Resonances determination in microstructured films embedded in multilayered stacks

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Abstract

Our approach consists in finding the eigenmodes and the complex eigenfrequencies of structures using a finite element method (FEM), that allows us to study mono- or bi-periodic gratings with a maximum versatility : complex shaped patterns, with anisotropic and graded index material, under oblique incidence and arbitrary polarization. In order to validate our method, we illustrate an example of a four layer dielectric slab, and compare the results with a specific method that we have called *tetrachotomy*, which gives us numerically the poles of the reflection coefficient (which corresponds to the eigenfrequencies of the structure). To illustrate our method, we show the eigenvalues of one- and two-dimensional gratings.

Methods

Diffraction problem :

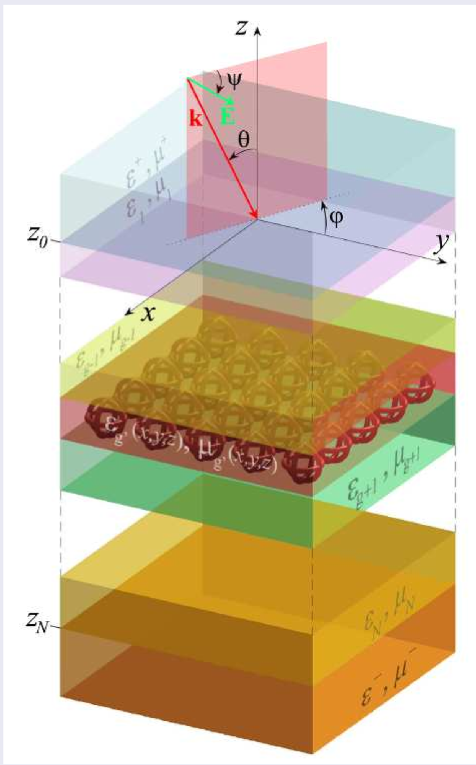
Formulation adapted to the FEM ([1, 2]).
Incident plane wave : wavevector $\mathbf{k}^+ = (\alpha, \beta, \gamma)^T$ of norm $k^+ = k_0\sqrt{\epsilon^+\mu^+}$ ($k_0 = \omega/c$), incidence angles (θ, φ), polarization angle ψ.
Find Maxwell's equation solutions $\mathbf{E}$ in harmonic regime :

$$-\mathbf{curl}(\mu_r^{-1}\mathbf{curl}\,\mathbf{E}) + k_0^2\epsilon_r\mathbf{E} = 0$$

Quasi-periodicity with respect to x and y co-ordinates :

$$\mathbf{E}(\mathbf{r}+\mathbf{d}) = \mathbf{E}(\mathbf{r})\exp(i(\alpha x + \beta y))$$

$\Rightarrow$ Extraction of transmission, reflection and Joule losses : global energy balance.



Schematic of the domain Ω

Eigenvalue problem :

Solutions of *source free* Maxwell's equations : find the complex eigenvalues $\omega_n = \omega_n' + i\omega_n''$ and the non vanishing fields $\mathbf{E_n}$ which are bi-pseudo-periodic in Ω (parameters $(\alpha, \beta) \in \mathbb{R}^2$) and such that :

$$\mathcal{M}_{\alpha,\beta}(\mathbf{E_n}) := c^2\epsilon_r^{-1}\mathbf{curl}(\mu_r^{-1}\mathbf{curl}\,\mathbf{E_n}) = \omega_n^2\mathbf{E_n}\,.$$

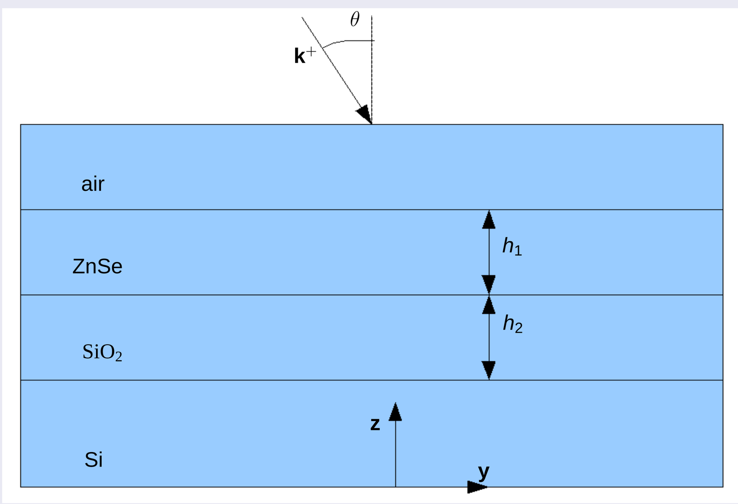
If ω_n'' small enough, $k_n^+ \simeq \sqrt{\epsilon^+\mu^+}\omega_n'/c$, angles given by $\alpha = k_n^+\sin\theta_n\cos\varphi_n$ and $\beta = k_n^+\sin\theta_n\sin\varphi_n$.
Quality factor : $Q_n = \omega'/2\omega''$.

Poles of the transmission coefficient ([3]) :

$$t(\omega) = \sum_{n\in\mathbb{N}} \frac{A_n}{\omega - \omega_n} + g(\omega), \quad A_n \in \mathbb{C},\ g \text{ holomorphic function.}$$

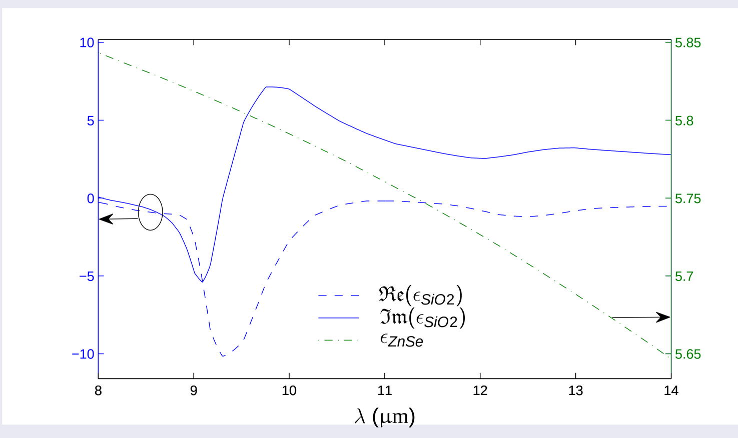
Robust numerical method based on complex analysis tools : tetrachotomy ([4]) $\Rightarrow$ ω_n and A_n.

Validation : slab

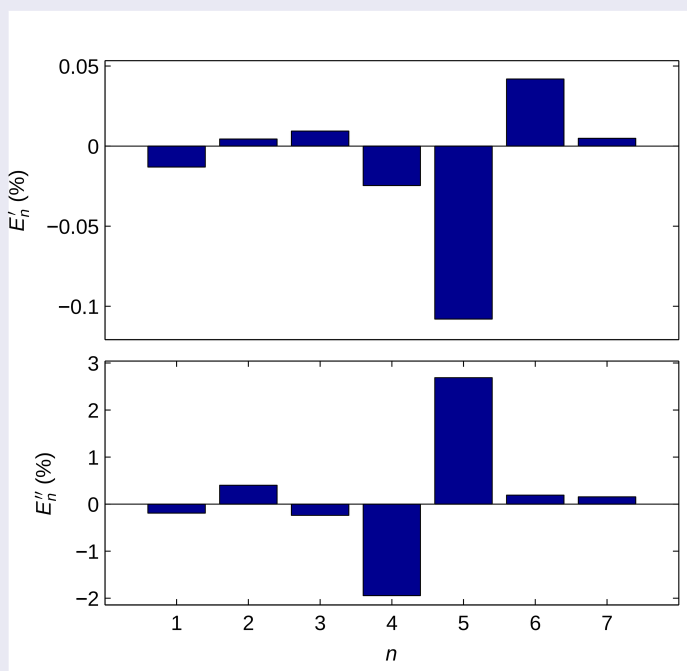


Schematic and notations of the slab under study.

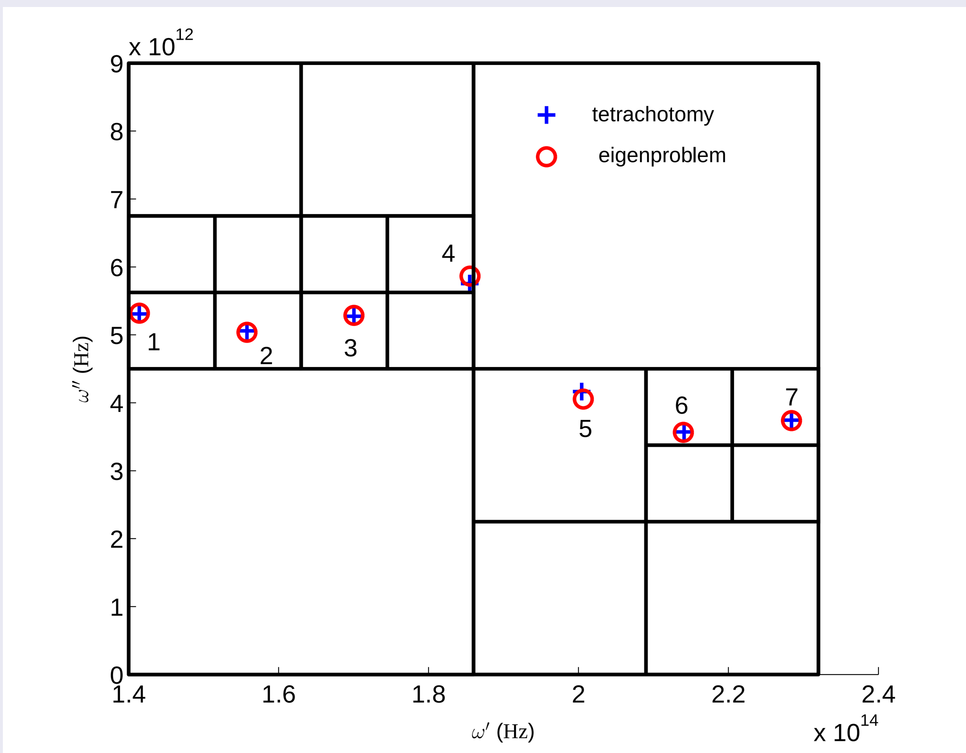
Parameters : $h_1 = 26\mu\mathrm{m}$, $h_2 = 0.5\mu\mathrm{m}$, $\epsilon_{air} = 1$, $\epsilon_{Si} = 11.7$, $\theta = 0$, TM polarization.



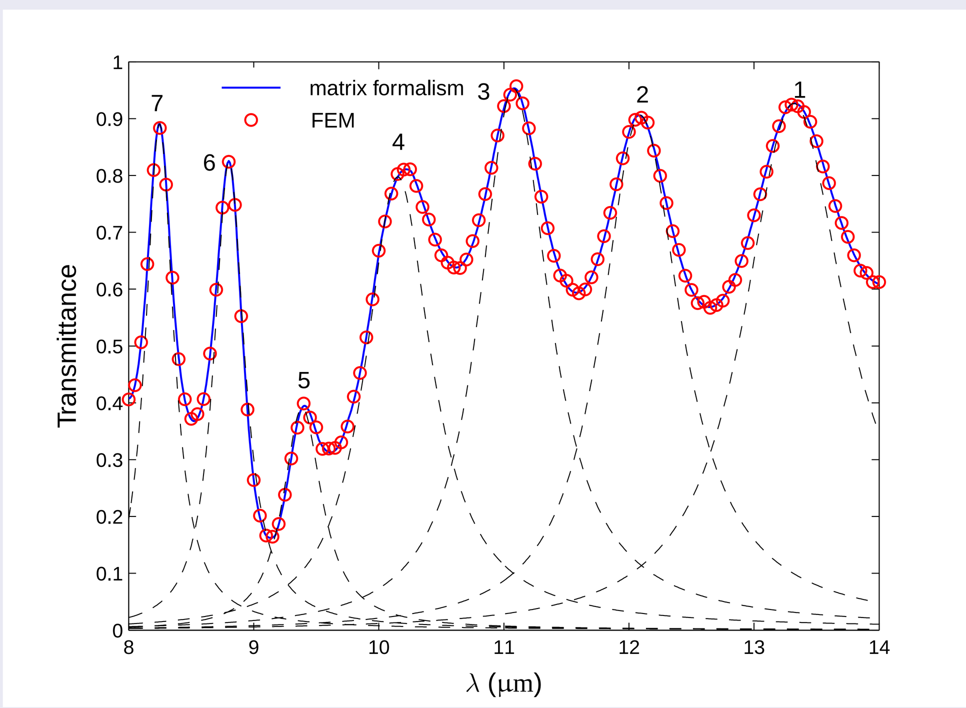
Relative permittivity of SiO$_2$ and ZnSe as a function of the wavelength λ.



Relative difference between the two methods for the n^{th} resonance (top : real parts, bottom : imaginary parts).



Loci of the resonance frequencies in the complex plane for the two methods.



Transmittance as a function of the wavelength λ ; solid line : tranfert matrix formalism [5] ; circles : FEM formulation ; dashed lines : single pole approximation.

Relative differences :

$$E_n' = \frac{\omega_n'^{,tetra} - \omega_n'^{,fem}}{\omega_n'^{,tetra}} \quad \text{and} \quad E_n'' = \frac{\omega_n''^{,tetra} - \omega_n''^{,fem}}{\omega_n''^{,tetra}}$$

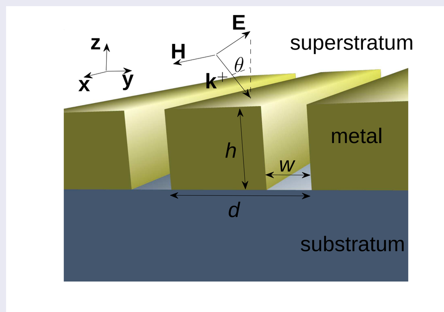
Single pole approximation around the pole ω_n :

$$t_n(\omega) = \frac{B_n}{\omega - \omega_n}$$

$B_n = -i\omega_n'' t(\omega_n')$, with $t(\omega_n')$ calculated by the FEM

$\Rightarrow$ Both methods in good agreement

Slit grating : example 1

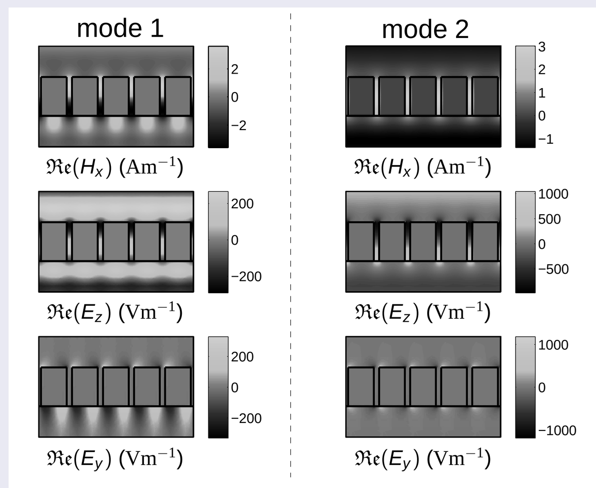


Schematic of the grating under study.

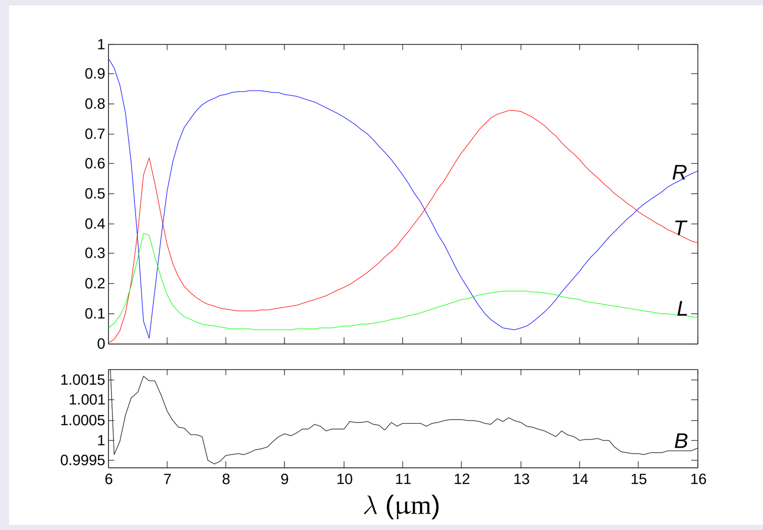
Parameters : $d = 4\mu\mathrm{m}$, $h = 5\mu\mathrm{m}$, $w = 0.7\mu\mathrm{m}$, metal : Cr, $\epsilon^+ = 1$, $\epsilon^- = 2.25$, $\theta = 0$, TM polarization.

n	λ_n	Q_n	λ_n^{fit}	Q_n^{fit}
1	6.63	12.48	6.7	12.5
2	12.77	3.26	12.8	3.3

Resonance features : λ_n and Q_n obtained by the resolution of the eigenproblem ; λ_n^{fit} and Q_n^{fit} extracted from a Gaussian fit (wavelength in µm).

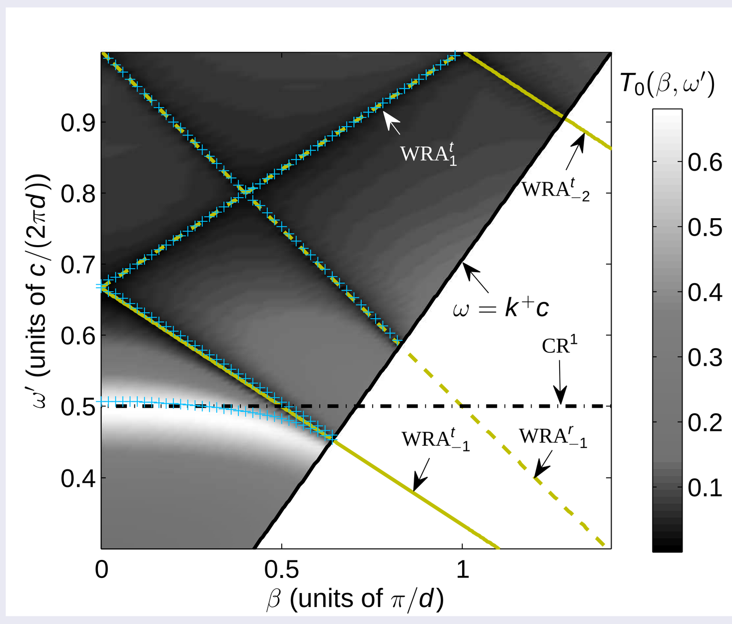


Spatial distribution of the real parts of H_x, E_y and E_z for the two eigenmodes.



Zeroth-order transmission T, zeroth-order reflection R, Joule loss L and energy balance B as a function of the wavelength λ.

Slit grating : example 2



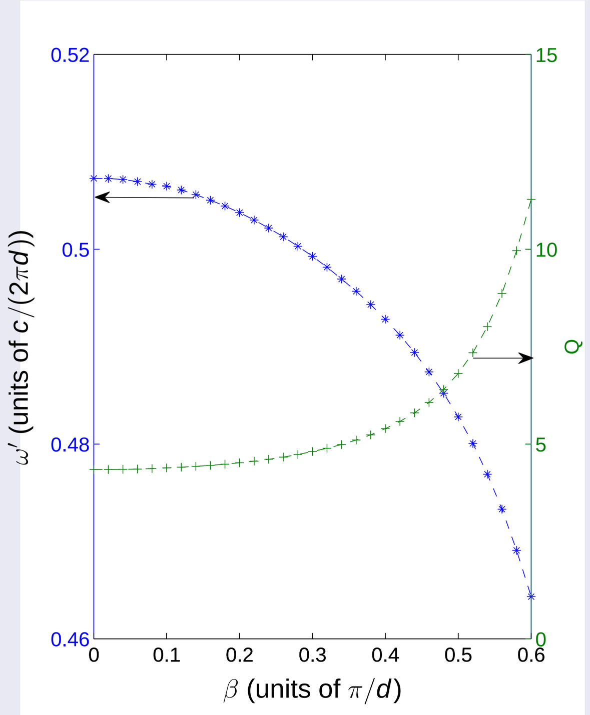
Colormap : zeroth-order transmittance $T_0(\beta, \omega')$; + : dispersion diagram $\omega'(\beta)$; — : n^{th} order Wood-Rayleigh anomalies in transmission WRA^t_n (solid) and reflection WRA^r_n (dashed) ; · - · - : cavity resonance CR^1.

Wood-Rayleigh anomaly ([6, 7]) of the n^{th} diffraction order :

$$\lambda_n^{\pm} = \frac{d}{n}(\sqrt{\epsilon^{\pm}} - \sin\theta).$$

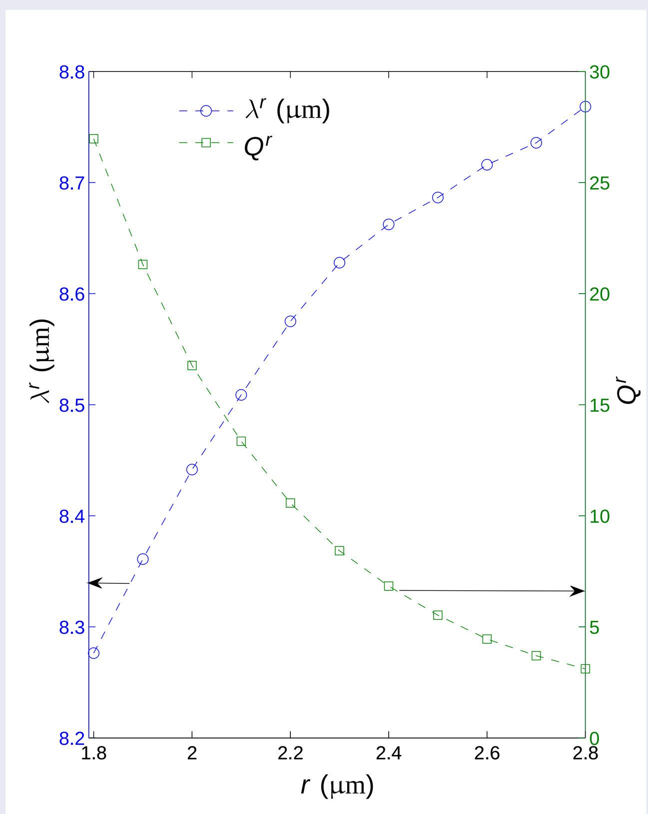
Cavity resonance : $\omega_m^{cav} = m\pi c/h$, for $m \in \mathbb{N}^*$

Same structure as example 1 with $d = 6\mu\mathrm{m}$, $h = 4\mu\mathrm{m}$ and $w = 1\mu\mathrm{m}$.

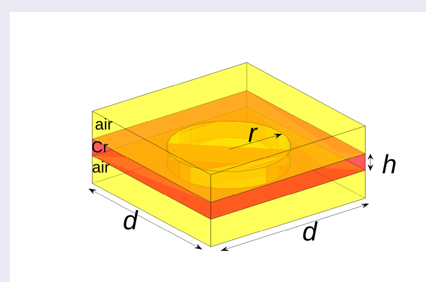


Lowest eigenfrequency and associated quality factor as a function of β.

Hole array

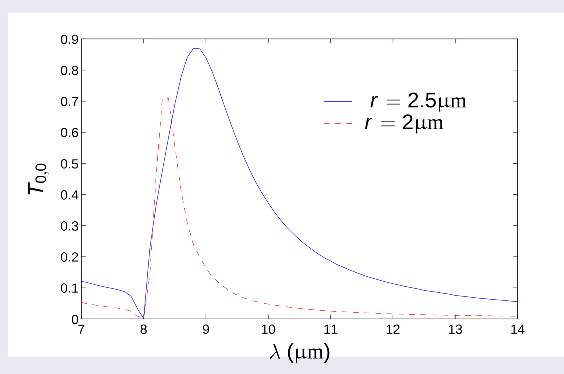


Resonance features λ^r and Q^r as a function of the hole radius r.



Schematic of the hole array under study.

Parameters : $h = 800\mathrm{nm}$, $d = 8\mu\mathrm{m}$



Zeroth-order transmittance $T_{0,0}$ as a function of the wavelength for $r = 2$ µm and $r = 2.5$ µm.

Refrerences

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