Total absorption of light by lamellar metallic gratings

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Abstract: Lamellar gratings illuminated in conical (off-plane) mounting can achieve with suitable optogeometrical parameters (grating profile, angle of incidence and wavelength) a total absorption of light for any polarization provided there is only the zeroth propagating order. A detailed analysis shows that electromagnetic resonances are involved and their nature strongly depends on the polarization. When the incident electric field is parallel to the cross-section of the grating, the resonance is provoked by the excitation of surface plasmons. For the orthogonal polarization, total absorption occurs for deep gratings only, when the grooves behave like resonant optical cavities. It is possible to reduce the optimal grating height by filling the grooves with a high refractive index material.

OCIS codes: (050.1950) Diffraction and gratings : Diffraction gratings; (240.6680) Optics at surfaces : Surface plasmons; (260.3910) Physical optics : Metal optics; (050.5745) Diffraction and gratings : Resonance domain

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1. Introduction

Reflection of light by metallic plane can be drastically reduced by structuring the metallic film at nanometer scales. Anomalies in reflection have been discovered one century ago by Wood [1] in the case of metallic gratings, and it is now established that surface plasmons polaritons are involved in the phenomenon of full absorption of light by metallic grating [2-4]. In the case of shallow grating, surface plasmons are delocalized over the metallic surface and can propagate over a distance of a few microns. Recently, full light absorption has been attained with extremely shallow gratings where surface plasmons are excited in the electrostatic regime [5]. In the case of deep metallic gratings, surface plasmons are coupled with transverse electric magnetic modes inside the groove and are highly localized on the grooves [6-11]. In the case of crossed gratings, surface plasmons are excited in both polarizations and, as a result, full light absorption is insensitive to the incident polarization [12]. It has been recently shown [13] that nanocavities in gold substrate sustain void plasmons and that full light absorption occurs independently of the angle of incidence. Moreover, it has been evidenced that such absorption occurs in off-plane incidence [13]. In the case of non crossed gratings, excitation of surface plasmons are highly dependent on the polarization of the incident light, and it is no more evident that it may be possible to manufacture gratings able to fully absorb light in both polarizations. However, in that case there exists another class of resonant phenomena that can contribute to the absorption, namely the so called cavity resonances [14].

This paper is dedicated to the study of light absorption by a bare metallic grating illuminated in conical mounting in both polarizations. We start from a numerical optimization of light absorption in both polarizations with respect to the geometrical parameters of the grating, in the case of deep bare metallic grating. Then a thorough study of the physical origin of the full light absorption in each polarization is carried out. It is the key point of the paper. Last, we show that similar results can be obtained with moderate groove heights, and the two different mechanisms of absorbance depending on the incident polarization are clearly evidenced.

2. Notations

Bare metallic lamellar gratings depicted in Fig. 1 are invariant with respect to the z axis. The groove height, groove width and period are denoted by h, c and d respectively. The filling factor c/d and the wavelength of light $\lambda = 2\pi/k$ are taken equal to 0.5 and 650 nm respectively. Fig. 1 shows the notations used to describe the incidence parameters. We denote by φ the angle between the xy plane and the plane of incidence. Except in the last part of the paper, we will deal with pure conical mountings, *i.e.* $\varphi = 90°$. The incident wavevector $\mathbf{k}^{\mathbf{i}}$ makes an angle θ with the normal (y-axis). The polarization angle δ is the angle between the electric field and the normal $\mathbf{n}$ to the plane of incidence. It is equal to zero or 90° according to whether the electric or magnetic field is perpendicular to the plane of incidence.

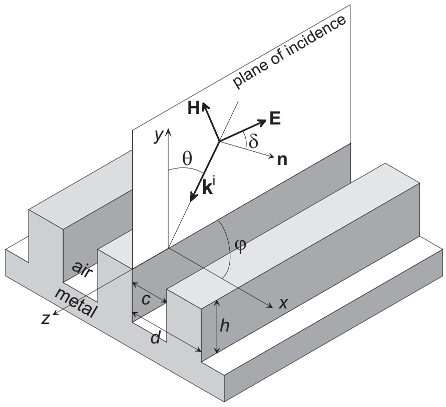


Fig. 1. Scheme of a bare metallic lamellar grating with parameters of the conical mount

In conical mount, it is well known that there exists a coupling between polarizations, except for perfectly conducting metals. This means that, in contrast with classical mounts, the fact that the incident electric (resp. magnetic) field lies in the plane of incidence does not entail that the total electric (resp. magnetic) field remains parallel to this plane. However, we still consider two fundamental cases of polarization ($\delta = 0°$ or $90°$). A total absorption for both cases involves total absorption for unpolarized light, and conversely.

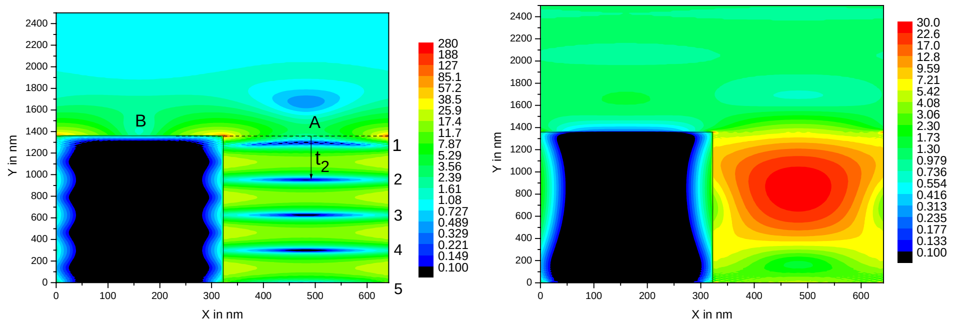
3. Total absorption of light by deep lamellar gratings in conical mounting: numerical optimization

In order to know whether the grating can absorb light totality for unpolarized light in pure conical mounting ($\varphi = 90°$), a thorough numerical optimization has been achieved using the modal method [15,16]. This method is based on a rigorous theory of diffraction and is specially designed for the study of lamellar gratings. It consists in representing the electromagnetic field inside the grooves and inside the lamellae as a linear combination of modes that are rigorous solutions of Maxwell equations and boundary conditions on the groove walls, and must not be confused with the so-called Fourier modal method (Rigorous Coupled Wave theory). The absorption rate is optimized with respect to the groove height h, the period of the grating d and the angle of incidence θ. We restrict ourselves to the case of a single reflected propagating order, which imposes limits on the wavelength-to-period ratio as a function of the incident angle. Numerical optimization consists in searching a set of parameters for which the reflectivity is minimal. For the best result, it turns out that an absorption rate larger than 99.9% for both fundamental polarizations is reached for d = 644.8 nm (= 0.992λ), h = 1360 nm, and θ = 30°. The results have been checked using two independent methods for modeling of diffraction by diffraction gratings. These are the integral and the differential methods. The differential theory [17] is based on a Fourier decomposition of the electromagnetic field, which transfers Maxwell equations into a system of ordinary differential equations, which is solved by the shooting method. In the case of lamellar grating, it reduces to the Fourier modal method. The integral theory [17] describes the electromagnetic field as unknown values taken on the grating surface and uses the Green-functions method to establish the field everywhere in space, resulting in a system of coupled integral equations, which require special analysis of singularities.

4. Physical origin of total absorption

In order to determine the origin of the total absorption appearing simultaneously for both cases of polarization, we have drawn in Fig. 2 the maps of the electric field intensity. In Fig. 2a (δ = 90°), one can observe a cavity resonance inside the groove, with an enhancement of the maximum field intensity close to 30 with respect to the intensity of the incident field. For that polarization, the incident electric field is parallel to the yz

plane, i.e. to the groove sides, and even though polarization states are coupled, it can be conjectured that the total electric field remains nearly parallel to the same plane (it is rigorously satisfied for the 0th order, due to the symmetry with respect to the *yz* plane). The groove can be considered as an air slab truncated at the top and filled with metal at the bottom. The cut-off of the fundamental mode is reached at a wavelength $\lambda = 2c = d =$ 644.8 nm for infinitely conducting metal but the cut-off wavelength is longer for real metals [19] because of the field penetration in the metal which can be observed in Fig. 2a. In the same way, the *x* and *z* components of the electric field vanish at the bottom of the groove (for perfectly conducting metals) and form interference pattern between the modes propagating down- and upwards which gives the maximum of light intensity in Fig. 2a. With a perfectly conducting grating, the distance between two successive nodes of the standing wave is given by $\lambda/(2\cos\theta)$. It must be stressed that in the case of real metal gratings, this distance is slightly shorter [20].

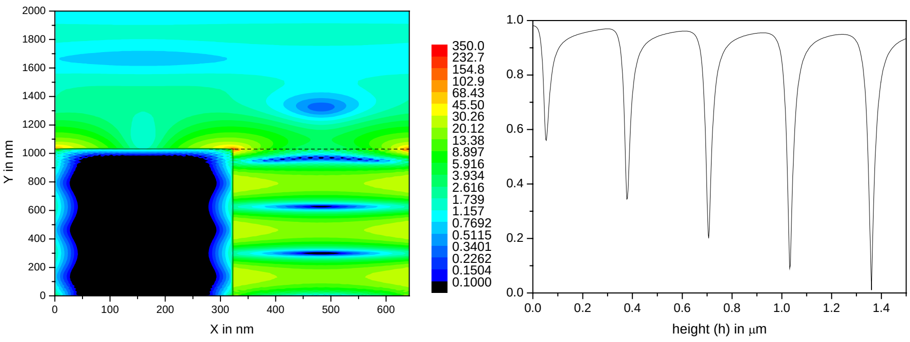


(a) (b)

Figs. 2. Map of the intensity $|E|^2$ on one period of the grating. Parameters are d = 644.8 nm, h = 1360 nm, c/d = 0.5, λ = 650 nm, refractive index of gold n = 0.142 + i3.374, θ = 30°. (a) δ = 90°, (b) δ = 0°. The dotted line in Fig. 2b shows the top of the groove. The different nodes are numbered on the right side. The fifth node lies in the metal, approximately 30 nm below the bottom of the groove as explained later in the text. The distance t_2 between the top of the groove and the second node is represented.

The map of the electric field intensity when δ = 0° is quite different from that obtained when δ = 90°. First, the electric field is maximum at the surface of the groove sides and at the edges of the groove top. Secondly, the enhancement of the electric field intensity is much higher and reaches a value close to 280. Finally, a standing wave including 4 nodes can be observed inside the groove. Indeed, in that case, the incident magnetic field is parallel to the groove sides and the fundamental mode of the air slab has no cut-off. So, the incident wave penetrates inside the groove and is reflected at the bottom. The field has almost the same values at points A and B, above the corrugation and above the lamella top (Fig. 2(b)). It is close to zero inside the metal but, more surprising, a minimum is observed very close to the point A, inside the groove. Fig. 2(b) inclines one to conjecture that for δ = 0° other resonance phenomena could occur by placing the bottom of the groove close to one of the nodes.

In order to verify this assumption, we first have drawn in Fig. 3(a) the modulus of the amplitude of the reflected wave as a function of *h*. Four other absorption peaks appear when the height of the grating is decreased, i.e. the number of nodes in Fig. 2(b), a fact which confirms our conjecture. Another confirmation can be found in Fig. 3(b) which presents the map of the electric intensity for *h* = 1032 nm, at the second minimum of the reflected efficiency. The nodes have been shifted upwards, the upper node has been cancelled from the groove and the number of nodes is reduced to 3 (plus the one present below the bottom of the groove).



(a) (b)

Figs. 3. (a) Reflected efficiency as a function of *h*. (b) Map of the electric intensity for h = 1032 nm. Parameters are λ = 650 nm, θ = 30°, refractive index of gold n = 0.142 + i 3.374, φ = 90°, δ = 0°, d = 644.8 nm, c/d = 0.5.

The comparison between Figs. 2b and 3b leads us to the conclusion that the minimum of the reflectivity is reached when the distance between the upper minimum of the field and the top of the groove is about t_1 = 65 nm. The necessary groove depth to achieve this with more nodes can easily be evaluated in the following way. At first, it is necessary to take into account that the bottom of the groove does not correspond to a node. Elementary calculations lead to a formula in closed form giving the shift between the metal surface and the node when a plane wave with electric field perpendicular to the plane of incidence is reflected by a plane metallic surface. It turns out from this formula that the node is located below the surface (here it is necessary to consider the continuation of the incident and reflected waves inside the metal). For a wavelength of 650 nm and an incidence of 30° on a gold plane, the shift t_0 reaches a value of 29 nm. Second, let us note with t_1 to t_5 the distances in y direction between the top of the groove and the corresponding node numbered in Fig. 2b. Using these values, the groove depth for which the upper node lies at the same distance from the top of the groove is simply given by: $h_n = t_n - t_0$, where $n = 1,\ldots,5$ corresponds to the node number.

Node number	Absorption peak	h_n (nm)
1	54 (|r|= 0.56)	36
2	378 (|r|= 0.34)	378
3	706 (|r|= 0.20)	705
4	1032 (|r|= 0.09)	1032
5	1360 (|r|< 0.01)	1360

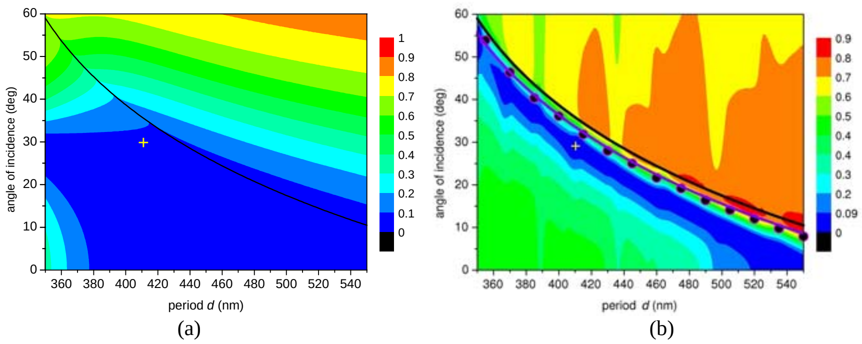
Table 1: Values of the grating depth for the different absorption peaks depending on the node number given in the first column. Second column: exact values of h corresponding to the absorption peaks in Fig. 3a (with the corresponding reflectivity). Third column: phenomenological value h_n explained in the text.

Table 1 makes a comparison between these phenomenological values (h_n) and the exact groove depth corresponding to absorption peaks in Fig. 3a. It can be concluded from Table 1 that the heights deduced from absorption peaks and from the distances h_n are very close to each other, except for the first resonance, which corresponds to a shallow grating. This shallow grating has a groove height/period ratio of the same order as the sinusoidal gold grating described in [4], at the discovery of total absorption by gratings. Table 1 clearly shows that for δ = 0°, a large absorption by deep gratings is obtained by generating at the vicinity of the top of the groove a field close to the field generated by a totally absorbing shallow grating. At the top of the deep grating, this field generates for the surface plasmon resonance conditions similar to those observed in the case of a shallow grating [21]: a field with close values above the top of the grooves and of the lamellae (points A and B in Figs. 2a and 2b). In such conditions, surface plasmons can propagate over deep gratings with propagating constants similar to those obtained with shallow gratings [21]. This absorption has been achieved with evanescent non-zero orders because it is easier to vanish only one order than 2 or more.

5. Total absorption of unpolarized light by lamellar gratings with moderate heights

It has been evidenced that deep metallic gratings illuminated in conical mounting allow the absorption of more than 99.9% of unpolarized light. But despite the progress of grating technology, deep metallic gratings are not so easy to realize. Thus it is worth finding similar results with more moderate groove heights. Our results have shown that for a magnetic field in the plane of incidence ($\delta = 0°$, $\varphi = 90°$), obtaining an almost total absorption with a shallow grating or a grating with moderate groove height does not make problem at all. On the other hand, when the electric field lies in the *yz* plane ($\delta = 90°$, $\varphi = 90°$) a resonance inside the groove must be excited and since the electric field must be small at the four sides of the groove, large groove heights and widths are needed. If one wants to reduce the groove height, two solutions can be envisaged. First, one can enlarge the groove width. However, since it is necessary not to increase significantly the period in order to maintain a single possible reflected order, we are led to use c/d ratios greater than 0.5 and obviously this condition entails for this first solution a strong limitation. On the other hand, it is well known that it is possible to reduce the geometrical size of a resonant cavity by increasing its optical index and this remark leads to a second solution.

We have filled the groove with silicon ($n = 3.5 + i\,0.02$), and, in normal incidence, the groove depth has been increased until a cavity resonance for $\delta = 90°$ is reached. This resonance has been obtained for a groove height close to $\lambda/5$. Then, the grating geometry has been optimized to achieve a good absorption for both polarizations. For the set of parameters $d = 542$ nm, $c = 287$ nm, $h = 120$ nm, the residual reflection in TE polarization (electric field parallel to the grooves) remains less than 5% and in TM polarization (magnetic field parallel to the grooves) the reflection is about 1.2%. These values can further be decreased if we use silver (refractive index n=0.07+i4.2) instead of gold for the grating materials. Grating parameters that give maximum absorption are quite similar, $d = 542$ nm, $c = 287$ nm, $h = 120$ nm and they lead to an absorption of 98.58% averaged on both fundamental polarizations in normal incidence.

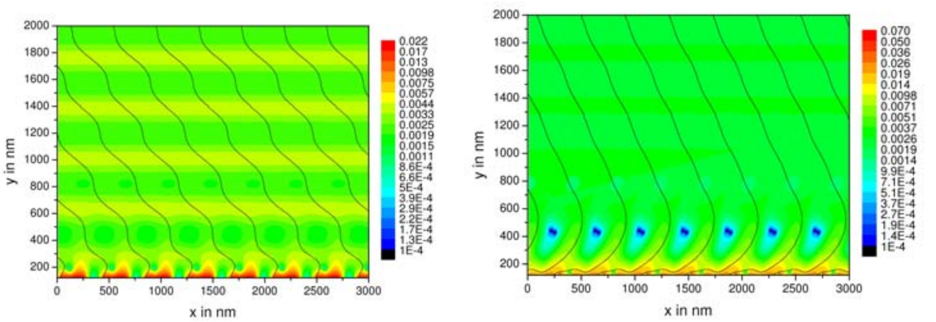


Figs. 4. Reflected efficiency in non-conical mount ($\varphi = 0$) as a function of the angle of incidence θ and the period with silver ($n = 0.07 + i\,4.2$). Groove is filled with silicon ($n = 3.5 + i\,0.02$), and its shape is kept constant (width $c = 287$ nm), $h = 120$ nm. (a) Electric field parallel to the groove, (b) magnetic field parallel to the groove. White crosses indicate the parameters d and θ chosen to plot the energy flow in Figs. 5, solid black line represents the cut-off position of order -1^{st}, the violet solid line in (b) gives the position of the plasmon propagating constant at $h = 0$, and the dark circles, at $h = 120$ nm.

Let us now clearly distinguish the two different resonances. First, keeping the same groove shape (groove width and height), the strong absorption is tracked in both polarizations with respect to angle of incidence in non-conical mount ($\varphi = 0$) and the period of the grating. Total reflected efficiency (order 0 plus order -1 when it is propagating) are displayed in Figs. 4, together with the cut-off of the -1^{st} order represented by a black line. When the electric field is parallel to the grooves (Fig. 4(a)), the absorption poorly depends on the grating period, which confirms that the resonance is linked to the groove dimensions. On the contrary, for the other polarization the resonance position strongly depends on both parameters d and θ. The plasmon surface wave that propagates along a flat silver surface has a normalized propagation constant $\alpha_{p,0}$ (= k_x/k^i) approximately equal to 1.032, and the position of its optimal excitation through order –1 is given by the equation $\theta = \text{asin}(\lambda/d - \alpha_{p,0})$, presented by a solid violet curve in Fig.4b. When the grating depth is varied, the plasmon propagation constant changes. In order to determine it, the pole of the scattering matrix S has been calculated. Let us remind that S is defined as: $S(\alpha)\ I = D$, where I and D represent column vectors made of the Fourier components of the x components of the incident (I) and diffracted (D) electric and magnetic fields. The so-called pole is the complex solution of the homogeneous problem [22]:

$$S^{-1}(\alpha_p)\ D = 0, \qquad (1)$$

The propagating constant of the surface plasmon satisfies Eq.(1) and can be identified with α_p. It has been calculated has a function of the period d for h = 120 nm and c = 287 nm, and the its values almost coincide with those determined for a flat surface, the curve $\theta = \text{asin}(\lambda/d - \alpha_p)$ has been superposed in Fig.4b (dark circles). It does not match exactly the maximum of absorption because the latter is determined by the zero of the reflected order, which differs slightly from the pole [22], but the behaviour of both of them stays the same as a function of d, as observed in Fig.4b.



(a) (b)

Figs. 5. Map of the modulus of the Poynting vector and lines of energy flow (black lines) on the top of the grating over 5 periods. The parameters are d = 410 nm, c = 287 nm, θ = 30°(crosses in Figs. 4), refractive index of silver is n=0.07+i4.2. (a) Electric field parallel to the grooves, the reflected efficiency is equal to 7.36%, (b) electric field perpendicular to the grooves, the reflected efficiency is equal to 1.47%.

Secondly, to clearly show the presence of a propagating surface wave when the electric field is perpendicular to the grooves, the lines of the Poynting vector, and thus the flow of energy, are reconstructed when the grating is illuminated in a classical mount (φ = 0) with an incidence θ = 30° (see crosses in Figs. 4). Inclined incidence is chosen to observe the propagation of a surface wave which is not possible in normal incidence where the interference between the two counter-propagating plasmons leads to a standing wave. The grating parameters have been chosen in order to generate a high absorption for both polarizations (see crosses in Figs. 4) and the lines of energy flow are displayed in Figs. 5. The colour map represents the modulus of the Poynting vector and the black lines are the lines of Poynting vector. For both polarizations, in the far field region, the vector lines show that the energy is impinging on the grating surface. When the electric field is perpendicular to the grooves (Fig. 5(b)), the excitation of a surface plasmon by the –1st order entails a bending of the lines toward the left in the near field region. The norm of the Poynting vector is maximum on the top of the grating surface. For the other fundamental polarization (Fig. 5(a)), the surface wave due to the propagation of the resonance from groove to groove is strongly localized and the bending of the Poynting lines is quite small.

6. Conclusion

As a conclusion, it is possible to achieve full light absorption independently of the incident polarization in conical mount with bare gratings. If surface plasmons are involved in both polarizations with crossed gratings, full light absorption in bare metallic grating is due to two different electromagnetic resonances depending on the polarization. In conical mounting ($\varphi = 90°$), it has been clearly evidenced in the last part of the paper that surface plasmons are responsible of the strong absorption when the incident electric field is perpendicular to the grooves. With deep gratings, surface plasmons are coupled with a transverse electric mode inside the grooves. A standing wave occurs in the grooves, with the presence of nodes whose number depends on the height of the grooves. The first node occurs inside the metal, approximately at 29 nm from the surface in the conditions of our example. The spacing between two successive nodes is close but shorter than $\lambda/(2 \cos\theta)$. As a consequence, for shallow grating, no node appears inside the groove, and when increasing the thickness of the grooves, nodes appear regularly spaced. When a node is present just below the top of the groove, the propagation of the surface plasmon is facilitated and absorption of light is strong. When the incident electric field is parallel to the grooves, a strong absorption is linked to the excitation of a cavity resonance inside the grooves. In this case, the light intensity is strong on the center of the cavity. This fact permits to clearly distinguish the resonances which occur for both polarizations since when the electric field is perpendicular to the grooves, the light intensity is maximum on the metallic surface and at the edges of the grooves. The presence of a cavity resonance implies large grooves since the electric field is minimum at the 4 sides of the cavity. However, the thickness of the grating can be decreased by increasing the refractive index of the dielectric that fills the grooves.