Dipole radiation into grating structures

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We present a detailed electromagnetic analysis for the radiation of an electric source located inside grating structures. Our analysis is based on the differential method and uses the scattering-matrix algorithm. We show that gratings that exhibit periodic modulations along two spatial directions (crossed gratings) enable one to couple out the totality of the light emitted by the source into the guided modes of the structure. This property is investigated through the computation of the far-field radiation patterns for crossed gratings with various etching depths. One key result is the possibility to confine the emitted light in a direction about the sample normal, a property that is of interest in the context of spontaneous emission control by microcavity structures. © 2000 Optical Society of America [S0740-3232(00)01506-4]


1. INTRODUCTION

For more than ten years now, many studies have been devoted to the modification of the spontaneous emission of luminescent species located in what is commonly called a microcavity. Since the first paper by Purcell,1 spontaneous emission control has been demonstrated for free atoms in high-Q cavities,2 organic molecules,3 and semiconductor devices.4 Two major effects can be distinguished. The first one is the spontaneous emission rate enhancement $\tau/\tau_0$ ($\tau$, free-space lifetime) related to the mode volume $V$ and to the cavity quality factor $Q = \lambda/\Delta\lambda$ ($\Delta\lambda$, cavity linewidth) through the Purcell factor $\tau/\tau_0 = 3/4\pi^2(Q\lambda^3/V)$. The second effect is the spatial distribution alteration of the emitted light, which is of great interest for extracting 100% of the electromagnetic power provided by the source. Such a solid-state device could be used to build high-brightness LED,5 high-sensitivity fluorescence biosensors,6 or single-photon sources.7 This problem of extracting the total amount of light emitted by a single source located inside a microcavity is far from being simple for at least three reasons:

1. The materials that constitute the microcavity have to present low loss at the optical frequency so that the provided electromagnetic power from the source equals the outgoing Poynting flux power that emerges outside the microcavity.

2. When the microcavity has at least one dimension that is larger than the emitted wavelength, trapped or guided electromagnetic modes usually exist and may carry an important part of the total provided power.8

3. When the structure is single mode such as in the micropillar case,9 the subwavelength dimension of the output surface leads to strong diffraction in free space, and the source-provided power is extracted, filling a large part of the $4\pi$ steradian of the entire free space. This wide angular radiation pattern is difficult to collect and requires large-numerical-aperture optics. However, this type of structure has the potential to reduce the radiative lifetime $\tau/\tau_0$.10

In addition to these reasons it is interesting to mention that efficient spontaneous emission coupling between a luminescent atom and an optical mode is usually achieved when the mode is well confined around the atomic position. This effect can be strong for sources interacting with closed rotating modes such as a whispering gallery modes in microspheres11 and has led to extremely low threshold in the case of a photonic wire laser.12 This enhanced source–field overlap is also the fundamental reason for the directive transverse emission from sources within a planar Fabry–Perot microcavity8; it is also responsible for the large part of the total spontaneous emitted power carried by the guided modes.13 More precisely, for this last case of sources located inside planar microcavities, it is now well established that, although the outgoing light can be directive, the total extracted light is usually less than a few tens of percent, with the remaining fraction of the source-provided power trapped in the substrate or guided modes3,8,13.

To increase the amount of extracted light from these planar microcavities, we can use corrugation to couple the guided light to running waves that propagate outside the structure. This idea was already presented and experimentally confirmed by Kitson et al. who showed that it is possible to scatter light from guided surface plasmon modes into running waves for dye molecules on a metallic grating.14 With a specific corrugation grating it is even possible to prohibit surface modes in a frequency range, causing a full photonic bandgap effect.15–17

Although corrugation can be applied in principle to any type of microcavity supporting trapped or guided modes, we restrict our analysis to planar structures for which coating techniques and etching processes are now well controlled at nanometer scales.

The use of gratings to extract guided light has been extensively treated in the domain of integrated optics.16,18 Less frequent, the study of active devices with sources directly located in the vicinity of corrugated surfaces can also be found.20 Although most of the reported studies deal with gratings with a periodicity along one direction,
it is necessary to consider crossed gratings (or doubly periodic gratings), which exhibit periodicity along two orthogonal directions, to couple out the total guided mode power regardless of the azimuthal direction $\phi$ of the guided mode. This point is discussed in Section 2, where we present the wave-vector diagram (WVD) analysis, which gives a simple graphic understanding for the light propagation into singly or doubly periodic gratings. In addition to these simple considerations, Section 3 presents an accurate electromagnetic theory for sources radiating into crossed gratings. This section is the key part of the paper and is divided into several subsections that present the source description and its radiation in terms of the differential method implemented with the $S$-matrix algorithm. Finally, Section 4 gives a numerical example for a localized source located in crossed gratings and emphasizes the amount of guided light coupled out by the gratings.

2. GUIDED-WAVE PROPAGATION INTO THE GRATING: WAVE-VECTOR DIAGRAM

In this section we present a physical insight of the radiation mechanisms for a source located in a periodic structure that supports guided modes. As presented by Zengerle, light propagation into planar structures with shallow corrugation can be physically understood from the WVD, which plots in the $k$ space the areas associated with the various kinds of modes existing in the structure of interest. If the wave-vector coordinates along the three axes of unit vectors $(\mathbf{x}, \mathbf{y}, \mathbf{z})$ of a right-hand Cartesian coordinate frame are denoted by $a$, $\beta$, and $\gamma$ so that $\mathbf{k} = a\mathbf{x} + \beta\mathbf{y} + \gamma\mathbf{z}$, the WVD in the $(a, \beta)$ plane of a simple single-mode slab waveguide coated on a substrate (see Fig. 1) is divided into three areas corresponding to the three types of electromagnetic modes taking place inside and outside the guide. We denote $\mathbf{k}_g$ as the planar part of the $k$-vector, $\mathbf{k}_g = a\mathbf{x} + \beta\mathbf{y}$. Throughout this paper a three-dimensional vector $\mathbf{u}$ is described by its planar component $\mathbf{u}_p$ and its vertical one $\mathbf{u}_z$ so that $\mathbf{u} = \mathbf{u}_p + \mathbf{u}_z$. The free-space disk corresponding to the running wave that propagates inside and outside the guide is defined for $0 < |\mathbf{k}_g| < k_0$ where $k_0 = 2\pi/\lambda = \omega/c$ and $\lambda$ is the wavelength of radiation. For $k_0 < |\mathbf{k}_g| < n_3k_0$ where $n_3$ is the refractive index of the substrate, the light remains trapped in the substrate, and for $|\mathbf{k}_g| = |\mathbf{k}_0|$ the light is guided into the fundamental guided mode with the specific wave vector $\mathbf{k}_g$. As can be seen from Fig. 1, there is no way to couple out the guided mode in this simple slab, since the $|\mathbf{k}_g|$ circle never intercepts the free-space disk.

To extract the guided mode, whatever its direction of propagation (i.e., for any azimuthal $\phi$ angle), we introduce a periodic modulation of the slab along both the $x$ and the $y$ axes with periods $d_x$ and $d_y$. Thus any wave vector $\mathbf{k}_g$ is coupled, through the grating, to all the waves of planar wave vectors $\mathbf{k}_{g, n}$ with $\mathbf{k}_{g, n} = \mathbf{k}_g + mK_x\mathbf{x} + nK_y\mathbf{y}$ ($m$ and $n$ positive or negative integers) where $K_x = 2\pi/d_x$ and $K_y = 2\pi/d_y$. Guided-mode extraction is possible if there is a couple $(m', n')$ of a free-space wave vector $\mathbf{k}_{g, mn}^\text{inc}(0 < |\mathbf{k}_{g, mn}^\text{inc}| < k_0)$ that satisfy $\mathbf{k}_g = \mathbf{k}_{g, mn}^\text{inc} + m'K_x\mathbf{x} + n'K_y\mathbf{y}$. This coupling phenomenon is illustrated in Fig. 2 where we duplicated periodically (with periods $K_x$ and $K_y$) the free-space disk along the $a$ and the $\beta$ axes. In our specific configuration we see that the guided-mode circle now always intercepts one of the duplicated free-space disks. Since our problem deals with a localized source in an infinite planar corrugated structure, this guided-mode coupling with running waves that propagate outside the structure will lead finally to the total extraction in free space of the guided-mode power (whatever its direction of propagation). Note that in this simple graphic representation, it is possible to obtain qualitatively the radiation pattern from a source located inside the grating. Assuming that the source emits most of its power into the fundamental guided mode, we know from Fig. 2(b) that this guided light is extracted in free space.
In what follows we assume that the radiation source inside an inhomogeneous structure that is not necessarily periodic. In what follows we assume that the radiation source can be adequately represented by an electric dipole oscillating at a frequency \( \omega \) (weak coupling between the source and the electromagnetic fields) and that a classical description of the electromagnetic fields is valid. Throughout this paper the \( \exp(\pm i \omega t) \) time dependence is assumed (and omitted). The method presented here is general and enables us to calculate the field radiated by the source everywhere in the structure (in particular, it permits us to obtain the electromagnetic field surrounding the source; i.e., extension to nonlinear coupling between the source and the local field is then conceivable). It is worth noting that, when we are interested solely in the field radiated in the far field outside the cavity, the reciprocity theorem\(^2\) enables us to obtain easily the radiated energy with the usual codes developed for passive structures (and a calculation of the field inside the structure). Here we propose a more direct estimation of the emitted light.

We seek the electromagnetic fields \((E, H)\) that are the solutions of the Maxwell equations in the harmonic regime,

\[
\begin{align*}
\nabla \times E(r) - i \omega \varepsilon_\infty H(r) &= 0, \\
\nabla \times H(r) + i \omega \varepsilon_\infty E(r) &= -i \omega \varepsilon_0 \delta(r - z_0 z),
\end{align*}
\]

which satisfy the outgoing wave-boundary condition at infinity. The relative dielectric constant \( \varepsilon \) is a function of the space variables and describes the geometry of the system. More precisely, we divide this system into five regions (see Fig. 4). For \( z > h_{\text{max}} \), the relative permittivity is a constant, and we are in the superstrate (in general, air), \( \varepsilon(r_p, z > h_{\text{max}}) = \varepsilon_1 \).

For \( z < h_{\text{min}} \), the relative permittivity is a constant, and we are in the substrate, \( \varepsilon(r_p, z < h_{\text{min}}) = \varepsilon_3 \). For \( h_a < z < h_b \) we are in the source region (i.e., \( h_a < z_0 < h_b \)), and the permittivity is also a constant \( \varepsilon(r_p, h_a < z < h_b) = \varepsilon_2 \). Hence we assume that there exists a homogeneous slab of finite thickness that surrounds the source: this is the main assumption of our model. Note however that the slab can be taken to be arbitrarily thin (this will be the case in the second part of this section). In the upper region \( h_a < z < h_{\text{max}} \) and the lower region \( h_{\text{min}} < z < h_a \), the relative permittivity varies along the vertical axis (if there is a multilayer) and varies in the \((0xy)\) plane (if there is a transverse modulation).

We first focus on the solution of the Maxwell equations inside the source region, i.e., for \( h_a < z < h_b \), and we seek a solution for the electric field (knowledge of the electric field is sufficient to determine the entire problem, the

\begin{align*}
\nabla \times E(r) - i \omega \varepsilon_\infty H(r) &= 0, \\
\nabla \times H(r) + i \omega \varepsilon_\infty E(r) &= -i \omega \varepsilon_0 \delta(r - z_0 z),
\end{align*}

}\]

3. ELECTROMAGNETIC THEORY

A. Radiation of an Electric Dipole into an Inhomogeneous Structure: Basic Steps

In this introductory part we sketch the main steps that permit us to calculate the radiation of a luminescent source inside an inhomogeneous structure that is not necessarily periodic. In what follows we assume that the radiating source can be adequately represented by an electric dipole oscillating at a frequency \( \omega \) (weak coupling between the source and the electromagnetic fields) and that a classical description of the electromagnetic fields is valid. Throughout this paper the \( \exp(-i \omega t) \) time dependence is assumed (and omitted). The method presented here is general and enables us to calculate the field radiated by the source everywhere in the structure (in particular, it permits us to obtain the electromagnetic field surrounding the source; i.e., extension to nonlinear coupling between the source and the local field is then conceivable). It is worth noting that, when we are interested

![Fig. 3](image-url)

**Fig. 3.** Radiation pattern in the WVD of a localized source located within doubly periodic grating. We assume dominant emission in the guided mode. \((m', n')\) are the multiplicities associated with each arc [see Fig. 2(b)].

![Free space disk](image-url)

**Fig. 4.** Source radiation in an inhomogeneous structure. The source is assumed to be located in a thin homogeneous material slab \((h_a < z < h_b)\) surrounded by inhomogeneous scatterers.
magnetic field being obtained through Eq. (1a)). It can be written as the sum of the particular solution (with the source term in the left-hand side of the equation) plus homogeneous solutions (obtained by removing the source term in the differential system), \( \mathbf{E} = \mathbf{E}_{\text{hom}} + \mathbf{E}_{\text{par}} \). In this region (slab), the homogeneous solutions for the electromagnetic field can be written as a sum of plane waves propagating downward and upward into the \([\mathbf{u}, \mathbf{d}]\) basis,

\[
E_{\text{hom}}(\mathbf{r}_p, z) = \int U(\mathbf{k}_p)\exp\left(i\mathbf{k}_p \cdot \mathbf{r}_p + i \gamma_2 z\right) + D(\mathbf{k}_p)\times \exp\left(i\mathbf{k}_p \cdot \mathbf{r}_p - i \gamma_2 z\right)\,dk_p,
\]

where \( \gamma_i = (\varepsilon_i k_0^2 - |\mathbf{k}_p|^2)^{1/2} \) and \( \mathbf{kp} = \alpha x + \beta y \).

The particular solution is simply the field radiated by a dipole inside an homogeneous region. It is given under the Weyl development, at the observation point \( \mathbf{r} \) different from \( z = z_0 \mathbf{z} \), by

\[
E_{\text{par}}(\mathbf{r}_p, z) = \int [U_s(\mathbf{k}_p)\exp\left(i\mathbf{k}_p \cdot \mathbf{r}_p + i \gamma_2(z - z_0)\right)\Theta(z - z_0) \\
+ D_s(\mathbf{k}_p)\exp\left(i\mathbf{k}_p \cdot \mathbf{r}_p - i \gamma_2(z - z_0)\right)\Theta(z_0 - z)]\,dk_p,
\]

with

\[
U_s(\mathbf{k}_p) = \frac{\omega^2 \mu_0}{8 \pi^2 \gamma_2}\mathbf{P} - (\mathbf{P} \cdot \mathbf{k}_p^+)\mathbf{k}_p^+,
\]

\[
D_s(\mathbf{k}_p) = \frac{\omega^2 \mu_0}{8 \pi^2 \gamma_2}\mathbf{P} - (\mathbf{P} \cdot \mathbf{k}_p^-)\mathbf{k}_p^-,
\]

where

\[
\mathbf{k}_p^+ = \frac{1}{(\varepsilon_2 k_0)^{1/2}}(\mathbf{k}_p + \gamma_2 \mathbf{z}), \quad \mathbf{k}_p^- = \frac{1}{(\varepsilon_2 k_0)^{1/2}}(\mathbf{k}_p - \gamma_2 \mathbf{z})
\]

and \( \Theta \) is the step function. Physically, the dipole radiates an ensemble of plane waves propagating upward for \( z > z_0 \) and propagating downward for \( z < z_0 \). The amplitudes of these plane waves are proportional to the projection of the dipole vector on the plane normal to the direction of propagation. Note that this representation is valid close to the surface source and includes evanescent waves. In this latter case, \( \mathbf{k}_p^+ \) and \( \mathbf{k}_p^- \) are complex vectors. Finally, when the observation point is taken at the source position, we add the Dirac contribution \( (z \cdot \mathbf{P})\omega^2 \mu_0 \delta(\mathbf{r} - \mathbf{r}_0)/\varepsilon_0 k_0^2 \). In the semi-infinite homogeneous regions \( z > h_{\text{max}} \) and \( z < h_{\text{min}} \) the Rayleigh development of the fields reads as

\[
E(\mathbf{r}_p, z) = \int R(\mathbf{k}_p)\exp\left(i\mathbf{k}_p \cdot \mathbf{r}_p + i \gamma_2 z\right)\,dk_p
\]

for \( z > h_{\text{max}} \),

\[
E(\mathbf{r}_p, z) = \int T(\mathbf{k}_p)\exp\left(i\mathbf{k}_p \cdot \mathbf{r}_p - i \gamma_3 z\right)\,dk_p
\]

for \( z < h_{\text{min}} \),

\[
E(\mathbf{r}_p, z) = \int S(\mathbf{k}_p)\exp\left(i\mathbf{k}_p \cdot \mathbf{r}_p + i \gamma_3 z\right)\,dk_p
\]

for \( z > h_{\text{max}} \),

Now the problem is to determine, through the boundary conditions at the interfaces, \( h_a, h_b, h_{\text{max}}, h_{\text{min}} \), the unknown vectors \( \mathbf{U, D, R, T} \) for each \( \mathbf{k}_p \) to get the field radiated by the electric dipole outside the cavity and close to the source. The upper inhomogeneous region \( h_b < z < h_{\text{max}} \) and the lower inhomogeneous region \( h_{\text{min}} < z < h_b \) can be viewed as two passive scatterers which are infinite in the \((0xy)\) plane, since they do not contain any source. Hence we can introduce their scattering matrices \( 5 \) matrices \( S_{h_b}, h_a \) and \( S_{h_{\text{min}}}, h_a \), which relate incident (in going) waves to outgoing (or scattered) waves.\(^{26}\)

In our geometry, incident waves for the upper scatterer (or upper region) correspond to outgoing waves at \( z = h_b \) and downgoing waves at \( z = h_{\text{max}} \). For the lower scatterer, incident waves correspond to downgoing waves for \( z = h_a \) and outgoing waves for \( z = h_{\text{min}} \). Note that the particular solution contributes to the upgoing (downgoing) waves only for \( z > z_0 \) \((z < z_0)\), because of the step function. We thus obtain a linear system in the plane wave (up and down) basis (in matrix form),\(^{25–27}\)

\[
\begin{bmatrix}
R \\
\mathbf{D}
\end{bmatrix} = S_{h_b} S_{h_{\text{max}}} \begin{bmatrix}
U_s + U \\
U_T
\end{bmatrix}, \quad \begin{bmatrix}
U \\
\mathbf{T}
\end{bmatrix} = S_{h_{\text{min}}} S_{h_a} \begin{bmatrix}
0 \\
\mathbf{D} + \mathbf{D}_s
\end{bmatrix},
\]

(5)

that relates the various unknowns of our problem and leads to a unique solution.

Once \( \mathbf{U, D, R, T} \) are known, we calculate the radiated intensity above and below the cavity. Applying the stationary phase theorem,\(^{26}\) we can show that the expressions of the electric field, Eqs. (4), at the observation point \( \mathbf{r} = r \mathbf{u}_r \), where \( r \) is the modulus of \( \mathbf{r} \) and \( \mathbf{u}_r \) is a unit vector, reduce to, when \( r \) tends toward infinity,

\[
E(\mathbf{r}) = -2\pi i \gamma_2 R(\mathbf{k}_p) \frac{\exp(ik_1 r)}{r} \quad \text{for } z > h_{\text{max}},
\]

\[
E(\mathbf{r}) = -2\pi i \gamma_3 T(\mathbf{k}_p) \frac{\exp(ik_3 r)}{r} \quad \text{for } z < h_{\text{min}},
\]

with \( k_j = \sqrt{\varepsilon_j k_0}, j = (1, 3) \), and \( \mathbf{k}_p \) is the projection of \( k_j \mathbf{u}_r \) onto the \((x, y)\) plane.

The power radiated in the direction of observation, given by the wave vector \( \mathbf{k} = \mathbf{k}_p + \gamma z \) in the superstrate and \( \mathbf{k} = \mathbf{k}_p - \gamma z \) in the substrate, per unit solid angle, is obtained by calculating the Poynting flux through the surface \( r^2 \, d\Omega \) normal to the direction of propagation. We get

\[
\frac{dr}{d\Omega} = \frac{4\pi^2}{2\eta_1} |\gamma_2 R(\mathbf{k}_p)|^2
\]

in the superstrate and

\[
\frac{dr}{d\Omega} = \frac{4\pi^2}{2\eta_3} |\gamma_3 T(\mathbf{k}_p)|^2
\]

in the substrate, where \( \eta_1 \) is the impedance of the medium, \( \eta_1 = (\mu_0 /\varepsilon_0\varepsilon_j)^{1/2} \).

The total radiated power is calculated by integrating the differential scattering cross section over the \( 4\pi \) steradian angle. Noting that \( d\Omega = d\mathbf{k}_p / (\gamma_2 k_j) \), the total radiated flux is
\[
\Psi_{\text{tot}} = \Psi_{\text{up}}^{\text{tot}} + \Psi_{\text{down}}^{\text{tot}}
\]

\[
= \int_{4\pi} d\sigma d\Omega + \int_{|k_p| < k_1} \frac{4\pi^2}{2\eta_1} |\gamma_1 R(k_p)|^2 \frac{dk_p}{\gamma_1 k_1}
\]

\[
+ \int_{|k_p| < k_3} \frac{4\pi^2}{2\eta_3} |\gamma_3 T(k_p)|^2 \frac{dk_p}{\gamma_3 k_3}
\]

(7)

\(\Psi_{\text{tot}}\) is the total power that emerges outside the corrugated structure. It may be different from the total source-provided power that includes \(\Psi_{\text{tot}}\) and an eventually absorbed power that is not radiated outside the structure. Therefore the present analysis can compute the dipole lifetime only if the structure is lossless and no trapped modes are present, i.e., if all the emitted electromagnetic power is coupled out of the structure. In this case \(\Psi_{\text{tot}}\) is related to the dipole lifetime \(\tau\) through \(\Psi_{\text{tot}}/\Psi_0 = \frac{\pi}{2\tau_0}\) where \(\Psi_0\) is the emitted power in free space and \(\tau_0\) the free-space dipole lifetime.

The most difficult step in this method is the calculation of the \(S\) matrix of the perturbed upper and lower regions in the plane-wave basis (i.e., for all wave vectors \(k_p\), including those contributing to evanescent waves). This difficult task can be reduced by noting that one needs to calculate solely the planar components [in the \((0xy)\) plane] of the vectors amplitude \((U, D, R, T)\). Indeed, in the homogeneous media, superstrate, substrate, and slab surrounding the source the vertical component of the electric field is deduced from the planar ones by invoking the null divergence of the electric field, \(\text{div} \, E = 0\). Assuming now that the permittivity of the perturbed regions is periodical further simplifies the numerical computation. Indeed, we will show that, in this case, the infinite double integral in the \(k\) space that describes the field in Eqs. (2)–(4) can be replaced with integrals over the finite interval \([(0,K_x),(0,K_y)]\) with discrete summation over the reciprocal space. Hence the calculation of the \(S\) matrices are easier.

### B. Radiation of a Dipole into a Periodically Inhomogeneous Medium: Detailed Analysis

In this subsection we present a more complete description of the numerical steps leading to the calculation of the field radiated by a source located into a periodical structure. Our approach is similar to that described in Subsection 3.A, but it is reformulated to account for the periodicity of the geometry.

#### 1. Structure and Coordinate Frame

We consider the type of structure depicted in Fig. 2(a). The structure consists of a corrugated homogeneous slab deposited onto a semi-infinite substrate. The corrugation exhibits a periodicity \(d_c\) along the \(x\) axis and \(d_y\) along the \(y\) axis. Note that Fig. 2(a) presents a square lattice that is only a specific example of doubly periodic structures. The thickness of the corrugated region is \(h'\), whereas \(d\) is the thickness of the homogeneous guiding layer in which the source is placed (at \(z_0\)). With our choice of axis origin, we have \(h_{\text{min}} = 0\) and \(h_{\text{max}} = h = h' + d\).

#### 2. Problem Reduction

The periodicity of the geometry enables us to simplify the problem greatly. By writing the Maxwell equations (1) in the two-dimensional Fourier space \((x, y) = (\alpha, \beta)\), bearing in mind the periodicity of the permittivity, we shall see that the Fourier component of the field \(\bar{E}(\alpha, \beta, z)\) radiated by the localized source,

\[
E(x, y, z) = \int_{-\infty}^{+\infty} d\alpha \int_{-\infty}^{+\infty} d\beta \bar{E}(\alpha, \beta, z)(i\alpha x + i\beta y),
\]

(8)

is related only to the Fourier components of the field \(\bar{E}_{\alpha,\beta}^m(z) = \bar{E}(\alpha + mK_x, \beta + nK_y, z)\) with \((m, n) \in \mathbb{Z}^2\) and to the Fourier components of the source \(\bar{P}_{\alpha,\beta}^{m,n} = \bar{P}(\alpha + mK_x, \beta + nK_y)\) with \((m, n) \in \mathbb{Z}^2\).

The electric field radiated in the periodic geometry by the pseudoperiodic source \(\bar{P}_{\alpha,\beta}(x, y, z)\),

\[
\bar{P}_{\alpha,\beta}(x, y, z) = \delta(z - z_0) \int_0^{2\pi/dx} \frac{d\alpha}{2\pi/d\alpha} \int_0^{2\pi/dy} \frac{d\beta}{2\pi/d\beta} \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \bar{P}_{\alpha,\beta}^{m,n} \times \exp(i\alpha m x + i\beta n y),
\]

(9)

where \(\alpha_m = \alpha + mK_x\) and \(\beta_n = \beta + nK_y\) and \(k_{\alpha,\beta}^{m,n} = \alpha_m x + \beta_n y\).

The electric field radiated in the periodic geometry by the pseudoperiodic source \(\bar{P}_{\alpha,\beta}(x, y, z)\),

\[
\bar{P}_{\alpha,\beta}(x, y, z) = \delta(z - z_0) \sum_{m=-\infty}^{+\infty} \sum_{n=-\infty}^{+\infty} \bar{P}_{\alpha,\beta}^{m,n} \times \exp(i\alpha m x + i\beta n y),
\]

(10)

is also pseudoperiodic and can be written as

\[
\bar{E}_{\alpha,\beta}(x, y, z) = \sum_{n=-\infty}^{+\infty} \sum_{m=-\infty}^{+\infty} \bar{E}_{\alpha,\beta}^{m,n}(z) \exp(i\alpha m x + i\beta n y).
\]

(11)

In particular, in the semi-infinite homogeneous medium above (below) the perturbed region, for \(z > h\) (for \(z < 0\)); the pseudoperiodic electric field can be written in the plane-wave basis restricted to the reciprocal space (i.e., restricted to \([k_p = (\alpha + mK_x)x + (\beta + nK_y)y\) with \((m, n) \in \mathbb{Z}^2\)] as
\[
E_{a,\beta}(x, y, z) = \sum_{n=-\infty}^{+\infty} \sum_{m=-\infty}^{+\infty} R_{a,\beta}^{m,n} \exp(i \alpha_m x + i \beta_n y + i \gamma_j^{m,n} z),
\]
(12a)
where
\[
E_{a,\beta}(x, y, z) = \sum_{n=-\infty}^{+\infty} \sum_{m=-\infty}^{+\infty} T_{a,\beta}^{m,n} \exp(i \alpha_m x + i \beta_n y - i \gamma_j^{m,n} z),
\]
(12b)

The total electric field is obtained by coherent superposition of the pseudoperiodic fields \(E_{a,\beta}\) following the integral (2),
\[
E(x, y, z) = \int_{0}^{2\pi/dx} \int_{0}^{2\pi/dy} \text{d}y \text{d}\beta E_{a,\beta}(x, y, z).
\]
(13)

From a numerical point of view the calculation of pseudoperiodic fields is much more interesting than a direct calculation of the total field. The calculation of \(E_{a,\beta}\) is completely independent of that of \(E_{a',\beta'}\) for two different couples, \([(\alpha, \beta), (\alpha', \beta')] \in [0, 2\pi/d_x] \times [0, 2\pi/d_y]\). Then the evaluation of the coefficients \(R_{a,\beta}^{m,n}\) and \(T_{a,\beta}^{m,n}\) yields directly the emitted light in the direction \((\alpha_m, \beta_n, \gamma_j^{m,n})\) through Eqs. (6). Hence, if we are interested in the far-field radiation of the dipole in certain directions, we restrict the pseudoperiodic calculations to a small set of \((\alpha, \beta)\). This is particularly convenient when we want to focus on a precise angular domain (where there is a resonant behavior, for example). In contrast, all \((\alpha, \beta)\) contributions are necessary to compute the electric field in the source vicinity.

Each calculation of \(E_{a,\beta}\) requires the evaluation of the \(S\) matrix of the system written on the plane-wave basis restricted to the discrete reciprocal space of the periodic structure. The convergence of the series in Eqs. (10)–(12) [truncation on \((m, n)\)] is rapidly obtained when the periods of the grating are small compared with the wavelength. Thus the size of the \(S\) matrix remains reasonable, and the resolution of the linear system can be achieved easily on a personal computer.

Finally, the symmetries of the structures under study enables us to limit the integration in Eq. (13) over the reduced Brillouin zone of the periodic geometry [in general, \((\alpha, \beta) \in [0, \pi/d_x] \times [0, \pi/d_y]\)].

3. Fields Radiated by a Pseudoperiodic Source \(P_{a,\beta}(x, y, z)\) in a Homogeneous Bulk Material

In this subsection we give the detailed expression of the electric field obtained in the homogeneous slab surrounding the pseudoperiodic source. For simplifying the notations we have omitted the suffix \((\alpha, \beta)\), which indicates the pseudoperiodicity of the source. Finally, we consider solely the planar components (projection onto the xy plane) of the \(U\) and the \(D\) vectors as inasmuch as they are sufficient to determine the electromagnetic fields entirely.

From Eq. (3) we obtain the electric field, the solution of the Maxwell equations with the pseudoperiodic source in the form

\[
E_{\text{par}}(x, y, z) = \sum_{n=-\infty}^{+\infty} \sum_{m=-\infty}^{+\infty} E_{\text{par}}^{m,n}(z) \exp(i \alpha_m x + i \beta_n y + i \gamma_j^{m,n} z),
\]
(14)
with
\[
E_{\text{par}}^{m,n}(z) = U_{m}^{n} \exp(i \gamma_j^{m,n} z) \Theta(z - z_0) + D_{a}^{m,n} \exp(-i \gamma_j^{m,n} z) \Theta(z_0 - z) + e^{m,n} \delta(z - z_0),
\]
\[
e^{m,n} = -(z \cdot \bar{P}^{m,n}) z, \quad e^{m,n} = \frac{1}{\varepsilon_0 \varepsilon_2},
\]
\[
D_{a}^{m,n} = D_{a}(k_{p}^{m,n}), \quad U_{m}^{n} = U_{a}(k_{p}^{m,n}),
\]
where \(k_{p}^{m,n} = \alpha_m x + \beta_n y\) and \(\gamma_j^{m,n} = (\epsilon_2 k_0^2 - \alpha_m^2 - \beta_n^2)^{1/2}\) with \(\text{Im}(\gamma_j^{m,n}) \geq 0\).

Solving Maxwell equations (1) we obtain explicitly, for the planar components of the field,

\[
\begin{cases}
U_{m}^{n} = 1 & C_{j}^{m,n} = \frac{1}{\varepsilon_0 \varepsilon_2} \left[ \frac{Y_{m}^{n}}{X_{m}^{n}} - C_{2}^{m,n} \right] - i \alpha_m, \\
D_{a}^{m,n} = 2 \varepsilon_0 \varepsilon_2 \left[ Y_{m}^{n} - C_{a}^{m,n} \right] - i \beta_n,
\end{cases}
\]
(15)
with
\[
C_{j}^{m,n} = \frac{i \alpha_m \beta_n / \gamma_j^{m,n}},
\]
\[
X_{j}^{m,n} = i[\alpha_m^2 + (\gamma_j^{m,n})^2]/\gamma_j^{m,n},
\]
\[
Y_{j}^{m,n} = i[\beta_n^2 + (\gamma_j^{m,n})^2]/\gamma_j^{m,n},
\]
(16)
where the suffixes \(x\) and \(y\) indicate a projection onto the \(x\) and the \(y\) axes of the vector.

To this particular solution we add the solutions of the homogeneous differential system, written in the plane-wave basis as

\[
E_{\text{hom}}(x, y, z) = \sum_{n=-\infty}^{+\infty} \sum_{m=-\infty}^{+\infty} U_{m}^{n} \exp(i \alpha_m x + i \beta_n y + i \gamma_j^{m,n} z) + D_{a}^{m,n} \exp(i \alpha_m x + i \beta_n y - i \gamma_j^{m,n} z).
\]
(17)

4. Fields Radiated by a Pseudoperiodic Source \(P_{a,\beta}(x, y, z)\) in a Modulated Structure

In a periodic or a doubly periodic structure the field radiated by a pseudoperiodic source \(P_{a,\beta}(x, y, z)\) is directly linked to the knowledge of two sets of data:

1. The field step that is due to the source \(P_{a,\beta}(x, y, z)\) expressed by Eq. (14) in the plane wave (\(u, d\)) basis.
2. The \(S\) matrices of the structure without any source.

In this subsection we do not address the issue of the \(S\)-matrix calculations; this is left to Section 5. We introduce the two \(S\) matrices, developed on the up and the down plane-wave bases, \(S_{h, u} = S_{h, \omega} = S_{h, b_{\max}} = S_{h, b_{\omega}} = S_{h, b_{\min}} = S_{h, b_{\min}}^*\) (the homogeneous slab surrounding the source taken to be as thin as possible in this case for more generality). \(S_{h, u}\) is the \(S\) matrix that links the electric fields
expressed in the plane-wave (up and down) bases between $z = 0$ (interface substrate–coating) and $z = z_0$ (location of the source). This matrix can be divided into four submatrices and is defined as

$$
\begin{pmatrix}
U \\
T
\end{pmatrix} =
\begin{bmatrix}
S^u_{0,z_0} & S^d_{0,z_0} \\
S^d_{0,z_0} & S^u_{0,z_0}
\end{bmatrix}
\begin{pmatrix}
0 \\
D + D_s
\end{pmatrix},
$$
(18)

where the column vector $[V]$, $[V] = \{[D_s], [U_1], [D], [U], [T], [R]\}$, is a column vector whose elements are the planar components of the vectors appearing in Eqs. (12), (14), and (17): $[V] = \{V_x^{m,n}, V_y^{m,n} \ (m, n) \in Z^2\}$. We recall that we need only the $(x, y)$ components of the electric plane waves to describe entirely the electromagnetic fields. Equation (18) is a simple notation for a matrix that is quite big. More precisely, if the computation takes into consideration $-M$ to $+M$ waves along the $x$ axis and $-N$ to $N$ waves along the $y$ axis, the $(U, D)$ vector, which includes the $U_x^{m,n}, U_y^{m,n}, D_x^{m,n}, D_y^{m,n}$ for every $(m, n)$ couple, is in fact a $4(2M+1)(2N+1)$ complex vector. For the same reason each of the submatrices $S^u_{z_0,h}, S^d_{z_0,h}$ links the fields between $z = z_0$ (location of the source) and $h = h$ (top interface between the structure and the air). Here again this matrix can be divided into four submatrices defined as

$$
\begin{pmatrix}
R \\
D
\end{pmatrix} =
\begin{bmatrix}
S^u_{z_0,h} & S^d_{z_0,h} \\
S^d_{z_0,h} & S^u_{z_0,h}
\end{bmatrix}
\begin{pmatrix}
U + U_s & 0
\end{pmatrix},
$$
(19)

The combination of Eqs. (18) and (19) leads to the linear system,

$$
\begin{pmatrix}
R \\
T
\end{pmatrix} =
\begin{bmatrix}
S^u_{z_0,h} & S^d_{z_0,h} \\
S^d_{z_0,h} & S^u_{z_0,h}
\end{bmatrix}
\begin{pmatrix}
(I + S^d_{z_0,h}) & (I + S^d_{z_0,h})
\end{pmatrix}
\begin{pmatrix}
U + U_s \\
-D_s
\end{pmatrix},
$$
(20)

where

$$
M = (I - S^d_{z_0,h}S^u_{z_0,h})^{-1}S^d_{z_0,h}.
$$
(21)

Once $R$ and $T$ are known, we can obtain the field close to the source and the energy radiated by the source outside the cavity. The final expression of the field radiated by the punctual source $P(x, y, z)$ given in Eq. (13) is obtained by summing the contributions of all the $(a, \beta)$ pseudoperiodic source functions $S_{a,\beta}(x, y, z)$ where $(a, \beta) \in [0, 2\pi/d_n] \times [0, 2\pi/d_q]$.

5. Energy Radiated by a Pseudoperiodic Source $S_{a,\beta}(x, y, z)$

In the superstrate the radiated power per unit solid angle obtained in the direction of the wave vector, $k = a_x x + a_y y + a_z z$, reads as [see Eq. (6a)]

$$
\frac{d\sigma}{d\Omega} = \frac{2\pi^2}{\eta_1} \left[ |X_1^{m,n}|^2 + |Y_1^{m,n}|^2 \right] + 2 \text{Re}(C_1^{m,n} R_x^{m,n} R_y^{m,n}),
$$
(22)

where $\bar{a}$ stands for the conjugate of $a$ and $\text{Re}(c)$ denotes the real part of $c$. In the substrate, we get, in the direction defined by the wave vector $k = \alpha_x x + \beta_y y + \gamma_z z$, Eq. (6b),

$$
\frac{d\sigma}{d\Omega} = \frac{2\pi^2}{\eta_3} \left[ |X_3^{m,n}|^2 + |Y_3^{m,n}|^2 \right] + 2 \text{Re}(C_3^{m,n} T_x^{m,n} T_y^{m,n}),
$$
(23)

Those expressions have meaning only if the wave vector $k$ is real, i.e., $\alpha_n^2 + \beta_n^2 < \varepsilon_1 k_0^2$ in the superstrate or $\alpha_n^2 + \beta_n^2 < \varepsilon_2 k_0^2$ in the substrate. It is worth noting that, when the period of the grating is much smaller than the wavelength, with $(a, \beta)$ taken in the radiative domain (see Fig. 2), this condition holds mainly for $(m, n) = (0, 0)$.

6. $S$ Matrix Calculation

The main numerical difficulty of this method is the calculation of the $S$ matrix of a periodic scatterer (located between two planes $z = z_p$ and $z = z_q$) under the condition of pseudoperiodicity of the field [given by the $(a, \beta)$ couple]. Many techniques have been developed to address this issue and can be found in the literature devoted to grating theories. Our approach is based on the well-known differential method.

The electric and the magnetic fields, $\mathbf{E}$ and $\mathbf{H}$, are expanded onto pseudoperiodic Fourier series (note the presence of $1/i\omega\mu_0$ factor in the magnetic field development),

$$
E(x, y, z) = \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} E^{m,n}(z) \exp(i \alpha_n x + i \beta_n y),
$$
(24a)

$$
H(x, y, z) = \sum_{i=1}^{i=\infty} \sum_{m=-\infty}^{m=-\infty} H^{m,n}(z) \times \exp(i (\alpha_n x + \beta_n y)).
$$
(24b)

Between $z_p$ and $z_q$, $\mathbf{E}$ and $\mathbf{H}$ satisfy the Maxwell equations, Eqs. (1), without the source term. Introducing Eqs. (24) into Eqs. (1) and eliminating the $z$ component of $\mathbf{E}$ and $\mathbf{H}$, we obtain an infinite set of ordinary first-order differential equations with respect to $z$.

$$
\frac{dE_z^{m,n}}{dz} = H_y^{m,n} - \alpha_n \sum_{p,q} \left[ \frac{1}{k^2} \right]_{m-p,n-q} (\alpha_p H_y^{p,q} - \beta_q H_x^{p,q}),
$$

$$
\frac{dE_y^{m,n}}{dz} = H_y^{m,n} - \beta_n \sum_{p,q} \left[ \frac{1}{k^2} \right]_{m-p,n-q} (\alpha_p H_y^{p,q} - \beta_q H_x^{p,q}),
$$

$$
\frac{dH_x^{m,n}}{dz} = \sum_{p,q} \left[ k^2 \right]_{m-p,n-q} E_y^{p,q} - \alpha_n (\alpha_p E_y^{m,n} - \beta_q E_x^{m,n}),
$$
\[
\frac{dH_{z}}{dz} = -\sum_{p,q} \left[ k^{2}\right]_{m-p,n-q} E_{z}^{p,q} - \beta_{n}
\]
\[
\times (a_{m} E_{y}^{m,n} - \beta_{n} E_{x}^{m,n}),
\]
(25)

where \(k^{2} \in m-p,n-q\) and \((1/k^{2}) \in m-p,n-q\) are the Fourier coefficients along \(x\) and \(y\) of
\[
\epsilon(x, y, z) \frac{d}{dz} + 1/[k^{2}]_{x,y}(x, y, z),
\]
\[
e(x, y, z) \frac{d^{2}}{dz^{2}} = \sum_{n=-\infty}^{\infty} \sum_{m=-\infty}^{\infty} \left[ k^{2}\right]_{m,n} \exp(\pm nK_{x} x + \pm iK_{y} y),
\]
(26)

similarly for \(1/[k^{2}]_{x,y}(x, y, z)\). We introduce the \(z\)-dependent column vectors \((E_{p}, H_{p})\) whose elements are the planar components of the fields, \(E_{x}^{m,n}, E_{y}^{m,n}, H_{x}^{m,n}, H_{y}^{m,n}(m, n) \in \mathbb{Z}\).

The integration of the differential system (25) between \(z = z_{p}\) and \(z = z_{q}\) is possible with use of a numerical algorithm such as Runge–Kutta or Adams–Moulton.3

This integration gives a matrix relation between the column vectors at \(z = z_{q}\) and \(z = z_{p}\) (see the shooting method in Ref. 29),

\[
\begin{pmatrix}
E_{p} \\
H_{p}
\end{pmatrix}(z_{p}) = [M] \begin{pmatrix}
E_{p} \\
H_{p}
\end{pmatrix}(z_{p}).
\]

(27)

Now, to introduce the \(S\) matrices, we assume that there exists a homogeneous thin slab surrounding the ordinate \(z_{p}\) and \(z_{q}\) (this is evidently the case when \(z_{p}\) and \(z_{q}\) are in the substrate, superstrate, or in the thin layer including the source); hence we decompose the field at \(z = z_{p}\) and \(z = z_{q}\) into upward and downward waves as in Section 4. This gives, at a particular \(z\) inside the homogeneous slab surrounding \(z_{p}\),

\[
E_{p}^{m,n}(z_{p}) = u_{p}^{m,n} \exp[i\gamma_{p}^{m,n}(z - z_{p})] + d_{p}^{m,n}
\]
\[
\times \exp[-i\gamma_{p}^{m,n}(z - z_{p})],
\]
\[
H_{p}^{m,n}(z_{p}) = u_{p}^{m,n} \exp[i\gamma_{p}^{m,n}(z - z_{p})]
\]
\[
+ d_{p}^{m,n} \exp[-i\gamma_{p}^{m,n}(z - z_{p})],
\]

(note the particular choice of the phase origin), where \(u_{p}\) and \(d_{p}\) are linked to \(u_{p}\) and \(d_{p}\) by

\[
u_{p}^{m,n} = -C_{j}^{m,n} u_{p}^{m,n} - Y_{j}^{m,n} u_{p}^{m,n},
\]
\[
u_{p}^{m,n} = Y_{j}^{m,n} u_{p}^{m,n} + C_{j}^{m,n} u_{p}^{m,n},
\]
\[
u_{p}^{m,n} = C_{j}^{m,n} d_{p}^{m,n} + Y_{j}^{m,n} d_{p}^{m,n},
\]
\[
u_{p}^{m,n} = Y_{j}^{m,n} d_{p}^{m,n} - C_{j}^{m,n} d_{p}^{m,n},
\]

and \(j = (1, 2, 3)\) depending on the position of \(z_{p}\).

We rewrite the matrix relation (27) in the \((u, d)\) basis thanks to Eqs. (28) and (29),

\[
\begin{pmatrix}
U^{v} \\
D^{v}
\end{pmatrix} = [T_{p,q}] \begin{pmatrix}
U^{p} \\
D^{p}
\end{pmatrix},
\]

(30)

where \((U^{v}, D^{v})\) is a column vector whose elements are \(u^{m,n}_{vx}, u^{m,n}_{vy}, d^{m,n}_{jx}, d^{m,n}_{jy}(m, n) \in \mathbb{Z}\), \(v = \{p, q\}\).

\[
[T_{p,q}] = \begin{pmatrix}
T_{uu, p,q}^{p,q} & T_{ud, p,q}^{p,q} \\
T_{du, p,q}^{p,q} & T_{dd, p,q}^{p,q}
\end{pmatrix},
\]

called the transfer matrix between \(z = z_{p}\) and \(z = z_{q}\) enables one to calculate the \(S\) matrix \([S_{p,q}]\) relating the inwardgoing waves to the outgoing waves through simple algebraic manipulations inasmuch as

\[
[U^{p}]^{d+1} = [T_{p,q}][U^{p}]^{d}.
\]

Unfortunately, it appears that in general the passive scatterer lying between \(z = z_{p}\) and \(z = z_{q}\) is too thick for this method to be numerically stable. Indeed, the presence of evanescent waves is poorly handled by the numerical integration along the \(z\) axis. To circumvent this problem, we use a recursive algorithm based on the \(S\)-matrix formalism.22 The interval \([z_{p}, z_{q}]\) is subdivided into \((q - p + 1)\) ordinates of increasing value \(z_{e}\), \(z_{p}, z_{p+1}, z_{p+2}, \ldots, z_{q-1}, z_{q}\). At each ordinate \(z_{e}\), we expand the field into upward- and downward-propagating waves \((U^{e}, D^{e})\),32 (as if there were an infinitely thin air layer). Each subinterval \([z_{e}, z_{e+1}]\) is sufficiently small for the transfer matrix \([T_{e}]\) linking the fields at \(z = z_{e} + 1\) to the fields at \(z = z_{e}\),

\[
[U^{e+1}]^{d+1} = [T_{e}]\begin{pmatrix}
U^{e} \\
D^{e}
\end{pmatrix},
\]

to be accurately calculated. Then we use a stable recursive algorithm22 to construct the total \(S\) matrix \([S_{p,q}]\). The recurrence system yielding \([S_{p,q}]\) from the transfer matrices \([T_{e}]\) is

\[
[S^{dd}_{p,p}] = 1, \
[S^{dd}_{p,q}] = [S^{dd}_{p,q}]^{-1}, [T_{p,q}],
\]
\[
[S^{dd}_{p,p}] = 0, \
[S^{dd}_{p,q}] = (T_{p,q}^{-1} S^{dd}_{p,q})^{-1} T_{p,q}^{-1} M_{q},
\]
\[
[S^{du}_{p,q}] = -S^{dd}_{p,q}^{-1} [T_{p,q}^{-1} H_{q-1} + T_{q}^{-1} G_{q-1}],
\]
\[
[S^{uu}_{p,p}] = 1, \
[S^{uu}_{p,q}] = T_{q}^{-1} H_{q-1} + T_{q}^{-1} G_{q-1},
\]
\[
[S^{uu}_{p,q}] = -S^{dd}_{p,q}^{-1} [T_{p,q}^{-1} H_{q-1} + T_{q}^{-1} G_{q-1}],
\]

(32)

with

\[
M_{q} = (T_{q}^{-1} S^{uu}_{p,q-1})^{-1} T_{q}^{-1} G_{q-1},
\]
\[
G_{q-1}^{-1} = (S^{dd}_{p,q-1})^{-1} S^{dd}_{p,q-1},
\]
\[
H_{q-1} = S^{uu}_{p,q-1} - S^{dd}_{p,q-1} (S^{dd}_{p,q-1})^{-1} S^{uu}_{p,q-1}.
\]

In short, we obtain the \(S\) matrices of the passive scatterers above and below the source with a recurrence formula involving transfer matrices. These transfer matrices are obtained by numerical integration of the set of coupled differential equations presented in Eqs. (25) over a sufficiently small interval.

Now that the main steps of the numerical technique have been presented, we turn to some numerical examples of the radiation pattern of a dipole into various periodic structures.
4. NUMERICAL EXAMPLE: POINTSOURCE RADIATION IN A DOUBLY PERIODIC SQUARE GRATING

The rigorous calculation of the field radiated by a point source located in a waveguide grating structure is of great interest for at least two reasons:

1. At first, the calculation gives the ratio of the energy radiated in the arcs as presented in the shallow grating case in Section 2. This ratio represents the percentage of the light coupled out through the grating.

2. The second point is to investigate the modification of the radiation pattern that is due to an increasing per-

Fig. 5. Results of the computation for the Poynting flux power density per unit solid angle $d\sigma/d\Omega$ in the $k_p/k_0$ plane for three different values of the perturbation parameter $\xi = 0.2$ (A) and (B), $\xi = 0.5$ (C) and (D), and $\xi = 1$ (E) and (F). (A), (C), and (E) are power density emitted in the air; (B), (D), and (F) are power density emitted in the substrate.

turbation of the guide. The first effect of a deeper grating is to broaden the arcs whose width depends on the leakage of the guided mode. Roughly, in the case of a weak perturbation, the leakage and the arc width are proportional to \( h^2 \) [Ref. 33] [see Fig. 2(a)]. In addition to this approximation, a rigorous calculation provides an accurate value of this width. When the perturbation becomes strong enough, the simple WVD analysis presented in Section 2 is not valid anymore, and we observe some modifications of the arc shapes as reported in Ref. 23.

Our goal in this section is to show the influence of the waveguide perturbation on the energy density pattern. To achieve this task, we chose a structure with two guided modes at \( \lambda = 650 \text{ nm} \). The substrate refractive index is \( n_3 = 1.46 \), whereas the film index is \( n_2 = 2 \). The thickness of the guide is \( d = 162.5 \text{ nm} \). The two effective indices of the guided modes are \( n_{\text{eff} \text{TE} 0} = 1.708 \) and \( n_{\text{eff} \text{TM} 0} = 1.553 \). We consider a biperiodic perturbation with an equal period along each axis (\( d_1 = d_2 \)) with a period \( d_0 = \lambda n_{\text{eff} \text{TE} 0} / 380.5 \text{ nm} \) so that \( K_x = K_y = k_j = 2\pi n_{\text{eff} \text{TE} 0} / \lambda \). Hence the TEO guided mode is coupled out at normal incidence (among others). To perform the calculation, we have to choose the values for \( a \) and \( b \) [see Fig. 2(a)]. They are related to the filling factors defined as \( a/d_1 \) and \( b/d_1 \) along each axis. The global filling factor \( f \) defined by the ratio of the groove area \( ab \) over the total unit surface \( d_1d_2 \) is chosen to be 0.5, and therefore we have \( a/d_1 = b/d_1 = \sqrt{0.5} \). This particular value of \( f \) maximizes the first-harmonic Fourier coefficient of the permittivity profile, and, as a matter of fact, the coupling between a guide mode and the grating. To compare accurately the radiation pattern for several values of the perturbation, it is important to keep the same value for the two guided modes’ effective indices. One of the solutions is to keep the total height of the structure constant (\( h = d + h' = 162.5 \text{ nm} \)) and to take the average permittivity of the modulated layer equal to that of the homogeneous guiding layer. As a result, the modulated structure is, on average, a planar guide with thickness \( (h' + d) \) and permittivity \( \varepsilon_g = 4 \) regardless of the groove depth. The average permittivity of the modulated layer composed by half of the air (\( \varepsilon_{\text{air}} = 1 \)) and half of the grooves (\( \varepsilon = \varepsilon_{\text{groove}} \)) is, with a crude approximation, \( (\varepsilon) = f\varepsilon_{\text{groove}} + (1 - f)\varepsilon_{\text{air}} \). Taking a permittivity \( (\varepsilon) = 7 \) for the grooves leads to \( (\varepsilon) = 4 \). Note that this approach is empirical and that, actually, the position of the resonance varies slightly with increasing modulation. The varying parameter characteristic of the perturbation is \( \xi = h'/(d + h') \). \( \xi = 0 \) corresponds to an unperturbed waveguide and \( \xi = 1 \) to a totally perturbed structure.

We can note that the dielectric contrast \( (\varepsilon_{\text{groove}} - \varepsilon_{\text{air}})/2(\varepsilon) = 0.75 \) is kept constant and is also an important parameter of the waveguide perturbation. The domain of validity of the WVD analysis presented in Section 2 is for small values of \( \xi \). To maximize the emission efficiency of the point source the guided modes, we placed the dipole at the guide center \( (d + h')/2 \) where electromagnetic fields are the most intense for the two fundamental modes.

Figure 5 shows the results of the computation for the radiated power \( d\sigma/d\Omega \) in the \( k_p/k_0 \) plane for three different values of the perturbation parameter \( \xi = 0.2 \) (A) and (B), \( \xi = 0.5 \) (C) and (D), and \( \xi = 1 \) (E) and (F). In these calculations the source is taken along the \( x \) axis \( (P = P_x) \) and therefore emits strongly in the \( (0, 1) \) and the \( (0, -1) \) multiplicities [see Fig. 2(b)]. Note that the TM arcs are not numerically visible, because their width is approximately ten times sharper than that of the TE. A structure equivalent to \( \xi = 0.1 \) was already reported in Ref. 34. In Fig. 5 the leftmost and the rightmost diagrams represent the energy radiated into the air and into the substrate, respectively. As foreseen, the first effect of the perturbation is to widen the arcs [Figs. 5(A) and 5(C)]. The simple WVD analysis presented in Section 2 remains valid for a remarkable domain. Even for \( \xi = 0.5 \), the arcs, which are broader than for \( \xi = 0.2 \), always have the same localization and radius of curvature. We checked numerically that the energy emitted along the arcs remains more or less constant: Sharper arcs are characterized by higher power densities (see the gray-scale in Fig. 5). In any case, the light emitted into all the arcs represents \( \sim 65\% \) of the total emitted light.

The effects of a strong perturbation are clearly visible in Figs. 5(E) and 5(F) \( (\xi = 1) \). The guide is totally dug, which corresponds to the maximal perturbation for our structure. This regime is far from being intuitive, since the WVD analysis is no longer valid. Nevertheless, from the calculations we can make the following comments:

- We can see the modification of the arc curvature, which are no longer circular. On top of that, energy is concentrated at the arc intersections, where two modes are simultaneously coupled.
- The strong emission near \( \alpha = \beta = 0 \) indicates that most of the emitted light is concentrated near the normal incidence. More precisely, if we consider a cone of half-angle 90 deg (upward half-space), we have ensured that the total emitted energy is constant for the three structures. But the power emitted into a 15-deg cone increases with \( \xi \) to reach, for \( \xi = 1 \), 25% of the power emitted into the 90-deg cone. More complex grating profiles \(^{35} \) should improve the energy concentration in specific directions.

This final point and the experimental confirmation of these predictions are under investigation.

5. CONCLUSION

We have presented an electromagnetic analysis of the far-field radiation pattern of an active source located inside a modulated structure. When the modulation is weak, we propose a simple interpretation of the radiation behavior based on geometric considerations in the wave-vector diagram (WVD). To obtain quantitative results even for strong modulations, we have developed a rigorous electromagnetic implementation that permits us to compute the fields radiated by the source inside and outside the modulated structure. Special emphasis has been given to cross gratings, which allow for a total coupling out for the light emitted into the guided modes of the grating guide.

We show that a strong corrugation can lead to energy concentration in directions close to the sample normal. This property is important in the context of spontaneous emission control with microcavity resonators and is of potential interest for building high-extraction-coefficient light-emitting devices.
REFERENCES


