

NANOSTRUCTURES

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Excitation of a plasmon resonance in metal cylinders by an evanescent wave

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Abstract. **The magnetic field distribution and electric-field amplification factor are found in the gap between periodically arranged parallel metal cylinders scattering an evanescent wave. Such a wave appears if an original plane wave is incident from the dielectric substrate onto the interface at an angle of total internal reflection. A substantial restructuring of the near-field distribution, which results from a small change in the angle of incidence, is revealed. Estimations of the angular dependence of the local field, explaining the shift and broadening of the plasmon resonance at a shorter wavelength, are presented.**

Keywords: *surface plasmon, array of nanowires, total internal reflection.*

1. Introduction

Nanophotonics investigates the interaction of radiation with the objects whose dimensions are much smaller than the wavelength of light. In this case, spatial frequency of the field inhomogeneity (e.g., of a scattered field near a small particle) exceeds the wavenumber in vacuum $k_0 = \omega/c$, and, as is known, such a perturbation cannot propagate in the form of a travelling wave. Therefore, evanescent waves, whose amplitude decreases exponentially along the wave vector, play a key role in nanophotonics. Thus, the optical processes turn out essentially localised in the area, the size of which is smaller than or of the order of the wavelength of light, i.e. in the near zone relative to the object under study.

The optical processes localised near metal objects are of particular interest. Localisation of excitation in one dimension takes place even in the simplest case of a planar interface between a metal and a dielectric: such waves, propagating along the interface, are called surface plasmons. At the same time, additional localisation occurs in the case of metal objects of small dimensions (significantly smaller than the wavelength of incident light) [1].

Plasmonic nanostructures have a variety of applications. In particular, a substantial local field amplification near roughened metal surfaces increases the sensitivity of the Raman spectroscopy [2, 3], whilst the concomitant large field gradients are used in optical micromanipulation [4–6]. Strong dispersion of the optical response of metal nanoparticles in the region of the plasmon resonance allows one to control the refractive index of composite materials over a wide range, and in particular, to create negative-index metamaterials [7, 8]. The critical dependence of the Fresnel coefficients on the frequency under conditions of total internal reflection at the metal–dielectric interface is widely used in plasmon ellipsometry [9, 10]. Novotny and van Hulst [11] discuss the concept of an optical nanoantenna that improves the detection efficiency of light emitted (or scattered) by the small objects, such as quantum dots or organelles of cells. Among the important applications of plasmonic structures, one can distinguish the local-field amplification near the surface to increase the efficiency of solar batteries [12, 13] or accelerate nonrelativistic particles [14].

Even in the simplest cases, the possibilities of analytical methods in consideration of plasmonic nanostructures are very limited (for example, scattering by metal objects on a dielectric substrate), which makes the development of efficient numerical methods rather urgent. Belai et al. [15] propose a modification of the boundary element method, which takes into account the presence of a dielectric half-space by means of a special-type Green function satisfying a boundary condition at the interface of the half-spaces. This allows reducing the problem in question to the problem of scattering by a body located in the homogeneous space. This approach has been subsequently generalised to the case of a periodic array of bodies located near the interface between two media [16], which allows scattering of an evanescent wave by an infinite grating.

The purpose of this work is to calculate a local field distribution in the gap between adjacent parallel cylinders of a periodic grating for different angles of the wave incidence from the dielectric. The tuning characteristics of a subwavelength grating are compared with those for a simplified model in which the grating is replaced by a metal layer. The results of numerical calculation of the local field amplification factor are given in Section 2. The estimates of light transmittance through a three-layer dielectric–metal–dielectric structure are presented in Section 3.

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2. Local field amplification

We consider the problem of interaction of an evanescent wave with a periodic system of parallel cylinders. An evanescent wave in medium 2 is generated by a plane wave from a substrate (medium 1) and is incident on the interface at an angle θ (Fig. 1). If the angle of incidence exceeds the angle of total internal reflection θ_0, only an evanescent wave exists in medium 2. Such a wave decays exponentially along the y axis and does not carry away the energy into infinity. In the presence of scatterers, such as thin metal cylinders, each of them generates a diverging cylindrical wave. The energy flow at $y \to +\infty$ appears, and the total internal reflection is violated. Below we present the solution to the scattering problem by means of the modified boundary element method that reduces the problem dimension and turns it into a one-dimensional problem because only the boundary integral equations are employed.

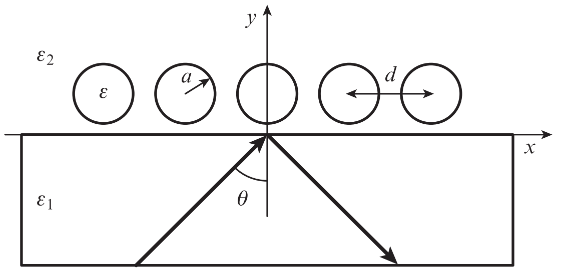

Figure 1. Statement of the problem: a is the cylinder radius; ε is its dielectric constant; d is the grating period; ε_1 is the dielectric constant of the substrate; ε_2 is the dielectric constant of medium 2; θ is the angle of incidence.

We seek the Green function $G(x, y; x', y')$ satisfying the inhomogeneous Helmholtz equation

$$\triangle G + k_{1,2}^2 G = \delta(x - x')\delta(y - y'), \tag{1}$$

where $k_{1,2} = \omega\sqrt{\varepsilon_{1,2}}/c$; ω is the frequency of light; and $\varepsilon_{1,2}$ are the dielectric constants of respective media. The function G only depends on the difference $x - x'$ due to translational symmetry of equation (1). The boundary condition at $y = 0$ for the case of a p-polarised wave appears as

$$[G(x, y; x', y')]_{y=0} = \left[\frac{1}{\varepsilon}\frac{\partial G(x, y; x', y')}{\partial y}\right]_{y=0} = 0, \tag{2}$$

where the square brackets denote the jump of the function at $y = 0$.

According to Floquet theorem [17], the magnetic field $H_z = H(x, y)$ as a function of coordinates in the grating having a period d represents the product of the periodic function and exponent:

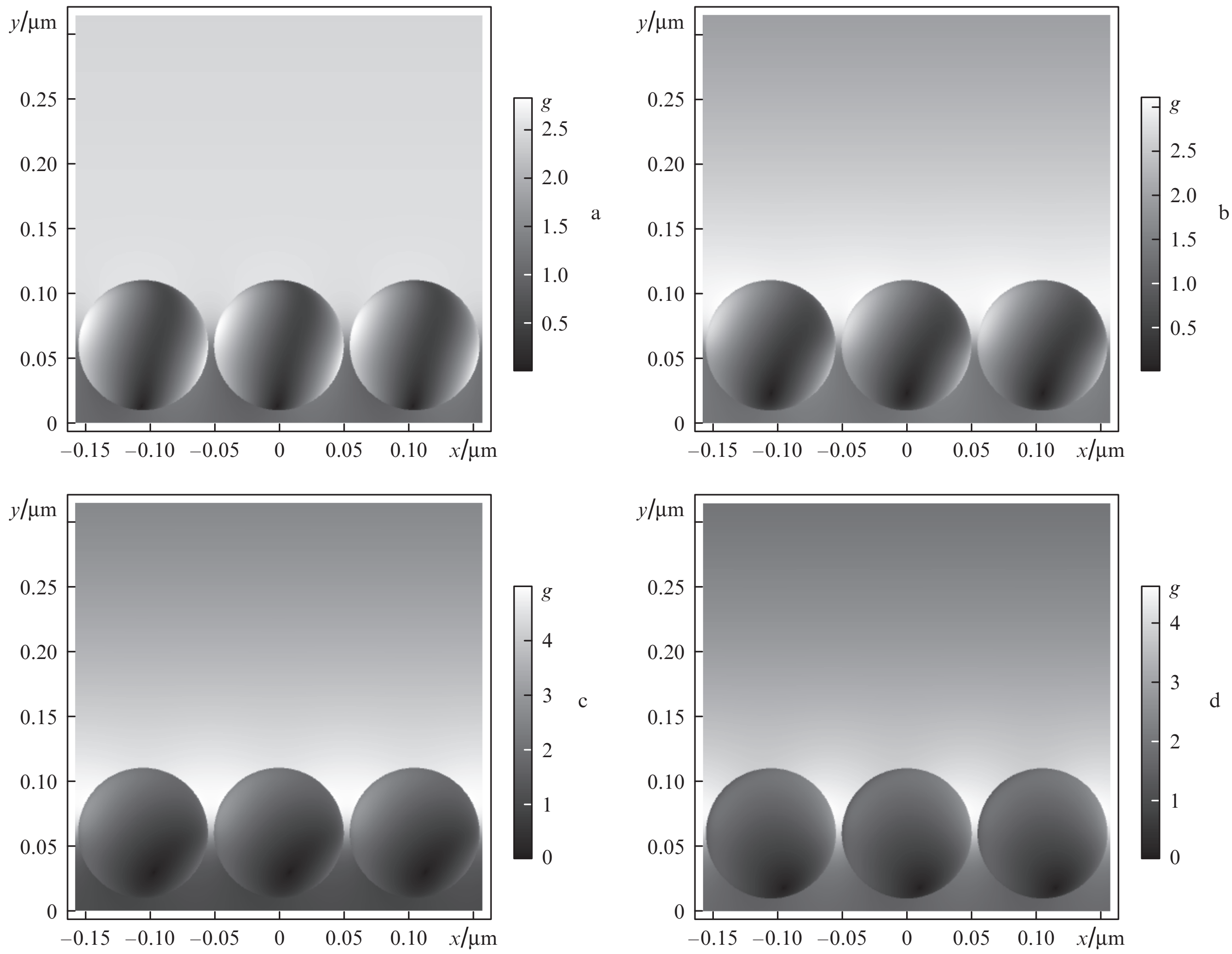

Figure 2. Distribution of the amplification factor of the local magnetic field in a p-polarized wave at λ = 652.6 nm, a = 50 nm and the gap size of 5 nm for θ = (a) 42°, (b) 43°, (c) 44° and (d) 45°.

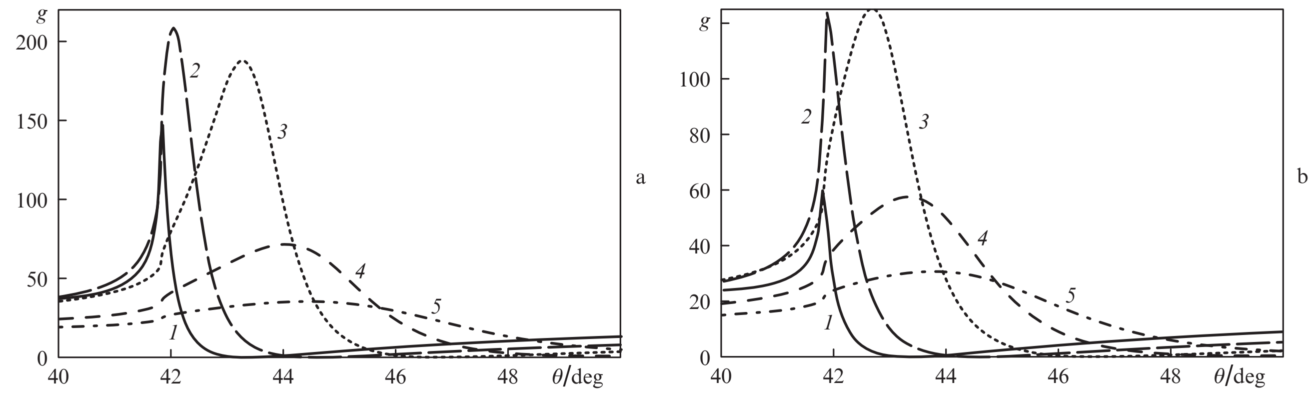

Figure 3. Local electric field amplification factor $g = |E/E_0|^2$ at the centre of the gap between gold cylinders as a function of the angle of incidence θ at λ = (*1*) 885.6, (*2*) 729.3, (*3*) 652.6, (*4*) 563.6 and (*5*) 539.1 nm. The gap size is (a) 7.5 nm and (b) 10 nm.

$$H(x+md, y) = H(x,y)\exp(\mathrm{i}k_x md),\ m = 0, \pm 1, \pm 2, \ldots. \quad (3)$$

Here, $k_x = \omega\sqrt{\varepsilon_1}\sin\theta/c$ is the tangential component of the wave vector in dielectric 1, which is conserved at the interface between media 1 and 2. Using equation (3), we can find the effective Green function, which takes into account the presence of a substrate, in the form of a series:

$$G(x,y;x',y') = -\frac{1}{2d}\sum_{m=-\infty}^{\infty}\mu_{2m}^{-1}\{\exp(-\mu_{2m}|y-y'|)$$
$$+\rho_m\exp[-\mu_{2m}(y+y')]\}\exp[\mathrm{i}(k_x+mk_\mathrm{d})(x-x')], \quad (4)$$

where $k_\mathrm{d} = 2\pi/d$ is the reciprocal grating vector of a periodic array of cylinders; and

$$\rho_m = \frac{\varepsilon_1\mu_{2m} - \varepsilon_2\mu_{1m}}{\varepsilon_1\mu_{2m} + \varepsilon_2\mu_{1m}};\ \mu_{1m,2m} = \sqrt{(k_x + mk_\mathrm{d})^2 - \omega^2\varepsilon_{1,2}/c^2}.$$

The first term in curly brackets describes the diverging cylindrical wave from the source at point (x', y'), whilst the second term corresponds to the image located at point $(x', -y')$. The use of the efficient Green function (4) allows the problem for an infinite structure to be reduced to the calculation of a single elementary cell containing one cylinder only. In particular, it is possible to find a solution for an arbitrary ratio of the tangential component of the wave vector k_x to the reciprocal grating vector k_d. In other words, it is possible to study a general non-periodic case, when the field period is not a multiple of the grating period. In [16], this method was tested on the well-known asymmetric resonances in the far field (the Rayleigh–Wood anomalies).

We solve the problem of a wave with the amplitude $\boldsymbol{E}_0$, incident onto the interface at an arbitrary angle θ. The distribution of the magnetic field amplification factor $g = |H/H_0|^2$ in the near field for three adjacent cylinders is shown in Fig. 2. The calculation is performed for a gold cylinder at the wavelength $\lambda = 652.6$ nm and $\varepsilon_1 = 2.25$, $\varepsilon_2 = 1$, $\varepsilon = -9.9 + 1.05\mathrm{i}$ [18]. It can be seen that the field in metal reaches its maximum near the lateral surface of the cylinder at points where the distance to the adjacent cylinder is small. The field minimum is located inside the cylinder near a point close to the substrate. A small change in the angle of incidence near the angle of total reflection θ_0 leads to radical restructuring of the near-field pattern. Consequently, in this range of angles the peculiarities of the local field amplification factor should be looked for.

The results of calculation of the electric field amplification factor for gold cylinders of radius $a = 50$ nm are shown in Fig. 3. The field was calculated at the centre of a gap 7.5 nm and 10 nm in width, depending on the angle of incidence. The dielectric constants $\varepsilon_2 = 1$ for air and $\varepsilon_1 = 2.25$ for a glass substrate were used; relevant data for gold (at different frequencies) were taken from the handbook [18]. A drastic field change can be seen near the angle of total internal reflection $\theta \approx \theta_0 = 42°$. In the long-wavelength case, for radiation with λ = 700–900 nm, the field changes especially dramatically. This feature makes promising the use of this resonance in tunable plasmonics devices. In the short-wavelength case, the reso-

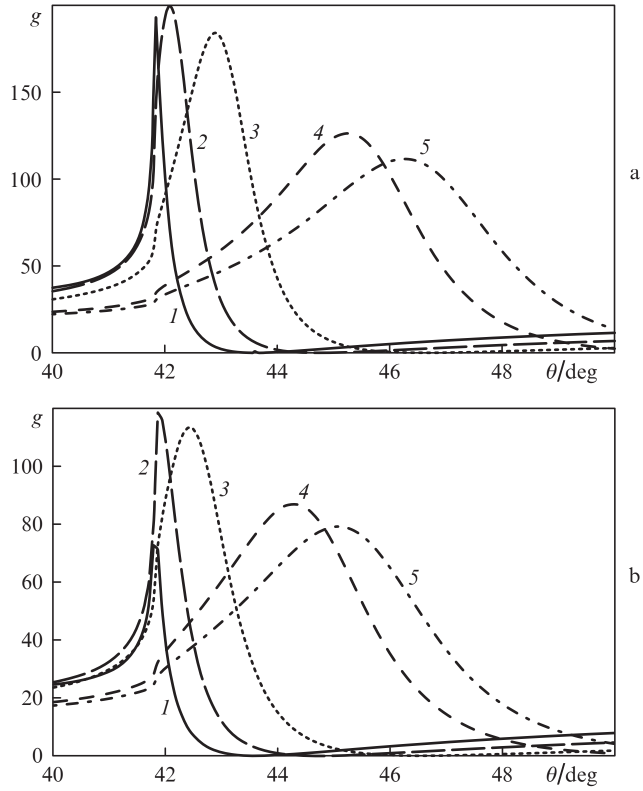

Figure 4. Local electric field amplification factor $g = |E/E_0|^2$ at the centre of the gap between silver cylinders as a function of the angle of incidence θ at λ = (*1*) 826.6, (*2*) 688.8, (*3*) 590.4, (*4*) 495.9 and (*5*) 476.9 nm. The gap size is (a) 7.5 nm and (b) 10 nm.

nance is shifted to higher angles and considerably broadened. Figure 3 also demonstrates that the local field almost doubles when the gap between cylinders decreases by 25%. A similar plasmon resonance manifests itself in the gap between silver cylinders (Fig. 4). As in the case of gold cylinders, the amplification factor considerably increases with decreasing gap.

The next section represents estimates of the plasmon resonance position and width, which allow qualitative interpretation of the dependences obtained. From the viewpoint of the general theory of diffraction gratings [19], the problem under consideration refers to the long-wavelength type if the dimensionless parameter $\varkappa = d/\lambda$ is small ($\varkappa \ll 1$). A grating without a substrate has been previously investigated in this limiting case in the electrostatic approximation when the two-dimensional Laplace equation can be solved by means of conformal mappings [20].

3. Plasmon excitation

Consider the simplest model, in which the grating of cylinders is replaced by a homogeneous metal layer. Since the distance between the cylinders is much smaller than the wavelength, the model should provide similar results. At the same time, the resonances in this model can be described by a simple formula and do not require numerical simulation. Let us verify whether this model gives the resonances in the angular dependence, which have been revealed in the preceding section by means of numerical simulation. Consider a metal layer with a dielectric constant ε located between dielectrics 1 and 2. Let us find the angular dependence of the coefficient of wave transmittance through the layer and compare the shape, width and position of relevant resonances with those found in the previous section. Generally speaking, if the layer is thin, the processes at the metal–air and dielectric–metal interfaces cannot be considered independently. In such a three-layer medium, the coefficients of reflection and transmittance can be found for an arbitrary polarisation of the incident wave. If the polarisation vector lies in the plane of incidence, the transmittance is given by the formula [21]

$$t = \frac{4\alpha}{(\alpha+\beta)(\mathrm{i}\alpha+1)\exp(h\kappa) - (\alpha-\beta)(\mathrm{i}\alpha-1)\exp(-h\kappa)}, \quad (5)$$

where

$$\kappa = \frac{\omega}{c}\sqrt{\varepsilon_1 \sin^2\theta - \varepsilon};$$

$$\alpha = \frac{\sqrt{\varepsilon_1(\varepsilon_1\sin^2\theta - \varepsilon)}}{\varepsilon\cos\theta}; \ \beta = \frac{\sqrt{\varepsilon_1\sin^2\theta - 1}}{\cos\theta};$$

h is the metal thickness; and $\varepsilon_2 = 1$. Plasmon interaction on the upper and lower boundaries of metal is determined by the parameter $\tau = \exp(-\kappa h)$ and has been studied in [22]. In this case, we have $|\tau| \lesssim 0.1$, so that plasmons can be treated independently in the estimates.

A plasmon can propagate along the metal–air interface ($\varepsilon_2 = 1$) if $\varepsilon_2\varepsilon < 0$ and $\varepsilon_2 + \varepsilon < 0$. In this case, the wave amplitude decays exponentially into the interior of metal and air, whilst the frequency ω and the wavenumber k are related by [23]

$$k^2 = \frac{\omega^2\varepsilon_2|\varepsilon|}{c^2(|\varepsilon| - \varepsilon_2)}. \quad (6)$$

Let us take into account the dependence of the dielectric constant ε on the frequency ω in the Drude model

$$\varepsilon(\omega) = \varepsilon_\infty - \frac{\omega_{\mathrm{p}}^2}{\omega(\omega + \mathrm{i}\gamma)}, \quad (7)$$

where ε_∞ is the limiting dielectric constant at high frequencies; $\omega_{\mathrm{p}} = (4\pi ne^2/m_{\mathrm{e}})^{1/2}$ is the plasma frequency; n is the concentration of free electrons; and m_{e} and e are the effective electron mass and charge. If we neglect the damping γ, relation (6) is reduced to a biquadratic equation, from which the dispersion law is obtained:

$$\omega_{1,2}(k) = \frac{\omega_{\mathrm{p}}}{2\sqrt{\varepsilon_\infty}}\left[\sqrt{1 + 2q\sqrt{\frac{\varepsilon_\infty}{\varepsilon_2}} + q^2\left(1 + \frac{\varepsilon_\infty}{\varepsilon_2}\right)} \pm \sqrt{1 - 2q\sqrt{\frac{\varepsilon_\infty}{\varepsilon_2}} + q^2\left(1 + \frac{\varepsilon_\infty}{\varepsilon_2}\right)}\right], \quad (8)$$

where $q = kc/\omega_{\mathrm{p}}$ is dimensionless wavenumber of the surface wave. The dispersion law is presented in Fig. 5. The lower branch corresponds to surface plasmon. The data taken from the literature were used in calculations: $\varepsilon_\infty = 9.84$, $\hbar\omega_{\mathrm{p}} = 9.1$ eV [24, 25].

It is seen from Figure 5 that the phase velocity of the exciting wave must not exceed a certain threshold value. That threshold can be found from formula (8) in the limit $q \to 0$: $\omega_2 = (kc/\sqrt{\varepsilon_2})(1 - q^2/2) + \mathrm{O}(q^4)$. Hence, at $\varepsilon_2 = 1$ we obtain $\omega_2/k \leqslant c$; therefore, only a wave incident from an optically denser medium, $\varepsilon_1 > \varepsilon_2$, can excite a surface plasmon. This scheme is called the Krechman excitation scheme [22]. The surface wave frequency coincides with the frequency of exciting light, while the wavenumber is determined by projection of the wave vector onto the boundary interface $\omega\sqrt{\varepsilon_1}\sin\theta/c$. Equation (6) gives the excitation angle:

$$\sin^2\theta_1 = \frac{|\varepsilon|}{\varepsilon_1(|\varepsilon| - 1)}. \quad (9)$$

The excitation angle θ_1 is always greater than the total internal reflection angle, for which $\sin^2\theta_0 = 1/\varepsilon_1$ (in the absence of a metal layer). Since for metal $|\varepsilon| \gg 1$, the excitation angle θ_1 slightly exceeds the total internal reflection angle θ_0. In particular, at $\varepsilon_1 = 2.25$ we obtain $\theta_0 = 42°$. Herewith, the excitation angle for $\mathrm{Re}\,\varepsilon = -25$ (in the case of a gold layer at $\lambda = 840$ nm) amounts to 43°.

Figure 6a shows the dependence of the transmittance in terms of intensity through a layer of gold on the incidence angle. Figure 6b demonstrates the angular dependence for the layer of silver. The layer thickness for the estimation is selected in accordance with the 'mass', i.e. from the condition of an equal amount of metal in the layer and array of cylin-

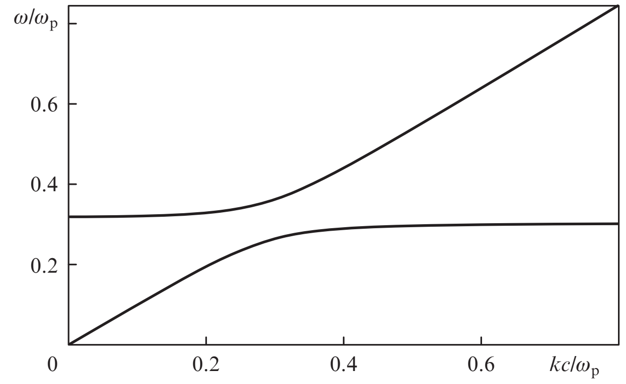

Figure 5. Dispersion law for plasma waves at the metal–air interface: volumetric (upper branch) and surface (lower branch) plasmons.

ders. We have obtained resonances in the angular dependence; herewith, their location, amplitude and width are dependent on the wavelength. Drastic behaviour of the coefficient of reflection from a metal film on a dielectric substrate and the field amplification factor as functions of the angle and wavelength, which is conditioned by excitation of the surface plasmon, has been experimentally studied in [22]. Goldina [26] proposes the use of a narrow resonance in the angular dependence of the coefficient of reflection from a film or a multilayer structure near the angle of total internal reflection to measure the refractive index of medium 2 with high sensitivity.

Figure 6 also shows that the plasmon resonance shifts to larger angles with decreasing wavelength. The same shift can be seen from formula (9). The dielectric constant of metal is reduced in absolute value at higher frequencies. In this case, in accordance with formula (9), the resonant excitation angle θ_1 increases. The effects of narrowing and shifting of resonances in a 70-nm-thick silver layer on a glass substrate have been experimentally tested at $\lambda = 514$, 633 and 670 nm using a scanning tunnelling optical microscope [27].

However, the resonance position for the metal layer is shifted relative to that for the subwavelength grating by a few degrees toward the region of larger angles of incidence. The comparison of Fig. 6 with Figs 3 and 4 shows that the shift constitutes 2° in case of a narrow long-wavelength resonance, whilst it amounts to 6° for wide short-wavelength resonances. The lesser value of the critical angle of plasmon mode excitation in the grating is apparently explained by the change in the dispersion law for surface plasmons in the periodic structure.

Thus, the metal layer model also reveals resonances in the angular dependence of the amplification factor. The model

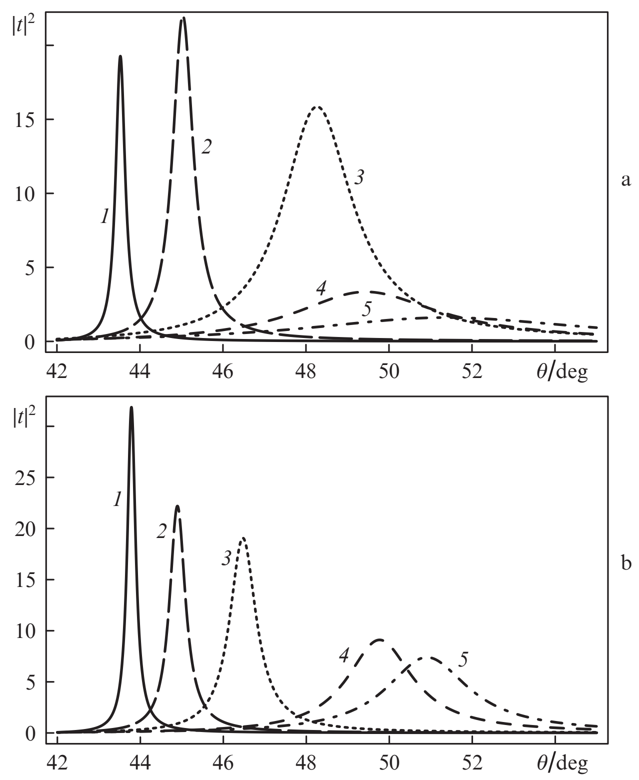

Figure 6. Transmittances $|t|^2$ through the (a) gold and (b) silver layers having the thickness $h = 72$ nm, calculated according to formula (5) as functions of the angle θ. The numbers of curves for gold are the same as in Fig. 3, whilst those for silver are the same as in Fig. 4.

explains qualitatively the angular shift of resonances with the change in the radiation wavelength. However, there is no quantitative agreement with numerical calculations because the dispersion law for a periodic chain differs from the dispersion law for a metal layer.

4. Conclusions

Thus, we have considered the problem of scattering of an evanescent wave by a system of parallel metal cylinders. Numerical simulations reveal a radical restructuring of the near-field as a result of a small change in the angle of incidence near the angle of total internal reflection. In particular, a drastic change in the local electric field in the gap between adjacent cylinders as a function of the angle of the wave incidence from dielectric is observed. Estimates of the shift and width of the resonance arising from excitation of the surface plasmon at the metal–air interface are presented.

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