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SUB-WAVELENGTH METALLIC GRATINGS OF VERY HIGH TRANSMISSION EFFICIENCY

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Metal transmission gratings with apertures much smaller than the wavelength used can exhibit very high transmission efficiency. We have performed numerical calculations for the transmission through lamellar silver gratings with very small slits and have shown how the geometrical parameters of slits contribute to the transmission enhancement. Such effect could be of great use in nano-optics and optical sub-wavelength lithography.

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1. Introduction

With nowadays fabrication facilities, metallic structures perforated with sub-wavelength apertures can be manufactured for visible light operation. These structures can be integrated into optoelectronic devices according to new trends of miniaturization toward a future nano-optics. Therefore the problem of light guiding through nanometer-size apertures has attracted considerable interest [1-5].

Recently it has been discovered that optically thick, metallic films perforated by cylindrical holes of sub-wavelength diameter can display highly unusual transmission in the visible and near-infrared region [1, 2]. For radiation of wavelength as large as ten times the diameter of the holes, the absolute transmission efficiency calculated by dividing the fraction of light transmitted by the fraction of the surface area occupied by holes, is ≥ 2. In other words, more than twice as much light is transmitted as impinges directly on the holes [1].

In this paper we theoretically report on the same effect observed in silver lamellar transmission grating of very narrow slits (a term which will become more precise later). We are able to interpret the high transmission as a resonance effect of the fundamental mode in the slit and to predict under what conditions high transmission through optically thick gratings is achieved. In order to study the propagation of light through metal transmission gratings we use a rigorous approach for solving the diffraction problem, known as the Rigorous Coupled-Wave Analysis (RCWA) [6,7].

2. Rigorous coupled-wave analysis

The grating considered here is a freestanding, mono-periodic metallic structure consisting of spatially vacuum separated silver rods of rectangular cross section (Fig. 1). The width of the gap (slit) between rods, the period and the thickness of the grating are w, Λ, and d, respectively. The grating is situated in the Oxy plane and extended along the Oz axis; its structural periodicity is only along the Ox axis. This metallic structure is illuminated at normal incidence by a plane electromagnetic wave of TM polarization (the magnetic-field vector is parallel to the metal rods and Oy axis). The wavelength is denoted by λ. As a response to the incident field, the grating will give rise to a diffracted field in the region above and below it and also a stationary field pattern inside it.

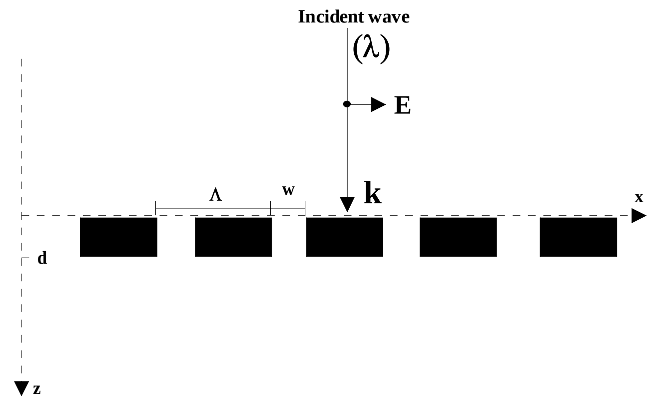

Fig. 1 Lamellar silver grating analyzed in this paper. The optical indices of the incident medium and of the substrate are both equals to unity (vacuum). In the grating region, the relative permittivity is alternatively 1 (vacuum) or ε (metal).

The RCWA is a versatile and efficient tool for describing the diffraction of electromagnetic waves in periodic structures. The relative permittivity ε(x) in the grating region is a periodic function along the Ox direction and therefore can be expanded in a Fourier series of the form:

$$\varepsilon(x) \quad = \quad \sum_m \varepsilon_m \exp[\, jm(\frac{2\pi}{\Lambda})x] \tag{1}$$

where ε_m is the m-th Fourier component of the relative permittivity.

Because of periodicity along Ox axis, the electromagnetic fields inside the grating region (0<z<d) can be also expressed as a Fourier expansion of space-harmonic fields:

$$H_y(x,z) = \sum_i U_{yi}(z)\, \exp(-jk_{xi}x)$$

$$E_x(x,z) = j(\frac{\mu_0}{\varepsilon_0})^{1/2} \sum S_{xi}(z)\, \exp(-jk_{xi}x) \tag{2}$$

where $U_{yi}(z)$ and $S_{xi}(z)$ are the normalized amplitudes of the i-th space-harmonic fields such that H_y (x,z) and E_x (x,z) satisfy Maxwell's equation in the grating region (near-field region).

Away from the grating (far-field region) the diffracted fields are taken as a superposition of plane waves (i.e. Rayleigh expansions):

$$H_y^1(x,z) = \exp(-j\frac{2\pi}{\lambda}z) \quad + \quad \sum_i R_i \exp[-j(k_{xi}x - k_{1,zi}z)] \quad in \quad the \quad input \quad region \quad z < 0$$

$$H_y^2(x,z) = \sum_i T_i \exp[-j(k_{xi}x - k_{2,zi}(z-d))] \qquad in \quad the \quad output \quad region \quad z > d \tag{3}$$

where the projections k_{xi} of **k**-vector are given by the Floquet condition [8]: $k_{xi} = -\,i(2\pi/\Lambda)$ and the projections k_{zi} can be calculated from:

$$k_{input,zi} = +\left(\sqrt{(\frac{2\pi}{\lambda})^2 - (k_{xi})^2}\right) \quad if \quad \frac{2\pi}{\lambda} > k_{xi}$$

$$k_{output,zi} = -j\left(\sqrt{k_{xi}^{\ 2} - (\frac{2\pi}{\lambda})^2}\right) \quad if \quad k_{xi} > \frac{2\pi}{\lambda} \tag{4}$$

We noted by R_i the normalized magnetic-field amplitude of the i-th backward-diffracted wave and by T_i the normalized magnetic-field amplitude of the i-th forward-diffracted wave. Introducing the Fourier expansions (Eq. 1 and Eq. 2) in the wave equation results a set of coupled-wave equations which alows to represent the electromagnetic field inside the grating (amplitudes U and S) as a function of the eigenvectors and eigenvalues of the coupled equation system:

$$S_i(z) = \sum_q C_q \quad A_{q,i} \quad \exp(B_q\ z) \tag{5}$$

where ($A_{q,i}$) and (B_q) are the eigenvectors and eigenvalues of the coupled equation system. Finally, the unknown coefficients (C_q) and the amplitude of reflected (R_i) and transmitted (T_i) waves are found by matching the electric and magnetic field components at the boundaries (z=0 and z=d).

The numerical implementation of the RCWA involves two steps: First, the eigenvalues and the eigenvectors of the matrix have to be computed and then a linear system of boundary equations has to be solved for finding R_i and T_i amplitudes. The diffraction efficiencies are defined:

$$\eta_i^{reflection} = R_i\ R_i^*\ \mathrm{Re}(k_{zi}^{input} / k_0\ )$$

$$\eta_i^{transmission} = T_i\ T_i^*\ \mathrm{Re}(k_{zi}^{output} / k_0) \tag{6}$$

where k_0 is the wave vector in vacuum ($2\pi/\lambda$).

The sum of the reflected and the transmitted diffraction efficiences given above must be unity for lossless gratings The dimension of the matrix associated with the eigenvalue problem is given by the number (N) of space harmonics taken to develop the field inside the grating. In order to get convergence, all propagating diffraction orders and a lot of evanescent waves have to be retained in the RCWA.

We should mention that it is not our objective to discuss the numerical implementation of the RCWA. Recently, the RCWA has been revisited by several authors and an enormous increase in the convergence speed for the computation of grating efficiencies has been reported [6,7]. Note that there are several other rigorous diffraction theories for periodic structures based on the differential formulation of the diffraction problem [8].

3. Results and discussions

Our results are with respect to the above example of lamellar silver grating with very narrow slits. We considered for silver a dielectric function that disperses with frequency $\varepsilon(\omega) = [n(\omega) + ik(\omega)]^2$. For the purpose of RCWA calculations the complex index of refraction of silver was interpolated from values tabulated in Ref [9]. Motivated by the results of Refs. [1,2], we investigate the optical response of a silver grating of fixed period (Λ=0.9 μm) in the near infrared region of the spectrum, namely between 0.9 μm and 2 μm. The grating in this region of the spectrum is a 'zero-order' diffraction grating because all diffracted orders, other than zero-th forward-transmitted and backward-reflected order are evanescent. Losses to metal associated with the imaginary part of the refractive index, physically manifested as carrier heating in the metal, can be extracted by the relation $A=1-\eta_{0,t}-\eta_{0,r}$, where $\eta_{0,t}$ and $\eta_{0,r}$ is the zero-order transmission and reflection efficiency, respectively.

The incident power is normalized to the unity. Fig. 2 and Fig. 3a show the transmission efficiency ($\eta_{0,t}$) of grating as a function of the slit width (other diffraction parameters, as the grating depth, period and light wavelength were fixed). For large slits (w > 100 nm), the grating exhibits a broad signal that goes to the unity. However, specific slit widths inferior to 100 nm produces a striking optical response: the grating exhibits very sharp transmission peaks where the absolute transmission efficiency is *greater than the unity*. This absolute transmission efficiency may be estimated by dividing the calculated zero-order transmission efficiency ($\eta_{0,t}$) of the grating to the transparency fraction (w/Λ) of grating. The transparent region is rigorously somewhat larger than the slit width (w) due to the skin effect (skin depth is around of 10 nm). In particular, the strongest peak where $\eta_{0,t}$=40% (see Fig. 3a) shows that this grating of geometrical transparency w/Λ = 3.6% transmits more than 10 times light of 1.433 µm wavelength than impinged directly on the slits. The slit has 32.4 nm width, which is nearly 45 times much smaller than the wavelength of incident light. That is what we call a very narrow slit.

Fig. 3b shows the transmitted efficiency ($\eta_{0,t}$) as a function of grating thickness (period, slit, and wavelength are fixed at Λ=0.9 µm, *w* = 90 nm and λ = 1.433 µm, respectively). Fig. 3c shows the spectral response of a silver grating between 0.9 < λ < 1.8 µm (period, thickness, and slit fixed at Λ=0.9 µm, d = 1.8 µm and *w* = 90 nm, respectively).

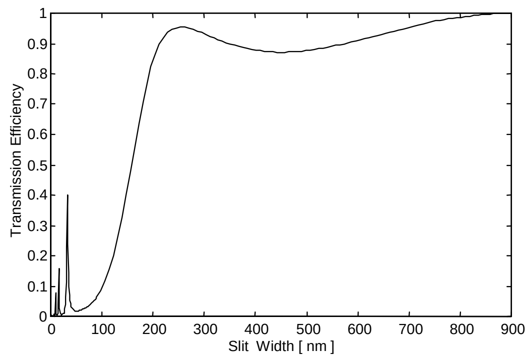

Fig. 2 Zero-order diffraction efficiency ($\eta_{0,t}$) of a lamellar silver grating illuminated normally with an incident TM-polarized plane wave as a function of the slit width (λ = 1.433 μm, d = 1.8 μm and Λ=0.9 μm).

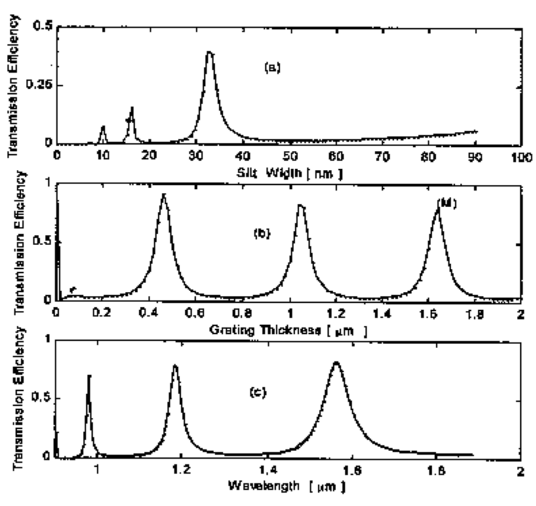

Fig. 3 Zero-order diffraction efficiency ($\eta_{0,t}$) of a 0.9 µm-period lamellar silver grating illuminated with a normally incident plane wave under TM polarization: (a) as a function of the slit width w (fixed parameters are λ = 1.433 μm and d = 1.8 μm); (b) as a function of the grating thickness d (fixed parameters are w = 90 nm and λ = 1.433 μm); (c) as a function of the wavelength of the incident wave λ (fixed parameters are w = 90 nm and d = 1.8 μm).

In order to analyze these results, we have investigated the propagation of electromagnetic eigenmodes inside the grating. The RCWA provides a direct method to find the wave-vectors (k_z) of eigenmodes [10,11]. In general the eigenmode is leaky and its wave-vector is a complex number. However, in our case (for slit width w<100 nm) we found that there is *only* one mode of real wave vector ($\mathrm{Real}(k_z) \neq 0$) which can propagate in the z-direction without significant heat losses (propagative mode). All the other high-order modes have imaginary wave vectors and are strongly evanescent ($\mathrm{Real}(k_z) \approx 0$). The normalized z-component of wave vector of the propagative mode plays the role of the *effective* refractive index of the grating ($n_{eff} = k_z/k_0$, where k_0 is the wave vector in vacuum $2\pi/\lambda$).

We found that the electrodynamical interaction between metallic walls in close distance strongly modify the phase constant of propagative modes. While the effective index is independent of the slit width for a perfect metal (no skin depth) being equal to the unity whatever the slit width is, for the real metallic case (our case), the effective index strongly depends on the slit width, especially for narrow slits. As the slit width becomes larger than about 200 nm the effective index of the slit goes to unity. So there is a strong difference between our real metal case and the perfect metal case [12].

In the following we will demonstrate that this effective refractive index is a very useful concept to predict the transmission peaks of metallic gratings of very narrow slits. We will provide that the transmission peaks occur whenever the *effective* slit cavity contains an integral number of half-wavelengths of the propagative mode, which is expressed by a Fabry-Pérot resonance condition: $m\,\lambda/n_{eff} = 2d$, where *m* is an integer. Indeed, the agreement between n_{eff} computed by the RCWA and those resulted from the Fabry-Pérot resonance condition is very good for the peak location in Fig. 3a (see Table 1).

Table 1
The modification of transmission efficiency and of the effective refractive index of the metallic grating as a function of slit width.

Slit width [nm]	Transmission efficiency ($\eta_{0,t}$)	n_{eff} (RCWA)	$n_{eff} = m\,\lambda/2d$
32.4	0.4	1.54	1.59 (m=4)
16.2	0.16	1.95	1.99 (m=5)
10	0.08	2.36	2.38 (m=6)

Moreover, the three locations resonance (d_1=0.59 μm, d_2=1.17 μm and d_3=1.76 μm) deduced from the resonance condition $m\,\lambda/n_{eff} = 2d$ for λ = 1.433 μm, n_{eff} = 1.22 (effective refractive index of the slit of width w = 90 calculated by RCWA), and m = 1, 2, and 3 are consistent with the peak positions in Fig. 3b. The resonance condition is confirmed in the case of peaks observed in Fig. 3c too.

We conclude that the very high transmission efficiency may be conceived as a *resonant effect* associated to the propagative mode supported by the grating waveguide structure. This observation clearly reveals that the electromagnetic field inside the slit is basically governed by the backward and forward propagation of one single mode. For a given depth not corresponding to a multiple of the half wavelength, no resonance occurs, and no transmission is obtained.

The metallic grating being an efficient converter of incident light to oscillatory energy of electrons it is not surprising that so efficient incoupling of light into waveguiding structure is observed. In a recent paper [5], we have demonstrated that the coupling between the incident light and the fundamental mode supported by the slit is strongly controlled by surface waves (plasmons). As a result, the collection of light into the slit is favored and an unusual optical transmission is achieved.

This paper is dealing with the calculation of optical responses which exhibit a resonant behavior where the signal quickly varies. Much care was taken to guaranty accurate computational results. Because eigenvalues are numerically obtained they are only approximate values and their accuracy increases with the number of retained orders for the eigenvalue problem (see Sec II).

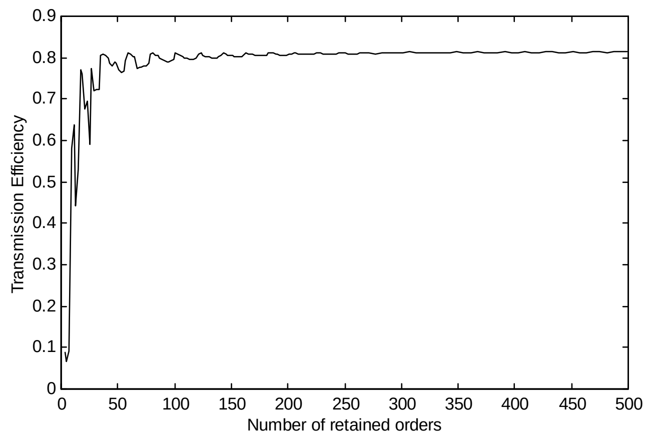

Fig. 4 Transmission efficiency calculated at the point M of Fig. 3b as a function of the number of retained orders. The grating depth is d = 1.637 μm.

Fig. 4 shows the zero-order transmission efficiency ($\eta_{0,t}$) as a function of the number of retained orders. As can be seen 200 retained orders guaranty the accuracy of our results with a relative error smaller than 1%.

4. Conclusions

We have introduced the concept of effective index to interpret the optical transmission of real metallic transmission gratings with very small slits. A simple model based on resonant propagation of the eigenmode inside the grating structure predicts the location of resonances, such as slit width and slit length at which the high transmission will occur.

We believe that the concept of effective index will be of great importance in evaluating the transport and optimum incoupling of light in metallic nanochannels. The result is of broad interest covering research work on metallic gratings, aggregates and colloidal media and may have important consequences for filtering with metallic plates in the near infrared, nanolithography or optical near-field microscopy.

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