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Analytical calculation of SPP generation with structured substrates

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Unusual optical properties of structured metal surfaces arise from plasmon resonances and interactions through surface plasmon-polariton waves (SPPs). Predicting these properties is generally challenging. However, simplifying the problem using harmonic Fourier components allows one to decompose the initial problem down to the problem of SPP generation by the finite-length sinusoidal grating. In this work, we propose an analytical method for the description of SPP generation with such gratings by utilising methods from the waveguide theory based on the Lorentz reciprocity theorem.

1 Introduction

Plasmonics is a rapidly growing field with significant contributions to scientific areas such as biosensing [1] and Raman spectroscopy [2]. One of the challenges in plasmonics is the efficient generation of surface plasmon polaritons (SPPs). Methods used to generate SPPs on flat metal surfaces have limited ability to control and manipulate the properties of SPPs [3]. Structured substrates have emerged as a promising approach to overcome these limitations.

Several analytical and numerical methods have been proposed to model the excitation of SPPs on structured substrates [3] or in the thin metallic films [4]. However, these methods often involve solving complex equations that require significant computational resources or sophisticated analytical techniques, limiting their practical applicability. Therefore, there is a need for simpler methods to model SPP generation.

In this work, we continue to develop the analytical model for the SPP generation [5, 6] and propose a simple and efficient approach that utilizes mode decomposition and the Lorentz reciprocity theorem [7] to describe the generation of SPPs on structured substrates. The proposed technique has the potential to contribute to the development of new SPP-based devices.

2 Results and discussion

In this paper, we aim to solve the following problem. Let us consider a sinusoidal grating of length z_0, period Λ and amplitude x_0 under the normal incidence of the plane electromagnetic wave (see Figure 1; the vacuum wavelength is λ). After the corrugated area, there is a planar semi-infinite interface. Hereinafter, the grating and the substrate are considered to be made of gold with the permittivity taken from [8].

According to the approach well-established in the waveguide theory, we are going to calculate the SPP

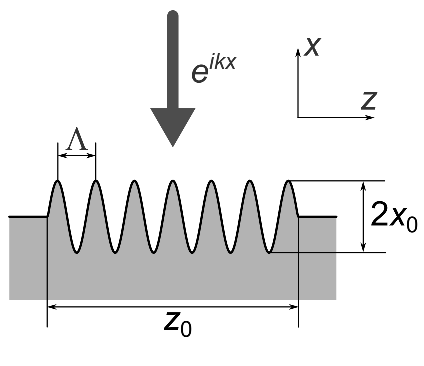

Figure 1: A sketch of the problem.

amplitude according to the relation [9]

$$a_{\mathrm{SPP}} = -\frac{1}{4N_0}\int_{(V)} (\mathbf{e}_{\mathrm{SPP}} \cdot \mathbf{J})\, e^{-ik_{\mathrm{SPP}} z} dV, \qquad (1)$$

where $\mathbf{e}_{\mathrm{SPP}} = e_x^{\mathrm{SPP}} \mathbf{n}_x + e_z^{\mathrm{SPP}} \mathbf{n}_z$ is the SPP mode's electric field with $e_z^{\mathrm{SPP}}(x) = e_0 e^{-\gamma(x)|x|}$ and $e_x^{\mathrm{SPP}}(x) = e_0 \frac{\sqrt{\varepsilon_{\mathrm{Me}}}}{\varepsilon_S(x)} e^{-\gamma(x)|x|}$; $e_0 = -h_0 \frac{\rho_V}{\sqrt{\varepsilon_{\mathrm{Me}}+1}}$; $\rho_V = \sqrt{\frac{\mu_0}{\varepsilon_0}}$; $\mathbf{h}_{\mathrm{SPP}} = h_y^{\mathrm{SPP}} \mathbf{n}_y$ is the SPP mode's magnetic field with $h_y^{\mathrm{SPP}} = h_0 e^{-\gamma(x)|x|}$;

$$\varepsilon_S(x) = \begin{cases} 1, & x \geqslant 0, \\ \varepsilon_{\mathrm{Me}}, & x < 0; \end{cases} \quad \gamma(x) = \begin{cases} \gamma_{\mathrm{Vac}}, & x \geqslant 0, \\ \gamma_{\mathrm{Me}}, & x < 0; \end{cases}$$

h_0 is an arbitrary constant of dimension A/m; $N_0 = \frac{1}{2}\left|\int_{(S)} \mathbf{e}_{\mathrm{SPP}} \times \mathbf{h}_{\mathrm{SPP}} \cdot \mathbf{n}_z \, dS\right|$; $\gamma_{\mathrm{Vac}} = k \frac{i}{\sqrt{\varepsilon_{\mathrm{Me}}+1}}$; $\gamma_{\mathrm{Me}} = -k \frac{i\varepsilon_{\mathrm{Me}}}{\sqrt{\varepsilon_{\mathrm{Me}}+1}}$; $k_{\mathrm{SPP}} = k n_{\mathrm{SPP}}$; $n_{\mathrm{SPP}} = \frac{\sqrt{\varepsilon_{\mathrm{Me}}}}{\sqrt{\varepsilon_{\mathrm{Me}}+1}}$; $\mathbf{n}_x$, $\mathbf{n}_y$ are the unit vectors in the X and Y directions respectively; $\mathbf{J}$ is the excitation current density distribution.

The only question here is the proper determination of the excitation current density $\mathbf{J}$. We will choose it as in [9]

$$\mathbf{J} = -ik(\varepsilon(x,z) - \varepsilon_s(x))\,\frac{\mathbf{E}}{\rho_V}, \qquad (2)$$

where $\mathbf{E}$ is the electric field amplitude; $\varepsilon(x,z)$ and $\varepsilon_s(x)$ set the permittivity as functions of spatial coordinates for the modified and the initial flat surfaces respectively; $k = 2\pi/\lambda$.

A straightforward choice of $\mathbf{E}$ as a superposition of the background (without the grating) and the overall scattered field specifies the self-consistent problem since both the left- and the right-hand sides of (2) depend on the SPP coefficient a_{SPP}. We are going to simplify our problem assuming the grating amplitude smaller than the wavelength λ and the grating period Λ.

2.1 Description of SPP generation within the Born approximation

One way of simplification of (1) stems from replacing the full electric field $\mathbf{E}$ in (2) by such a field that does not include the SPP contribution. According to this suggestion, let us set the electric field as follows:

$$\mathbf{E} = E_{0\_\mathrm{ins}} \mathbf{n}_z \begin{cases} e^{ikx} + re^{-ikx}, & x \geqslant 0, \\ (1+r)e^{\gamma^0_{\mathrm{Me}} x}, & x < 0, \end{cases}$$

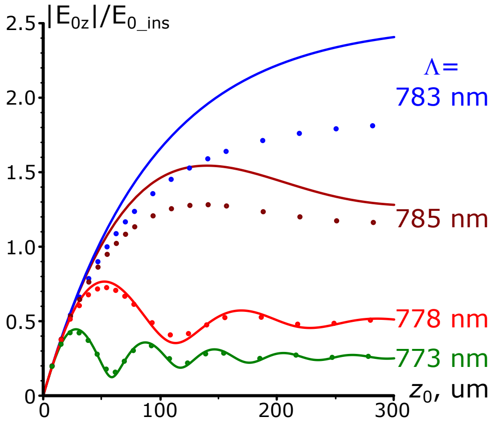

Figure 2: Comparison of the analytically calculated Z component of the electric field at the end of the grating and the results of the full-wave numerical simulations. The grating amplitude is 10 nm; the solid lines represent the analytical results while the dotted ones correspond to the numerical simulations. The wavelength $\lambda = 800$ µm.

where E_{0_ins} is the incident wave field amplitude, $r = \left(1 - \sqrt{\varepsilon_{\mathrm{Me}}}\right)/\left(1 + \sqrt{\varepsilon_{\mathrm{Me}}}\right)$ the reflection coefficient from the flat metal surface, and $\gamma^0_{\mathrm{Me}} = ik\sqrt{\varepsilon_{\mathrm{Me}}}$. For the sake of simplicity, only the linear term of the power series by the small parameter kx_0 is considered.

Figure 2 shows the results of the electric field calculations right after the grating for different grating lengths and grating periods. It demonstrates the essential properties of the desired solution: if the grating is resonant (i.e., the SPP wavelength and the grating period coincide), the electric field is maximal; while the discrepancy between the grating period and the SPP wavelength is getting larger, the generation efficiency drops and the picture of beats appears.

Despite these advantages, this figure also highlights a limitation of the described approach. Indeed, the analytical results agree well with the numerical calculations for the short or non-resonant gratings. Meanwhile, the divergence of the predicted dependence with the calculated one is fairly high for the case of long ($z_0 > 50$ µm) resonant gratings.

Figure 3 suggests another issue with the found solution. Comparison of the analytically calculated amplitude of the electric field produced by the resonant grating with the numerical one pronounces the

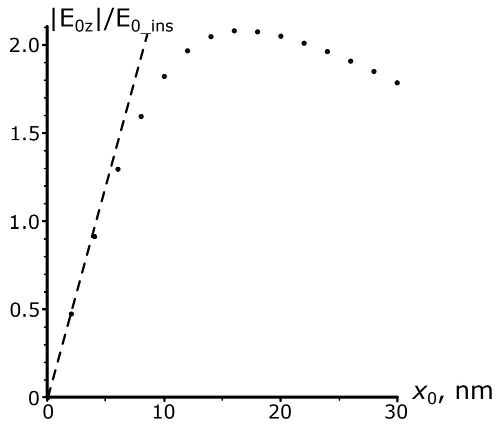

Figure 3: Dependence of the normalized Z component of the electric field near the end of the grating on the grating amplitude x_0 for the resonant SPP excitation. The dashed line shows the analytical dependence; the dots are for numerical calculations. For both cases, the total length of the grating is kept constant and equal to 400.5 grating periods (≈ 313 μm).

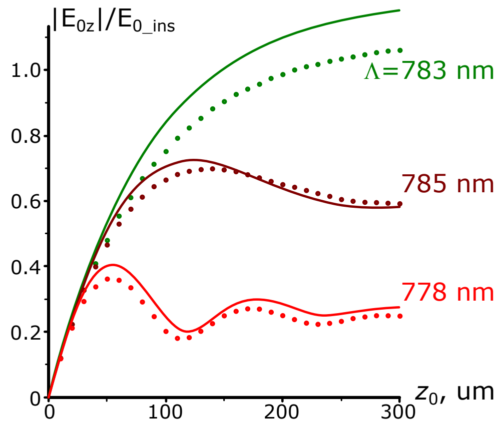

Figure 4: Dependence of the SPP amplitude on the grating length z_0 with variation of the latter's period. The height of the grating profile $x_0 = 5$ nm. The wavelength of radiation incident on the grating is $\lambda = 0.8$ μm ($\lambda_{\text{SPP}} = 0.783$ μm). The solid curves are the results of analytical calculations, the colored dots are the numerical results.

significant disagreement between two curves albeit the grating amplitude keeps being relatively small.

The roots of these problems lie in the Born approximation's limitations. Indeed, one can expect a satisfactory agreement between the exact solution and the approximation as long as the SPP-related and other scattering terms can be treated as a small perturbation. This assumption is no longer true if the SPP impact is not negligible (as for the long resonant gratings) or when the real electric field is essentially non-zero while the background field exponentially decays (if the grating amplitude is larger than the penetration depth in metal). Therefore, we need to correct this approach to mitigate these effects.

2.2 Description of SPP generation within the corrected Born approximation

First, let us suggest the simpler yet more powerful substitution for $\mathbf{E}$ in (2). Here we use the constant electric field taken at the position of the planar interface without the grating:

$$\mathbf{E} = E_{0\_\text{ins}}(1 + r)\mathbf{n}_z.$$

It must describe the SPP generation by the gratings with larger grating amplitudes more accurately as it does not decay exponentially for $z < 0$.

One more correction aims to account for the SPP radiative losses, which are more pronounced for long gratings. In the linear approximation, the radiative losses must be proportional to the SPP electric field:

$$E_{\text{lkg}} = \kappa E_{0z}.$$

The symmetry of the problem allows one to determine the value of the parameter κ as in [10].

Ultimately, the Z component of the electric field at the end of the grating reads as

$$E_{0z} = i\gamma_E \frac{1}{\Delta k + i(k_I + \gamma_{\text{rad}})} \times \left(1 - e^{-z_0(k_I+\gamma_{\text{rad}})+i\Delta k z_0}\right) E_{0\_\text{ins}},$$

where

$$\gamma_E = \gamma_0 \left(x_0 - i\frac{2}{3\pi} k x_0^2 \sqrt{\varepsilon_{\text{Me}} + 1} \right)$$

with

$$\gamma_0 = -i(\varepsilon_{\text{Me}} - 1)\,(1 + r)\frac{k_{\text{SPP}}^2}{2\varepsilon_{\text{Me}}} \left| \frac{\varepsilon_{\text{Me}}^{3/2}}{\varepsilon_{\text{Me}}^2 - 1} \right|;$$

the radiation decay

$$\gamma_{\text{rad}} = \frac{|\kappa|^2}{2N_1} = \frac{N_1}{2}|\gamma_E|^2$$

with

$$N_1 = \frac{1}{2k}\left|(\varepsilon_{\mathrm{Me}}+1)\,\frac{\varepsilon_{\mathrm{Me}}^2-1}{\varepsilon_{\mathrm{Me}}^{3/2}}\right|;$$

and

$$k_{\mathrm{SPP}} = \left(\frac{2\pi}{\Lambda}+\Delta k\right)+ik_I.$$

Figure 4 confirms the validity of the suggested corrections. The curves still exhibit monotonic growth until it saturates for the resonant excitation, and the non-resonant curves show decreased generation efficiency with the presence of oscillations. However, the degree of divergence between the analytical and numerical dependencies is smaller compared to the one for the Born approximation. Therefore, while the found solution retains the obtained advantages of the Born approximation, it introduces a finer agreement for the broader range of grating lengths and periods.

3 Conclusion

The proposed approach provides a simple and efficient way to describe the SPP generation by finite-length grating. We illustrated this method by calculating the SPP generation with the sinusoidal corrugation. While any profiled surface can be decomposed to the set of sinusoidally profiled surfaces and incident fields allow one to represent them as a set of plane waves, our results are useful for modelling excitation of surface waves with various configurations of the incident fields and metasurfaces.

Acknowledgements

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