Metal–dielectric photonic crystal superlattice: 1D and 2D models and empty lattice approximation

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1. Introduction

Nowadays, a lot of research is focused on photonic crystals and metamaterials. In most cases these structures consist of metal–dielectric nanostructured slabs. Defining a proper geometry, it becomes possible to control their optical properties [1]. The so-called soft lithography method (SLM) [2] allows to grow such structures with a period down to a few hundred nanometers and with an additional superperiodicity on a larger scale. Extra (superlattice) periodicity gives an additional instrument to control the optical properties such as resonance position and linewidth in these structures [3–7].

Metal–dielectric structures have very rich and interesting optical properties due to plasmon resonances, i.e., collective oscillations of conduction electrons. There are two different types of plasmon resonances: the localized and delocalized ones. Each type of plasmon influences the properties of the structure with superlattice via its own characteristic way. In this paper we propose and discuss simplified approaches to understand the optical properties of a superperiodic structure grown by SLM.

2. Metal–dielectric superlattice

The center of interest of this work is a 2D metal–dielectric photonic crystal structure. A modulated gold layer of thickness 80 nm was grown on a glass substrate using the SLM. The unit cell of the metal is 6 by 6 µm including a region of 4 by 4 µm with square air holes of 0.1 by 0.1 µm. The range between the centers of the air holes is 0.4 µm. The electron microscope view of this structure and the schematics of the unit cell are shown in Fig. 1. The insert in panel (b) shows the reference frame used in this paper.

We investigate the optical response of the structure, illuminated by P-polarized light ($\mathbf{H} \perp \mathbf{OY}$), the plane of light incidence is $X0Z$. The dependence of the transmission spectra on the polar incidence angle $\phi$ was measured for this structure, while the azimuthal angle $\psi$ remained constant. Fig. 2 shows the transmissivity plotted as a function of energy and in-plane momentum $k = (\omega/c) \sin \phi$.

3. Theory and simplified models

The calculations in this paper were done with a Fourier modal decomposition method based on the scattering matrix ($S$-matrix) approach. Discussion of the methods and its improvements can be found in Refs. [8–11]. The precision of this method depends on the number of harmonics describing the structure.

The calculation time grows as $N^3$, where $N$ is the number of harmonics. Furthermore $N = (2g_x + 1) \times (2g_y + 1)$ with $g_{xy}$ as the number of Bragg's harmonics for $X$ and $Y$ directions. In case of the 1D model, $N=301$ (we can take into account only one direction); in case of the 2D model, $N \approx 441$, which means that for each direction $g \approx 10$. 

**References**

This method cannot describe precisely the structure of interest with the superlattice owing to a large CPU-time consumption caused by the large complex 2D supercell. Therefore, it is essentially important to develop reliable simplified models to describe qualitatively the superlattice structures.

For the calculations was used a gold dielectric permittivity from Johnson and Christy [12].

3.1. Simplified 1D model of superlattice

For the numerical simulations, the original 2D structure was substituted by two simplified models, see Fig. 3 a.

First, we consider a 1D model with the same periodicity and superperiodicity along 0X as the original structure. The calculated transmission spectra of this structure is plotted in Fig. 4 a as a function of the incoming photon energy and in-plane momentum.

The anomalies that look like sharp ridges in the optical spectra of the periodic structures are called Wood's anomalies [13]. The series of ridges with a main one surrounded by satellite ridges can be found in Fig. 2 as well as in Fig. 4 a. We can also observe a horizontal nondispersive mode located between 2.4 eV and 2.5 eV. Presumably, this mode can be attributed to a localized Mie resonance. In the case of a 1D model this resonance (between 2.5 and 2.6 eV) is a Mie resonance in an individual metal wire [14], and it differs from the 2D case. In case of the 2D model this resonance (between 2.4 and 2.5 eV) is a Mie resonance in an individual hole in the metal film [15,16], what coincides with the situation we have in the experiment.

3.2. Simplified 2D model of superlattice

Another numerical calculation was made for a simple 2D model without superperiodicity, with the unit cell 0.4 by 0.4 μm and a square air hole 0.1 by 0.1 μm in the center. The result of this calculation is shown in Fig. 4 b.
These calculations confirm that the additional set of satellite ridges exists completely due to superperiodicity effects. Some correspondence between Fig. 4a and b is clearly seen. The main dispersive ridges are on the same places in both panels, 1D as well as 2D, shown as functions of wavevector along ΓX direction in the first Brillouin zone. New less dispersive features are seen in the case of the 2D model (starting at ~1.8 eV at the Γ-point and ending at ~2 eV at the X-point).

4. Physical origin of Wood’s anomalies

To understand the origin of Wood’s anomalies let us consider that the incoming light is treated as a plane wave with a frequency ω and a wavevector

\[ \mathbf{k} = (k_x, k_y, k_z) = k_0 (\sin \beta \cos \phi, \sin \beta \sin \phi, \cos \beta), \] (1)

where \( k_0 = \omega / c \), and \( \beta \) and \( \phi \) are polar and azimuthal angles of the light incidence.

If the dielectric function is periodic, \( \varepsilon(X, Y, Z) = \varepsilon(X + d_x, Y + d_y, Z) \), and the electric field can be expressed in the Bloch–Floquet form as a sum over the Bragg harmonics:

\[ E(X, Y, Z) = \sum_{s_x = -\infty}^{\infty} \sum_{s_y = -\infty}^{\infty} E_s(Z) \times \exp \left[ i \left( k_x + \frac{2\pi g_s}{d_x} \right) x + \left( k_y + \frac{2\pi g_s}{d_y} \right) y \right]. \] (2)

Henceforth, we will analyze the different types of Wood’s anomalies for our structure in details.

4.1. Rayleigh anomalies in a lattice and superlattice

The simplest Wood’s anomalies are the Rayleigh anomalies (RAs). They occur due to the openings or closings of diffraction orders [17].

In the 1D periodic case the incoming wave is coupled with all Bragg harmonics, outgoing into superstrate (air in our case) and substrate. The reflected main harmonic (\( g = 0 \)), diffracted and evanescent harmonics (\( g_{x,y} = \pm 1, \pm 2, \ldots \)) in \( X \)-direction into superstrate and substrate are

\[ k_{g_{\text{sup/sub}}}^{\text{sup/sub}} = (k_{x,g_{x,y}} + k_{z}^{\text{sup/sub}}), \]

\[ k_{g_{x,y}} = k_{x,y} + \frac{2\pi g_{x,y}}{d_{x,y}}, \] (3)

\[ k_{k_{g}^{\text{sup/sub}}}^{\text{sup/sub}} = \sqrt{k_0^2 \varepsilon_{\text{sup/sub}} - \left( k_x + \frac{2\pi g_x}{d_x} \right)^2 - \left( k_y + \frac{2\pi g_y}{d_y} \right)^2}, \] (4)

where \( \varepsilon_{\text{sup/sub}} \) is the dielectric constant of the substrate and superstrate, respectively.

The RA appears at a given frequency when the light field of some Bragg harmonic changes its character from evanescent to radiative (in the superstrate or substrate) [15]. This happens when the term under the square root in Eq. (4) changes its sign.

The Rayleigh anomalies are connected with the radiating conditions, so they depend only on the dielectric constants of the substrate and the superstrate and on the period. There is no dependence of the RA position on the near-field and, thus, on the polarization state of the incoming light or the dielectric susceptibilities of the PCS itself. Only the shape of the RA depends on the PCS structure.

4.2. Surface plasmon–polariton

The other dispersive Wood’s anomalies in the transmission spectra originate from the excitation of surface plasmon–polaritons (SPPs) on the metal/dielectric interfaces [18]. Starting from Maxwell’s equations, the SPP dispersion law can be derived for the SPP of an unmodulated metal surface [19]

\[ k = \frac{\omega}{c} \sqrt{\frac{\varepsilon_m \varepsilon_1}{\varepsilon_1 + \varepsilon_m}}, \] (5)

where \( \varepsilon_m \) is the permittivity value of the metal and \( \varepsilon_1 \) is that of the dielectric. An SPP is a wave propagating along the interface and evanescent into the metal and dielectric. The evanescent decay exponents in these two media (perpendicular to the...
interface) are found as
\[ k_1 = \frac{\omega}{c} \sqrt{-\varepsilon_1}, \quad k_m = \frac{\omega}{c} \sqrt{-\varepsilon_0}, \]

SPPs can appear only when \( \text{Re}(\varepsilon_1 + \varepsilon_0) < 0 \), i.e., one of the media is a metal and another is a dielectric. SPPs may not be optically excited at a planar metal surface by incident plane waves without some method of increasing the wave vector of the incident light since the wavevector of the SPP is beyond the maximum wavevector available to the incident light. Also, an SPP can only be excited with P-polarized light (magnetic field parallel to the interface), since an orthogonal component of the incident E-field at the surface is required to excite the surface charge density oscillation.

Eq. (5) is the eigenvalue equation describing the SPP. It can be solved either as a complex function \( \omega(k) \) of a real in-plane momentum \( k \), or as a complex function \( \tilde{k}(\omega) \) of real frequency \( \omega \).

These two possible solutions of the eigenproblem (5) correspond to two physically different situations. A dispersion law \( k(\omega) \) corresponds to the excitation of the plasmon wave with a fixed frequency \( \omega \) at some spatial point; \( \text{Re}(\omega(k)) \) gives the wavenumber of the resulting surface wave, and \( \text{Im}(k) \) is the inverse SPP propagation length along the interface.

It is obvious that it is not our case of the SPP excitation by an infinite plane wave, incoming from the outside. In this case the in-plane projections \( k_1, k_2 \) are real, so we need a complex solution of Eq. (5).

The permittivity \( \varepsilon_1 = \varepsilon_{\text{sub}} = 2.32 \) (\( \varepsilon_0 = 1 \)) was taken for the glass substrate (air). In order to find the SPP dispersion law \( \omega(k) \) it is not sufficient to know only \( \varepsilon_1(\omega), \varepsilon_0(\omega) \) on the real frequency axis only. We have to perform the analytical continuation of these functions into the complex energy plane. In the case of gold with d-band we use the Lorentz–Drude approximation [20]:

\[ \varepsilon_m(\omega) = 1 - \frac{\Omega_p^2}{\omega(\omega + i\Gamma)} + \sum_{j=1}^{M} \frac{f_j\Omega_p^2}{(\omega^2 - \omega_j^2) - i\omega \Gamma_j}, \]

where \( \Omega_p = \sqrt{\omega_p^2} \) is plasma frequency, \( \omega_p = 9.03 \text{ eV} \), see other parameters in Eq. (7) in Table 1.

It appears that a simple Drude approximation (the first two terms in Eq. (7)) does not describe adequately the gold dielectric susceptibility starting from \( \omega > 1.4 \text{ eV} \).

Fig. 5 compares the calculated \( \text{Re}(\omega(k)) \) for a gold/air interface in the case of the Lorentz–Drude model (7) with the dependence \( \text{Re}(\tilde{k}(\omega)) \), drawn in the same axes. We can see that there is a large difference between them, especially in the region of 2.4–2.6 eV.

In addition, Fig. 5 shows the plasmon dispersions derived using the Drude model. At the higher energies above 2.2 eV a large difference between the SPP dispersions calculated in the Drude and Lorentz–Drude models can be clearly seen. It is the energy of the d-band of gold, and the Drude model fails here.

Red lines in Fig. 5 show the imaginary part of the SPP dispersion \( \text{Im}(\omega) \) as a function of \( \text{Re}(\omega) \) (i.e., the implicit function of \( k \)). The gaps in red lines correspond to d-band gaps in the SPPs’ dispersions (from 2.5 to 2.57 eV for gold/air and from 2.4 to 2.57 eV for gold/glass interfaces). The gaps mean that there is no

### Table 1

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**Fig. 5.** Calculated SPP dispersion \( \omega(k) \) on the gold/air (a) and the gold/glass (b) interfaces. Blue (green) symbols show the calculated \( \text{Re}(\omega(k)) \) for LD (Drude) model, red symbols are \( \text{Im}(\omega(k)) \) for LD. Black arrow shows that the upper axes belongs to the red dashed line. Black thick symbols show \( \text{Re}(\tilde{k}(\omega)) \), black thin solid (dash/point) symbols show the air (glass) cone. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)
solution of Eq. (5) with real \( k \) and complex \( \omega \). As to the \( \text{Re}(k) \) dependence, it has a negative slope here, which indicates a gap in \( k \), also due to d-band in gold.

It is expected that in transmission the Bragg resonances of the SPPs’ look like dips, i.e., they correspond to the minima of transmission at the corresponding \( k \) and \( \omega \), because the incoming light energy goes into the SPP excitation.

4.3. Empty lattice approximation and folding of SPP

The complicated dispersions of Wood’s anomalies especially in the case of a superlattice structure can be understood within the empty lattice approximation (ELA), see, e.g., in Refs. [8,21]. The latter is merely a folding of the dispersion laws of the unmodulated structure into the first Brillouin zone of the relevant lattice, according to the rule \( \omega(k_{xG},k_{yG}), k_{i}=(k_{xG},k_{yG}) \in \text{BZ} \). The main features in the measured as well as calculated spectra correspond to folding into the 1BZ of the lattice (with small period) and the satellite features correspond to a smaller 1BZ of the superlattice (with a large period). In our case the periods are multiple. Fig. 6 shows the ELA for the smaller period.

5. Discussion

Fig. 7 shows the calculated as well as measured spectra with folded light and SPP cones. The plasmon modes are shown in Fig. 7 with white lines. The SPP dispersion shown by solid white line is clearly observed. The theoretical line, however, is shifted to lower energies. It can occur because \( e_{\text{metal}} \) was used in the calculation, but, in principle, some effective \( e_{\text{eff}} \) should be taken, because of the presence of air holes in the metal layer. Dips can be observed for \( G_{y} = \pm 1 \), shown as a dotted line, white for the plasmon, black for the RAs’. Some darker (than the average background) spot can be noticed near this theoretical line, but it is very weak. It is emphasized more clearly in Fig. 4b for the simplified 2D model. Plasmons that occur on the metal/air interface are shown with the white dashed line. Such plasmons are clearly seen in the experiment as well as in all two calculated spectra.

In the measurements, these RAs’ are not seen clearly. It can be due to the measurement error or insufficient sensitivity of the measurement equipment. The RAs’ are well observable in all calculated figures. The theoretical lines for the RAs’ for a 6 \( \mu \text{m} \)
superperiod are located closer to each other. They form series of satellite ridges.

As discussed in Section 4.2, the Lorentz–Drude model of gold permittivity gives an absorption band between 2.4 and 2.6 eV (corresponding to the d-band of gold). According to this we may expect a decreased transmission here. However, it appears that the effect of the localized plasmon is stronger, and we do observe bright lines in Figs. 2 and 4.

6. Conclusion

We have shown that the 1D model of a photonic crystal slab with superlattice allows to explain the physical origin of dispersive (vs. angle of incidence) Wood’s anomalies in the optical spectra. The localized plasmons cannot be described well in the 1D model. On the other hand, it is possible to describe them within a simplified 2D model without the superperiodicity. The superperiodicity does not influence the localized plasmons significantly. Finally, the folding of the light and SPP cones into the 1BZ of the lattice (superlattice) allows to explain the observed Wood’s anomalies as RAs' and SPPs'.

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