Analysis of diffraction gratings via their resonances

Benjamin Vial[a,b], Mireille Commandré[a], Frédéric Zolla[a], André Nicolet[a] and Stéphane Tisserand[b]

[a]*Institut Fresnel UMR CNRS 6133, Aix-Marseille Université, Ecole Centrale de Marseille, Campus de Saint-Jérôme, 13013 Marseille, France,*
[b]*Silios Technologies, France*

Abstract. We analyze diffraction gratings via their resonances by a direct determination of the eigenmodes and the complex eigenfrequencies using a finite element method (FEM), that allows 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).

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The field of application of diffraction gratings has been extended over the past decades. For spectral filtering applications, one should determine the line shape of the transmission or reflection spectra in order to fit the required features. To avoid the calculation of diffracted efficiencies for a wide range of wavelengths, resonances of the structures should be found. This can be done by searching for complex eigenfrequencies : the real parts correspond to the resonant frequencies and the imaginary parts are related to the damping factors.
This paper is devoted to the study of resonances in different structures by solving an eigenvalue problem with a FEM. It is validated by an independent method that we have called *tetrachotomy* on an example of a four layer dielectric slab. Then the eigenproblem solved by a FEM is applied to one- and two-dimensional gratings. The originality of our approach is that it works irrespective to the geometry and material properties. We denote by **x**, **y** and **z** the unit vectors of an orthogonal co-ordinate system *Oxyz*. We deal with time-harmonic fields, so that the electric and magnetic fields are represented by complex vector fields **E** and **H** with a time-dependence in $\exp(-i\omega t)$.

We deal with stacks of different layers that may be periodically structured. The materials in this paper are assumed to be isotropic and their optical behaviour is characterized by their relative permittivity ε_r and relative permeability μ_r. Note that these scalar fields can be complex-valued, allowing the study of lossy materials, and can vary spatially continuously or discontinuously (graded or step index structures). The domain Ω under study can be divided into several sub-domains (See Refs.[1, 2, 3, 4]):

- *The superstratum* ($z > z_0$) which is supposed to be homogeneous, isotropic and lossless and characterized solely by its relative permittivity ε^+ and its relative permeability μ^+ and we denote $k^+ := k_0\sqrt{\varepsilon^+\mu^+}$, where $k_0 := \omega/c$.
- *The multilayered stack* ($z_0 < z < z_N$) composed of N layers which are supposed to be homogeneous and isotropic and therefore characterized by their relative permittivity ε_n and their relative permeability μ_n and we denote $k_n := k_0\sqrt{\varepsilon_n\mu_n}$
- *The substratum* ($z < z_N$) which is supposed to be homogeneous and isotropic and therefore characterized by its relative permittivity ε^+ and its relative permeability μ^- and we denote $k^- := k_0\sqrt{\varepsilon^-\mu^-}$
- *The groove region* ($z_{g-1} < z < z_g$) which is embedded in the layer numbered g of the domain under study, which can be heterogeneous and then characterised by the scalar fields $\varepsilon_g(x,y,z)$ and $\mu_g(x,y,z)$. The periodicity of the grooves along *Ox* (resp. *Oy*) is denoted d_x (resp. d_y).

The grating is illuminated by an incident plane wave of wave vector defined by the angles θ and ϕ : $\mathbf{k}^+ = k^+(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)^T = (\alpha,\beta,\gamma)^T$. Its electric field $\mathbf{E^0}$ is linearly polarized along the direction defined by the unit vector $\mathbf{A^0}$: $\mathbf{E^0} = \mathbf{A^0}\exp(i\mathbf{k}^+\cdot\mathbf{r})$, with $\mathbf{r} = (x,y,z)^T$ and $\mathbf{A^0} = (\cos\psi\cos\theta\cos\phi - \sin\psi\sin\phi, \cos\psi\cos\theta\sin\phi + \sin\psi\cos\phi, -\cos\psi\sin\theta)^T$. The problem of diffraction is to find Maxwell's equation solutions in harmonic regime *i.e.* to find the unique solution **E** of :

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

such that the diffracted field satisfies an Outgoing Wave Condition and where $\mathbf{E}$ is quasi-periodic with respect to x and y coordinates, *i.e.* :

$$\mathbf{E}(\mathbf{r}+\mathbf{d}) = \mathbf{E}(\mathbf{r})\exp(i\mathbf{k}^+ \cdot \mathbf{d}) = \mathbf{E}(\mathbf{r})\exp(i(\alpha d_x + \beta d_y)) \tag{2}$$

with $\mathbf{d} = (d_x, d_y, 0)^T$.

A method [1, 2, 3, 4] based on the resolution of the diffraction problem defined by Eq.1, and adapted to the FEM, allows us to extract the transmission, reflection, Joule losses and to obtain a global energy balance.

The eigenvalue problem

The eigenvalues of the structure, which can be complex, are denoted $\omega_n = \omega_n' + i\omega_n''$. The real part is the resonant frequency and the imaginary part is the damping ratio. We define the quality factor of the resonance as $Q_n := \omega_n'/(2\omega_n'')$. These eigenvalues are also the poles of the reflection coefficient of the device [5]. The first method consist in finding the eigenmodes of our structures by the FEM. The second one (called tetrachotomy), based on tools of complex analysis, gives us numerically those poles.

The eigenvalue problem we are dealing with consists in finding the solutions of Maxwell's equations *without sources*. We want to find the complex eigenvalues ω_n and the non-zero fields $\mathbf{E_n}$ which are bi-pseudo-periodic in Ω, such that :

$$\varepsilon_r^{-1}\mathbf{curl}(\mu_r^{-1}\mathbf{curl}\ \mathbf{E_n}) = c^{-2}\omega_n^2\mathbf{E_n} \tag{3}$$

In fact, there is no incident plane wave, but nevertheless the coefficients of quasi-periodicity α and β are parameters (via Eq. 2) and are forced to be real valued. Note that α and β given do not allow to recover θ and ϕ since k^+ is not known. It will be given by the eigenvalue ω_n : if ω_n'' is small, we can set $k_n^+ \simeq \sqrt{\varepsilon^+\mu^+}\omega_n'/c$, and deduce the corresponding angles for which a resonance may occur from $\alpha = k_n^+(\sin\theta_n \cos\phi_n)$ and $\beta = k_n^+(\sin\theta_n \sin\phi_n)$.

The FEM formulation

The eigenproblem defined by Eq. 3 is then solved by the FEM, using both PML at the bottom and at the top of the meshed domain and by taking into account the quasi-periodicity conditions on lateral bounds on the same area. Finally, Neumann homogeneous conditions are imposed on the outward edge of each PML. Note that the eigenvectors $\mathbf{E_n}$ we are looking for are not of finite energy, but the use of PMLs makes them of finite energy, which is a necessary condition for the weak formulation associated with the FEM [5, 6, 7]. The cell is meshed using 2^{nd} order edge elements. In the numerical examples of the sequel, the maximum element size is set to $\lambda/(N_m\sqrt{\mathfrak{Re}(\varepsilon_r)})$, where N_m is an integer (between 6 and 10 is usually a good choice). The final algebraic system is solved using a direct solver (PARDISO).

The tetrachotomy

As previously said, the eigenvalues of the structure are also the poles of the reflection $r(\omega)$ (or transmission $t(\omega)$) coefficient for the amplitude. Searching for poles is a rather difficult problem, since we do not know *a priori* their number nor their positions in the complex plane. The transmission coefficient can be cast in the following form [5] :

$$t(\omega) = \sum_{n\in\mathbb{N}} \frac{A_n}{\omega - \omega_n} + g(\omega) \tag{4}$$

where the residues $A_n \in \mathbb{C}$ and g is an holomorphic function representing the non-resonant process. Let Γ be a Jordan curve in the complex plane containing solely the pole ω_m. We define the following complex line integrals I_k for $k = 0, 1, 2$:

$$I_k = \frac{1}{2i\pi}\oint_\Gamma \omega^k t(\omega)\mathrm{d}\omega = \frac{1}{2i\pi}\oint_\Gamma \omega^k \frac{A_m}{\omega-\omega_m}\mathrm{d}\omega \tag{5}$$

since, invoking Cauchy's theorem, the integral of g on a closed loop is null. Applying the residues theorem to $f_k : \omega \mapsto \omega^k \frac{A_m}{\omega-\omega_m}$ leads to :

$$I_k = \mathrm{Res}_{\omega_m} f_k = \lim_{\omega\to\omega_m} (\omega-\omega_m) f_k(\omega) = A_m\omega_m^k$$

Hence, we know the value of $A_m = I_0$ and the pole ω_m is precisely given by :

$$\omega_m = \frac{I_2}{I_1} = \frac{I_1}{I_0} \tag{6}$$

The algorithm of tetrachotomy consists in calculating the poles one by one by dividing sets of rectangular domains (starting with a single initial one) in four isometric parts until we "surround" every pole (see Fig. 3). We distinguish 3 cases :

- $I_0 = I_1 = 0$: no pole,
- $\frac{I_2}{I_1} = \frac{I_1}{I_0}$: a single pole given by Eq. 6,
- $\frac{I_2}{I_1} \neq \frac{I_1}{I_0}$: several poles.

The performance of the method is linked to the calculus of the integrals defined by Eq. 5. The details of the method can be found in Ref. [8].

Validation : example of a dielectric multilayered stack

In order to validate the two methods and to compare them, we search for the resonances of a four layer slab, as shown in Fig. 1. The problem is invariant in the (Ox) direction the plane of incidence is $(0xz)$ $(\phi = 0)$. We search for TM polarized fields (the only non-zero component of the magnetic field is H_x), *i.e.* we search for eigenvectors in a subspace such that $\psi = \pi/2$. Under these conditions, the vectorial problem reduces to a scalar one. We are looking for resonances at normal incidence $(\theta = 0)$, so we set $\beta = 0$ (and hence $\gamma = k^+$). The parameters for the following example are $h_1 = 26\mu m$, $h_2 = 0.5\mu m$, $\varepsilon_{air} = 1$, $\varepsilon_{Si} = 11.7$, and the relative permittivity [9] of SiO_2 and ZnSe are plotted in Fig. 2. Note that we work in the absorption band of SiO_2, its relative permittivity varies quickly with the wavelength.

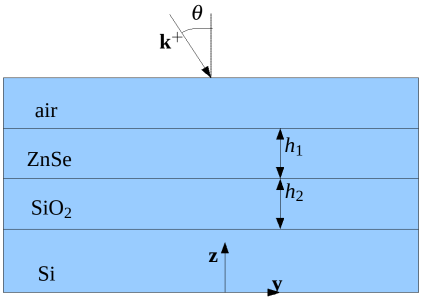

FIGURE 1. The multilayered slab under study.

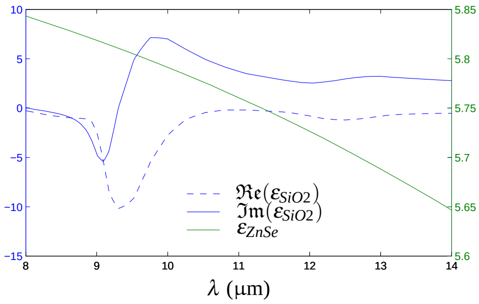

FIGURE 2. Relative permittivity of SiO_2 and ZnSe as a function of the wavelength λ.

Dealing with dispersive materials makes the eigenvalue problem not directly tractable with standards solvers, as the operator of which we want to find the eigenvalues depends itself on the eigenvalue ω via $\varepsilon_r(\omega)$. In practice, the permittivity is supposed constant : we search N_{eig} eigenvalues $\omega_n^{(1)}$ around the frequency $\omega^{(0)}$ fixed arbitrarily. Then, for $n = 1, 2, \ldots N_{eig}$ we search one eigenvalue $\omega_n^{(2)}$ around $\omega_n^{(1)}$ with updated $\varepsilon_r(\omega_n^{(1)})$, and iterate by computing $\omega_n^{(k)}$ until we converge to a fixed point on the value of $\omega_n^{(k)}$. Here we obtain the transmission coefficient of the slab by a transfer matrix formalism [10, 11]. The numerical scheme used to calculate the integrals defined by Eq. 5 requires to evaluate the transmission coefficient at a number of points proportional to the requested accuracy. The method used to calculate the transmission coefficient needs therefore to be low memory consuming in order to be able to use the tetrachotomy in a workable way. Fig. 3 shows the loci in the complex

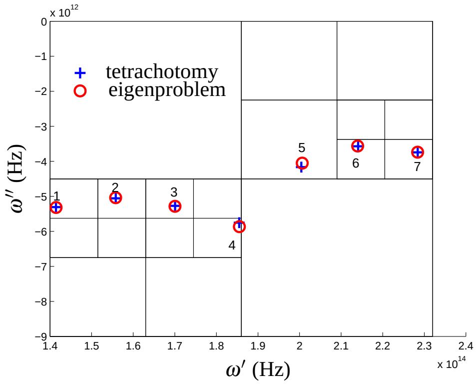

FIGURE 3. Loci of the resonance frequencies in the complex plane for the two methods.

plane of the resonances found by the tetrachotomy and the eigenvalue problem. The two methods are in good agreement : the maximum absolute value of the relative difference is of 0.1% for the real parts and of 2.7% for the imaginary parts. Note that these maxima occurs for the resonance numbered 7, which real part is near 10.6μm, where ε_{SiO_2} shows a resonant behaviour, and corresponding to the resonant frequency of Si-O bound.

In the full paper, examples of gratings (2D modeling) and crossed gratings (3D modeling) will be given.

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