k gaps for multimode waveguide gratings

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Eigenmodes (plasmons or guided modes) in dielectric or metallic gratings can be excited by an incident free space wave. This excitation yields an anomaly in the reflectivity curves with respect to the incident wavelength or angle. The anomaly is often used experimentally to exhibit the mode dispersion relation. By studying the reflectivity of a weakly corrugated dielectric waveguide, we show that, at the crossing of two independent mode dispersion relations, the anomaly disappears for a wide range of incident angles, thus forming a k gap. We point out that, in this case, the loci of the anomaly differ strongly from the dispersion relation of the modes. We derive a simple model that accounts for this phenomenon.

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Dielectric or metallic multilayer stacks can support eigenmodes (guided modes or plasmons) that can be excited with an incident plane wave provided that a suitable grating is included in the structure. The coupling and decoupling of the mode induces rapid variations, from a minimum to a maximum, of the grating reflected orders with respect to the wavelength and angle of incidence. These are the so-called Wood anomalies.[1] Experimentally, the dispersion relation of the eigenmode is inferred from the reflectivity maximum (for dielectrics) or minimum (for metals or dielectrics), with respect to the incident temporal frequency ω and spatial frequency k (hereafter, k is the projection of the incident wave vector on the plane of the layers).[2–4] This approach is in general accurate. Yet, for some metallic configurations,[5] the reflectivity minimum locus revealed the existence of a k gap at the crossing point of the dispersion relation of the plasmon, instead of an ω gap.[6–8] After some confusion,[9] theoretical works pointed out that the opening of the k gap in the reflectivity extrema locus was connected to a weak direct coupling between the two modes,[10,11] hence to a small ω gap in the mode dispersion relation. In this case, the dispersion relation of the mode cannot be inferred simply from the reflectivity anomaly. In this paper, we point out the nontrivial link between the radiative properties and the mode dispersion relation when two modes are excited simultaneously in the structure. We consider a weakly periodically perturbed waveguide and we study the excitation of guided modes instead of plasmons. Taking advantage of the absence of loss, of the symmetry properties of the structure and of the possibility of exciting independent modes, we are able to exhibit well-pronounced k gaps both for the reflectivity and transmittivity minima. We provide a simple model that explains thoroughly this phenomenon. The surprising radiative behavior of these multimode structures could be used for designing new optical functions.

Since the 1970s, an important theoretical work has been performed to show that the Wood anomalies can be interpreted in terms of poles and zeroes of the reflection and transmission coefficients of the resonant grating, in the special case where only the specular order is propagative.[12] More precisely, when only one eigenmode is excited, with a fixed incident temporal frequency ω, and a varying incident spatial frequency k the reflection and transmission coefficients of the structure can be written as

$$R = r_{ref}\frac{k-k_{zr}}{k-k_p} \quad \text{and} \quad T = t_{ref}\frac{k-k_{zt}}{k-k_p}, \tag{1}$$

where r_{ref} and t_{ref} are the reflection and transmission coefficients away from the resonance, and k_{zr}, k_{zt}, and k_p are *a priori* complex zeroes and pole. It has been shown[13] that curves obtained from Eq. (1) fit perfectly the reflectivity and transmittivity curves obtained from rigorous numerical calculation. Hence the knowledge of the pole and zeroes is sufficient to account for the reflectivity and transmittivity properties of the resonant grating. Note that the pole and zeroes can be obtained numerically by studying R and T for complex incident spatial frequencies k. In this Brief Report, we derive expressions of k_{zr} and k_{zt} in relation to k_p, thanks to an approached model. We consider a dielectric multilayer stack, with relative dielectric constant $\epsilon_{ref}(z)$. We assume that this reference structure supports one or several guided modes in the range of wavelengths under study. In the following, we will consider only TE modes (electric field perpendicular to the direction of propagation). We introduce a periodic perturbation to the reference structure. The period d is small enough as compared to the wavelength, so that solely the specular order is propagative in the substrate and superstrate. Due to the periodic perturbation, the guided modes of the reference structure become leaky and they can be excited with an appropriate incident wave, and decoupled into free space. In this Brief Report, we assume that the structure is periodic along one direction (Ox), with spatial frequency $K = 2\pi/d$, and invariant along the orthogonal direction (Oy) (Fig. 1). We call $\epsilon(x,z)$ the relative dielectric constant of the structure, and we introduce the dielectric constant of the perturbation,

$$\epsilon_{per}(x,z) = \epsilon(x,z) - \epsilon_{ref}(z), \tag{2}$$

and Ω the domain where ϵ_{per} is nonzero. We consider an incident monochromatic plane wave coming from the superstrate (dielectric relative permittivity ϵ_a), whose wave vector in the (Oxz) plane is described by its spatiotemporal frequencies (k,ω). The incident wave is TE polarized, and its electric field along (Oy) is $E_{inc}(x,z)=\exp(ikx-i\gamma^a z)$, where $\gamma^a = \sqrt{(\epsilon_a k_0^2 - k^2)}$, and $k_0=\omega/c$ is the wave number in vacuum (c is the celerity of light in vacuum). Hereafter, the $\exp(-i\omega t)$ dependency is omitted. We note $E(x,z)$ and $E_{ref}(z)$ the elec-

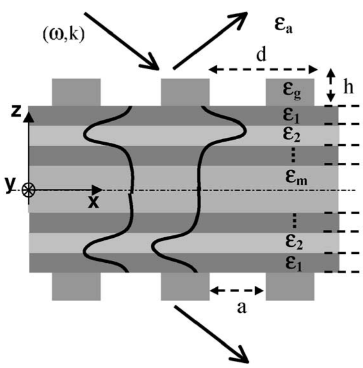

FIG. 1. Geometry of the studied configuration. The structure is invariant along (Oy) and symmetrical with respect to the (Oxy) and (Oyz) planes. The periodicity of the structure and the spatial frequency of the incident wave are chosen in order to excite two independent eigenmodes.

tric fields solutions of the diffraction problems for the whole structure, and the reference (planar) structure, respectively. Hence the field $E-E_{ref}$ is the solution of the equation

$$\Delta(E-E_{ref})+k_0^2\epsilon_{ref}(E-E_{ref})=-k_0^2\epsilon_{per}E, \qquad (3)$$

that satisfies an outgoing-wave boundary condition. Due to the periodicity along (Ox), the field E is pseudoperiodic: it can be written as a Floquet-Bloch expansion $E(x,z)=\Sigma_n e_n(z)\exp[ix(k+nK)]$. To solve Eq. (3), we introduce the pseudoperiodic Green function $G(k,x-x',z,z')$, the solution of Eq. (3) with the right-hand side equal to the Dirac distribution sum $\Sigma_n\delta(x-x'-nd,z-z')\exp[ik(x-x')]$.[14] Finally, we can show that the coefficients e_n are the solution of a coupled set of equations

$$e_n(z)=\delta_{n,0}e_{ref}(z)+\int_\Omega dz' G_n(z,z')\sum_m \tilde{\epsilon}_{n-m}(z')e_m(z'), \qquad (4)$$

where $\tilde{\epsilon}_m$ are the coefficients of the Fourier expansion of ϵ_{per}, $G_n(z,z')$ are the coefficients of the Floquet-Bloch expansion of G, and e_{ref} is defined by $E_{ref}(x,z)=e_{ref}(z)\exp(ikx)$. In the superstrate, $e_{ref}(z)=r_{ref}\exp(i\gamma^a z)+\exp(-i\gamma^a z)$, and in the substrate (dielectric relative permittivity ϵ_s), $e_{ref}(z)=t_{ref}\exp(-i\gamma^s z)$, where $\gamma^s=\sqrt{(\epsilon_s k_0^2-k^2)}$. From Eq. (4), it is possible to derive an analytic expression for e_0, which yields the reflection and transmission coefficients as functions of the temporal frequency ω and spatial frequency k. Indeed, in the superstrate, $e_0(z)=R\exp(i\gamma^a z)+\exp(-i\gamma^a z)$, and in the substrate, $e_0(z)=T\exp(-i\gamma^s z)$. In the following, we choose to keep ω real constant, and to search for the complex spatial frequency k such that the reflectivity or transmittivity of the structure is null.

First, we choose the period of the structure and the incident wave in such a way that only one leaky eigenmode, with spatial frequency k_m at the incident temporal frequency ω, is excited through the qth grating order. In other words, the incident spatial frequency k varies in the vicinity of $k_p=k_m-qK$. As a consequence, the field in the qth order of the grating is prevailing when k is in the vicinity of k_p. Hence, in our perturbative calculation of e_0, we will take into account only the term coming from the decoupling of the mode (the qth order), plus the reference field, and neglect the other terms:

$$e_0(z)\simeq e_{ref}(z)+\int_\Omega dz' G_0(z,z')\tilde{\epsilon}_{-q}(z')e_q(z'), \qquad (5)$$

where $e_q(z)\simeq\int_\Omega dz' G_q(z,z')\tilde{\epsilon}_q(z')e_{ref}(z')$.[15] To take into account the existence of the resonance, we write the qth coefficient of the Green function as

$$G_q(z,z')\simeq\frac{A_q(z,z')}{k-k_p}, \qquad (6)$$

for k in the vicinity of k_p. Injecting Eq. (6) into Eq. (5), we obtain the following expressions for the reflection and transmission coefficients:

$$R\simeq r_{ref}+\frac{X_q}{k-k_p} \quad \text{and} \quad T\simeq t_{ref}+\frac{Y_q}{k-k_p}, \qquad (7)$$

where

$$X_q=\int_\Omega dz' g_{0r}(z')\tilde{\epsilon}_{-q}(z')\int_\Omega dz'' A_q(z',z'')\tilde{\epsilon}_q(z'')e_{ref}(z''), \qquad (8)$$

and Y_q is obtained by replacing g_{0r} with g_{0t} in Eq. (8). To obtain Eq. (7), we used the following property of the Green function: $G_0(z,z')=g_{0r}(z')\exp(i\gamma^a z)$ for z in the superstrate

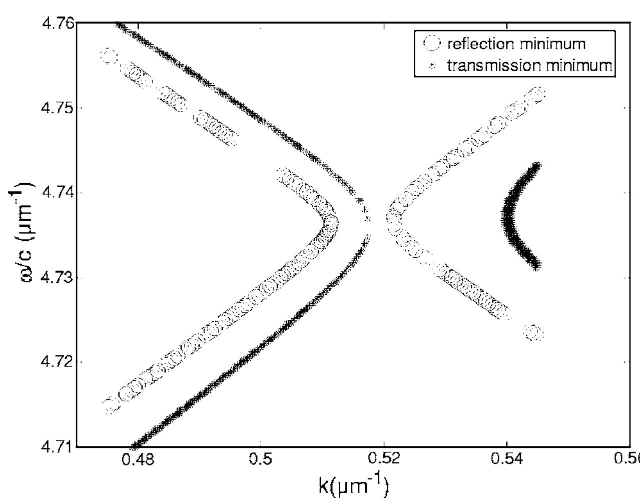

FIG. 2. Trajectory of the minimum of reflectivity (void circles) and the minimum of transmittivity (black stars) with respect to the temporal and spatial frequencies ω and k (criterion: $|R|^2$ and $|T|^2$ are less than 10^{-4}). A wide k gap is observed in both trajectories. The grating parameters are (see Fig. 1) $h=300$ nm, $d=1076$ nm, $a=538$ nm, and $\epsilon_g=2.1609$. The thickness and relative permittivity of the layers are ($t_1=187$ nm, $\epsilon_1=4.2849$), ($t_2=264$ nm, $\epsilon_2=2.1609$), ($t_3=187$ nm, $\epsilon_3=4.2849$), ($t_4=264$ nm, $\epsilon_4=2.1609$), ($t_5=187$ nm, $\epsilon_5=4.2849$), ($t_6=264$ nm, $\epsilon_6=2.1609$), ($t_7=1000$ nm, $\epsilon_7=2.0967$) from top to the middle layer. The surrounding media is air, $\epsilon_a=1$. In all figures, the calculations are performed with a rigorous Fourier modal method (Ref. 16).

and $G_0(z,z')=g_{0t}(z')\exp(-i\gamma^s z)$ for z in the substrate.[18] We deduce from Eq. (7) the expressions of the zeroes:

$$k_{zr} \simeq k_p - \frac{X_q}{r_{ref}} \quad \text{and} \quad k_{zt} \simeq k_p - \frac{Y_q}{t_{ref}}, \tag{9}$$

where r_{ref} and t_{ref} are the reference planar structure reflection and transmission coefficients (e.g., the reflection and transmission coefficient away from the resonance). In Eq. (7), it appears that the field diffracted by the structure is the sum of the field diffracted by the planar structure and the field coming from the coupling and decoupling of the eigenmode. Hence the zeroes in reflection and transmission can be interpreted in terms of destructive interferences between these two fields. Note that these results are available whatever the structure symmetry. In the particular case when the structure is symmetrical with respect to the (Oxy) and (Oyz) plane (see Fig. 1), it can be shown from Eq. (8) that X_q and Y_q are not proportional to r_{ref} and t_{ref}. Hence, from Eq. (9), we note that the zeroes k_{zr} and k_{zt}, in general complex, follow the pole k_p, and that the zero of reflection (transmission) will be all the farther from the pole than the reference structure reflectivity (transmittivity) is low. Similar expressions are obtained for the temporal frequency of the zeroes ω_{zr} by fixing the spatial frequency k (real).

Now, we consider a structure presenting a plane of symmetry parallel to the plane of the layers (Fig. 1), and we choose the grating period and the incident wave in such a way that a symmetric and an antisymmetric mode are simultaneously excited, in opposite directions, through the orders q_+ and q_- of the grating, respectively. We note k_m^+ and k_m^- are the spatial frequencies of the symmetric and antisymmetric modes at the incident temporal frequency ω, and we introduce the notations $k_{p+}=k_m^+-q_+K$ and $k_{p-}=-k_m^-+q_-K$. In other words, the incident spatial frequency k varies in the vicinity of $k_p^+\simeq k_p^-$. Taking inspiration from Eq. (7), and reminding that the two modes are independent, it can be shown that the reflection coefficient takes the following form:

$$R \simeq r_{ref} + \frac{X_{q+}}{k-k_p^+} + \frac{X_{q-}}{k-k_p^-}, \tag{10}$$

where the expression of the numerator $X_{q\pm}$ is the same as that obtained when exciting one eigenmode independently of the other. Hence it is easy to show that, at a given ω, when both modes are excited, the zero of reflectivity is obtained for two spatial frequencies,

$$k_{zr}^j \simeq \frac{k_{zr}^+ + k_{zr}^-}{2} \pm \frac{1}{2}\sqrt{(k_{zr}^+ - k_{zr}^-)^2 + 4(k_{zr}^+ - k_p^+)(k_{zr}^- - k_p^-)}, \tag{11}$$

where $j=1$ or 2 according to the sign before the square root, and k_{zr}^+ and k_{zr}^- are given by Eq. (9), with k_p^+ and k_p^- replacing k_p. Similarly, when the spatial frequency k is fixed, one finds two temporal frequencies at which the reflectivity is null,

$$\omega_{zr}^j \simeq \frac{\omega_{zr}^+ + \omega_{zr}^-}{2} \pm \frac{1}{2}\sqrt{(\omega_{zr}^+ - \omega_{zr}^-)^2 + 4(\omega_{zr}^+ - \omega_p^+)(\omega_{zr}^- - \omega_p^-)}, \tag{12}$$

where $\omega_{zr}^\pm$ are the zeroes obtained when only one mode is excited. Similar expressions are obtained for the zeroes in transmission, k_{zt} and ω_{zt}, by replacing the index r by t in Eqs. (11) and (12). In the following, we limit our discussion to the zeroes in reflection, but the same properties apply to the zeroes in transmission.

First of all, we note that when two independent modes are excited simultaneously, we can no more differentiate the zero of the symmetric mode from the zero of the antisymmetric mode: a coupling occurs between the zeroes, whereas there is no coupling between the modes. Second, it can be shown, for resonant grating presenting a plane of symmetry parallel to the plane of the layers, and when only one mode is excited, that the zeroes in reflection (k_{zr}^+ and k_{zr}^-) and (ω_{zr}^+ and ω_{zr}^-) are real,[13] and that it is the same for the zeroes in transmission. In this case, the loci of the zeroes are easily seen in the

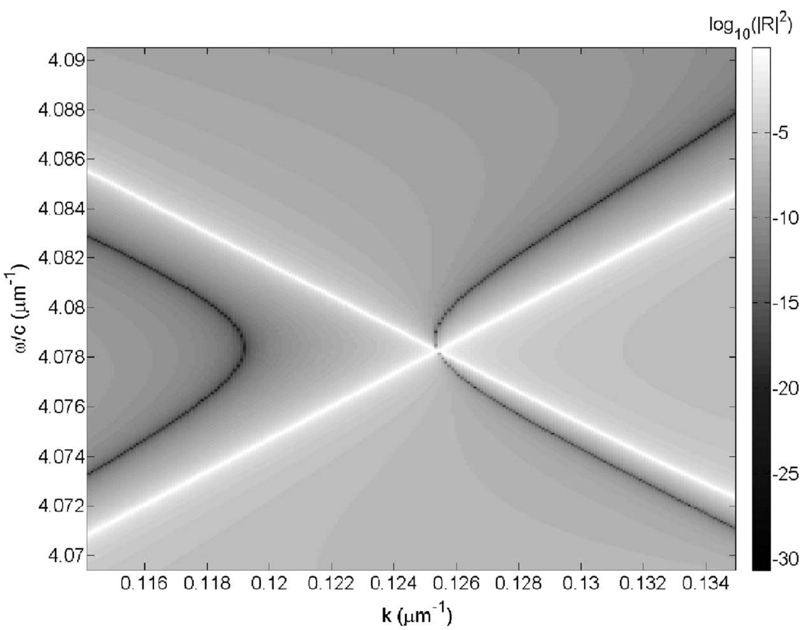

FIG. 3. Reflectivity with respect to the incident temporal and spatial frequencies ω and k. The grating parameters (see Fig. 1) are $h=50$ nm, $d=1076$ nm, $a=269$ nm, and $\epsilon_g=2.1609$. The thickness and relative permittivity of the layers are ($t_1=349$ nm, $\epsilon_1=2.1609$), ($t_2=70.1$ nm, $\epsilon_2=4.2849$), ($t_3=3000$ nm, $\epsilon_3=2.0967$) from top to the middle layer. The surrounding media is air, $\epsilon_a=1$. A wide k gap is observed in the trajectory of the minimum of reflectivity (in black).

reflectivity map $R(k,\omega)$, since it corresponds either to a null or 100% reflectivity. The demonstration[13] is based on the reciprocity theorem and the conservation of energy. Using the same arguments, one can easily show that when two modes are excited, the two coupled zeroes k_{zr}^1 and k_{zr}^2 [Eq. (11)] or ω_{zr}^1 and ω_{zr}^2 [Eq. (12)] are either real or complex conjugate. Then, reminding that the real and the imaginary parts of k_m are positive, simple arithmetic leads to the conclusion that $(k_{zr}^+ - k_p^+)(k_{zr}^- - k_p^-)$ is always positive. This means that, for a fixed temporal frequency, the zeroes k_{zr}^1 and k_{zr}^2 are always real, and split-up on each side of a mean value. This is the proof of the forming of a k gap. In Fig. 2, we plot the reflectivity maximum and minimum (calculated thanks to a rigorous Fourier modal method[16]) of a structure depicted in Fig. 1. We observe that the loci of the zeroes of reflection and transmission present a k gap. Moreover, from Eq. (9) and (11), we note that the weaker the reflectivity r_{ref} of the reference structure, the larger the k gap between the zeroes in reflection, and the smaller the k gap between the zeroes in transmission. This can be seen in Fig. 3, where we plot the reflectivity of a resonant grating depicted in Fig. 1 with $r_{ref} \simeq 0$ (antireflection coating). The structure being symmetrical with respect to the (Oxy) plane and the material lossless, the reflectivity minimum (in black) and maximum (in white) loci correspond to the trajectories of the zeroes of reflection and transmission, respectively. The k gap between the zeroes in reflection is wide, while the k gap between the zeroes in transmission is much narrower, it is not visible on the figure. We have conducted a similar study of the zeroes ω_{zr}^1 and ω_{zr}^2 obtained for a fixed spatial frequency. Contrary to the previous case, one can show that $(\omega_{zr}^+ - \omega_p^+)(\omega_{zr}^- - \omega_p^-)$ is always negative, thus ω_{zr}^1 and ω_{zr}^2 can be complex conjugate. In Fig. 4, we plot the real and imaginary part of ω_{zr}^1 and ω_{zr}^2 obtained numerically with respect to k real, for the same structure as in Fig. 3. We observe that the zeroes become complex, for k values belonging to the k gap observed in Fig. 3. Note that when two counterpropagative modes are excited with a strong direct coupling between them, an ω gap occurs both for the poles and for the zeroes.[17] More precisely, in this case, the zeroes for ω are real and split on each side of a mean value, while the zeroes for k are complex conjugate.

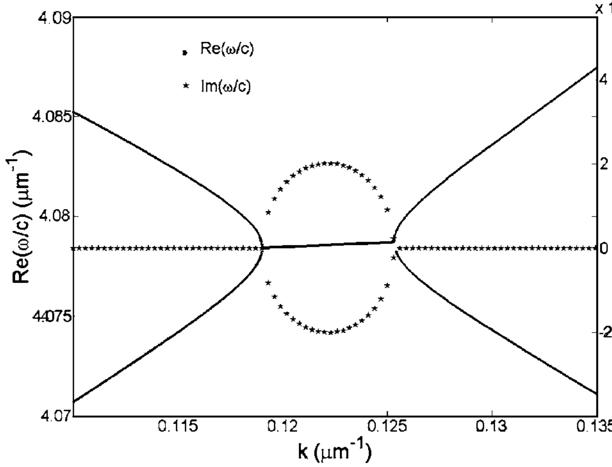

FIG. 4. Trajectory of the complex zeroes of reflection ω_{zr}^1 and ω_{zr}^2 [obtained numerically (Ref. 16)], real part (dark points) and imaginary part (stars) with respect to k for the structure of Fig. 3.

As a conclusion, we have shown that the loci of the Wood anomalies of a weakly periodically perturbed waveguide can strongly differ from the dispersion relation of the excited mode. More precisely, when two independent modes are excited, we have demonstrated the existence of a well-pronounced k gap for the loci of the reflectivity and transmittivity minima. From a practical point of view, the existence of k gaps may be interesting, since it provides broadband devices (filters, sensors,...) with high angular selectivity. In our opinion, the optical properties of structures in which several eigenmodes of different kinds, guided waves, plasmons, and cavity modes, are excited simultaneously, could be explained with an extension of the simple model presented here. Such a tool should permit the tailoring of nanostructures with ultraspecific and requested optical properties.

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