Description of the modes governing the optical transmission through metal gratings

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Abstract: An analytical model based on a modal expansion method is developed to investigate the optical transmission through metal gratings. This model gives analytical expressions for the transmission as well as for the dispersion relations of the modes responsible for high transmission. These expressions are accurate even for real metals used in the visible – near-infrared wavelength range, where surface plasmon polaritons (SPP’s) are excited. The dispersion relations allow the nature of the modes to be assessed. We find that the transmission modes are hybrid between Fabry-Pérot like modes and SPP’s. It is also shown that it is important to consider different refractive indices above and below the gratings in order to determine the nature of the hybrid modes. These findings are important as they clarify the nature of the modes responsible for high transmission. It can also be useful as a design tool for metal gratings for various applications.

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1. Introduction

The observation of enhanced optical transmission (EOT) through a periodic array of subwavelength holes in a metal film was reported more than ten years ago by Ebbesen et al. [1]. This observation has lead to many studies exploring the complex process responsible for EOT as well as its potential for various applications [2]. To clarify the EOT process observed in Ref. [1], many theoretical studies considered metal lamellar gratings, i.e. the one dimensional equivalent of a periodic array of holes. As pointed out in several studies [3,4], care must be taken in the analogy between one and two dimensional structures. In the one dimensional case there is always a propagating mode inside slits for TM polarization (electric field perpendicular to the slit), whereas in the two dimensional case a cut-off wavelength exist for holes. Consequently, the transmission process for the two types of structures is different. However, even one dimensional gratings show complex transmission properties.

Several past studies observed transmission peaks following the surface plasmon polariton (SPP) dispersion curves and consequently attributed the high transmission to SPP excitation [3,5,6]. Other high transmission peaks presenting no dispersion with respect to the incident angle where attributed to Fabry-Pérot (FP) resonances inside slits [5,7,8]. In fact, there is a continuous change from FP related peaks to SPP related peaks, as reported by several studies [4,9,10]. This has been explained by Marquier et al. as coupled SPP-FP modes [10].

The exact role of SPP in the transmission process has been controversial. Several studies observed that the transmission at the SPP condition is close to zero [11,12]. Also, peaks observed in close proximity to the SPP condition were sometimes not attributed to SPP excitation but to the discontinuity observed when a diffracted order passes from evanescent to propagating [13,14], i.e. at the Rayleigh anomaly. We see from this brief résumé that the nature of the coupled modes responsible for the transmission peaks is not clear.

In the present work, an analytical model derived from the work of Lochbihler et al. [15] is developed in Sect. 2. From this analytical model, accurate analytical formula for the transmission and for the dispersion relations of the transmission resonances are obtained in Sect. 3. This allows the nature of the modes responsible for high transmission to be determined. Also, it is shown in Sect. 4 that the controversy regarding the role of the SPP modes in the transmission process can be lifted by considering asymmetric gratings (i.e. with a different refractive index above and below the grating) instead of symmetric ones (i.e. with the same refractive index above and below the grating). In light of this discussion, the symmetric grating is revisited in some details. Finally, the low transmission observed at the SPP condition is discussed.
2. Theoretical formalism

2.1 Structure under study

We study the transmission of a plane wave through an infinite metal lamellar grating of period $p$, thickness $h$ and slit width $w$, see Fig. 1. The metal permittivity is denoted $\varepsilon$ while the permittivity above the grating, inside the slits and below the grating is denoted $\varepsilon_1$, $\varepsilon_2$ and $\varepsilon_3$ respectively. The incident wave, with wavevector $k_0 = \frac{2\pi}{\lambda}$, propagates in a direction contained in the $(x, y)$ plane and forms an angle $\theta$ with the $y$ axis. With these conditions, the grating does not mix polarization so the two different polarizations can be treated independently. Only TM polarization (magnetic field in the $z$ direction) is considered as TE polarization (electric field in the $z$ direction) does not excite SPP.

\[ H_z(x, y) = \exp \left\{ i \left[ k_{x,0} x - k_{y,0} (y - h/2) \right] \right\} + \sum_{n=\infty}^{\infty} r_n \exp \left\{ i \left[ k_{x,n} x + k_{y,n} (y - h/2) \right] \right\} \text{ for } y \geq h/2, \]

\[ H_z(x, y) = \sum_{n=\infty}^{\infty} t_n \exp \left\{ i \left[ k_{x,n} x - k_{y,n} (y + h/2) \right] \right\} \text{ for } y \leq -h/2, \]

where $k_{x,n} = (\sqrt{\varepsilon_1})k_0 \sin \theta + n(2\pi/p)$, $n$ is an integer related to the $n^{th}$ diffracted order, $k_{y,d,n} = (\varepsilon_d k_0^2 - k_{x,n}^2)^{1/2}$ where $d = 1$ or 3. $r_n$ and $t_n$ are respectively the amplitudes of the reflected and transmitted fields. Inside the apertures, i.e. for $-h/2 \leq y \leq h/2$ and $0 \leq x \leq w$, the magnetic field is expressed as a sum of waveguide modes:

Fig. 1. A schematic of the studied structure and definitions used in this article for the structure dimensions and incident field directions.

2.2 Theoretical development

The model used to calculate the optical properties of metal lamellar gratings are detailed here. As a starting point, the method of Lochbihler et al. [15] is considered. In this method, surface impedance boundary conditions (SIBC) are used at metal dielectric interfaces. SIBC have been used successfully for gold gratings in the visible to infrared wavelength range [16,17]. Using SIBC, the electromagnetic field in the metal is not calculated. Therefore, this model assumes there is no evanescent tunnelling through the metal and is limited to metal walls with thickness greater than the metal skin depth, as is the case in the present study.

The magnetic field above and below the grating is rigorously expressed as a Rayleigh (or plane wave) expansion:

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\[ H_j(x, y) = \sum_{m=0}^{\infty} X_m(x) [a_m \exp(i\beta_m y) + b_m \exp(-i\beta_m y)], \]  
(3)

with \(a_m\) and \(b_m\) respectively the amplitudes of backward and forward propagating waves inside the slit related to the mode number \(m\) \((m\) being an integer), \(X_m(x) = \cos(\mu_m x) + \sin(\mu_m x)\eta_2\beta_m\) where \(\mu_m\) is the \(m\)th eigenvalue of the transcendental equation \(\tan(\mu_m w) = 2 \eta_2 \mu_m (\mu_m^2 - \eta_2^2)\), \(\beta_m = (k_0 - \mu_m^2)^{1/2}\) and \(\eta_2 = -i\varepsilon_0 k_0 \mu_0^{1/2}\).

To satisfy the continuity of tangential components of electric and magnetic fields, the continuity of \(H_j\) and its normal derivative are considered. Matching \(H_j\) at \(y = \pm h/2\), multiplying for any \(m = j\) the resulting equations by \(X_j(x)\) and integrating over the region \(0 \leq x \leq w\) as done in Ref. [15], the following set of equations is obtained for any \(m = j\):

\[ I_j \left[ a_j \exp(i\beta_j h/2) + b_j \exp(-i\beta_j h/2) \right] = \sum_{n=-\infty}^{\infty} (r_n + \delta_{n,0}) K_{j,n}, \]  
(4)

\[ I_j \left[ a_j \exp(-i\beta_j h/2) + b_j \exp(i\beta_j h/2) \right] = \sum_{n=-\infty}^{\infty} t_n K_{j,n}, \]  
(5)

where the overlap integrals are defined by:

\[ I_j = \int_0^w X_j(x) X_j(x) \, dx = \left[ 1 + \left( \frac{\eta_2}{\mu_j} \right)^2 \right] \frac{w + \eta_2}{2}, \]  
(6)

\[ K_{j,n} = \int_0^w \exp(ik_{x,\pm x} x) X_j(x) \, dx. \]  
(7)

In a similar way, the normal derivative of \(H_j\) are matched at \(y = \pm h/2\) for \(0 \leq x \leq w\) and SIBC is considered at metal - dielectric interfaces at \(y = \pm h/2\) for \(w \leq x \leq p\). The obtained equations are multiplied for any \(n = q\) by \(\exp(-i\varepsilon_{x,q} x)\) and integrated over the region \(0 \leq x \leq p\). This gives the following set of equations for any \(n = q\):

\[ ik_{y,\pm q} \left( r_q - \delta_{q,0} \right) = i \frac{\varepsilon_1}{\varepsilon_2} \sum_{m=0}^{\infty} \beta_m \left[ a_m \exp(i\beta_m h/2) - b_m \exp(-i\beta_m h/2) \right] J_{q,m}, \]  
(8)

\[ + \eta_1 \sum_{n=-\infty}^{\infty} (r_n + \delta_{n,0}) Q_{q,n}, \]

\[ ik_{y,\pm q} t_q = -i \frac{\varepsilon_1}{\varepsilon_2} \sum_{m=0}^{\infty} \beta_m \left[ a_m \exp(-i\beta_m h/2) - b_m \exp(i\beta_m h/2) \right] J_{q,m}, \]

\[ + \eta_1 \sum_{n=-\infty}^{\infty} t_n Q_{q,n}, \]  
(9)

where \(\eta_d = -i\varepsilon_0 k_0 \mu_0^{1/2}\) \((d = 1 \text{ or } 3)\) and the overlap integrals are defined by:

\[ J_{q,m} = 1/p \int_0^w \exp(-i\varepsilon_{x,q} x) X_m(x) \, dx, \]  
(10)

\[ Q_{q,n} = 1/p \int_0^w \exp[i(k_{x,n} - k_{x,q}) x] \, dx. \]  
(11)

The calculation of the unknown coefficients \(r_n\), \(t_n\), \(a_m\) and \(b_m\) can then be performed after truncation and writing Eqs. (4), (5), (8), (9) into a matrix equation.

In order to have a better understanding of the transmission properties of the grating, two simplifications are made here as compared to the model described in Ref. [15]: (i) The
fundamental slit mode $\beta_0$ is the only one considered as it is the only propagating mode for narrow slits, the others being evanescent. This approximation has already been made for narrow slits (i.e. $w < \lambda/10$) to study light transmission through slit arrays [4,11,13,18,19] but also hole arrays [20]. (ii) The $Q_{q,q}$ matrix defined by Eq. (11), which represents the overlap between plane waves, is considered as the identity matrix. This approximation, also valid for narrow slits, means that the plane waves do not mix via scattering from the slits. With these two approximations, Eqs. (4), (5), (8), (9) lead to analytical expression of $r_n$, $t_n$, $a_m$ and $b_m$. The transmission amplitude of order $q$ $t_q$ is expressed as:

$$t_q = \frac{4(e_1/e_2) J_{0,0} K_{0,0} \left(k_{1,0} + k_0 e^{-i}\right)^{-1} \left(k_{1,0} + k_0 e^{-i}\right)^{-1} k_{1,0} Y_2}{\sum_{n=-\infty}^{\infty} (Y_{n+2} + Y_2) \sum_{n=-\infty}^{\infty} Y_{n+2} - Y_2 \sum_{n=-\infty}^{\infty} Y_{n+2} - Y_2} e^{i\beta_0 h}, \quad (12)$$

where $Y_{d,n} = (e_d e_2) J_{0,0} K_{0,0} (k_{d,0} + e_d k_0 e^{-i\lambda/2})^{-1}$ for $d = 1$ or 3 and $Y_2 = I_d/\beta_0$. The transmission through the grating is then obtained summing the transmission intensities $T_q$ of any propagating diffracted orders where $T_q = \left(\sqrt{\epsilon_1 \cos \theta_{out,q}}/\sqrt{\epsilon_1 \cos \theta}\right)^2$ with $\theta_{out,q}$ the angle of the $q^{th}$ outward propagating order.

### 2.3 Comparison with other models

To show the validity of Eq. (12), transmission spectra of a gold grating are plotted in Fig. 2 for: (i) the rigorous coupled wave analysis [21] (RCWA, green dashed curve); (ii) the modal expansion method described in Ref. [15]. (red solid curve); (iii) Eq. (12) (blue dotted curve). The chosen parameters for the grating are $w = 50$ nm, $p = 1000$ nm, $h = 600$ nm, $\epsilon_1 = \epsilon_2 = \epsilon_3 = 1$ and normal incidence. Visible to near infrared wavelengths are considered, a range where SPP excitation is observed for gold. For all the calculations done in this paper, the permittivity of gold is taken from the Sopra database [22]. Excellent agreement is observed for the three different spectra, validating the use of the above method. The spectra have also been compared with results obtained from a finite difference time domain (FDTD) code [23] and show excellent agreement in the range of parameters used in the present paper (not shown here).

![Fig. 2. Transmission spectra of a gold grating with $p = 1000$ nm, $w = 50$ nm, $h = 600$ nm, $\epsilon_1 = \epsilon_2 = \epsilon_3 = 1$ and normal incidence obtained from: modal expansion method described in Ref. [15]. (red solid curve), RCWA (green dashed curve) and Eq. (12) (blue dotted curve).](image-url)
RCWA which does not give analytical formulas [13]. As a consequence, it was only possible to obtain either analytical formulas or accurate results. In the present case, results are accurate and can be calculated fully analytically when we use the analytical expression for \( \beta_0 \) as developed by Collin \textit{et al.} [24]. Equation (12) provides also analytical formulae of the dispersion relation of the transmission resonances, as shown in the following section.

3. Dispersion relation of transmission resonances

3.1 Derivation

The dispersion relations of the transmission resonances can be obtained analytically from Eq. (12). Resonant transmission is obtained by computing the poles of \( t_n \) in the complex frequency domain [6,13]. Poles of \( t_n \) correspond to zeros of the determinant in Eq. (12), i.e.:

\[
\sum_{n=-\infty}^{\infty} Y_{\ell,n} + Y_2 \left( \sum_{n=-\infty}^{\infty} Y_{\ell,n} + Y_2 \right) e^{-i\beta_0 h} - \left( \sum_{n=-\infty}^{\infty} Y_{\ell,n} - Y_2 \right) \sum_{n=-\infty}^{\infty} Y_{\ell,n} - Y_2 \right) e^{i\beta_0 h} = 0. \quad (13)
\]

The above equation is very similar to the one describing the modes of a slab waveguide [25] when re-written:

\[
\tan(\beta_0 h) = -i \frac{G_1 + G_3}{\beta_0^2 + G_1 G_3}, \quad (14)
\]

with \( G_d = I_d / \sum_{n=-\infty}^{\infty} Y_{d,n} \). In the particular case of a symmetric grating, \( Y_1 = Y_3 \) and the following two transcendental equations are obtained from Eq. (13):

\[
\sum_{n=-\infty}^{\infty} Y_{\ell,n} + i Y_2 \cot(\beta_0 h/2) = 0, \quad (15)
\]

\[
\sum_{n=-\infty}^{\infty} Y_{\ell,n} - i Y_2 \tan(\beta_0 h/2) = 0. \quad (16)
\]

The case of symmetric gratings allows the term \( \sum_{n=-\infty}^{\infty} Y_{\ell,n} \) related to the periodicity to be separated from the term \( Y_2 \tan(\beta_0 h/2) \) related to the slit. This can be useful to simplify the interpretation of the relative role of each geometrical parameter on the transmission process. Note also that the above equations are very similar to the one describing the symmetric and antisymmetric modes of a slab waveguide [25] when re-written:

\[
\beta_0 \tan(\beta_0 h/2) = -i G_1, \quad (17)
\]

\[
\beta_0 \cot(\beta_0 h/2) = i G_1. \quad (18)
\]

It will be shown later that solutions to Eq. (15) and Eq. (16) correspond to symmetric and antisymmetric modes respectively.

3.2 Validity of the mode equation

Equation (13) reduces the transmission problem to a set of modes and gives the position of the transmission peaks. As an example, the total transmission of a gold grating for \( w = 50 \text{ nm} \), \( h = 600 \text{ nm} \), \( \varepsilon_1 = \varepsilon_2 = 1 \), \( \varepsilon_3 = 2.25 \) and normal incidence as a function of \( p \) and \( \lambda \) is plotted in Fig. 3(a). Note that plotting the transmission as a function of \( k_{x,0} \) and \( \lambda \) would lead to similar observations. It is however more convenient to plot the transmission as a function of \( p \) and \( \lambda \) for an easier identification of the grating resonances which appear close to \( \lambda = (\sqrt{\varepsilon_2}) p n \) (\( d = 1 \) or 3). For the same set of parameters as in Fig. 3(a), solutions to Eq. (13) are represented by the blue and red dashed curves in Fig. 3(b). The SPP dispersion relations for the top and
bottom interfaces are represented by cyan and green solid curves. All transmission maxima observed in Fig. 3(a) match with the dispersion curves plotted in Fig. 3(b). This shows that the excitation of the modes whose dispersion relations are given by Eq. (13) leads to the transmission peaks.

Fig. 3. (a) Transmission of a gold grating for \( w = 50 \) nm, \( h = 600 \) nm, \( \varepsilon_1 = \varepsilon_2 = 1, \varepsilon_3 = 2.25 \) and normal incidence in function of \( p \) and \( \lambda \). The brighter the region, the larger is the transmission. (b) Dispersion relations of the modes obtained from the solutions of Eq. (13) (blue and red dashed curves) for the same set of parameters as in Fig. 3(a). The cyan and green solid lines correspond to the dispersion relations of SPP modes excited at the top and bottom of the grating respectively.

4. Description of the modes responsible for high transmission

The nature of the modes responsible for the high transmission is determined in the present section. At first, the dispersion relations of the uncoupled modes are extracted from Eq. (13).

4.1 Periodicity related effects

Observing Fig. 3, one sees that high transmission is strongly dependant on period. The only terms dependant on period in Eq. (13) are the \( Y_{d,n} \) terms. These terms present two critical points: (i) at Rayleigh anomalies, \( Y_{d,n} \) terms are discontinuous; (ii) at SPP conditions, \( Y_{d,n} \) terms present poles. \( Y_{d,n} \) is rewritten here for clarity:

\[
Y_{d,n} = \frac{\varepsilon_d}{\varepsilon_2} \frac{j_{w,0} K_{0,n}}{k_{id,n} + \varepsilon_d k_a e^{-\gamma_2^2}}.
\]
Rayleigh anomalies occur when a diffracted order above or below the grating passes from evanescent to propagating, i.e. at $k_{d,n} = 0$. At this condition, $k_{d,n}$ is discontinuous as it abruptly changes from an imaginary to a real value, this in turn causes a discontinuity of the $Y_{d,n}$ terms. At normal incidence, this condition is expressed as:

$$\lambda_{Rd,n} = \frac{\rho}{n} \sqrt{\varepsilon_d}. \quad (20)$$

As an example, the term $Y_{1,1}$ is plotted in Fig. 4(a) for a gold grating with $w = 50$ nm, $p = 1000$ nm, $\varepsilon_1 = \varepsilon_2 = 1$ and normal incidence. It shows that $Y_{1,1}$ presents a discontinuity at $\lambda_{R1,1}$, see the abrupt change in the phase of $Y_{1,1}$, $\text{arg}(Y_{1,1})$.

SPP modes are excited when $k_{x,n} = k_{SPPd}$ where $k_{SPPd}$ is the SPP wavevector. Under SIBC, $k_{SPPd} = k_0 \left[ (\varepsilon_d - \varepsilon_0^2) / \varepsilon_d \right]^{1/2}$ [26] and SPP modes are excited at:

$$\lambda_{SPPd,n} = \frac{\rho}{n} \sqrt{\varepsilon_d} \left[ \frac{\varepsilon_d - \varepsilon_0^2}{\varepsilon} \right]. \quad (21)$$

The above equation corresponds to the condition at which the denominator of $Y_{d,n}$ in Eq. (19) is zero, hence producing a pole. This is what is observed in Fig. 4(a) where $Y_{1,1}$ presents a pole at $\lambda_{SPP1,1}$.

![Fig. 4. Real (blue curves) and imaginary part (red curves) of the terms (a) $Y_{1,1}$; (b) $\Sigma Y_{n}$ (solid lines) and $Y_2$ (dashed lines) for a gold grating for $w = 50$ nm, $h = 600$ nm, $\rho = 1000$, $\varepsilon_1 = \varepsilon_2 = 1$ and normal incidence. In panel (a) $\lambda_{R1,1}$ and $\lambda_{SPP1,1}$ are represented by vertical dashed lines and the phase of $Y_{1,1}$ is represented by the violet curve and the right hand axis corresponds to the phase of $Y_i$. $\lambda_{Rd,n}$ and $\lambda_{SPPd,n}$ appear each time in pair as they both depend linearly on period and incident angle. $\lambda_{SPPd,n}$ is red shifted as compared to $\lambda_{Rd,n}$. In the case of a PEC, $\lambda_{Rd,n} = \lambda_{SPPd,n}$, i.e. both the resonance and the discontinuity due to the periodic structure appear under the same condition.](image)
4.2 Fabry-Pérot resonances

Far from $\lambda_{\text{SPP}_{nl}}$, $Y_{dL}$ terms are small as compared to $Y_2$. This is what is observed in Fig. 4(b). Solutions to Eq. (13) can then be approximated by wavelengths $\lambda_{\text{FP},l}$ which fulfill the condition:

$$\beta_l h = \pi l,$$

where $l$ is an integer. At these conditions, FP resonances are excited inside the slits. In analogy with waveguides, it will be shown later that the integer $l$ corresponds to the number of field maxima inside the slits.

4.3 Coupled modes

The goal of this section is to determine the nature of the modes responsible for high transmission. To this aim, it is shown here that it is easier to consider asymmetric gratings than symmetric ones as the top and bottom SPP modes are well separated.

It was shown in Sect. 4.1 and 4.2 that both FP and SPP modes are contained in the dispersion relation given by Eq. (13). Also, Fig. 3 shows that the coupled modes are asymptotic to SPP modes at long wavelength. This agrees with the description made by Marquier et al. [10] who described the modes of the grating as a coupling between FP and SPP modes. However, several past studies attributed the high transmission observed to the discontinuity produced by the Rayleigh anomaly instead of the excitation of SPP modes [11,13,14]. A point which could have lead to some ambiguity regarding the respective role of SPP and Rayleigh anomaly is the fact that most of the past study considered symmetric environment, i.e. $\epsilon_1 = \epsilon_3$. The symmetric grating is a very particular case.

To show this, schematics of the mode coupling for three different types of gratings are shown in Fig. 5. Although these schematics could appear oversimplified as compared to the case of Fig. 3, it helps to give a general idea of the coupling mechanism. The system is composed of 3 types of modes, each one being represented in Fig. 5: (i) SPP modes excited above the grating $\lambda_{\text{SPP}_{nl}}$ (cyan lines); (ii) SPP modes excited below the grating $\lambda_{\text{SPP}_{nl}}$ (green lines); (iii) FP modes $\lambda_{\text{FP},l}$ (black lines). The coupling of these modes leads to new modes represented by red and blue lines. In Fig. 5(a), $\epsilon_1 < \epsilon_3$ and the top and bottom SPP modes are well separated. As the contrast between $\epsilon_1$ and $\epsilon_3$ is decreased, $\lambda_{\text{SPP}_{nl}}$ and $\lambda_{\text{SPP}_{nl}}$ become closer [cf. Fig. 5(b)] until $\lambda_{\text{SPP}_{n1}} = \lambda_{\text{SPP}_{n1}}$ for $\epsilon_1 = \epsilon_3$. The top and bottom SPP modes couple together via the slits, which creates two degenerated SPP modes: a symmetric low frequency mode $\lambda_{\text{SPP}_{n1}}$ and an antisymmetric high frequency mode $\lambda_{\text{SPP}^*_{n1}}$. This degeneracy of the SPP modes is discussed in the Appendix. The band structure of the symmetric case is then strongly modified as compared to the asymmetric one, see Fig. 5(c). For example, both $\lambda_{\text{FP}1}$ and $\lambda_{\text{FP}2}$ modes in Fig. 5(c) couple to $\lambda_{\text{SPP},1}$ as the period is increased. The mode corresponding to the coupling between $\lambda_{\text{FP}2}$ and $\lambda_{\text{SPP},1}$ represented in red crosses the SPP line. This crossing could be interpreted as if this mode was not a hybrid FP-SPP mode. But this crossing occurs because we are in the presence of the two degenerated SPP modes $\lambda_{\text{SPP}^*_{n1}}$ and $\lambda_{\text{SPP}_{n1}}$. Increasing the contrast between $\epsilon_1$ and $\epsilon_3$ removes any ambiguity regarding the nature of the coupled modes. Note also that it is easier to determine graphically the nature of the coupled modes in a $(p, \lambda)$ diagram as done in Fig. 3 rather than in a $(\lambda, h)$ diagram as in Ref. [13].

In the next section, the mode symmetry of symmetric grating is investigated by plotting the field profiles at transmission maxima. We will refer to FP-like behaviour when the transmission peaks are independent on $p$ and the field is mainly localized inside the slits, whereas SPP-like corresponds to transmission peaks following the dispersion of SPP modes and where the field is partly localized on the grating surface.
Fig. 5. Schematic of the coupling mechanism between SPP and FP modes in metal gratings. In panel (a) and (b) $\varepsilon_1 < \varepsilon_3$ and the difference between $\varepsilon_1$ and $\varepsilon_3$ is reduced from (a) to (b). In panel (c), $\varepsilon_1 = \varepsilon_3$.

5. The symmetric grating case

The transmission of a symmetric gold grating for $w = 50$ nm, $h = 600$ nm, $\varepsilon_1 = \varepsilon_2 = \varepsilon_3 = 1$ and normal incidence is plotted in Fig. 6 together with the mode dispersion. As the SPP modes excited at each interface appear at the same condition, there are half as many SPP lines as compared to the asymmetric case shown in Fig. 3. As a consequence, it is easier to distinguish the horizontal lines close to $\lambda_{FP}$.

5.1 High transmission far from SPP conditions

From the FP condition given by Eq. (22), high transmission far from SPP conditions is expected at $\lambda_{FP,1} \approx 1700$ nm, $\lambda_{FP,2} \approx 845$ nm and $\lambda_{FP,3} \approx 620$ nm for the slit parameters of Fig. 6. Indeed, broad transmission maxima are observed in Fig. 6(a) close to these three wavelengths for any period except when in close proximity with $\lambda_{SPP,n}$. For example, for $p$ ranging from 500 to 1500 nm, high transmission is observed close to $\lambda_{FP,1}$.

Maps of the magnetic field intensity at each peak position close to $\lambda_{FP,1}$ with $l = 1, 2$ and 3 are shown in Fig. 7(a)–7(c) for $p = 500$ nm. Each figure is plotted in the $(x, y)$ plane over one period in the $x$ direction. Grey rectangles represent the metal regions. In each case, the field is strongly localized inside the slit with $l$ field maxima. This shows that the slit is acting as a FP cavity. When $l$ field maxima are observed in the slit with $l$ odd, the transmission peak position is predicted from Eq. (15), whereas it is obtained from Eq. (16) for $l$ even. Plotting the field amplitude [Fig. 7(d)–7(f)], one sees that the field is symmetric and antisymmetric with respect to the $y = 0$ axis for $l$ odd and even respectively.
Fig. 6. (a) Transmission of a gold grating for $w = 50$ nm, $h = 600$ nm, $\varepsilon_1 = \varepsilon_2 = \varepsilon_3 = 1$ and normal incidence in function of $p$ and $\lambda$. The brighter the region, the larger is the transmission. (b) Dispersion relations of the modes obtained from the solutions of Eq. (15) (blue dotted curves) and Eq. (16) (red dashed curves) for the same set of parameters as in Fig. 6(a). The green solid curves correspond to the SPP dispersion relations.

5.2 High transmission near SPP conditions

The different branches constituting the dispersion relations of symmetric gratings are labeled $\lambda(n,l)$ in Fig. 6(b), i.e. poles for which $\lambda_{SPP,n+1} < \lambda < \lambda_{SPP,n}$ and $\lambda_{FP,l+1} < \lambda < \lambda_{FP,l}$. Only the first five branches are labeled for clarity.

Focusing on the $\lambda(0,1)$ branch, the mode is red-shifted as the period is increased. Mathematically, this is due to the resonance of $Y_{1,1}$ occurring at $\lambda_{SPP,1,1}$ which is red-shifted as the period is increased. The mode continuously evolves from a FP-like mode in the 500 - 1500 nm period range with nearly flat dispersion to an SPP-like one for periods ranging from 2000 to 3000 nm, where $\lambda(0,1)$ is asymptotic to $\lambda_{SPP,1,1}$. Whereas the magnetic field intensity is mainly confined inside the slit for the $\lambda(0,1)$ branch at small periods [see Fig. 7(a)], an intense field is present on the surface for larger periods, whilst a FP character remains inside the slit, see Fig. 8(a) for $\lambda = 3000$ nm and $p = 2977$ nm. Figure 8(b) shows that the magnetic field amplitude along $\lambda(0,1)$ keeps a symmetric profile for large periods.
The \( \lambda(0,2) \) branch is also red-shifted as the period is increased. It crosses \( \lambda_{SPP,1,1} \) and merges to the \( \lambda(1,0) \) branch which stays asymptotic to \( \lambda_{SPP,1,1} \) for large periods. The two maxima of the FP cavity become less confined into the slit as \( p \) is increased along the \( \lambda(0,2) \) branch and afterwards the \( \lambda(1,0) \) branch. In Fig. 8(c), the field is no longer confined inside the slit for \( p = 2999.6 \text{ nm} \) and \( \lambda = 3000 \text{ nm} \) but it extends in the \( y \) direction above and below the
grating. As shown in Fig. 8(d), the magnetic field amplitude of the $\lambda(1,0)$ branch keeps the antisymmetric profile of the $\lambda(0,2)$ branch.

The transmission peak related to the $\lambda(1,0)$ mode is very narrow and not visible in Fig. 6(b) due to the figure resolution. To show that this mode effectively gives a transmission peak, a transmission spectrum is plotted in Fig. 9 for $\lambda = 3000$ nm and periods close to the $\lambda(1,0)$ branch. A narrow transmission peak is observed close to $\lambda_{R1,1}$.

At long wavelengths, the $\lambda(0,1)$ and $\lambda(1,0)$ modes present similarities with the symmetric and antisymmetric SPP modes observed with thin metal films. In both thin metal films and metal gratings, symmetric modes are red-shifted as compared to $\lambda_{SPP1,n}$, whereas the antisymmetric modes are blue-shifted. Also, the antisymmetric modes correspond to the long range SPP’s, which give sharp resonances [see the $\lambda(1,0)$ mode in Fig. 9], whereas the symmetric modes correspond to the short range SPP’s, presenting broader resonances [the $\lambda(0,1)$ mode in Fig. 9]. The difference here as compared to a flat metal film is that SPP’s are coupled on both sides of the film for any thickness due to the presence of slits.

As the two SPP modes couple together via the slits and creates two SPP modes, the first FP mode, which is symmetric, couples with the symmetric SPP mode of order $n = 1$. Similarly, the second FP mode, which is antisymmetric, couples with the antisymmetric SPP mode of order $n = 1$. Finally, it can be said that Eq. (15) and Eq. (16) give the dispersion relation of respectively symmetric and antisymmetric hybrid “FP-SPP” modes.

6. Minimum in transmission at the SPP condition

It has been shown previously that high transmission is induced by the excitation of hybrid “FP-SPP” modes. We want to clarify here what exactly happens at the SPP resonance.

At $\lambda = \lambda_{SPPd,n}$, $Y_{d,n}$ is resonant and one sees from Eq. (12) that the transmission amplitude $t_q$ is nearly zero for any propagating diffracted order, i.e. for $q < n$. Consequently, the total transmission is always minimal at $\lambda_{SPPd,n}$, as observed in Fig. 3 and Fig. 6. This is in agreement with Cao et al. who already observed that the transmission is nearly zero at the SPP condition [11]. It also explains why transmission peaks are hardly observed in transmission spectra when the dispersion relations predict transmission resonances that are too close to the SPP conditions. Lalanne et al. investigated in a past study the zero observed at the SPP condition in terms of reflected and transmitted intensities of single interfaces [13]. They found that the transmitted intensity of the incident wave into the fundamental mode is close to zero at $\lambda_{SPPd,n}$. This means that there is no coupling into or out of the slit at the SPP resonance.
Physically, this low transmission can be understood as the fact that at the SPP condition, the field is bounded at the metal interface but not above the slit, as seen from Fig. 10 at the crossing of the $\lambda(0,2)$ branch with $\lambda_{\text{SPP},1}$ for $p = 1693$ nm and $\lambda = 1700$ nm. This inhibits light from coupling into the slit mode. Note that the degeneracy of the top and bottom SPP modes in the case of symmetric grating leads to two transmission minima. This is discussed in the Appendix.

Fig. 10. Map of the magnetic field intensity plotted as in Fig. 7 for $\lambda = 1700$ nm and $p = 1693$ nm.

7. Conclusion

To conclude, an analytical model based on a modal expansion method has been derived to study the light transmission through metal gratings for TM polarization. This model gives accurate analytical expressions for the transmission and the dispersion relations of the modes responsible for high transmission. Both FP and SPP modes are contained in the dispersion relations of the transmission resonances. In addition, it is observed that in the case of asymmetric grating, transmission peaks stay asymptotic to SPP modes at long wavelengths. It is then established that the modes responsible for high transmission are hybrids between SPP and FP modes. In the case of symmetric gratings, the top and bottom SPP modes are degenerate, complicating the interaction between the modes of the system. With symmetric gratings, two types of modes are identified: symmetric and antisymmetric ones. Finally, it is shown that transmission is suppressed at the SPP condition. These findings give a unifying picture regarding the transmission properties of metal gratings. The observations made in the present paper are useful in designing metal gratings for various applications.

8. Appendix: Coupled SPP modes and photonic bandgap

This section is dedicated to the degenerated SPP modes of symmetric gratings. It is shown that the degenerated SPP modes lead to two transmission minima. This should also be useful in order to avoid confusion with photonic bandgaps observed in the propagation of surface plasmon polaritons on corrugated surfaces [27].

The degeneracy of the top and bottom SPP modes in the case of symmetric grating cannot be observed considering only one mode inside the slit. Due to symmetry reasons, it is necessary to consider at least three slit modes. Therefore, the model of Ref. [15], is now used.

The transmission spectrum of a gold grating is plotted in Fig. 11(a) on a log scale for $p = 1750$ nm, $w = 700$ and $h = 600$ nm. Two minima, labeled $\lambda_{\text{SPP},1}$ and $\lambda_{\text{SPP,1}}$, are observed between $\lambda_{\text{R}1,1} \approx 1750$ nm and $\lambda_{\text{SPP},1} \approx 1757$ nm. This shows that there is a coupling between the two SPP modes excited on both sides of a symmetric grating. The amplitude of the magnetic field for the transmission minima $\lambda_{\text{SPP,1}}$ and $\lambda_{\text{SPP,1}}$ are plotted in Fig. 11(b) and 11(c) respectively. The field profile is similar to the one already shown in Fig. 10 at the SPP condition. The field appears saturated above the grating in Fig. 11 because the scale has been
adjusted such that the weak field amplitude below the grating can be observed. The low
frequency mode \( \lambda_{SPP, n} \) presents a symmetric profile and the high frequency mode \( \lambda_{SPP, n}^+ \) an antisymmetric one. This is in agreement with what is said in Sect. 4.3.

![Fig. 11](image)

Fig. 11. (a) Transmission spectrum of a gold grating for \( w = 600 \text{ nm}, h = 600 \text{ nm}, \lambda = 1750 \text{ nm}, \epsilon_1 = \epsilon_2 = \epsilon_3 = 1 \) and normal incidence. The magnetic field amplitudes at \( \lambda_{SPP, n} = 1750.5 \text{ nm} \) and \( \lambda_{SPP, n}^{-1} = 1751.9 \text{ nm} \) are plotted in panel (b) and (c) respectively.

The derivation of an analytical formula considering perturbation induced by the slit width and film thickness in the SPP dispersion relation is out of the scope of the present work. Plotting transmission spectra for different slit widths and film thicknesses gives however general trends of these perturbations. The total transmission of a gold grating for \( p = 1750 \text{ nm}, \epsilon_1 = \epsilon_2 = \epsilon_3 = 1 \) and normal incidence in function of \( w \) and \( \lambda \) is plotted in Fig. 12(a) for \( h = 600 \text{ nm} \). For a better observation of the minima in transmission resulting from the SPP excitation, metal losses are removed and the transmission intensity is represented with a logarithmic color scale. Two lines of low transmission are observed, corresponding to \( \lambda_{SPP, n}^+ \) and \( \lambda_{SPP, n}^- \).

As the slit width is reduced, the two lines merge to the SPP condition \( \lambda_{SPP,1,1} \approx 1757 \text{ nm} \) defined by Eq. (21) and the SPP splitting is indistinguishable. Increasing the slit width decreases the amount of metal. As a consequence, the SPP modes become closer to air modes and the two transmission minima are blue shifted towards \( \lambda_{RL,1} \approx 1750 \text{ nm} \). The interaction between the electromagnetic field on top and bottom of the grating increases with the slit width. This increases in turn the splitting between the two transmission minima. On Fig. 12(b), the film thickness is reduced to \( h = 200 \text{ nm} \) as compared to Fig. 12(a). It shows that the splitting between the two transmission minima increases as the film thickness decreases. This is again attributed to an increased interaction between the electromagnetic field on top and bottom of the grating as the film thickness is reduced, as is the case for thin metal films [28].

It should be noted that the SPP splitting observed here occurs due to the finite grating thicknesses and coupling between the two grating surfaces. Consequently, the analogy with photonic crystals as done by Barnes et al. cannot be used for the splitting observed here [27].
Fig. 12. Transmission of a gold grating for $p = 1750$ nm, $\varepsilon_1 = \varepsilon_2 = \varepsilon_3 = 1$ and normal incidence in function of $w$ and $\lambda$. The film thickness is (a) $h = 600$ nm; (b) $h = 200$ nm. The brighter the region, the larger is the transmission.

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