# Refining the model of light diffraction from a subwavelength slit surrounded by grooves on a metallic film

Changtao Wang, Chunlei Du, and Xiangang Luo*

*State Key Laboratory of Optical Technologies for Microfabrication, Institute of Optics and Electronics, Chinese Academy of Sciences, Chengdu, China 610209*

(Received 19 December 2005; revised manuscript received 7 October 2006; published 1 December 2006)

By considering the surface plasmon mode in metallic grooves for true metals, we proposed a revised version of the analytical and numerical model on the light diffraction from a subwavelength slit surrounded by finite number grooves on a metallic film, originally published in Phys. Rev. Lett. **90**, 167401 (2003). In comparison to numerical simulations by the finite difference time domain (FDTD) method, the revised model proves more accurate in describing the light diffraction behavior in the case of narrow grooves. A factor concerning the excitation efficiency of surface electromagnetic mode is proposed to measure the grooves' ability of tailoring diffraction patterns. Also discussed are the general characteristics of its dependence with geometrical structure parameters.

DOI: 10.1103/PhysRevB.74.245403 PACS number(s): 42.70.Qs, 73.20.Mf

## I. INTRODUCTION

The dependence of apertured light diffraction on the surface features around the vicinity of aperture edge has never been expected so great until Lezec *et al.*[1] reported experimentally the light beaming from a subwavelength aperture surrounded by surface corrugations on a thin metallic film. The unexpected diffraction phenomena with similar metallic structure have also been observed for microwaves.[2] Its unique diffraction-reducing property provides a unique way to achieve photonic miniaturization in the subwavelength regime.[1,3,4] Although the physical origin of these phenomena has not been fully understood, surface plasmons (SPs) or surface electromagnetic (EM) waves are generally believed to play an important role in governing the unexpected behavior of EM waves. The momentum conservation principle associated with SP diffraction is utilized to explain the beaming direction of light.[1] This is further demonstrated by Liangbin Yu *et al.*[5] with rigorous coupled wave analysis (RCWA) and experimental test. By assuming the perfect conductor condition and fundamental mode approximation, Martín-Moreno *et al.*[6] proposed the first theoretical framework describing the beaming phenomena of slit aperture with finite number of grooves. The interactions among grooves and central slit are fully considered and described with a set of linear equations derived from the EM matching conditions at grooves and slit openings. The anomalous diffraction behavior is regarded as the coherent combination of emissions from the central slit and surrounding grooves. This theory is also employed to explore the enhancement of optical transmission through a grooves-surrounded subwavelength slit[7] and scattering of SP from one-dimensional periodic nanoindented surfaces.[8] In addition, the similar diffraction phenomena are also observed in the light emission from photonic crystal waveguides with proper surface corrugations,[9,10] which provides extra illustrations for the excited surface EM wave affecting the diffraction behavior of apertured light.

In this paper, we investigated the light diffraction from slit aperture with finite metallic grooves for true metals. First, an improved version of the diffraction theory in Ref. 6 is derived through the Raleigh-Sommerfeld diffraction formalism and the coupled SP mode in grooves. In Sec. III, the validity of the improvement is justified by comparing it with the finite difference time domain (FDTD) simulation. The following section introduces a factor concerning the magnitude of excited surface EM wave. It is used to discuss the grooves' ability for tailoring diffraction patterns of slit-groove structures, as well as the diffraction dependence with variant geometrical parameters. A brief summary is given at the end.

## II. THEORETICAL FORMALISM

In this section, we will propose a refinement of the theoretical formalism[6] on the light diffraction from a slit-grooves metallic structure. To keep the integrity of the formalism, a derivation by use of conventional diffraction theory is presented. Another benefit of this dealing is that we can clearly see the difference between apertures with subwavelength structured screen surface and conventional diffraction problems, such as a circular hole with opaque and smooth screen,[11] when applying the scalar diffraction theory.

Considering a subwavelength slit aperture symmetrically surrounded by $2N$ grooves on the exit side of a metallic film (Fig. 1). The slit and grooves, all with a width of $a$, are positioned periodically with a space of $d$ and a constant groove depth of $h$. The monochromatic and TM polarized illuminating light is incident from the left side. The TE polarization case is not considered here due to its weak ability of tailoring light diffraction.[1,6] The used coordinate and polarization are depicted in Fig. 1.

According to the Kirchoff's diffraction theory, the field at any point $P$ can be determined by some form of integration with the appropriate Green function over a surface enclosing the point. Here we assume the second class of Raleigh-Sommerfeld diffraction equation[11] as

 

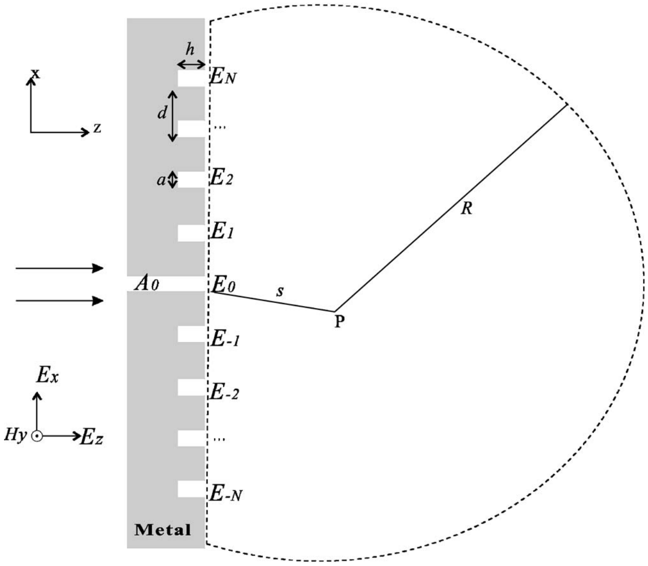


FIG. 1. Schematic of light diffraction from a metallic slit surrounded by grooves corrugation. The dashed line represents the integral surface of the Kirchoff's diffraction theory. The origin of the coordinate is in the middle of the slit's right opening.

$$U(P) = -\frac{1}{2\pi}\int\int \frac{\exp(iks)}{s}\frac{\partial U}{\partial z}dS, \quad (1)$$

where $U$ is the scalar variable of the EM field, $k=2\pi/\lambda$, $\lambda$ is the light wavelength in vacuum and $s=\sqrt{(x-x')^2+(y-y')^2+z^2}$. The rigorous integration region is a closed surface including the opening of the central slit aperture, the portion of being not directly an illuminated side of metal screen and a large semisphere of radius $R$ centered at $P$. In much the same way in Kirchhoff's diffraction theory, the contribution from the sphere can be neglected if $R$ is sufficiently large. But the contribution from the screen should not be arbitrarily regarded unimportantly here because some form of surface EM wave may be excited along corrugations. Note that the flat metal screen without corrugation would not deliver considerable change to the diffraction pattern of slit aperture, it is reasonable to assume that the disturbance mainly comes from the openings of corrugations. So the integration is further restricted to the regions of grooves and central slit openings. In some sense, this assumption can be viewed as the perfect conductor approximation at the output metal surface. If we let $U$ denote the EM field component $H_y$ then

$$H_y(P) = -\frac{ik}{2\pi\mu_0 c}\int\int_{\text{openings(grooves+slit)}} E_x(x,y,z = z_0)\frac{\exp(iks)}{s}dS, \quad (2)$$

where $\mu_0$ and $c$ is the magnetic permeability and the velocity of light in the vacuum. Considering the infinity of slit-grooves aperture in the $y$ direction, the above equation can be further reduced to a simplified form

$$H_y(x,z) = \frac{-ik}{2\mu_0 c}\int_{\text{openings(grooves+slit)}} E_x(z=z_0)H_0^{(1)} \times (k\sqrt{(x-x')^2+z^2})dx', \quad (3)$$

where $H_0^{(1)}$ is the zero-order first class Hankel function.

Now we encounter the difficulty of how to determine the $E_x$ at the openings of each groove and slit. Usually, the rigorous analytical solution of this problem is hard to obtain and numerical method, $x'$FDTD for instance, is often recommended. But some form of approximated analytical solution is available with EM matching condition, if appropriate approximation is introduced.

First, it is necessary to know the EM field or the surface EM admittance at the two sides of groove and slit openings. Usually, only the fundamental mode is considered in a subwavelength metal groove due to the evanescence property for modes of higher order. Instead of the approximation of TEM mode for perfect conductor case,[6,7] we introduce a TM mode of combined SPs in subwavelength grooves for true metal materials. The reason for this treating can be well understood from the following analysis.

Considering an air channel sandwiched between two semifinite metal plates with a space of $a$. By the similar analytical derivation for planar dielectric waveguides,[12] the general fundamental TM mode inside grooves can be expressed as

$$E_x = \beta T\cosh(Tx)\exp(\pm j\beta z), \quad (4)$$

$$E_z = -jT^2\sinh(Tx)\exp(\pm j\beta z), \quad (5)$$

$$H_y = \frac{k}{\mu_0 c}T\cosh(Tx)\exp(\pm j\beta z), \quad (6)$$

where $T^2=\beta^2-k^2$, $\beta$ is the propagation constant which can be calculated in an explicit way from the following expression:

$$\varepsilon_m\sqrt{\beta^2-k^2}a\tanh\lfloor\sqrt{\beta^2-k^2}a/2\rfloor = -\sqrt{\beta^2-\varepsilon_m k^2}a. \quad (7)$$

$\varepsilon_m$ is the dielectric coefficient for true metal and its value can be calculated from the Drude formalism $\varepsilon_m(\omega)=\varepsilon_\infty-\frac{\omega_p^2}{\omega(\omega+i\kappa)}$, where $\omega_p$ is the plasma frequency, $\kappa$ is the absorption, $\omega$ is the frequency, and $\varepsilon_\infty$ comes from the contribution of the bound electrons to the polarizability.

Generally, $\beta$ is a complex number and its real and imaginary part represents propagation constant and absorption loss respectively. As stated by some papers,[13] the TM mode displays a greater propagation constant than the TEM mode, especially for much narrower grooves. Since the imaginary part of $\beta$ is usually much smaller than the real part for the groove width with practical implication, we neglected it in the following analysis. So we can assume the standing wave of the fundamental TM mode, Eqs. (4)–(6), in the grooves due to the total reflection at the groove bottom. The effective surface EM admittance at groove openings, if the disturbance at groove openings contributed from higher order modes is neglected, can be expressed as

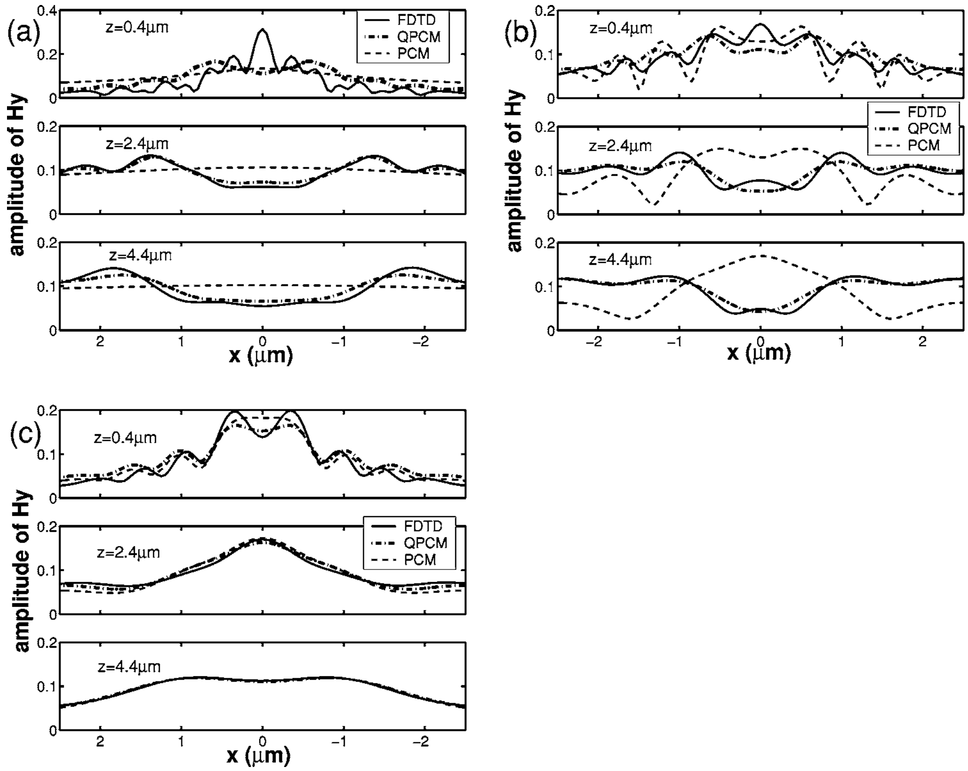


FIG. 2. Calculated diffraction patterns (time averaged $H_y$ distribution) at certain $z$ (0.4 $\mu$m, 2.4 $\mu$m, and 4.4 $\mu$m) by use of FDTD, PCM, and QPCM. The parameters are as follows: (a) $a=0.1$ $\mu$m, $h=0.25$ $\mu$m, $\lambda=0.5$ $\mu$m; (b) $a=0.05$ $\mu$m, $h=0.1$ $\mu$m, $\lambda=0.6$ $\mu$m; (c) $a=0.25$ $\mu$m, $h=0.2$ $\mu$m, $\lambda=0.8$ $\mu$m.

$$Y = j\frac{k}{\beta\mu_0 c}\cot(\beta h + \phi_0), \tag{8}$$

where $\phi_0$ is the phase shift due to the slight penetration into the metal at the bottom of the grooves. For the simplicity of computation, it is approximated as the case of plane wave normally incident on planar metallic surface, namely

$$\phi_0 = \frac{1}{2}\arg\left(\frac{{\varepsilon_m}^{1/2} - 1}{{\varepsilon_m}^{1/2} + 1}\right). \tag{9}$$

Here arg is the phase angle of a complex number.

Now we apply the EM matching condition to solve the coupling of grooves and central slit, as presented in Ref. 6. Let $E_\alpha$ denotes the magnitude of $E_x$ at groove openings with $\alpha$ running over all grooves and $\alpha=0$ for the central slit. The integration averaged $H_y$ component outside the grooves matches that associated with the fundamental groove mode, i.e.,

$$E_\alpha Y_\alpha = \sum_\gamma G_{\alpha\gamma}E_\gamma,\ (\alpha \neq 0), \tag{10}$$

where $G_{\alpha\gamma}E_\gamma$ represents the averaged integration of $H_y$ at the opening of groove $\alpha$ contributed from groove $\gamma$

$$G_{\alpha\gamma} = \left(-\frac{k}{2a\mu_0 c}\right)\int_{\text{opening}\to\alpha} dx \int_{\text{opening}\to\gamma} dx' H_0^{(1)}[k|x - x'|]. \tag{11}$$

In some sense, $G_{\alpha\gamma}$ can be regarded as the effective coupled surface admittance between groove $\alpha$ and $\gamma$. For the central slit, the EM matching equation becomes

$$E_0 Y_0 = \sum_\gamma G_{0\gamma}E_\gamma + A_0. \tag{12}$$

Because the EM field in the slit takes the form between traveling and standing state, the surface EM admittance $Y_0$ at opening has complicated expression. However, it can be proved that changing the value of $Y_0$ would not deliver the change to the solution of Eqs. (10) and (12) except that it is multiplied by a constant complex number.[14] Since we are mainly discussing the diffraction pattern, $Y_0$ can take any value in the following calculation and analysis, for instance $\sqrt{\frac{\varepsilon_0}{\mu_0}}$ for traveling plane wave in vacuum. Note that the model presented here can be reduced to that in Ref. 6 by replacing the admittance Eq. (8) with $Y=j\sqrt{\frac{\varepsilon_0}{\mu_0}}\cot(kh)$ for a perfect conductor. It is appropriate to name them the quasiperfect conductor model (QPCM) and the perfect conductor model (PCM), respectively.

## III. ILLUSTRATIVE EXAMPLES OF COMPARISON TO FDTD RESULTS

In order to illustrate the validity of the theoretical model, numerical calculations of slit-grooves diffraction pattern are performed in the near field region by QPCM proposed in this paper, the model in Ref. 6 (PCM) and FDTD method. The common parameters of calculated slit-grooves structure are as follows: space between grooves $d=0.5$ $\mu$m, four grooves are positioned on both sides of the central slit. The used metal is Ag with $\omega_p=1.346\times 10^{16}$ Hz, $\kappa=9.617\times 10^{13}$ Hz, $\varepsilon_\infty=4.2$. These parameters are also shared by the numerical calculations of the following sections. The calculation region of FDTD is set to be

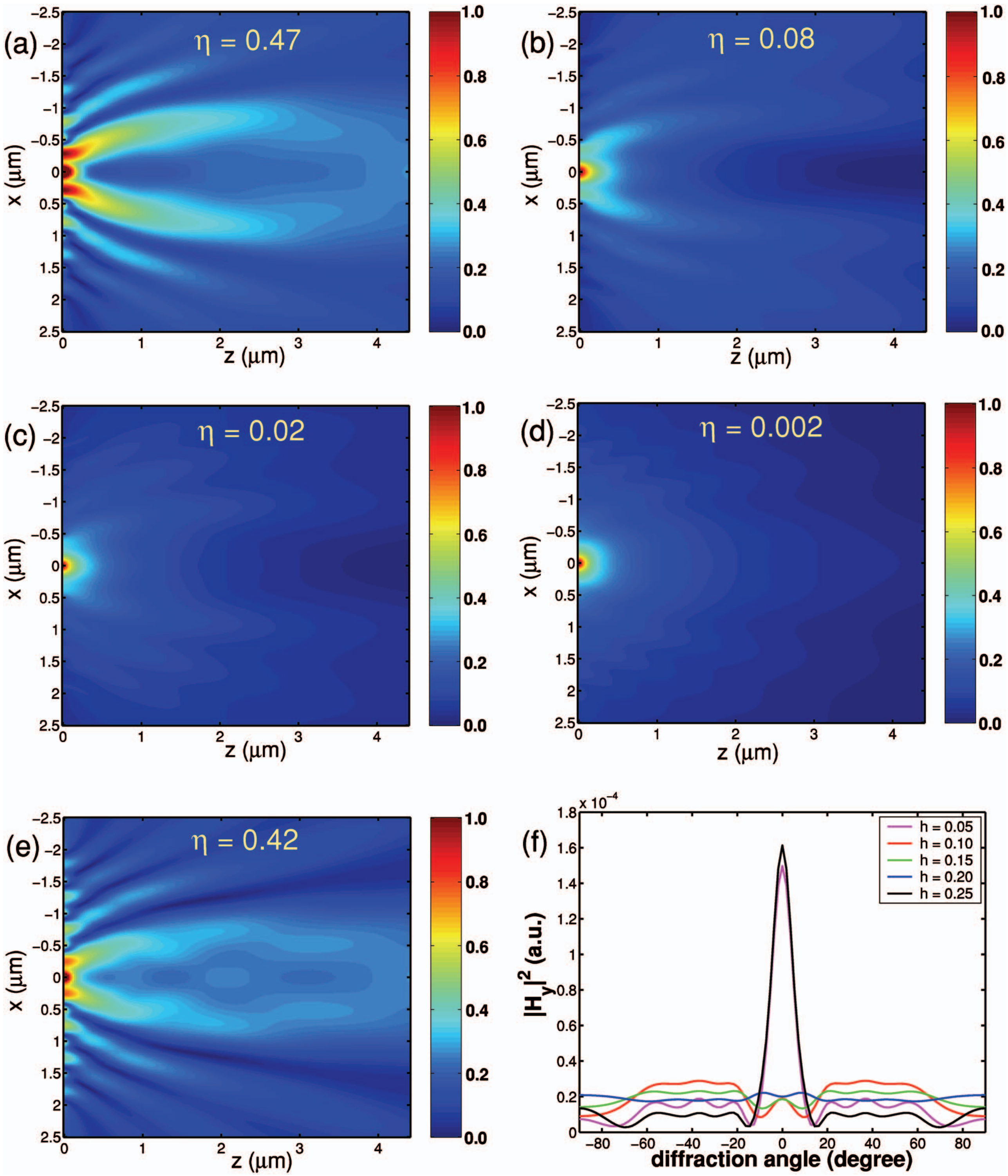


FIG. 3. (Color) Illustrative examples of surface EM wave excitation factor indicating the magnitude of deviation of diffraction behavior from conventional subwavelength diffraction. (a), (b), (c), (d), and (e) are time averaged Hy for groove depth ranging from 0.05 $\mu$m to 0.25 $\mu$m with a step of 0.05 $\mu$m. Plotted in (f) are the calculated diffraction angle spectra in the far field region. The other parameters here are $d=0.5$ $\mu$m, $a=0.05$ $\mu$m, and $\lambda=0.6$ $\mu$m. The model used here is QPCM.

5 $\mu$m $\times$ 5 $\mu$m and the grid cell is 0.005 $\mu$m $\times$ 0.005 $\mu$m. Moreover, a perfect matching layer is positioned around the computation region.

Figure 2 presents three groups of calculated diffraction pattern (amplitude of time averaged $H_y$) at certain $z$ (0.4 $\mu$m, 2.4 $\mu$m, and 4.4 $\mu$m) with different geometrical groove parameters and wavelength (see caption). Since undetermined constant maybe exist between FDTD and PCM and QPCM, all the data are scaled with the square integration along $x(-2.5\ \mu\text{m} \sim 2.5\ \mu\text{m})$ being 1. From these figures, we

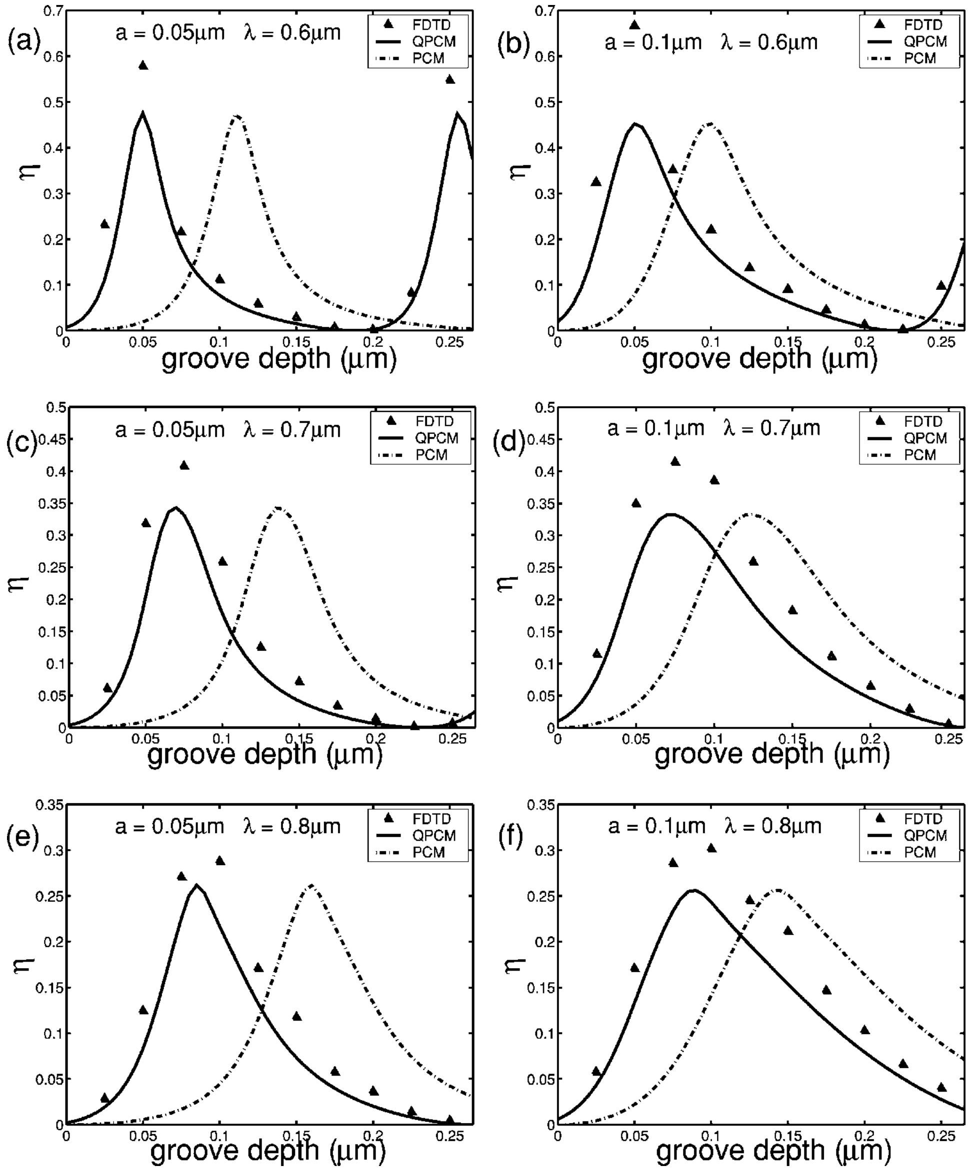


FIG. 4. Dependence of excitation efficiency of surface EM field on groove depth for groove width $a=0.05$ $\mu$m and 0.1 $\mu$m and $\lambda=0.6$ $\mu$m, 0.7 $\mu$m, and 0.8 $\mu$m. The other parameters are the same as those in Fig. 3.

can see that the QPCM presented in this paper is more accurate than the PCM in describing the diffraction pattern in the specific case of narrow groove width. For the case of wide grooves, however, both PCM and QPCM show good agreement with FDTD. This can be well understood because the fundamental TM mode in this case is close to the TEM mode for perfect conductor and similar surface admittance is observed at openings. Admittedly, great deviations with FDTD are observable, especially at surfaces ($z=0.4$ $\mu$m) close to the slit and groove openings. This, we believe, mainly arises from the assumption that the $E_x$ field at the grooves-patterned integral surface (Fig. 1) is zero for regions not localized at groove and slit openings.

## IV. DISCUSSIONS

### A. Origin of unexpected diffraction phenomena

Clearly, the origin of unexpected diffraction behavior is the excited surface EM wave at the grooves-patterned metallic output surface.[6,7] Accordingly, the contributions from all the aperture screen including grooved parts and non-grooved parts have to be included in the computation of scalar diffraction integration.[11] This point is crucial and of great significance for the analysis of subwavelength photonic devices. Since it is the surface structures that govern the light diffraction behavior, light beaming observed for dielectric photonic crystals waveguide featured with specifically designed corrugation at output surface which resembles metallic grooves and plays the same role,[9,10] is reasonably possible.

One point worth highlighting is the physical insight delivered by the two models. PCM assumes perfect conductor approximation everywhere for the total metallic structure.[3,6,7] Not only does it provide us the simplified analytical and numerical model for designing structures related to SP resonance, the physical insight of these anomalous diffraction phenomena is revealed as well. It convinces us that the subwavelength structures dominate the exciting and scattering surface EM waves and hence change the diffraction behavior. QPCM, however, provides improved accuracy in describing the diffraction behavior by applying the perfect conductor condition to the output metal surface and considering the optical property of groove mode with true metals. This improvement is especially obvious for the cases of narrow grooves because the penetration depth of light into metals with finite admittance becomes comparable with the size of groove structures. In some sense, the dominating role of subwavelength structures is further demonstrated through QPCM. More importantly, it shows that the optical property of true metals, even for good conductors such as Ag and Au, may strongly influence the diffraction behavior and should be fully considered in the definite design of photonic devices using these phenomena.

### B. Dependence of diffraction with geometrical parameters

In addition to the complete quantitative description of diffraction pattern, it would be very useful to find a simple way in evaluating the influence of grooves imposed on the diffraction pattern. From the above analysis, we know the disturbance to normal diffraction behavior comes from the excited electronic field at each groove opening. So the portion of electronic energy at groove openings along the total output surface can be regarded as a good measurement for its ability of tailoring diffraction pattern. We refer to it as surface EM wave excitation efficiency and its definite expression is $\eta=\Sigma_{grooves}|E_\alpha|^2/\Sigma_{slit+grooves}|E_\alpha|^2$. $\eta$ can also be related with the confinement factor which is commonly used in describing the waveguide mode's ability of confining energy.[15] $\eta$, however, describes the opposite effect of distracting energy from central slit to groove openings.

As an example of demonstrating the $\eta$'s fidelity of evaluating the diffraction disturbance, Fig. 3 presents the evolution of diffraction pattern for groove depth varying from 0.05 $\mu$m to 0.25 $\mu$m, both in the near field and in the far field. The other parameters can be seen in the figure caption. For high valued $\eta$ with $h=0.05$ $\mu$m and $h=0.25$ $\mu$m in Figs. 3(a) and 3(e), $H_y$ is mainly localized in two branches. Slowly, the magnetic field spreads and merges at the distance of about 3 $\mu$m from the slit, indicating a great deal of the portion of the field is confined to the propagation direction with a small divergence. This is further confirmed with a peak around zero degree of angle spectra in Fig. 3(f). With decreased $\eta$ in Figs. 3(b) and 3(c), the diffraction from central slit becomes dominating and more energy is diffracted into wide space and directions. For groove structures exhibiting nearly zeroed surface EM wave excitation, as shown in Fig. 3(d), weak and even no disturbance is observed to the diffraction pattern of the slit aperture and light is diffracted almost uniformly into all directions.

Figure 4 plots the functions of $\eta$ with groove depth ranging from 0 $\mu$m to 0.25 $\mu$m for different groove width and wavelength calculated by FDTD, QPCM, and PCM. For FDTD, $E_\alpha=\frac{1}{a}\int_{opening\to\alpha}E_x(x)dx$. Obviously, the QPCM results exhibit better agreement with FDTD. $\eta$ oscillates with $h$ and reaches maximum at certain values of $h$. At the same time, for some groove depth, the surface EM wave excitation is damped to zero and the light diffraction from the central slit is featured with a nearly 180° divergence, as conventional diffraction theory predicts. This can be well understood from Eqs. (8) and (10) that the surface admittance at groove openings governs the surface mode excitation, which is a cotangent function with $h$. Accordingly, the oscillation period is half the wavelength in the groove. In this case, the surface EM admittance reaches infinity and the diffraction behaves like that of smooth metallic surfaces. Thus no tailoring of diffraction pattern occurs. Moreover, we can also see that small groove width helps to obtain narrower resonance excitation peak with shortened oscillation period due to increased propagation constant in grooves.

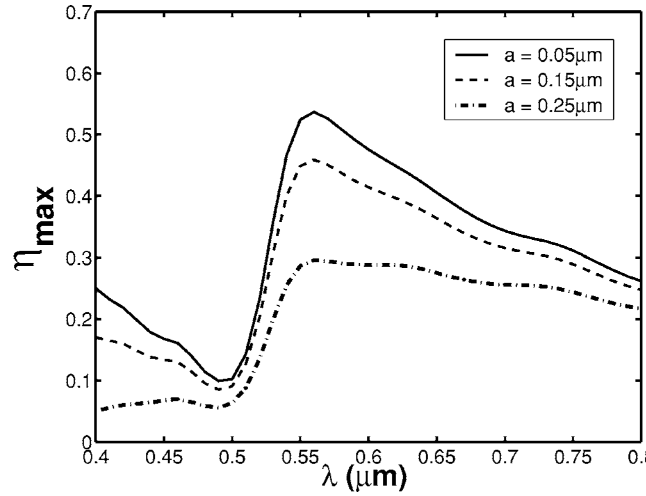


FIG. 5. Maximum surface mode excitation efficiency versus wavelength for fixed $d=0.5$ $\mu$m and variant groove width of 0.05 $\mu$m, 0.15 $\mu$m, and 0.25 $\mu$m.

The wavelength of light $\lambda$ and groove space $d$ between grooves and central slit display **a** dominating role in governing the behavior of diffracted light.[3,6] They give maximum excitation efficiency $\eta_{max}$ by tuning groove depth if the other parameters are fixed, as shown in Fig. 5. The maximum $\eta_{max}$ occurs around the wavelength of about $1.1d$ and the minimum value appears at wavelength around $d$. This can be related with the analysis of SP scattering by one-dimensional periodic nanoindented surfaces in Ref. 8, which indicates the scattering is most strongly damped and intensified at the lower and upper edge of a band gap for groove structures. We also see that wide grooves display decreased excitation efficiency and slowly sloped variance than narrow grooves. Similar results are also observed in the investigation of angular spectra with this type of metallic structures.[16]

## V. CONCLUSION

In summary, we proposed a refinement to the numerical model in Ref. 6 which can be successfully used to describe the light diffraction behavior of slit-grooves structures for true metals in the case of narrow groove width. The revised model indicates that the optical property of true metals, even for good metals such as Ag and Au, may possess great influence to the light diffraction as the size of subwavelength structure is comparable to the depth of light penetration into metal. A factor of surface EM wave excitation efficiency at groove openings was introducedto measure the grooves' ability of tailoring diffraction pattern. By use of the above results, we also discussed the general characteristics of diffraction dependence on the geometrical parameters, which would help to design subwavelength metallic photonic devices.[17,18] Our discussion is limited to the one dimensional case with slit-grooves structures, but some ideas and conclusions may be extended to the two-dimensional case with different groove shapes and complicated distributions.

## ACKNOWLEDGMENTS

This work was supported by the National Basic Research Program of China (2006CB302900) and the Chinese Nature Science Grant (No. 60507014/F05 and No. 60528003).

---

*Author to whom correspondence should be addressed. Electronic address: lxg@ioe.ac.cn

[1] H. J. Lezec, A. Degiron, E. Devaux, R. A. Linke, L. Martín-Moreno, F. J. García-Vidal, and T. W. Ebbesen, Science **297**, 820 (2002).

[2] A. P. Hibbins, J. R. Sambles, and C. R. Lawrence, Appl. Phys. Lett. **81**, 4661 (2002).

[3] F. J. García-Vidal, L. Martín-Moreno, H. J. Lezec, and T. W. Ebbesen, Appl. Phys. Lett. **83**, 4500 (2003).

[4] L. A. Blanco and F. J. García de Abajo, Opt. Lett. **29**, 1494 (2004).

[5] Liang-Bin Yu, Ding-Zheng Lin, Y. C. Chen, Y. C. Chang, K. T. Huang, J. W. Liaw, J. T. Yeh, J. M. Liu, C. S. Yeh, and C. K. Lee, Phys. Rev. B **71**, 041405(R) (2005).

[6] L. Martín-Moreno, F. J. García-Vidal, H. J. Lezec, A. Degiron, and T. W. Ebbesen, Phys. Rev. Lett. **90**, 167401 (2003).

[7] F. J. García-Vidal, H. J. Lezec, T. W. Ebbesen, and L. Martín-Moreno, Phys. Rev. Lett. **90**, 213901 (2003).

[8] F. López-Tejeira, F. J. García-Vidal, and L. Martín-Moreno, Phys. Rev. B **72**, 161405(R) (2005).

[9] P. Kramper, M. Agio, C. M. Soukoulis, A. Birner, F. Müller, R. B. Wehrspohn, U. Gösele, and V. Sandoghdar, Phys. Rev. Lett. **92**, 113903 (2004).

[10] Esteban Moreno, F. J. García-Vidal, and L. Martín-Moreno, Phys. Rev. B **69**, 121402(R) (2004).

[11] Max Born and Emil Wolf, *Principles of Optics* (Cambridge University Press, Cambridge, 7th expanded edition).

[12] H. A. Haus, *Waves and fields in optoelectronics* (Prentice-Hall, Englewood Cliffs, NJ, 1984).

[13] H. Shi, C. Wang, C. Du, X. Luo, X. Dong, and H. Gao, Opt. Express **13**, 6815 (2005).

[14] The relation of two sets of solution $E_\alpha$ and $E'_\alpha$ with different impedance $Y_0$ and $Y'_0$ at central slit opening can be obtained with simple algebra manipulation as $\frac{E_\alpha}{E'_\alpha}=1+\frac{(Y'_0-Y_0)E_0}{A_0}$.

[15] H. Kogelnik, "Theory of dielectric waveguides," in *Integrated Optics*, edited by T. Tamir (Springer-Verlag, Berlin, 1975).

[16] C. Wang, C. Du, Y. Lv, and X. Luo, Opt. Express **14**, 5671 (2006).

[17] X. Luo, H. Wang, J. Shi, and H. Yao, Mod. Phys. Lett. B **18**, 1181 (2004).

[18] X. Luo and T. Ishihara, Appl. Phys. Lett. **84**, 4780 (2004).