Numerical simulation of the interaction of terahertz waves with metal diffraction gratings

Oleg Kameshkov[1, a)], Boris Knyazev[1,2] and Vasily Gerasimov[2 b)]

[1] *Novosibirsk State University, 630090, Russia, Novosibirsk Region, Novosibirsk, 1, Pirogova St;*
[2] *Budker Institute of Nuclear Physics of Siberian Branch Russian Academy of Sciences (BINP SB RAS) 11, Acad. Lavrentieva Pr., Novosibirsk, 630090 Russian Federation.*

[a)]*Corresponding author: o.kameshkov@g.nsu.ru*

Abstract. In the terahertz plasmonics, it is widely used wavelength 1D grooved metal gratings for excitation of surface plasmon polaritons (SPPs). SPPs are traveling charge density waves at the surface of conducting materials. Since these modes have a non-radiative nature, it is possible to excite them only if the configuration providing the wavevector-matching condition between the incident light and SPP dispersion law. The wavelength gratings are the most suitable and cheaper solution to satisfy this requirement. The careful optimization of the most suitable experimental parameters by the numerical simulations leads to the enhancement of surface plasmon resonance response. In this paper, numerical results of grating optimization with different groove profiles are discussed.

INTRODUCTION

Terahertz (THz) waves are within the frequency range of 0.1–10 THz and lie between the microwave and infrared frequencies of the electromagnetic spectrum. Due to their unique properties, researchers expect to find many cutting-edge applications for them including sensors, high-resolution radar and imaging, nondestructive evaluation, and many others. In particular, THz technology has great potential for the development of ultra-high-speed communications. In particular, THz technologies have great potential for the development of next-generation ultra-fast communications due to its wide frequency band and ability to carry ultra-large amounts of information. To develop terahertz technologies, it is desirable to develop THz sources, detectors and devices with high efficiency and performance [1]

Surface plasmon polaritons (SPPs) arising as a result of collective oscillation of electrons are a special type of electromagnetic wave propagating along a “metal-dielectric” interface. The replacement of the free-space waves by SPPs can significantly reduce the design of devices and systems from three-dimensional to two-dimensional space. Due to this, SPPs components have great potential for integration in communication and photon circuits for control and signal processing. The interaction between photons and electrons makes the SPP wave vector larger than that of waves in free space. This leads to the limitation of the field and its exponential decay from the boundary of the media. Propagating along the surface, SPPs interact strongly with the material, which makes them promising for surface sensing and nonlinear applications.

A general problem of using THz-SPPs is the low efficiency for the transfer of free-space wave energy to the surface plasmons. The SPP has a wave vector larger than that of a free space wave of the same frequency. In the THz frequency range, several SPP excitation methods were reported such as attenuated total internal reflection method, end-fire coupling, grating coupling, waveguide matching method and others.

In this paper, we optimize the groove profile of diffraction gratings for the effective excitation of THz plasmons. Blazed and rectangular gratings are considered. It is shown that for efficient excitation of plasmons it is necessary to use gratings with a rectangular profile of grooves coated with a dielectric.

TERAHERTZ PLASMONS ON FLAT METAL SURFACE

Surface plasmon-polaritons wave propagating along a “metal-dielectric” interface are two-dimensional waves. Their confinement on the surface is achieved due to the fact that the propagation constant $k_{spp} = k_0\sqrt{\dfrac{\varepsilon_d \varepsilon_m}{\varepsilon_d + \varepsilon_m}}$ is greater than the wave number k in the dielectric and this leads to the formation of exponentially decay oscillations on both sides of the interface [2]. The dispersion curve of SPPs lies to the right of the light line ($\omega = ck_0$) and the excitation of a surface wave by a three-dimensional light field is directly impossible unless special phase matching methods are used. For instance, if we have a photon with energy $\hbar\omega$ and a wave vector $\hbar\omega / c$, its value must be increased by Δk in order to transform photons into SPPs [3].

One of the methods for satisfying the phase matching condition is the grating coupling. Light diffracted on a reflective periodic grating can have wave vectors

$$\vec{k}_m = \vec{k}_{inc} + m\vec{K} = n_d k_0 \sin\theta + \frac{2\pi m}{p},$$

where n_d is the refractive index of the medium above the grating, $\vec{K}$ is the grating wave vector.

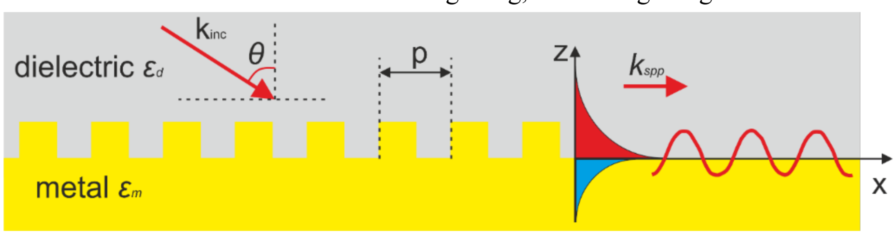


FIGURE 1. Schematic representation of the method of excitation of plasmon polaritons by grating coupling method.

The condition for matching wave vectors is rewritten in the form

$$\vec{k}_{spp} \simeq k_0\sqrt{\frac{\varepsilon'_d \varepsilon'_m}{\varepsilon'_d + \varepsilon'_m}} = n_d k_0 \sin\theta + \frac{2\pi m}{p} \tag{1}$$

or

$$\sin\theta = -\left(\frac{m\lambda}{n_d p}\right) \pm \sqrt{\frac{\varepsilon'_m}{\varepsilon'_d + \varepsilon'_m}}, \tag{2}$$

where the signs + and – correspond to diffraction orders $m > 0$ and $m < 0$. For efficient excitation of plasmons, it is necessary to satisfy the conditions $\varepsilon'_m \gg n_d^2$, then

$$\sin\theta + m\frac{\lambda}{n_d p} = \pm 1 \tag{3}$$

This leads to the determination of diffraction orders which is controlled by the grating period

$$\begin{aligned} &\frac{p}{\lambda} > \frac{m}{n_d} \qquad m > 0 \\ &\frac{|m|}{2n_d} < \frac{p}{\lambda} < \frac{|m|}{n_d} \qquad m < 0 \end{aligned} . \tag{4}$$

Gratings that have only three diffraction orders (including zero) are most preferred. The generation efficiency of surface plasmons is affected not only by the correctly selected polarization, materials, or grating period, but also by the profile of the grooves themselves. The optimization of the profile of the grating grooves will be considered below.

PHYSICAL STATEMENT OF THE PROBLEM

It is necessary to optimize the profile of the grating grooves to efficient generation of plasmons. Before setting the modeling, we define a more detailed physical statement of the problem. In our work, the Novosibirsk free-electron laser [4] will be used as a source of terahertz radiation. The radiation will be transformed into conically converging plane waves (Bessel beam) and incident on the cylindrical coupler at the angle of $\theta = 45^{\circ}$. For our operating frequencies, the dispersion equations for cylindrical surfaces are exactly the same as for flat ones. Any changes in the dispersion relations are not expected when folding a flat linear lattice into a cylinder, therefore, to reduce the computational resources spent in calculations, we used linear gratings [5].

In the calculations, the plane TM wave was taken at an angle of $\theta = 45^{\circ}$ as an incident wave. We will try to find the grating resonance condition for a wavelength of $\lambda_{inc} = 141\ \mu m$. As part of our analysis, we will vary the dielectric. In one case, the dielectric is air ($\varepsilon_{air} = 1$), in the other case it is ZnS ($\varepsilon_{ZnS} = 8.7 + i \cdot 0.059$). Moreover, for simplicity in the calculations, we assume that ZnS does not have absorption. Assuming that $m = 1$ and substituting all the parameters in the equation (3) , we find the grating period

$$p_{ZnS} = \frac{141}{\sqrt{8.7} \cdot \left(1 - \sin 45^{\circ}\right)} \approx 159 \mu m \quad p_{air} = \frac{141}{1 \cdot \left(1 - \sin 45^{\circ}\right)} \approx 470 \mu m \tag{5}$$

In our calculations, we will analyze rectangular gratings and blazed gratings. From the condition of matching wave vectors, it is possible to get the grating period, but other parameters also affect the efficiency of plasmon coupling. For a rectangular grating, we will find the depth d and width of the slit w, or more precisely, the fill factor FF ($w = FF \cdot p$). For a blazed grating, we will vary the blaze angle α. Optimization stages are demonstrated in table 1.

TABLE 1. Optimization stages

Stage	Rectangular grating	Blazed grating
1	Fill factor (FF) variation	Blaze angle (α) variation
2	Depth (d) variation	

MODEL DEFINITION

We used the COMSOL Multiphysics software to perform the modeling. The program solves the two-dimensional scattering problem. To determine it, it is necessary to define the port, boundary conditions and the material of the grating. The virtual experiment schemes, which depicts Floquet cells, are shown in fig. 2.

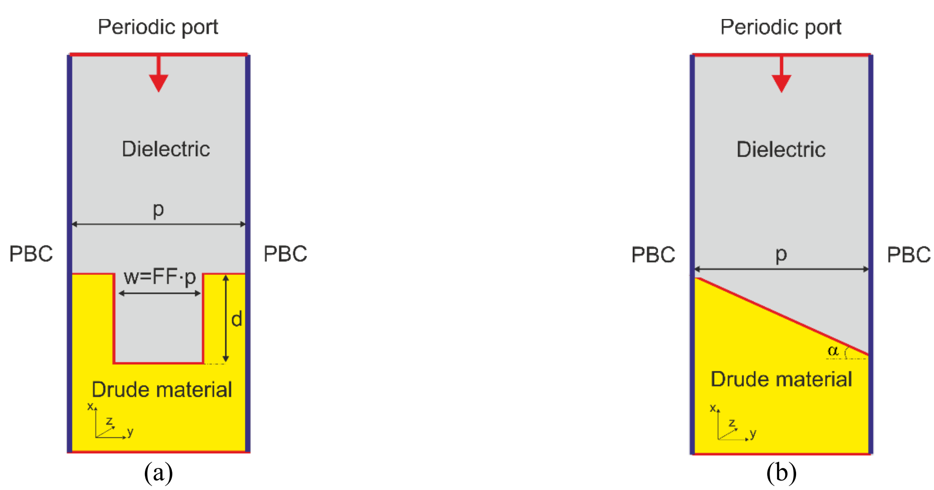


FIGURE 2. Floquet cell of (a) rectangular grating and (b) blazed grating.

The left and right cell boundaries are determined using periodic boundary conditions (Floquet conditions). As applied, this condition states that the solution on one side of the cell is equal to the solution on the other side multiplied by the complex phase coefficient. The phase shift between the boundaries is estimated by the perpendicular component of the wave vector. Since the periodic boundaries are parallel to the y-axis, only the x-component is required. The port is also periodic $\begin{pmatrix} H_x & H_y & H_z \\ 0 & 0 & 1 \end{pmatrix}$ and excites a plane TM wave at an angle of $\theta = 45^{\circ}$. Ports are used both to determine the incident wave, and to ensure that the resulting solution "leaves" the model without any non-physical reflection. To achieve this, each port (diffraction order) must have its own port. Estimate their number. Constructive interference condition is

$$m\lambda_{inc} = pn_d\left(\sin\theta_m - \sin\theta\right). \tag{6}$$

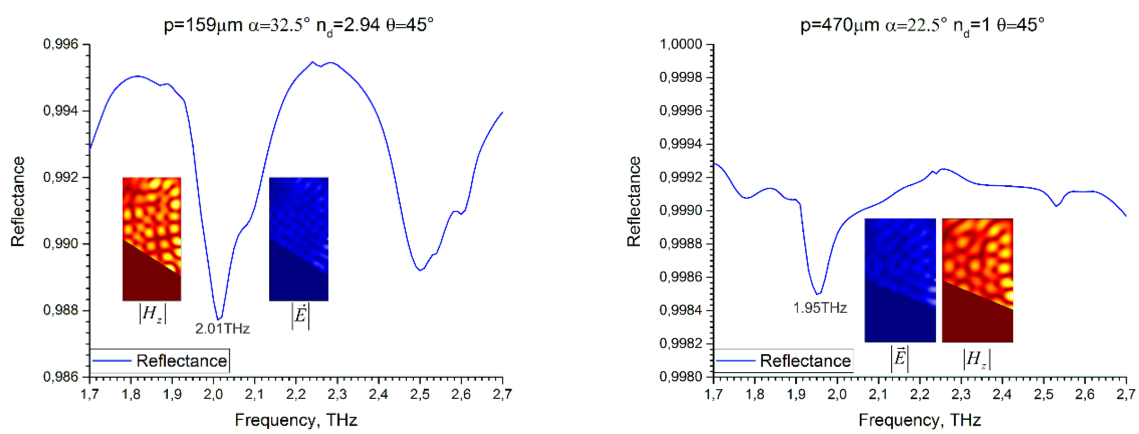
The maximum value of m is determined from condition $\left|\sin\theta_m\right| \leqslant 1$ i.e.

$$\left(-1-\sin\theta\right)\frac{pn_d}{\lambda_{min}} \leqslant m \leqslant \left(1-\sin\theta\right)\frac{pn_d}{\lambda_{min}}. \tag{7}$$

Simulation is occurred in the frequency range of $f = 1.7 - 2.7$ THz. Thus, substituting $\lambda_{\min} = 111\ \mu m$ and grating parameters into the equation, we obtain that $-7 \leqslant m \leqslant 1$. As a result, we obtain 9 modes so it is needed to install 9 ports.

SIMULATION RESULTS

In the simulation, it was expected to observe a dip in the region of the assumed plasmon resonance. The goal of the grating optimization is to maximize the dip in the reflection spectrum. Blazed gratings are much easier to manufacture on CNC machines. Such gratings also have an advantage over rectangular grating when optimizing them with COMSOL. So, it is needed to vary only one parameter. In the first assumption, we thought that these gratings would effectively excite plasmons. However, calculations show that the efficiency of plasmon excitation by such grating should be extremely low as demonstrated in fig. 3.



(a) (b)

FIGURE 3. Optimal parameters of blazed gratings (a) coated with a dielectric and (b) without dielectric

It turned out to be a little more difficult to analyze the results of modeling rectangular gratings, but the results were much more interesting. Analysis of the calculations was carried out in two stages. At the first stage FF is fixed then the minimum reflectivity and the frequency at which the plasmon dip is located are obtained from all possible graphs of the reflectivity R versus frequency for different d. According to these data, two graphs of $\min R\left(d\right)$ and $\min R\left(f\right)$ were plotted. Examples of the graphs are presented in fig.4.

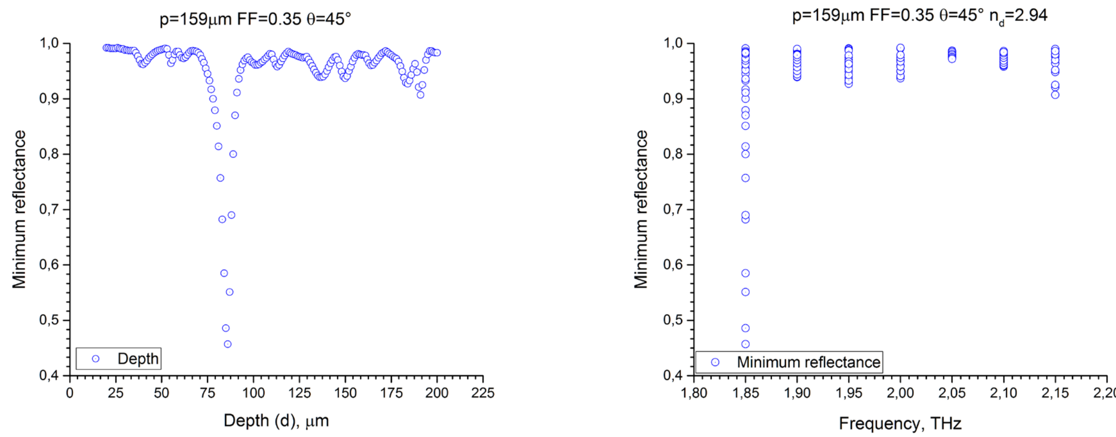


FIGURE 4. Examples of graphs to analyze rectangular gratings.

From such graphs, it is possible to obtain data on the extent to which there may be an error in the manufacture of the depth of the grating grooves or how the frequency of the dip depends on the groove depth. Based on such plots, stable resonances for rectangular gratings were determined.

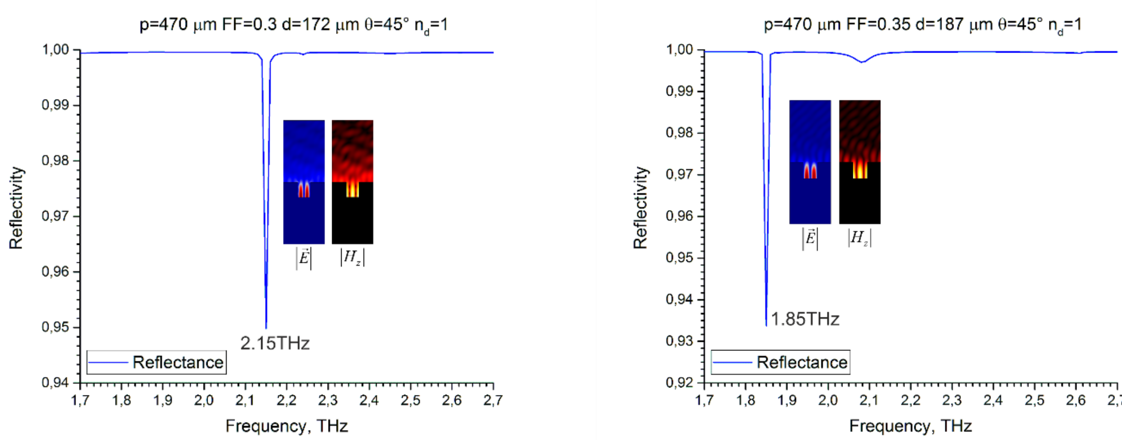
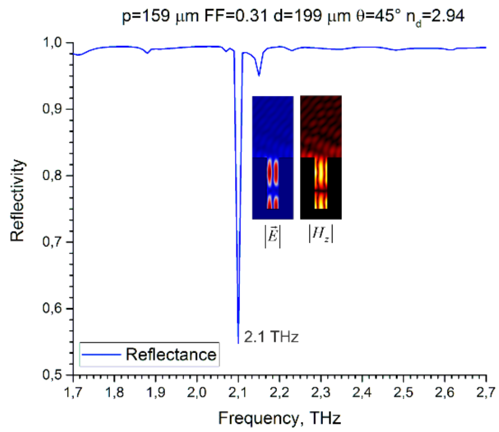
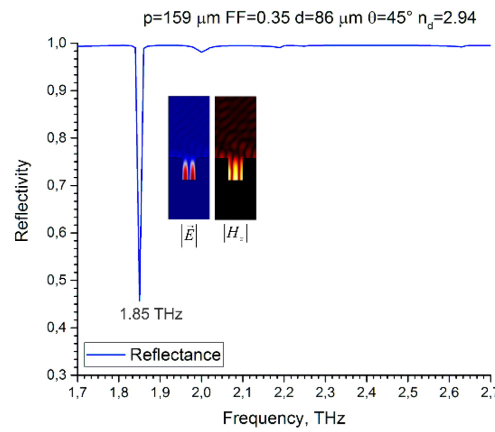


FIGURE 5. Optimal parameters of gratings.



(a)



(b)

FIGURE 6. Optimal parameters of dielectric coated rectangular gratings.

Without dielectric, the plasmon generation efficiency is much lower ($5-10\%$) than in the case of gratings coated dielectric ($>50\%$) after optimization. Thus, the optimal parameters for the gratings are shown in table 2.

TABLE 2. Optimization stages

f_{res}, ТГц	p, мкм	FF, мкм	d, мкм	n_d	θ, °
2.15	470	0.3	172	1	45
1.85	470	0.35	187	1	45
2.1	159	0.31	199	1	45
1.85	159	0.35	86	1	45

CONCLUSION

Diffraction metal blazed gratings and rectangular grating for efficient excitation of plasmons were investigated. The optimal parameters of depth, width and blaze angle were found. It has been found that for excitation of plasmons, rectangular gratings coated with a dielectric are most preferable.

ACKNOWLEDGMENTS

The work was supported in parts by the RSF grant No. 19-12-00193. The experiments were carried out using the infrastructure of the shared research facility 'Siberian Synchrotron and Terahertz Radiation Center (SSTRC)' based on 'NovoFEL' of BINP SB RAS.

REFERENCES

1. Zhang, X., Xu, Q., Xia, L., Li, Y., Gu, J., Tian, Z., Zhang, W. Terahertz surface plasmonic waves: a review. Advanced Photonics, 2(1), 014001.
2. Maier, Stefan A. "Excitation of surface plasmon polaritons at planar interfaces." *Plasmonics: fundamentals and applications*. Springer, New York, NY, 2007. 39-52.
3. Sarid D., Challener W. Modern Introduction to Surface Plasmons: Theory, Mathematica Modeling and Applications. — Cambridge: Cambridge University Press, 2010. — ISBN: 978-1-139-19484-6.
4. Knyazev, Boris A., et al. "Novosibirsk free electron laser as a user facility." *Physics Procedia* 84 (2016): 27-34.
5.