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Effects of relief gratings, light characteristics and material properties to the emission resonance region

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ABSTRACT

We present numerical simulations in order to investigate the coupling of the incident radiation to Surface Plasmon polaritons (SPPs) by metallic relief gratings. When the frequency of the SPPs is coincident with the electromagnetic waves, there is a strong absorption of the electromagnetic waves. This phenomenon is called surface Plasmon resonance (SPR). The effects of surface materials, characteristics of incident light and the geometrical shapes on the SPR are studied by using the rigorous coupled-wave algorithm (RCWA). The results reveal that a peak of high emissivity is obtained for Au compared with W, Cu and Al. This explained that the gold is the best transition metal used for the excitation of SPPs. At the resonance the absorption of light by the (Au) grating is greater for grazing than normal incident light. Every considered transition material has the particular wavelength emission region and the period emission region. The influence of gratings geometric parameters on the SPR is also presented.

Keywords

Diffraction; Metallic gratings; Surface Plasmon resonance; Emission.

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INTRODUCTION

The SPPs are electromagnetic waves localized on the surface of a metal or a doped semiconductor and dielectric interface and coupled to the collective oscillations of free charges [1]. In recent years, the research of SPPs in the near-infrared and visible ranges has received much attention. It has attracted considerable attention due to their application in optical sensor devices [2, 3]. In attempts to excite the SPPs by transverse magnetic polarized light incident on a metal grating from the adjacent dielectric medium, the frequency of the incident light must be equal to the frequency of the SPPs. The direct excitation of SPPs by light beams is not possible unless special techniques to achieve phase matching are employed such as total internal reflection geometry (Kretschmann and Otto configurations [4-6]), waveguide coupling [7] and grating coupling method [1]. Recently, A. Dhawan et al. [8] have presented a novel SPR configuration based on narrow groove plasmonic nano gratings without the use of Kretschmann configuration.

The study of radiative properties of surface-relief gratings based on SPPs excitation is important for both academic researches and practical applications [9-14]. Several numerical and experimental methods are essential in the design and analysis of grating structures. The last several decades, many rigorous numerical methods have been developed for solving the diffraction grating problem [15-34] such as the analytic modal method [17], the differential method [18], the integral equation method [19-21], the coordinate transformation method (C method) [22, 23], the finite element method (FEM) [24, 25], the finite-difference time-domain method (FDTD [10], a method of variation of boundaries [27], the method of fictitious sources (FS) [28] and the RCWA [29-34]. Currently, the RCWA method has been widely used in optical critical dimension (OCD) metrology for the optical modeling of grating structures. Over the last years, the RCWA become one of the most popular methods for grating diffraction simulation. In the RCWA algorithm, the permittivity of the grating region is first expanded into a series of Fourier harmonics and then the electromagnetic field is expressed as a Fourier expansion with a corresponding order of harmonics [35]. Schuster et al. achieved a better convergence than the conventional formulations [36], by combining the classic RCWA with Popov and Neviere`s general equations [37].

In this paper, we aim at discovering the effects of the geometrical and optical parameters on the radiative properties of surface gratings. These parameters are involved in several application areas ranging from the calculation of energy exchange by radiation in the design of selective rough surfaces, applications on the semiconductor industry and the solar energy. In addition with the recent development of micromaching techniques a number of reports have been published. They have study the interaction between thermal radiation and SPPs [38, 39], the microcavity effect [40, 41], and photonic crystals [42**]**. In addition, the effects of various geometrical and physical parameters on the excitation of SPPs is a subject of many authors. F. Marquier et al. [11] have quantified the thermal emission of highly doped silicon grating surfaces in the near field and the far field. M. Kreiter et al. [38] have reported the emission of light at two different wavelengths, 710 and 810 nm, from the gold-covered grating. Recently, A. Dhawan et al. [8] have employed RCWA calculations to study the effect of the nano-gratings parameters on their plasmon resonance wavelengths.

In the present paper, firstly, we introduce the RCWA theory, which is proposed by Chateau and Hugonin [29]. Secondly, we report the numerical study of the scattering of electromagnetic waves by metallic gratings by using the RCWA. The effects of geometrical and physical parameters on the transverse magnetic polarized emissivity are of interest. Finally, many results and discussions are presented. The position and shape of the resonance of the SPPs is extremely sensitive to both the roughness of the interface profile and the characteristic of incident light. In the context, we aim is to determine the ERR and the resonance peak (RP) for various transition metals such as Au, Cu, Al, and W. The second goal is to quantify the influence of the relief morphology (period, depth and geometrical shape) on the SPR, within the visible range, impinging at a given incidence angle. The third goal is to study the effects of the characteristics of incident light on the excitation of SPPs. At the end, the comparisons are performed and restricted between Au and W.

THEORY

Because the excitation of the SPPs is not detected by TE polarization case, a simple compact formulation of the RCWA is presented only for TM polarization. The general three-dimensional binary grating diffraction problem is depicted in Fig. 1. A linearly polarized electromagnetic wave is obliquely incident at an arbitrary angle of incidence θ_{inc} and at an azimuthally angle $\emptyset$ upon a binary dielectric or lossy grating. We consider the case of planar diffraction ($\emptyset = 0$). Here all the forward and the backward diffracted orders lie in the same plane of incidence (the x-z plane). The grating is bound by two different media with refractive indices n_I and n_{II}.

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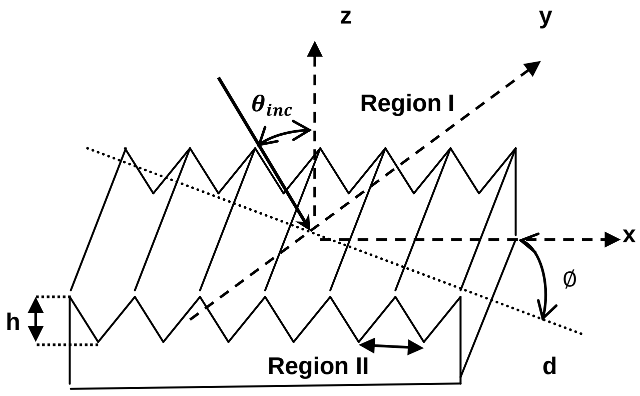

Fig1. Geometry for the binary rectangular-groove grating

In the grating region ($0 < z < d$), the periodic relative permittivity associated with the surface-relief is expandable in a Fourier series as:

$$\varepsilon(x) = \sum_{h=-\infty}^{+\infty} \varepsilon_h \exp(j\frac{2\pi h}{d}), \quad (1)$$

Where ε_h is the hth Fourier component of the dielectric function in the grating region, which is complex for lossy or non symmetric dielectric gratings. In this study, we have assumed that the incident light has transverse magnetic (TM) polarization.

A detailed formulation for a stable and efficient numerical implementation of this analysis technique was presented for one-dimensional binary gratings for both TE and TM polarization and for the general case of conical diffraction in reference 30.

Using the RCWA technique, we calculate diffraction efficiencies up to $\pm 7\ th$ diffraction orders. The emissivity of the grating sample is estimated from the following equation:

$$\xi(\lambda.\theta_{\text{inc}}) = 1 - \sum_i (DE_{ri} + DE_{ti}) \quad (2)$$

Where DE_{ri} and DE_{ti} are the diffractions efficiencies in region I and II.

This condition is necessary but not sufficient for the success of the numerical algorithm. The RCWA converges to the proper solution for metallic binary gratings [43]. Convergence for incident TE polarization is efficient, requiring a small number of field harmonics. However, a significantly larger number of field harmonics are required for the case of TM polarization, and convergence is very slow [30].

RESULTS AND DISCUSIONS

The emissivity of periodic rough surfaces are the radiation properties of interest, with ranging from $0.1\,\lambda$ to $100\,\lambda$. The effects of the geometrical and physical parameters on surface emission are interesting. The RCWA has been used to compute the emission of transverse magnetic polarized plane wave. The results demonstrate that by the variation of several parameters (roughness, geometrical shape, characteristics of incident light and surface materials) we can control the properties of grating in emission.

The contribution of various geometrical and physical parameters to the plasmon resonance phenomena is the subject of interest. Also, we define two parameters. The first is called the resonance region (RR), detected by an increase brusque of the emissivity, signaled by a strong emission ξ_0 at particular parameter. The second is called the resonance peak (RP). Consequently, we can define the geometrical parameter called the period resonance region (PRR) and the physical parameter called the wavelength resonance region (WRR). The period resonance peak (PRP) is defined by: $\text{PRP}(\text{d}_0/\lambda, \xi_0)$ at fixed depth, and the wavelength resonance peak (WRP) is defined at fixed depth and period $\left(\text{WRP}(\lambda_0(\mu\text{m}),\ \xi_0)\right)$.

Effects of surface materials and incident light characteristics to the emission resonance region

In this subsection, we study the effects of surface materials and the characteristic of incident light on the behavior of the emissivity. Figure 2 shows curves displaying behavior of the emissivity of triangular grating (TG) versus the ratio d/λ at fixed h/λ and incidence angle, characterized by the function $\text{z} = \text{h}(\text{x})$, for various materials (Au, W, Cu and Al). Figure 3 shows curves displaying behavior of the emissivity of TG versus the ratio d/λ at fixed h/λ for various incidence angles. Figure 4 shows curves displaying behavior of the emissivity of TG characterized by the geometrical parameters: $\text{h}/\lambda = \text{d}/\lambda = 0.1$, versus the wavelength raging from $0.4\ \mu\text{m}$ to $0.8\ \mu\text{m}$, at fixed emission angle ($\theta_{\text{inc}} = 1^{\text{o}}$).

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• Effects of surface materials

Figure 2a and Figure 2b (zoom) show curves displaying behavior of the emissivity of TG versus the ratio d/λ. For each one of curves of Figure 2a, the asymptotic behavior is obtained for the greater values of the d/λ. The horizontal asymptote is defined by the value of the emissivity of the plane surface of the considered material. Table I shows, for all materials at the resonance peak approximately the half of the energy is absorbed by the triangular grating. The maximum of the emissivity at the (RP) is the greater for the (Au) material, and the lesser for the (W) material. The (Au) and the (Cu), which have the same configuration (n d^{10} (n+1) s^{1}), have the same value of d_0/λ.

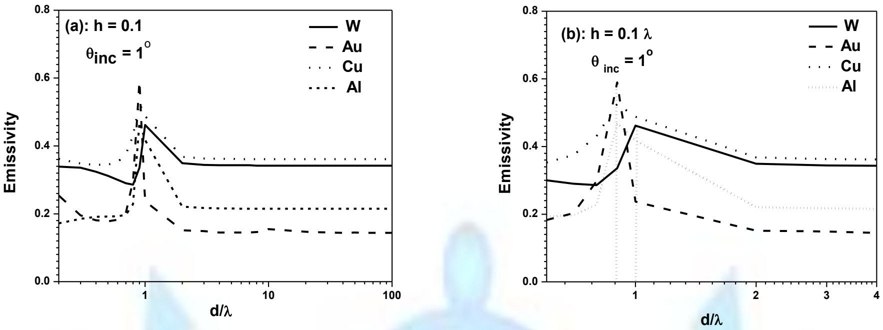

Fig 2. Dependence of the TG emissivity on the period of microstructure for various materials. Parameters: $\theta_{inc} = 1^o$, $\lambda = 0.55\ \mu m$ and $h/\lambda = 0.1$

The table below resume the results for the ERR of the considered transition metals.

Table 1. The PRR and the coordinates of PRP for W, Au, Cu and Al materials

Material	**W**	**Au**	**Cu**	**Al**
PRR	[0.6. 2]	[0.5. 1]	[0.5. 2]	[0.6. 2]
d_0/λ	**1**	**0.9**	**0.9**	**0.9**
$\xi_0(\lambda.\theta_{inc})$	0.462	0.59	0.526	0.469

• Effects of incident light characteristics

In the subsection, we examine the effects of characteristic of the incident light on the (RD) and the (RP). Firstly we investigate the effects of the direction of incident light, we consider three incidence angles 1°, 20° and 80°. Figure 3b shows, for triangular gold grating at fixed h/λ, the peak of resonance is moved from $d_0 = 0.9\,\lambda$ at normal incident ($\theta_{inc} = 1°$ to $d0{=}0.5\ \lambda$ at oblique incident $\theta inc{=}80°$ and the emissivity is decreased (table II).This resume the resonance phenomena at oblique incident need narrow grating. It is found that, the excitation of SPPs is depended on the direction of light. For the oblique incident light, Figure 3 shows, the excitation of the SPPs needed deep gratings for the two materials.

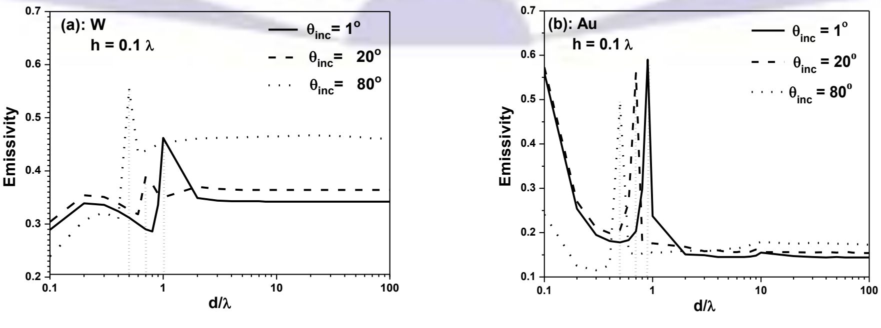

Fig 3. Variation of the emissivity versus the ratio d/λ for two materials Au and W. Parameters: $\lambda = 0.55\ \mu m$ and $h/\lambda = 0.1$

Table 2. The RR and RP for Au and W materials for various incidence angles

θ_{inc}	RR of Au	RR of W	$d_0/\lambda\,(Au)$	$d_0/\lambda\,(W)$	$\xi_0(\lambda.\theta_{inc})$ of Au	$\xi_0(\lambda.\theta_{inc})$ of W
1°	[0.5; 1]	[0.6; 2]	0.9	1	0.59	0.462
20°	[0.5 ; 0.9]	[0.6 ; 1]	0.7	0.7	0.56	0.39
80°	[0.4 ; 0.7]	[0.4 ; 0.7]	0.5	0.5	0.495	0.555

Secondly, we examine the effects of the wavelength of the incident light to the behavior of the emissivity of the TG for various materials, versus the wavelength ranging from $0.4\,\mu m$ to $0.8\,\mu m$. Results are displayed in Figure 4, at incidence angle ($\theta_{inc} = 1°$) and small slopes ($h = d = 0.055\,\mu m$). For all the considered materials, the wavelength at normal incident light, which excite the (SPPs) is in the visible domain. Table III shows that, every material has the particular excitation wavelength.

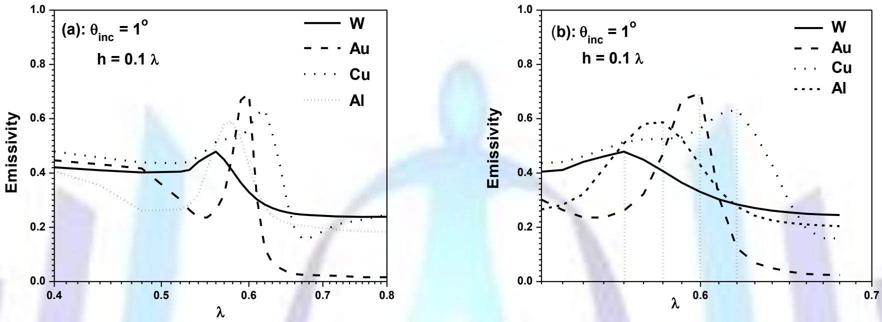

Fig 4. Dependence of the TG emissivity on the wavelength for several materials.

Parameters: $\theta_{inc} = 1°$ and $h = d = 0.055\,\mu m$

TABLE 3. RR and RP for wavelength for Au and W materials

Material	(W)	(Au)	(Cu)	(Al)
WRR	[0.52, 0.58]	[0.55, 0.62]	[0.58, 0.66]	[0.53, 0.62]
$\lambda_0(\mu m)$	0.55	0.60	0.623	0.574
$\xi_0(\lambda.\theta_{inc})$	0.449	0.694	0.634	0.587

Effects of geometrical shapes

For three geometrical shapes: triangular, rectangular and sinusoidal, we study the variation of the emissivity versus the ratio d/λ, for fixed depth and incident angle. Figure 5 shows that the (PRR) for the two materials is approximately the same for different geometrical shapes, and the greatest value of the emissivity at the PRP is for rectangular grating. For (Au) material the PRR and the PRP are approximately the same for the triangular and sinusoidal. But is not the same for the rectangular grating geometrical shape. The resonance domain is from 0.1 to 1, and the peak of resonance is at $d_0/\lambda = 0.8$ of the grating. At the RP approximately 70% of the incident energy is absorbed by the rectangular grating. The table V resumes the effects of the geometrical shapes of grating on the ERR.

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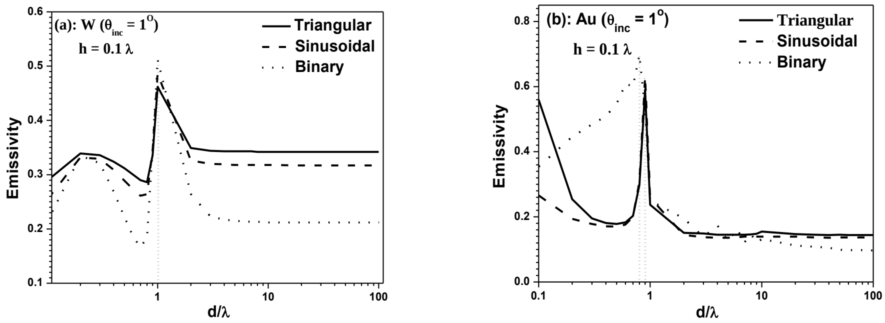

Fig 5. Effects of the geometrical shapes of grating on the emissivity of surfaces for (Au) and (W) materials.

TABLE 4. Effects of the geometrical shapes of grating on the emissivity of surfaces for W and Au materials

Grating	PRR (Au)	PRR (W)	d_0/λ (Au)	d_0/λ (W)	$\xi_0(\lambda.\theta_{inc})$ (Au)	$\xi_0(\lambda.\theta_{inc})$ (W)
Triangular	[0.5; 1]	[0.6; 2]	0.9	1	0.59	0.462
Sinusoidal	[0.5; 1]	[0.6; 2]	0.9	1	0.63	0.486
Rectangular	[0.1; 1]	[0.1; 3]	0.8	1	0.697	0.512

CONCLUSIONS

The emission of one-dimensional metallic gratings with various depths and periods of grooves was investigated by means of RCWA method. The effects of the surface morphologies of gratings, light characteristic and the material surfaces properties on the excitation of SPPs are quantified. From the results obtained in this paper, some important conclusions can be drawn:

(1) Shallow Gold gratings with small $h/\lambda = 0.1$ showed a strong absorption peak at $d/\lambda = 0.9$ due to SPPs. On the other hand, deep gratings with wide grooves showed a different absorption.

(2) At the resonance the absorption of light by the (Au) grating is greater for normal incident angle than azimuthally incident angle.

(3) For the three geometrical shapes: triangular, rectangular and sinusoidal, the two materials (Au and W) showed the greater strong absorption at resonance peak for rectangular shape.

(4) For all geometrical shapes of grating and incident angles the absorption and of light at the peak of resonance is greater for (Au) than all considered materials.

(5) For all the considered materials, the wavelength of the incident light, which excite the (SPPs) is in the visible domain.

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