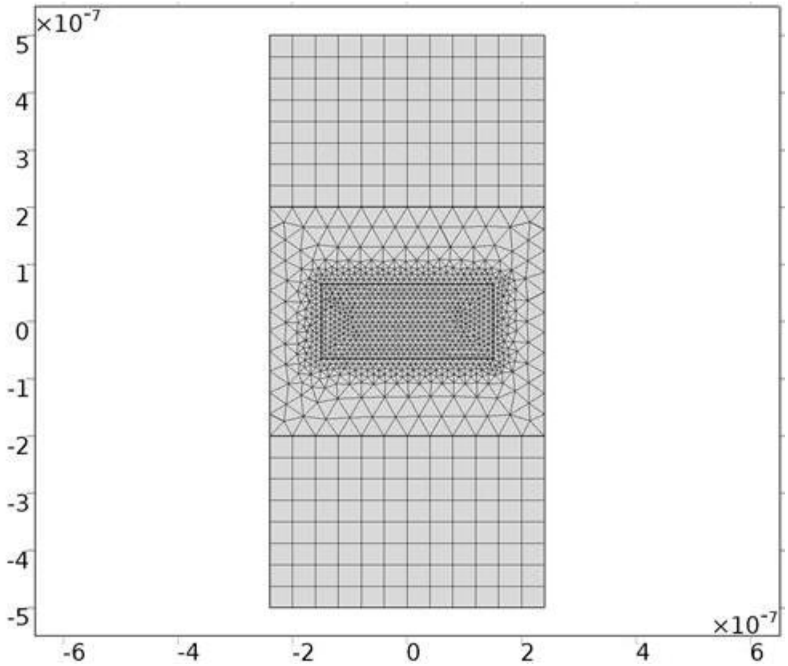
DP1y=epsilon0_const*(emw.epsilonryx*P1x+emw.epsilonryy*P1y) .

4 Two integration operators: **intAll,** integration over all domains including PML domains; **intMetal**, integration over the Ag domain.

5 One linear extrusion operator, **linext1**, which maps the fields, e.g., ***E***(*x,y*), to ***E***(−*x,y*).

6 QNM normalization factor, **QN.** For a short description of the normalization of Bloch modes , we refer to Section 4 ''**Normalization of Bloch Modes"**.

MESHES



ELECTROMAGNETIC WAVES, FREQUENCY DOMAIN (EWV)

1 We add one weak contribution in the Ag domain:

mu0_const*QNM_omega^2*(test(emw.Ex)*DP1x+test(emw.Ey)*DP1y))*pml1.detInvT

2 We impose the **Floquet periodicity** condition for the left and right boundaries of the unit cell. We specify the Bloch-wavevector components [Kx Ky] as

Kx	kb
Ky	0

WEAK FORM PDE FOR AUXILIARY FIELDS P1x, P1y

The input weak formulation is

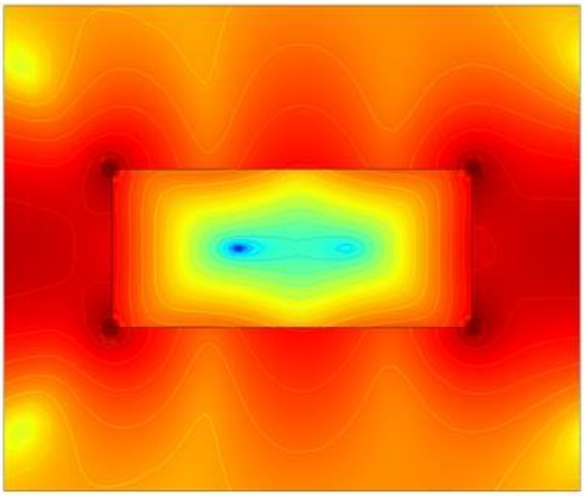
1/lambda_N^2*((test(P1x)*P1x+test(P1y)*P1y)*(QNM_omega^2-j*gamma_Ag*QNM_omega-omega0_Ag^2)/omegap_Ag^2+(test(P1x)*emw.Ex+test(P1y)*emw.Ey))

STUDY 1

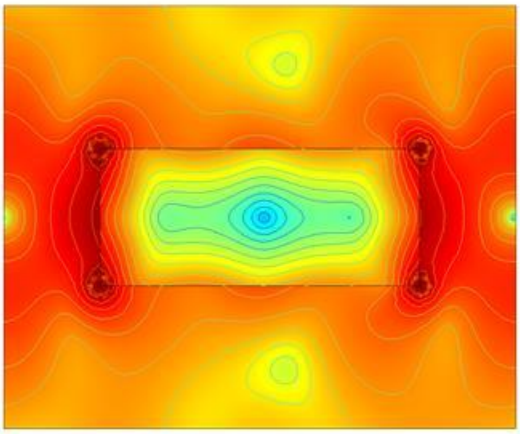
We ask the eigensolver to compute 80 QNMs around $0.2 \times \omega_{\mathrm{p,Ag}}/(2\pi)$.

RESULTS

Eigenfrequency=8.7238E14+8.8110E12i Surface: log(emw.normE)
Contour: log(emw.normE)



Eigenfrequency=1.1029E15+7.1210E12i Surface: log(emw.normE)
Contour: log(emw.normE)



4. Normalization of Bloch Modes

The normalization of a Bloch mode $\tilde{\boldsymbol{E}}_{k_b}$ involve another Bloch mode with the opposite Bloch wavenumber and the same eigenfrequency, $\tilde{\boldsymbol{E}}_{-k_b}$. Specifically, the normalization factor *QN* (see subsection "***DEFINITIONS (Local)***" in "***Modelling Instructions***") is

$$QN = \iint [\tilde{\boldsymbol{E}}_{k_b} \cdot \frac{\partial \omega \boldsymbol{\varepsilon}(\omega)}{\partial \omega} \tilde{\boldsymbol{E}}_{-k_b} - \tilde{\boldsymbol{H}}_{k_b} \cdot \frac{\partial \omega \boldsymbol{\mu}(\omega)}{\partial \omega} \tilde{\boldsymbol{H}}_{-k_b}] d^2\boldsymbol{r}, \tag{4}$$

which, for non-dispersive $\boldsymbol{\mu}$, could be simplified to

$$QN = \iint [2\tilde{\boldsymbol{E}}_{k_b} \cdot \frac{\partial \omega^2 \boldsymbol{\varepsilon}(\omega)}{\partial \omega^2} \tilde{\boldsymbol{E}}_{-k_b}] d^2\boldsymbol{r}. \tag{5}$$

For our Ag grating that has inversion symmetry in the *x* direction, $\tilde{\boldsymbol{E}}_{k_b}$ and $\tilde{\boldsymbol{E}}_{-k_b}$ are linked by a simple relation

$$\tilde{E}_{-k_{b,x}}(x,y) = -\tilde{E}_{k_{b,x}}(-x,y), \tilde{E}_{-k_{b,y}}(x,y) = \tilde{E}_{k_{b,y}}(-x,y), \tilde{E}_{-k_{b,z}}(x,y) = \tilde{E}_{k_{b,z}}(-x,y), \tag{6}$$

where the subscripts "x", "y", "z" specify the *x, y, z* components of the electric fields. Thus, knowing $\widetilde{\boldsymbol{E}}_{k_b}$, $\widetilde{\boldsymbol{E}}_{-k_b}$ is straightforwardly computed from Eq. (6). Technically, Eq. (6) is implemented by defining a linear extrusion operator, **linext1,** see subsection "***DEFINITIONS (Local)***" in "***Modelling Instructions***"; that is $\tilde{E}_{-k_{b,x}} = -\mathbf{linext1}(\tilde{E}_{k_{b,x}})$ **,** $\tilde{E}_{-k_{b,y}} = \mathbf{linext1}(\tilde{E}_{k_{b,y}})$**,** $\tilde{E}_{-k_{b,z}} = \mathbf{linext1}(\tilde{E}_{k_{b,z}})$**.**

5. References

[1] P. Lalanne, W. Yan, A. Gras, C. Sauvan, J.-P. Hugonin, M. Besbes, G. Demésy, M. D. Truong, B. Gralak, F. Zolla, A. Nicolet, F. Binkowski, L. Zschiedrich, S. Burger, J. Zimmerling, R. Remis, P. Urbach, H. T. Liu, and T. Weiss, "Quasinormal mode solvers for resonators with dispersive materials," J. Opt. Soc. Am. A **36**, 686-704 (2019).