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Grating diffractive behavior of surface plasmon wave on meta-surface

WANG Xue-fei[1,2], LU Zhen-wu[1], WANG Tai-sheng[1], YU Wei-xing[3*]
(1. *Changchun Institute of Optics, Fine Mechanics & Physics, Chinese Academy of Sciences, Changchun* 130033, *China*;
2. *University of the Chinese Academy of Sciences, Beijing* 100049, *China*;
3. *Xi´an Institute of Optics and Precision Mechanics, Chinese Academy of Sciences, Xi´an* 710119, *China*)
* *Corresponding Author, E-mail: yuwx@opt.ac.cn*

Abstract: In this paper, a rigorous numerical simulation method(FDTD) is employed to study the grating diffractive behavior of surface plasmon polariton(SPP) waves on meta-surface excited by the incident visible light through metallic grating coupler in 550 – 700 nm waveband. The simulation results indicate that the diffraction of SPP waves on meta-surface is quite different from that of free space light. Due to the near-field characteristics, the SPP wave shows obvious diffractive effect in near field when it interacts with a metallic grating. However, the different diffracted orders will merge into one after propagating some distances. Nevertheless, the diffractive behavior in near-field is similar to that in free space. In near field, only the 0th order light is transmitted when metallic gratings have a sub-wavelength period and higher diffraction orders appear when the period of metallic gratings is larger than the wavelength of SPP waves. The research results of this paper are of great significance for designing spectroscopic devices or systems on meta-surface with a micronscale.
Key words: surface plasmon polariton(SPP) wave; metallic grating coupler; near field diffraction; micro/nano-scale

超表面上表面等离激元波的光栅衍射行为研究

王雪飞[1,2],卢振武[1],王泰升[1],鱼卫星[3*]
(1. 中国科学院 长春光学精密机械与物理研究所,吉林 长春 130033;
2. 中国科学院大学,北京 100049;
3. 中国科学院 西安光学精密机械研究所,陕西 西安 710119)

摘要: 本文利用严格数值仿真研究了 550 ~ 700 nm 波段的可见光通过金属光栅耦合方式激发的表面等离激元(SPP)波在金属表面的光栅衍射行为与现象。研究结果表明: SPP 波在金属表面的衍射行为与自由空间光相比有极大不同,由于

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SPP 波的近场属性,经金属光栅衍射后在近场可表现出明显的光栅分光现象,但经过一段传输距离后则分光现象消失而表现为不同级次的光合为同一束光;在近场衍射情况下,其情况与自由空间光衍射行为类似,对 SPP 亚波长金属光栅来说同样只有零级透射光;而当金属光栅周期大于 SPP 波长时,高级衍射级次则开始出现。研究结果对下一步在金属表面上实现微米级片光谱仪器具有重要借鉴意义。

关　键　词:表面等离子体波;金属光栅耦合;近场衍射;微纳尺度
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1　Introduction
引　言

Surface Plasmon Polariton wave (SPP) is an electron density wave with collective oscillation generated by the interaction between photons and free electron on the metal surface. It can gather electromagnetic field energy in a small space[1], which has shown great potential in the field of nanophotonics and has become a hotspot in the research of nanophotonics[1]. SPP has been hailed as the most promising information carrier for integrated nano-photonic devices and has been widely used in many fields such as nano-lithography, new energy sources, highly sensitive biochemical sensing, solar cells and high-efficiency photonic components[2-5]; SPP has also an important application in the area of super-resolution imaging. Yang Jingzhong, use light soure with wavelength of 7 μm to illuminate a graphene nanocavity on metasurface to excite the SPP wave, and generate a standing wave with wavelength of 52 nm by interference. When this standing wave is applied to a microscope illumination source[6], the resolution of the microscope can reach 26 nm, which is nearly 100 times of the conventional fluorescent microscope.

表面等离激元激化波(Surface Plasmonic Polariton Wave,SPP)是光子和金属表面的自由电子相互作用所产生的集体振荡的电子疏密波,它能够将电磁场的能量聚集在一个很小的空间范围内[1],在纳米光子学领域显示出了巨大的应用潜力,并成为当前纳米光子学研究的热点。SPP 被誉为当前最有希望的纳米集成光子器件的信息载体,并已被广泛地应用在纳米光刻、新型能源、高灵敏生物化学传感、太阳能电池以及高效光子元器件等诸多领域中[2-5]。SPP 在超分辨成像中也有重要应用,杨靖忠利用波长 7 μm 的光源入射到超表面的石墨烯纳米腔结构激发 SPP 波,干涉产生了波长为 52 nm 的驻波。将该驻波应用到显微镜的照明光源时,显微镜分辨率可达到26 nm,比传统荧光显微镜提高了近 100 倍左右[6]。

As a device to excite SPP, the metal grating has a simple structure and is easy to control, so it is widely used to generate SPP waves[7].

金属光栅作为激发 SPP 的器件,结构简单且易于控制,被广泛应用于 SPP 波的产生[7]。

The SPP wave is an electromagnetic wave and is essentially the same as the spatial light wave thus possess characteristics of interference and diffraction. A number of nanodevices, such as super-lenses, have been developed by using the diffractive properties of SPP waves. In recent years, the research on the diffraction of SPP waves has been increasing. R. Zia *et al*. studied the effects of the width of the metallic waveguide on the diffraction of the SPP wave at the waveguide end when they conducted Young's double-slit experiment of SPP waves and found that the SPP wave is not diffracted at the waveguide end face if the waveguide width is smaller than a critic value[8]. Feng Liang *et al*. focused SPP wave on the metal surface by using its near-field diffractive property, and found that the electric field strength of the focusing point was increased by three times[9].

SPP 波在本质上与空间光相同,为电磁波,因此具有干涉及衍射特性。利用 SPP 波的衍射特性已经制作出了很多纳米器件,例如超透镜等。

近年来对 SPP 波衍射特性的研究不断增多。R. Zia 等人在做 SPP 波的杨氏双缝实验时,研究了金属波导的宽度对 SPP 波在波导端部衍射现象的影响,并发现存在一个极限值,当波导宽度小于这个值时,SPP 波在波导端面不发生衍射[8]。冯亮等人在金属表面上利用 SPP 波的近场衍射现象对其进行聚焦,使聚焦点的电场强度增大了 3 倍之多[9]。

The near-field diffraction phenomenon of SPP waves on the metal surface is mainly affected by the structural parameters such as the period and filling factor of the diffraction grating. However, only few work have been reported in this area. In this paper, we use the metallic grating couple method to excite SPP waves, and studied the influence of diffraction grating on the near-field diffraction phenomenon of SPP wave. We found that of SPP wave has an obvious diffractive effect in near-field. The spatial light is transformed into SPP wave, and the spectral signal can be separated at the micro-nanoscale by optimizing the structural parameters of the diffraction grating.

SPP 波在金属表面的近场衍射现象主要受衍射光栅的周期、占空比等结构参数的影响,然而鲜见关于这方面的公开报道。本文利用金属光栅耦合方式激发 SPP 波,研究了衍射光栅对 SPP 波近场衍射现象的影响,并发现 SPP 波的近场衍射有分光作用。将空间光转变成 SPP 波,通过优化衍射光栅的结构参数,可以实现在微纳尺度上对光谱信号的分离。

2 Surface plasmon resonance theory and three characteristic lengths of SPP waves
表面等离子体共振理论及 SPP 波的 3 个特征长度

SPP wave is a kind of electromagnetic wave propagating along the metal/dielectric interface formed by the coupling of the surface charge group´s oscillation and the electromagnetic field on the metal/dielectric interface[10]. The SPP field intensity component is maximum at the metal/dielectric interface and decays exponentially on both sides of the interface. In the visible and near-infrared wave bands, the real part of the dielectric constant of most metals is negative, so the sign of dielectric constant of the metal and its neighboring dielectric medium is opposite, and only P-polarized light(TM) can excite SPPs. As shown in Fig. 1, when light(including P-polarized light) is incident on the metallic grating, diffraction occurs on the grating surface, and different diffraction angles correspond to different diffraction orders. According to the grating equation, it can be seen that the component of the wave vector of the m-th($m = \pm 1, \pm 2, \pm 3, \cdots, \pm n$) order diffracted light in the direction parallel to the interface is

SPP 是金属/介质界面上由表面电荷的集体震荡与电磁场耦合所形成的沿着金属/介质界面传播的一种电磁波[10]。SPP 的场分量在金属/介质界面上取得最大值,在金属两侧的介质中场分量呈 e 指数衰减。在可见光及近红外波段内,绝大多数金属介电常数的实部为负数,因此金属的介电常数与其相邻介质的介电常数异号,只有 P 偏振光(TM)才能激发出 SPP。如图 1 所示,当光

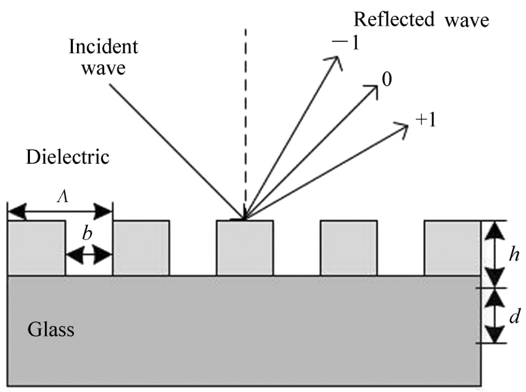

Fig. 1 Cross section of rectangular metal gratings in one-dimension

图 1 一维矩形金属光栅横截面

波（含 P 偏振光）入射到金属光栅时，在光栅表面将发生衍射现象，不同的衍射角度对应于不同的衍射级次。根据光栅方程可知第 m（$m = \pm 1, \pm 2, \pm 3, \cdots, \pm n$）级衍射光的波矢在平行于界面方向上的分量如式（1）。

$$k_x = k_0 \sqrt{\varepsilon_2} \sin\theta \pm m \frac{2\pi}{\Lambda}, \quad (1)$$

Where k_0 is the light wave vector in free space, θ is the incident angle of the light wave, ε_2 is the dielectric constant of the medium, and Λ is the grating period. It can be seen from equation (1) that the wave vector of the diffracted light can be increased due to the diffraction of the grating so that the wave vector of the m-th order diffracted light parallel to the interface can be equal to the wave vector of the SPP wave at the interface, that is

式中，k_0 是自由空间光波波矢，θ 为光波的入射角，ε_2 为介质的介电常数，Λ 为光栅周期。从式（1）可知，光栅的衍射作用可以使衍射光的波矢得到增大，从而可以使平行于界面的第 m 级衍射光波矢分量与界面上 SPP 波的波矢相等，即有式（2）。

$$k_x = k_0 \sqrt{\varepsilon_2} \sin\theta \pm m \frac{2\pi}{\Lambda} = k_0 \left(\frac{\varepsilon_1 \varepsilon_2}{\varepsilon_1 + \varepsilon_2} \right)^{1/2}, \quad (2)$$

Where $k_0 \left(\frac{\varepsilon_1 \varepsilon_2}{\varepsilon_1 + \varepsilon_2} \right)^{1/2}$ is the wave vector of the SPP wave at the metal/dielectric interface and ε_1 is the dielectric constant of the metal [11]. When the equation (2) is satisfied, the incident light is coupled to the SPP wave so that it is excited, and the surface plasmon resonance (SPR) phenomenon occurs.

式中，$k_0 \left(\frac{\varepsilon_1 \varepsilon_2}{\varepsilon_1 + \varepsilon_2} \right)^{1/2}$ 为金属/介质界面处 SPP 波的波矢，ε_1 为金属的介电常数[11]。当满足式（2）时，入射光就会与 SPP 波相耦合而获得激发，产生表面等离子体共振（SPR）现象。

As can be seen from the formula (2), the surface plasmon wave wavelength is as follows:

由公式（2）可知，表面等离激元波的波长为：

$$\lambda_{spp} = \lambda_0 \sqrt{\frac{\varepsilon_1 + \varepsilon_2}{\varepsilon_1 \varepsilon_2}} \quad (3)$$

where, λ_0 is incident wavelength.

式中，λ_0 为入射光波长。

SPP 波有 3 个特征长度，分析如下。

Three characteristic lengths of SPP wave are analyzed as follows.

The SPP wave propagation distance at the metal/dielectric interface is defined as the distance traveled of the SPP wave when the electric field decreases to $1/e$ of the initial value, denoted as δ_{spp}, which is mainly determined by the imaginary part k''_{spp} of the wave vector and

SPP 波在金属/介质交界面的传播距离定义为电场强度减小为初始值的 $1/e$ 时 SPP 波的传播距离，记为 δ_{spp}，它主要决定于波矢的虚部 k''_{spp}，且有如式（4）所示关系。

$$\delta_{spp} = \frac{1}{2k''_{spp}} = \lambda_0 \frac{\varepsilon'^2_m}{2\pi \varepsilon''_m} \sqrt{\frac{\varepsilon_d + \varepsilon'_m}{\varepsilon_d \varepsilon'_m}}, \quad (4)$$

Where ε'_m and ε''_m are respectively the real and imaginary parts of the complex dielectric constant of the metal respectively, λ_0 is the wavelength of the incident light, and the penetration depth of the SPP wave in the medium and the metal is respectively

式中，ε'_m、ε''_m 分别为金属的复介电常数的实部和虚部。λ_0 为入射光波长。SPP 波在介质与金属中的穿透深度分别为式（5）、（6）所示。

$$\delta_d = \frac{1}{k_0} \left| \frac{\varepsilon'_m + \varepsilon_d}{\varepsilon_d^2} \right|^{1/2}, \quad (5)$$

$$\delta_m = \frac{1}{k_0} \left| \frac{\varepsilon'_m + \varepsilon_d}{\varepsilon'^2_m} \right|^{1/2}, \quad (6)$$

Where, k_0 is the incident light wave vector [12]. From equation (4) to (6), the distance of light in 550 – 700 nm waveband propagating on the silver surface is in the range of 12.5 – 60 μm, the penetration depth of SPP in air and silver is in the range of 279 – 500 nm and 22.7 – 29.5 nm, respectively.

式中，k_0 为入射光的波矢量[12]。由式（4）～（6）可得，550～700 nm 波长的光波在金属银表面的

传播距离为 12.5 ~ 60 μm 时,SPP 在空气和银中的穿透深度分别为 279 ~ 500 nm 和 22.7 ~ 29.5 nm。

3 Determination of optimal structure of metallic grating coupler 最优激发金属光栅结构的确定

Fig. 2 shows the model for studying the near-field diffraction of SPP waves. The left metal grating is used to as grating coupler to excite the SPP wave, the right metal grating serves as the diffraction grating. When light is incident on the metal grating structure, an SPP wave is generated on the metal surface and propagates to both left and right along the metal surface. Near-field diffraction occurs when a diffraction grating is encountered.

图 2 是研究 SPP 波超表面近场衍射的模型。左侧是激发 SPP 波的金属光栅结构,右侧是衍射光栅。当光入射到金属光栅结构上时,会在金属表面产生 SPP 波,产生的 SPP 波将沿着金属表面向右传播,遇到衍射光栅时便会发生近场衍射现象。

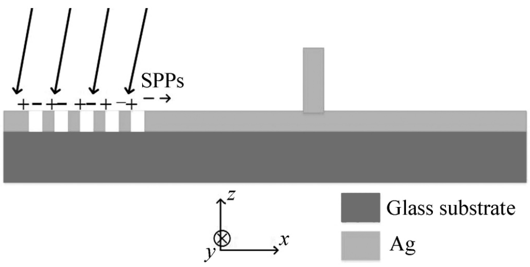

Fig. 2 Theoretical model of near-field diffraction for the SPP wave on meta-surface

图 2 SPP 波超表面上近场衍射的模型图

In this paper, the near-field diffraction of SPP waves excited by incident light with wavelength in the range of 550 - 700 nm and the central wavelength of 625 nm is studied. The coupling efficiency of incident light to SPP wave is mainly related to the structure parameters of metal grating coupler such as cycle, filling factor and modulation depth. The material of the metal grating coupler is set as silver, and it can be seen from equation (2) that for the incident light with a wavelength of 625 nm, the coupling efficiency of the incident light is the highest when the grating period Λ is 607 nm. The grating filling factor D is set to 0.5 and the grating depth h is 200 nm. By emplaying the rigorous coupled wave theory, the reflectivity of the incident light against the wavelength ranging from 550 - 700 nm, and the incident angle ranging from 10 - 15° was calculated by using the SPR angle scanning method [13]. Fig. 3(a) shows the three-dimensional map of the reflectivity and against the wavelength and the angle of incidence. Fig. 3(b) illustrates the relationship of the reflectivity and wavelength for different incident angles.

本文主要研究中心波长为 625 nm,波段为 550 ~ 700 nm 的入射光激发的 SPP 波近场衍射现象。而入射光耦合激发 SPP 波的效率主要与金属光栅的面型参数如周期、占空比及调制深度等有关。设定耦合金属光栅的材料为银,通过式(2)可知,对于波长为 625 nm 的入射光,光栅周期 Λ 为 607 nm 时,入射光的耦合率最高。光栅占空比 D 设为 0.5,光栅厚度 h 设为 200 nm。根据严格耦合波理论,利用 SPR 角度扫描方法[13],计算入射光波长为 550 ~ 700 nm、入射角在 10° ~ 15°范围内入射光的反射率,得到反射率与波长及入射角度的三维关系图,如图 3(a)所示。图 3(b)为反射率与波长及入射角的关系曲线图。

It can be seen from Fig. 3(a) that for the above mentioned metal grating structure, the reflectivity is lower for 625 nm wavelength when incident angle falls on the range of 12.5° - 15°. It can be further deduced from Fig. 3(b) that when the incident angle is about 14°, the reflectivity is the mimimum, that means the coupling efficiency is the highest, about 35%. At this incident angle, the coupling ratio is 25% and 10% for 550 nm and 700 nm respectively.

由图 3(a)可以看出,在上述金属光栅结构下,波长为 625 nm 的光以 12.5° ~ 15°入射时,反射率较低。由图 3(b)进一步可得,当入射角约等

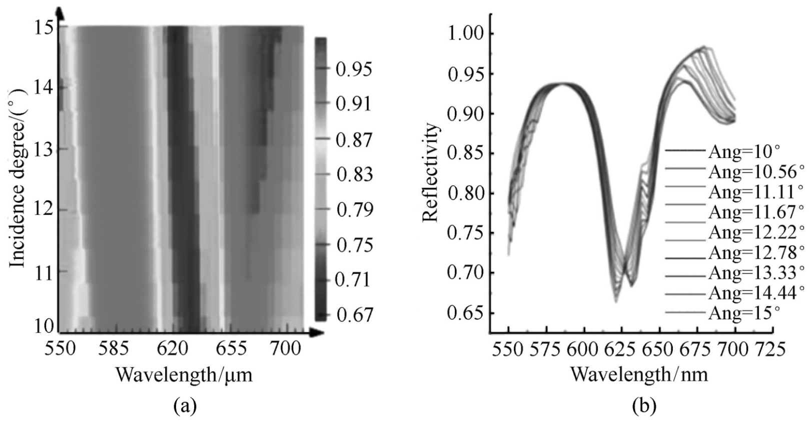

Fig. 3　Relationship between the reflectivity of the metal grating structure and wavelength for different incident angles for the wavelength in the range of 550 – 700 nm and the incident angle in the range of 10° – 15°. (a) 3D Diagram; (b) 2D curve

图 3　波长在 550 ~ 700 nm 内，入射角度在 10° ~ 15°范围内时，金属光栅结构的反射率与波长和入射角的关系图: (a) 三维关系图; (b) 反射率曲线图

于 14°时，反射率最小，即耦合成 SPP 波的效率最高，大约在 35% 左右。在此入射角下，550 nm 波长的入射光的耦合率为 25% ，700 nm 波长的入射光的耦合率在 10% 左右。

4　Diffraction results and analysis 衍射结果与分析

When the period of the metal silver grating is 607 nm, the wavelength of SPP waves excited by the incident light with a wavelength ranging from 550 – 700 nm is in the range of 525 to 683 nm. As shown in Fig. 2, the metal grating coupler has a period of 607 nm, filling factor of 0. 5 and a groove depth of 200 nm. The right diffractive metal grating located on the metal surface has a height of 600 nm and a thickness of 200 nm in the *X* direction. When studying the diffractive behavior of SPP waves through a metal grating, two cases are considered: one is the case where the grating height and filling factor keep no change but the grating period changes; the other case is that the grating height and period keep no change but the filling factor changes. At the same time, the excitation wavelength and the incident angle are fixed at 625 nm and 14°.

当金属银的光栅周期为 607 nm 时，波长为 550 ~ 700nm 的入射光激发出的 SPP 波波长在 525 ~ 683 nm 之间。设定图 2 所示的近场衍射模型中激发 SPP 波的金属光栅周期为 607 nm，占空比为 0. 5，凹槽深度为 200 nm。右方衍射金属光栅位于金属表面上，高度为 600 nm，在 *X* 方向上的厚度为 200 nm。当研究 SPP 波经过其的衍射行为时，对以下两种情况分别研究: 一种是光栅高度和占空比不变，而光栅周期发生变化时的情况; 另一种是光栅高度和周期不变，占空比发生改变的情况。同时激发光波长和入射角度固定为 625 nm和 14°。

4. 1　Diffraction situation by fixed diffraction grating filling factor but different period 衍射光栅占空比固定，周期不同时的衍射情况

Figs. 4(a) – 4(e) show the near-field diffraction of the SPP wave excited by the incident light with the wavelength of 625 nm when the filling factor of the diffraction grating is constant(0. 5) and the period is different. In the figures, *XY* plane is the metal film surface, and the diffraction grating is located on the *Y*-axis.

图 4(a) ~ 4(e) 是波长为 625 nm 的入射光所激发的 SPP 波在衍射光栅占空比一定(0. 5) 而周

期不同时的近场衍射现象。图中 XY 平面为金属薄膜表面，衍射光栅位于 Y 轴上。

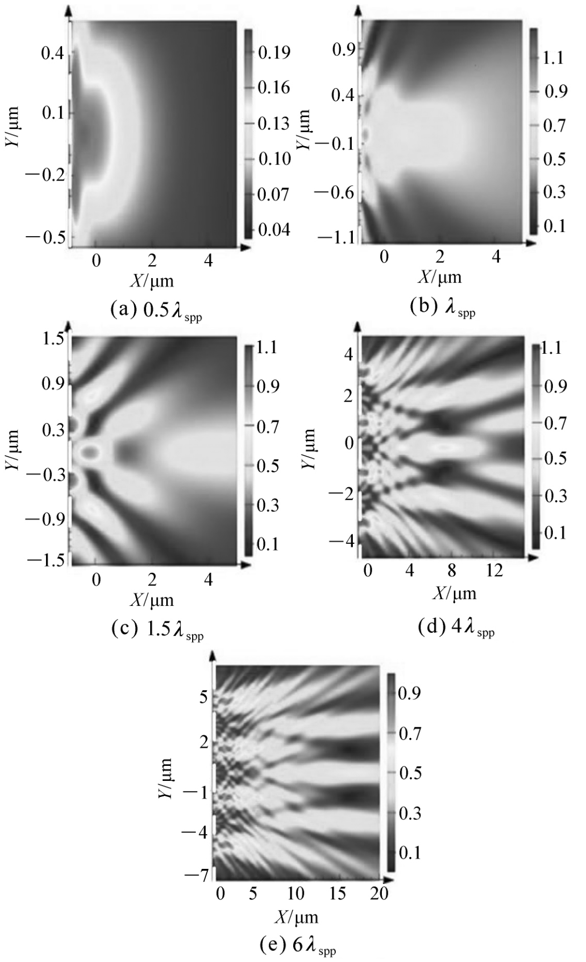

Fig. 4 Diffraction phenomenon of SPP wave of incidence light with wavelength of 625 nm when diffraction grating with different period but the same filling factor(It should be noted that the white dashed line represents the location of the diffraction grating)

图4 波长 λ =625 nm 的入射光激发的 SPP 波在周期不同，占空比一定的条件下的衍射现象(图中白色断线表示金属衍射光栅的位置)

It can be seen that there is only the 0th diffraction order at this time. The transmitted light intensity is quite weak, below 0. 2, and the transmission distance is only about 2. 3 μm after passing through the diffraction grating; Fig. 4(b) is the case when the period of the diffraction grating is λ_{spp}. In this case, the diffraction phenomenon can be observed and one can see that besides the 0th order, ±1 storders are also appear. The light intensity at this time also increases significantly with the maximum reaches to about 1, while the transmission distance also increases to about 4 μm; Figs. 4(c) -(e) depict the diffraction of the SPP wave when the diffraction grating period is $1.5\lambda_{spp}$, $4\lambda_{spp}$ and $6\lambda_{spp}$, respectively. It can be seen that the diffraction order increases correspondingly as the period of the diffraction grating increases. When the diffraction grating period is 1. 5 times of the SPP wavelength, the highest order of the diffraction is ±2nd and the distinction of diffraction fringes is relatively clear. When the grating period is 4 -6 times of the SPP wavelength, the distribution of diffraction fringes becomes more disordered due to even higher diffraction orders appear.

图4(a) 为当衍射光栅周期为 $0.5\lambda_{spp}$ 时 SPP 波的衍射情况。可以看到此时只有零级衍射，且透射光强较弱，在 0. 2 μm 以下，入射光透过衍射光栅后传播距离在 2. 3 μm 左右; 图4(b) 为衍射光栅周期为 λ_{spp} 的情形，此时已有明显的衍射现象，可以看到 0 级和 ±1 级衍射，并且此时光强有明显的增强，最大达到了 1 左右，同时透过衍射光栅后 SPP 光的传播距离在 4 μm 左右; 图4(c) ~4(e) 为衍射光栅周期分别为 $1.5\lambda_{spp}$、$4\lambda_{spp}$ 和 $6\lambda_{spp}$ 时 SPP 波的衍射情形。可以看到，随着衍射光栅的周期不断增大，衍射级次相应地增多。当衍射光栅周期为 SPP 波长的 1. 5 倍时，最高衍射级次为 ±2 级，并且衍射条纹的分布比较清晰; 而当光栅周期为 SPP 波长的 4 ~6 倍时，由于更高衍射级次的出现使得衍射条纹的分布变得较为紊乱。

4.2 Diffraction behavior of diffraction grating with fixed period but different filling factor 衍射光栅周期固定，占空比不同时的衍射情况

Figs. 5(a) -5(e) show the near-field diffraction of the SPP wave at the metaface with a constant period of the diffraction grating of 910 nm, but the filling factor changes. In the Fig. 5, the XY plane is the metal film surface, and the diffraction grating is located on the Y-axis. Fig. 5(f) illustates the electric field intensity distribution corresponding to the Fig. 5(a) -5(d) near field diffraction on the surface of the metal thin film at $x=0$.

图 5(a)~5(e)为衍射光栅周期固定为 910 nm不变，占空比变化时 SPP 波在超表面的近场衍射情形。图中 XY 平面为金属薄膜表面，且衍射光栅位于 Y 轴上。图 5(f)为对应于 5(a)~5(d)金属薄膜表面直线 $x=0$ 上近场衍射的电场强度分布图。

As can be seen from the graphs in Figs. 5(a) -(e), the SPP wave finally converges on the metal surface after passing through the diffraction grating, and the diffraction order does not change substantially, but the intensity changes as the filling factor of the diffraction grating changes. When the filling factor of the grating changes from 0.1 to 0.7, the diameter of the converging light beam gradually becomes smaller. When the grating filling factor is 0.9, the light transmittance has become very low, so that the maximum electric field intensity is only about 0.3. It can be seen from Fig. 5(f) that the diffraction angle the SPP wave in of near-field also varies when the filling factor of grating is different. The diffraction angle of the ±1 storderis in the range of 39.79° to 42.67° for different filling factors. When the filling factor is 0.1, the diffraction angle is the smallest, i.e. 39.79°. The diffraction angle is the largest at 42.67° when the filling factor is 0.5. The diffraction angle is very close, i.e. about 41°, when the filling factor ranges from 0.3 to 0.7. The light field intensity of ±1 diffraction order varies with different filling factor, which is related to the different intensity of the SPP wave passing through the diffraction grating.

从图 5(a)~5(e)可以看到，SPP 波透过衍射光栅后，在金属表面上最终都汇聚到一起，衍射级次基本不发生变化，但强度随着衍射光栅占空比

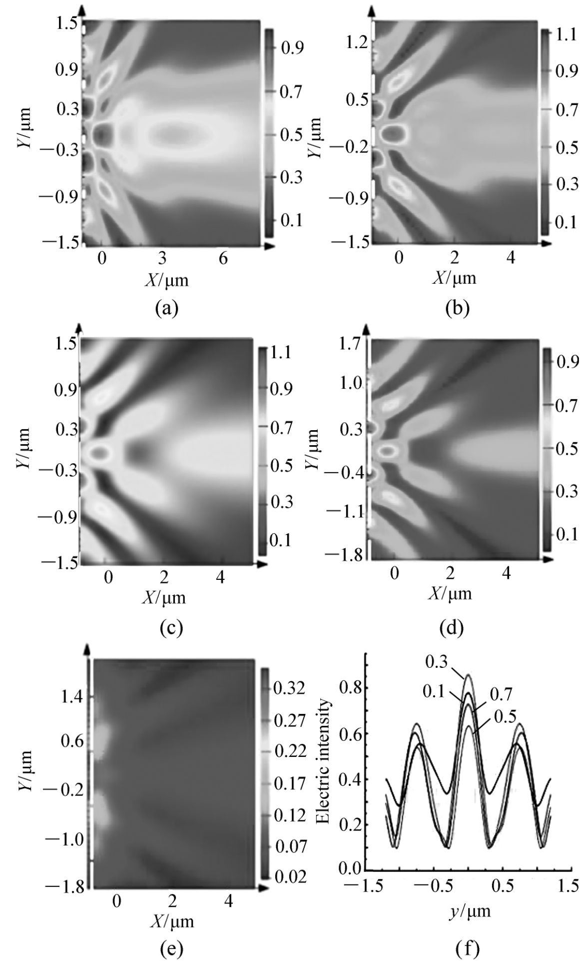

Fig. 5　Diffraction phenomenon of SPP wave for an incidence light with wavelength of 625 nm for diffraction grating with different duty ratios and the fixed grating period. (a) Duty radio is 0.1; (b) Duty radio is 0.3; (c) Duty radio is 0.5; (d) Duty radio is 0.7; (e) Duty radio is 0.9; (f) Electric field intensity distribution of the diffraction patterns along y axis under different duty radio at $x=0$

图 5　入射光波长 $\lambda=625$ nm，衍射光栅周期为 910 nm，占空比不同时的衍射现象，其中白色虚线表示金属光栅的位置。(a)占空比为 0.1；(b)占空比为 0.3；(c)占空比为 0.5；(d)占空比为 0.7；(e)占空比为 0.9；(f)衍射光栅占空比不同时，金属薄膜表面上 $x=0$ 直线上的近场衍射电场强度曲线图

的变化而变化。当光栅占空比从 0.1 变化到 0.7 时，汇聚光束的直径逐渐变小。当光栅占空比为

0.9 时，光的透过率已经变得非常低，电场强度最大只有 0.3 左右。从图 5(f) 中可以看出，光栅占空比不同时，SPP 波的近场衍射角也有所变化，几种不同占空比的衍射光栅对应的 ±1 级衍射角在 39.79°~42.67°内，其中：当占空比为 0.1 时，衍射角最小，为 39.79°；占空比为 0.5 时，衍射角最大，为 42.67°；占空比为 0.3 或 0.7 时，衍射角接近，在 41°左右。占空比不同，±1 级的光场强度也不同，这也与 SPP 波透过衍射光栅的光强不同有关。

4.3 Comparison of diffraction behaviors of metal gratings in free space and on meta-surface 自由空间中与超表面上金属光栅衍射行为比较分析

To further illustrate the difference between the grating diffraction behavior of SPP waves on the meta-surface and that in free-space light, we also calculated the diffraction effect of metal gratings in free space and compared them with those on the meta-surface. Fig. 6(a) shows the free space grating diffraction model. Here for the convenience of comparison, let the incident light wavelength and SPP wavelength to be 607 nm as well, and let the thickness of the metal grating also equal to 200 nm. However, the difference is that the height of the metal grating on the meta-surface is limited to 600 nm in the direction perpendicular to the period, while the size of the metal grating in the free space in the direction perpendicular to the period is infinitely large.

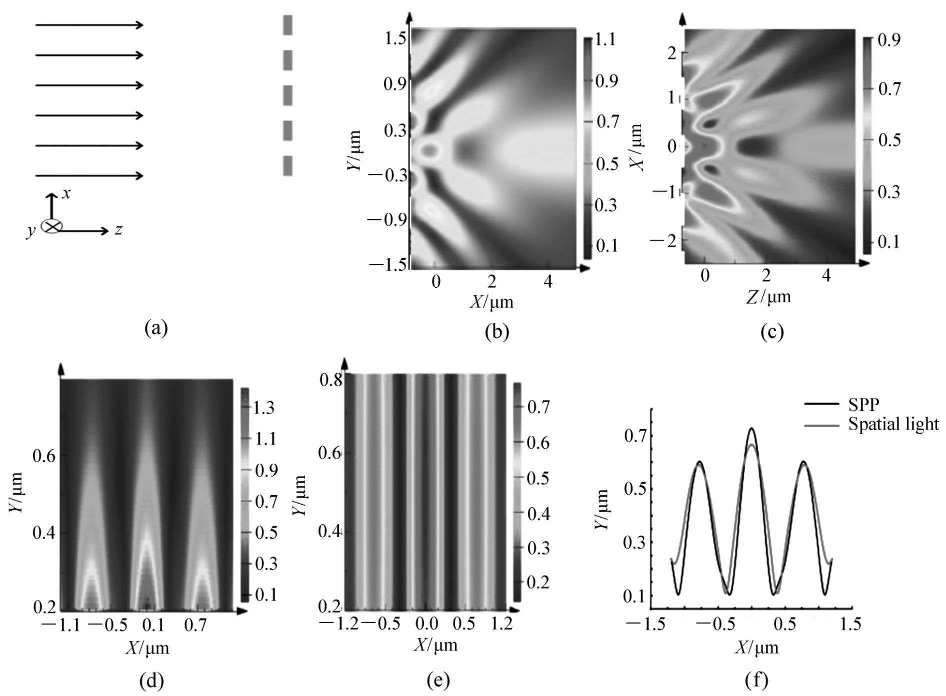

Fig. 6 Comparison of near field diffraction of SPP wave and free space light: (a) theoretical model for near field diffraction of free space light; (b) near field diffraction of SPP on meta-surface; (c) near field diffraction in free space light; (d) electric field distribution in X direction at 0.95 μm from diffraction grating corresponding to (b); (e) electric field distribution in Z direction at 0.95 μm corresponding to (c); (f) electric field intensity at the surface of the metal film corresponding to (d), (e)

图 6 自由空间光与超表面上光栅近场衍射行为对比结果图：(a) 空间光的近场衍射装置图；(b) SPP 波超表面上的光栅近场衍射图；(c) 自由空间光的光栅近场衍射图；(d) 对应(b) 在距衍射光栅 0.95 μm 处 X 方向上的电场分布图；(e) 对应(c) 在距衍射光栅 0.95 μm 处 Z 方向上的电场分布图；(f) 对应(d)、(e) 在金属薄膜表面处的电场强度曲线

为进一步说明超表面上 SPP 波的光栅衍射行为和自由空间光的光栅衍射行为的区别。本文对自由空间中金属光栅进行了计算，并和超表面上的情况进行比较。图 6(a) 所示为自由空间光栅的衍射模型图。这里为方便比较，使入射光波长和 SPP 波波长相等，都为 607 nm，并且金属光栅厚度相等，皆为 200 nm，但不同之处在于超表面上金属光栅在和周期垂直方向上高度有限制，为 600 nm，而自由空间中的金属光栅在和周期垂直方向上的尺寸取无限大。

Fig. 6(b) shows the grating near-field diffraction of the SPP wave for an incident wavelength of 625 nm. The wavelength of the SPP wave excited at this time is 607 nm and the period of the diffraction grating is 910 nm, which is about $1.5\lambda_{spp}$, the filling factor is 0.5. Fig. 6(c) shows the near-field diffraction of the space light with an incident wavelength of 607 nm. In order to compare the diffraction phenomenon on the metasurface to that in free space, the period, filling factor and thickness of the diffraction grating is set to 910 nm、0.5 and 200 nm respectively.

图 6(b) 是入射光波长为 625 nm 时激发的 SPP 波在超表面上的光栅近场衍射情形，此时激发的 SPP 波波长为 607 nm，衍射光栅周期设为 910 nm，约为 $1.5\lambda_{spp}$，占空比为 0.5。图 6(c) 为入射光波长为 607 nm 的空间光的近场衍射情形。为了对比分析空间光与 SPP 波在超表面的衍射现象，设衍射光栅周期为 910 nm，占空比为 0.5，金属光栅厚度为 200 nm。

Comparing Fig. 6(b) and 6(c), one can see that the diffractive behavior of SPP wave is similar to the phenomenon when space light is diffracted in the near field. Fig. 6(d) and 6(e) correspond to the electric field intensity plots for $Z > 0$ (i. e SPP waves in air) at $X = 0.95$ μm in Fig. 6(b) and 6(c). The SPP wave exponentially decays in the medium and in the metal, so that on the metal film surface, the electric field intensity reaches its maximum value and decays rapidly in the Z direction. Where as space light propagates uniformly in the medium [14], the intensity of the electric field in the Z-direction is uniformly distributed. Fig. 6(c) is light intensity distribution curve on the metal surface corresponds to Fig. 6(d) and 6(e). As can be seen from the figure, in addition to the difference in field intensity, the position of 0th and ±1th diffraction orders are basically the same.

比较图 6(b) 和 6(c) 可以看出，SPP 波与空间光在近场衍射现象类似。图 6(d) 和 6(e) 为对应图 6(b)、6(c) 中 $X = 0.95$ μm 处，$Z > 0$ 部分(即 SPP 波在空气中)的电场强度图，SPP 波在介质和金属中光强呈指数衰减，因此在金属薄膜表面上，电场强度取得最大值，在 Z 轴方向迅速衰减。而空间光在介质中是均匀传播的[14]，所以在 Z 轴方向电场强度是均匀分布的。图 6(c) 对应图 6(d)、6(e) 在金属表面上光强分布曲线图，从图中可以看出，二者除了在强度上有所区别外，0、±1 衍射级的位置基本一致。

In addition, it is clear that the near-field diffraction angles of the SPP waves excited by different incident wavelengths on the meta-surface are also different after diffraction by metal grating on meta-surface. It is known from equation (3), when the incident light wavelengths is 550 nm, 581 nm, 616 nm, 655 nm and 700 nm respectively, the wavelength of SPP waves excited by the device in Fig. 2 is 524.7 nm, 557.9 nm, 594.8 nm, 635.8 nm and 682.9 nm, and the ±1 order near-field diffraction angles after metal grating diffraction on the metasurface is 35.737°, 36.966°, 38.157°, 39.311° and 41.507°, respectively. For diffraction of light in free space, when light with a wavelengths of 524.7 nm, 557.9 nm, 594.8 nm, 635.8 nm and 682.9 nm respectively is incident on the diffraction grating with the same structural parameters as shown in Fig. 6(a), the resulting far-field diffraction angle can be determined by:

此外，很显然超表面上不同入射波长所激发的 SPP 波经光栅衍射后的近场衍射角也不同，由式(3)可知，当入射光波长分别为 550、581、616、655 及 700 nm 时，利用图 2 的装置激发出的 SPP

波波长依次为 524.7、557.9、594.8、635.8 及 682.9 nm，且经过超表面上金属光栅衍射后的 ±1 级的近场衍射角分别为 35.737°、36.966°、38.157°、39.311°及 41.507°。而对于自由空间中光的衍射，将波长分别为 524.7、557.9、594.8、635.8 及 682.9 nm 的光入射到图 6(a) 所示具有相同结构参数的衍射光栅上时产生的远场衍射角可由下面式(7) 决定:

$$d\sin\theta = k\lambda . \tag{7}$$

By using this formula, the corresponding diffraction angles are determined to be 31.653°, 33.916°, 36.503°, 39.485° and 43.071° respectively. In comparison with the case on meta-surface, it can be found that the near-field diffraction angle is almost the same, and the maximum error is only about 5°. This means that the diffraction angle of the SPP wave after transmitted through the metal grating on the meta-surface can be roughly estimated by using the conventional grating diffraction formula in free-space-of, but more accurate results have to be obtained by rigorous numerical calculations.

利用该公式可计算得出所对应的衍射角分别为 31.653°、33.916°、36.503°、39.485° 及 43.071°。两相对比，可发现其与 SPP 波透过衍射光栅后的近场衍射角相差不大，最大误差仅约 5°。这说明，采用常规的用于自由空间光光栅衍射公式，可以对超表面上光栅的衍射角度进行粗略估计，但更准确的结果必须通过严格数值计算来获得。

4.4 Comparison of diffraction of two kinds of diffraction gratings on metasurface 超表面上两种衍射光栅衍射情况的对比

Figs. 7(a) and 7(b) show two kinds of diffraction gratings on the meta-surface, Fig. 7(a) shows the case where the diffraction grating protrudes on the metal surface; and Fig. 7(b) shows the case where the diffraction grating is recessed on the metal surface. In Fig. 7(a), in order to avoid the influence of stray light on the diffraction of near-field SPP wave, the height of the diffraction grating is set to be 600 nm, which is equal to the penetration depth of the SPP wave in the air and the width is 200 nm. In order to compare the near-field diffraction of the two kinds of diffraction gratings, the depth of the diffraction grating grooves in Fig. 7(b) is set to be 600 nm and the width is set to be 200 nm which is the same as that in Fig. 7(a). The two kinds of diffraction gratings are set to have the same period and filling factor.

图 7(a)、7(b) 为超表面上两种衍射光栅示意图，图 7(a) 为衍射光栅凸起于金属表面的情形；图 7(b) 为衍射光栅凹进金属表面的情形。图 7(a) 中，为了避免杂散光对 SPP 波近场衍射的影响，设衍射光栅的高度为 600 nm，与 SPP 波在空气中的穿透深度相等，宽度为 200nm。为对比两种衍射光栅的近场衍射情况，取图 7(b) 中衍射光栅凹槽深度为 600 nm，宽度为 200 nm，与图 7(a) 相同，且设定两种衍射光栅的周期和占空比均相同。

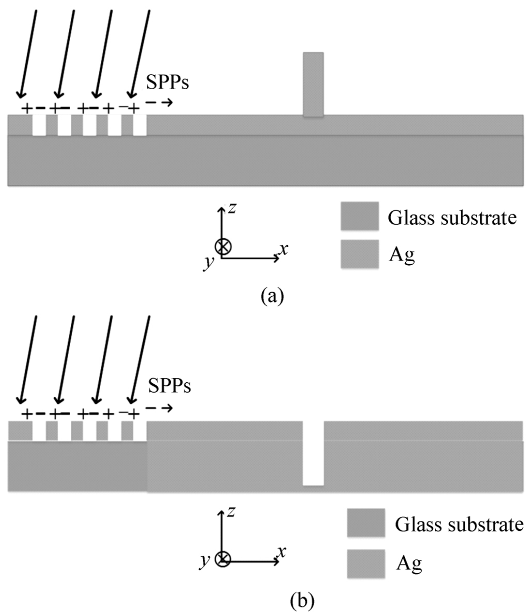

Fig. 7 Schematic diagrams of two kinds of diffraction gratings

图 7 两种衍射光栅的示意图

The grating period, the filling factor and depth of grating coupler of excitation SPP wave on the left of the above two structures is set to be 607 nm, 0.5, 200 nm respectively, the incident light wavelength is in the range of 550 – 700 nm and the incident angle is 14°. Figs. 8(a) and 8(b) show the near-field diffraction of SPP waves under the above mentioned two grating structures, respectively. In Fig. 8, *XY* plane is the metal film surface, the diffraction grating is located on the *Y*-axis.

设定上述两种结构左侧激发 SPP 波的光栅周期为 607 nm,占空比为 0.5,光栅深度为 200 nm,入射光波长为 550 ~ 700 nm,入射角度为 14°。图 8(a)、8(b) 分别为在上述两种光栅结构下,SPP 波的近场衍射情况。图中 *XY* 平面为金属薄膜表面,衍射光栅位于 *Y* 轴上。

Fig. 8(c) shows the near-field diffraction curve with an incident light wavelength of 550 – 700 nm corresponding to the structure shown in Fig. 7(b). As can be seen from the figure, the zero-th diffraction order of each wavelength center is located at $y = 0$, but for diffraction orders of ±1, ±2, there have been obvious diffractive effect. The reason is that the intensity of the electric field diffracted by the SPP wave is different that for the fixed metal grating coupling structure there is only one optimal incident wavelength, and at this wavelength, the light is coupled into the SPP wave most efficiently [15].

图 8(c) 为对应图 7(b) 所示结构,入射光波长为 550 ~ 700 nm 的近场衍射曲线图。从图中可以看出,各波长的零级衍射的中心均在 $y = 0$ 上,但在 ±1、±2 衍射级时已经有明显的分光现象。不同波长的入射光所激发的 SPP 波衍射后的电场强度不同,原因是,固定的金属光栅耦合结构只对应一个最佳的入射波长,这个波长的光耦合成 SPP 波的效率最高 [15]。

In Fig. 8(d), the incident light of 550 – 581 nm is separated by 1.23° and the incident light of 581 – 616 nm is separated by 1.20° on the metal surface. The incident light of 616 – 655 nm is separated by 1.15° and the incident light at 655 – 700 nm is separated by 2.20° on the metal surface due to the near-field diffraction of the SPP wave. Since the excitation and propagation of SPP waves in near-field diffraction are on the order of micrometers [15], the signal of incident light can be separated by the near-field diffraction of SPP wave to realize micron-scale spectrometer.

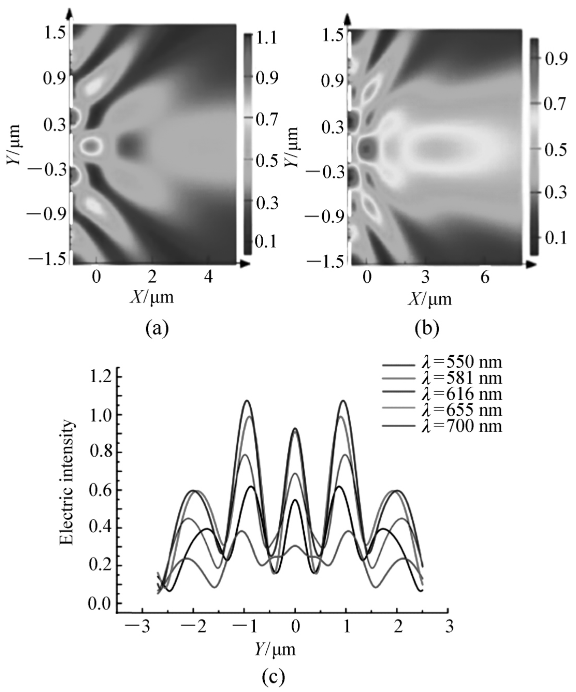

Fig. 8 (a) Near field diffraction of the incident light at 625 nm Corresponding to Fig. 7(a); (b) near field diffraction of the incident light at 625 nm Corresponding to Fig. 7(b); (c) curve of near field diffraction of the incident light at 550 – 700 nm corresponding to Fig. 7(b). White dashed line in the figure(ieft sode) represents the grating location

图 8 (a) 对应图 7(a) 所示结构,入射波长为 625 nm 的近场衍射;(b) 对应图 7(b) 所示结构,波长 625 nm 时近场衍射;(c) 对应图 7(b) 所示结构,入射光波长为 550 ~ 700 nm的近场衍射曲线图。图中左侧白色虚线表示衍射光栅所在位置

图 8(d) 中由于 SPP 波的近场衍射,550 ~ 581 nm 的入射光在金属表面上分开 1.23°,581 ~ 616 nm 的入射光在金属表面上分开 1.20°,616 ~ 655 nm 的入射光在金属表面上分开 1.15°,655 ~ 700 nm 的入射光在金属表面上分开 2.20°。在近场衍射中由于 SPP 波的激发和传播都在微米量级 [15],可以利用 SPP 波的近场衍射现象对入射光的信号进行分离,制备微米量级的光谱仪器。

5 Conclusions
结 论

In this paper, the near-field diffraction of SPP waves excited by visible light incident on metal grating structures in the wavelength range of 550 - 700 nm is studied by a method of metal grating coupling. First of all, according to the rigorous coupling wave theory, the SPR angle scanning method is used to find the optimal metal grating structure with the highest coupling efficiency for the incident light with the central wavelength of 625 nm. Then the effect of metal grating structure parameters on the near-field diffraction of SPP wave is studied. The results show that the diffraction effect of SPP is most pronounced when the period of the diffraction grating is 1.5 times the wavelength of SPP and the filling factor is 0.5. Finally, using the phenomenon of SPP wave near-field diffraction, the incident light of 550 - 558 nm can be separated by 1.23° on the metal surface, the incident light of 581 - 616 nm is separated by 1.20° on the metal surface and the incident light of 616 - 655 nm can be separated by 1.15° on the metal surface, the 655 - 700 nm incident light can be separated by 2.20° on the metal surface. Finally, the diffraction of SPP wave and the diffraction of free space light are compared. We discover that the diffraction angle calculated from the free-space grating diffraction formula is similar to that of the SPP wave. The formula can be used to make a rough estimate of the diffraction angle of a grating on a meta-surface.

本文利用金属光栅耦合方式,对波长在550 ~ 700 nm 范围内的可见光入射到金属光栅结构上激发的 SPP 波的近场衍射现象进行了研究。首先根据严格耦合波理论,利用 SPR 角度扫描方法,找出中心波长 625 nm 的入射光耦合效率最高的金属光栅结构。然后研究了金属光栅结构参数对 SPP 波近场衍射的影响。结果表明,当衍射光栅的周期为 SPP 波波长的 1.5 倍、占空比为 0.5 时,SPP 波的衍射效果最明显。最后,利用 SPP 波的近场衍射现象,可将 550 ~ 581 nm 的入射光在金属表面上分开 1.23°,581 ~ 616 nm 的入射光在金属表面上分开 1.20°,616 ~ 655 nm 的入射光在金属表面上分开 1.15°,可将 655 ~ 700 nm 的入射光在金属表面上分开 2.20°。最后将 SPP 波的衍射情况和自由空间光的衍射情况进行比较,发现根据自由空间光栅衍射公式计算出的衍射角度和 SPP 波的情况相差不大,可以用该公式对超表面上光栅的衍射角度进行粗略估算。

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作者简介：

WANG Xuefei (1990—), master's degree candidate, obtained her bachelor's degree from Northeast Forestry University in 2013. Her main research interest focuses on surface plasmon waves. E-mail: wangxuefeizb@163.com

王雪飞(1990—)，女，吉林长春人，硕士研究生，2013 年于东北林业大学获得学士学位，主要从事表面等离子体波方面的研究。E-mail: wangxuefeizb@163.com

YU Weixing (1975—) received his bachelor's degree from Northwestern Polytechnical University in 1998, a master's degree from Changchun Institute of Optics, Fine Mechanics and Physics, Chinese Academy of Sciences in 2001. In 2004, he received his Ph. D. from Nanyang Technological University in Singapore. In recent years, he is mainly engaged in research on the fields of subwavelength optics, micro/nano optics, surface plasmonic optics, microfabrication technology and 3D micro/nano fabrication technology. E-mail: yuwx@opt.ac.cn

鱼卫星(1975—)，男，陕西临潼人，博士，研究员，1998 年于西北工业大学获学士学位，2001 年于中国科学院长春光学精密机械与物理研究所获得硕士学位，2004 年于新加坡南洋理工大学获得博士学位，主要从事亚波长光学、微纳光学、表面等离子体光学、微细加工技术、三维微纳加工技术等方面的研究。E-mail: yuwx@opt.ac.cn