ISSN 0735-2727, Radioelectronics and Communications Systems, 2015, Vol. 58, No. 5, pp. 201–211. © Allerton Press, Inc., 2015.
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Scattering of Light Waves by Finite Metal Nanostrip Gratings: Nystrom-Type Method and Resonance Effects

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Received in final form September 25, 2014

Abstract—Efficient and rapidly convergent numerical algorithm for the simulation of the scattering of light waves by a finite gratings consisting of thin (thinner than the wavelength in the free space) metal nanostrips is presented. The model is based on the utilization of generalized boundary conditions (GBC), which allow one to exclude from consideration the field inside each strip and to reduce the two-dimensional boundary problem to one-dimensional systems of singular/hypersingular integral equations (IE). The obtained IE are solved numerically using the Nystrom-type method and the quadrature formulas of interpolation type, that provides guarantee convergence and controlled accuracy. The article presents the results of characteristics calculations for optical scattering and absorption by the gratings, which consist of silver nanostrips, as dependences on the width and on the thickness of the strips, and on the grating period. The nature of resonance phenomena has been investigated, namely the article presents the analysis of intensive optical scaterring and absorption in the case of excitation of plasmonic modes (plasmons) and of grating modes, which are induced by the periodicity.

DOI: 10.3103/S0735272715050027

1. INTRODUCTION

Nanoscale materials, devices and technologies is permanently developing and expanding range of science and industry, which rapidly generates new areas, such as nanophotonics and nanooptics. Resonance effects in the scattering and absorption of light waves by metal nanoobjects are associated with surface plasmon resonances and have a wide range of practical applications. For example, in the case of biosensors designing the plasmon effects allow one significantly improve the efficiency of detection, identification and diagnostics of biological objects by increasing the intensity of fluorescence.

Due to modern technologies of sputtering, deposition and etching the nanowires and thin nanostrips made of precious metals (silver, gold) have permanently become a part of many devices for terahertz and optical wave bands (for instance, nanoantennas and biosensors) [1–5]. Periodic gratings of nanowires and nanostrips attract particular attention. This is connected with the newly discovered phenomena of anomalous reflection, transmission, radiation and amplification of the near field [3–6]. Such phenomena are observed near the so-called Rayleigh anomalies for the corresponding infinite gratings [6] and, in the most general case, they possess the form of Fano-type resonances in the spectra of corresponding characteristics.

The techniques for the numerical simulation of optical properties of nanostrips include the techniques of volume [7] and boundary integral equations (IE) [8]. Boundary IE are more efficient due to the fact that it is necessary to discretize only the strip's contour instead of its volume. Secondly, the boundary IE often have smooth or integrable kernels, which ensures a more reliable discretization. It should be noted that the number of unknown quantities, even when calculating characteristics for one nanostrip, is equal to several thousand for the volume IE and it equals to hundreds for the boundary IE.

In contrast to [7, 8], in this paper the two-dimensional problems for scattering of electromagnetic waves by finite gratings made of thin silver strips in the optical range are studied by means of dual-sided generalized boundary conditions (GBC) [9] and they are reduced to systems of singular and hypersingular IE. They are solved by the Nystrom-type method with the utilization of quadrature formulas of interpolation type [10, 11].

Note that the Nystrom-type technique has recently attracted particular attention in the simulation of wave scattering by perfectly conducting and infinitely thin planar and curved strips. This article is related to the development of such a mathematical model, of the numerical algorithm for solving the problems of light

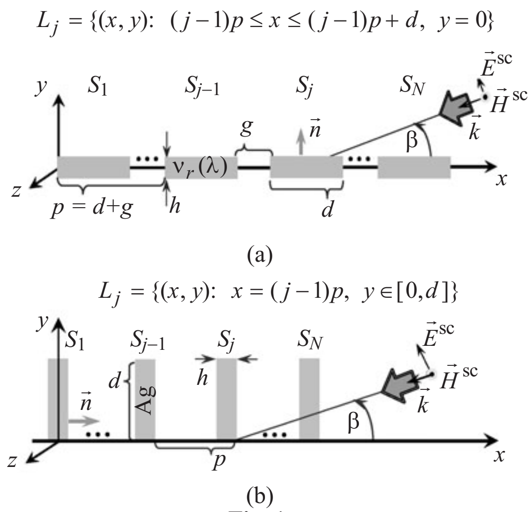


Fig. 1.

scattering by finite gratings of thin planar silver nanostrips in the optical wavelength range and to the investigation of observed resonance phenomena.

2. PROBLEM STATEMENT

Let us consider the two-dimensional problem for the scattering of a plane *H*-polarized electromagnetic wave by the multiple-element strip gratings in free space. Time dependence is given by the factor $e^{-i\omega t}$. The geometry of the two investigated gratings, namely of a planar and of a blade one, is demonstrated in Fig. 1a,b, respectively.

It is assumed that each of them consists of the finite number N of identical silver planar nanostrips, which are infinite along the OZ axis. The width of each strip equals d, the thickness is h, the grating period equals p. The refraction index of silver is given as a function of wavelength $\nu_r(\lambda) = \sqrt{\varepsilon_r(\lambda)}$ in the optical wavelength range. Note that in this range silver possess a complex permittivity $\varepsilon_r(\lambda)$, where its real part takes negative values. The experimental data from [12] has been used for the refractive index of silver.

It should be noted that in the case of *H*-polarization the vectors of electric and magnetic fields take the form $\vec{E} = (E_x, E_y, 0)$, $\vec{H} = (0, 0, H_z)$. On account of superposition, the only nonzero z component of the magnetic field can be represented in the form of sum

$$U_{\mathrm{tot}}(\vec{r}) = U_0(\vec{r}) + U_{\mathrm{sc}}(\vec{r}),$$

where $U_0(\vec{r}) = e^{-ik(x\cos\beta + y\sin\beta)}$ designates the known field of the incident plane wave, $U_{\mathrm{sc}}(\vec{r})$ stands for the sought field, which is scattered by the grating.

In this case the total field must satisfy the two-dimensional Helmholtz equation outside the grating

$$(\Delta + k^2)U_{\mathrm{tot}}(\vec{r}) = 0, \quad \vec{r} = (x, y) \in \mathbb{R}^2 \setminus S, \tag{1}$$

where $S = \bigcup_{j=1}^{N} S_j$, S_j denotes the contour of the jth strip, $k = \omega / c$ is the wave number of free space.

Assume that the thickness of each strip is sufficiently small ($h << \lambda$), then based on [9–11] the cross section of each strip can be replaced by its corresponding center line

$$L_j = \{(x, y)\colon\ (j-1)p \le x \le (j-1)p + d,\ y = 0\}$$

or

$$L_j = \{(x, y):\ x = (j-1)p,\ y \in [0, d]\}$$

for a planar or a blade grating, respectively.

In turn, on the assembly of these center lines $L = \bigcup_{j=1}^{N} L_j$ one can determine the dual-sided GBC, which connect the boundary values of the tangential field components (subscription "tan")

$$[E_{\tan}^{+} + E_{\tan}^{-}] = 2Z_0 R \cdot \vec{n} \times [H_{\tan}^{+} - H_{\tan}^{-}],$$

$$[H_{\tan}^{+} + H_{\tan}^{-}] = -2Z_0^{-1} Q \cdot \vec{n} \times [E_{\tan}^{+} - E_{\tan}^{-}], \tag{2}$$

where $\vec{n}$ denotes a unit vector of the normal to the grating's surface.

These GBC have been originally derived for a thin planar dielectric layer [9]. In point of fact, the conditions (2) represent Ohm's law for effective surface electric $\vec{n} \times [H_{\tan}^{+} - H_{\tan}^{-}]$ and magnetic $\vec{n} \times [E_{\tan}^{+} - E_{\tan}^{-}]$ currents. Finally, for $U_{\text{tot}}(\vec{r})$ GBC (2) take the form:

$$\frac{\partial}{\partial \vec{n}} [U_{\text{tot}}^{+}(\vec{r}) + U_{\text{tot}}^{-}(\vec{r})] = -2\mathrm{i}kR[U_{\text{tot}}^{+}(\vec{r}) - U_{\text{tot}}^{-}(\vec{r})],$$

$$[U_{\text{tot}}^{+}(\vec{r}) + U_{\text{tot}}^{-}(\vec{r})] = \frac{2\mathrm{i}Q}{k} \frac{\partial}{\partial \vec{n}} [U_{\text{tot}}^{+}(\vec{r}) - U_{\text{tot}}^{-}(\vec{r})], \quad \vec{r} \in L, \tag{3}$$

where R and Q stand for relative electric and magnetic resistivity,

$$R = \mathrm{i}\cot(kh\nu_r / 2) / (2\nu_r),$$

$$Q = \mathrm{i}\,\nu_r \cot(kh\nu_r / 2) / 2. \tag{4}$$

Note that such GBC with resistivities, which are defined by (4), allow one to simulate a uniform metal layer in the optical wavelength range with the thickness smaller as well as larger than the skin layer is. This follows from the fact that for metals in the optical band $-\varepsilon_r \approx |\varepsilon_r| >> 1$, and for $k_0 h |\sqrt{\varepsilon_r}| >> 1$ cotangents may be replaced by "–i". A detailed investigation of the applicability limits of GBC in the problems of the scattering for plane waves by metal and dielectric strips is presented in [14].

An additional point is that the scattered field must also satisfy the Sommerfeld radiation condition at the infinity

$$\frac{\partial U_{\text{sc}}(x, y)}{\partial r} - \mathrm{i}kU_{\text{sc}}(x, y) = \bar{o}\left(\frac{1}{\sqrt{r}}\right),$$

$$r = (x, y) = |\vec{r}| \to \infty, \tag{5}$$

and the condition of local boundedness of energy

$$\int_{\Omega} \{k^2 |U_{\text{tot}}|^2 + |\nabla U_{\text{tot}}|^2\} \mathrm{d}\sigma < \infty, \tag{6}$$

where Ω designates an arbitrary bounded region in $\mathbb{R}^2$.

The formulated boundary problem (1)–(6) has a unique solution [9].

3. DERIVATION OF SINGULAR AND HYPERSINGULAR INTEGRAL EQUATIONS

Let us represent the scattered field outside the grating in the form of a linear combination of potentials for a single and a double layer

$$H_z^{\mathrm{sc}}(\vec{r}) = \sum_{j=1}^{N}\left[k\int_{S_j} v_j(\vec{r}\,')G(\vec{r},\vec{r}\,')\mathrm{d}\vec{r}\,' + \int_{S_j} w_j(\vec{r}\,')\frac{\partial G(\vec{r},\vec{r}\,')}{\partial n(\vec{r}\,')}\mathrm{d}\vec{r}\,' \right], \tag{7}$$

where $G(\vec{r},\vec{r}\,') = (\mathrm{i}/4)H_0^{(1)}(k|\vec{r}-\vec{r}\,'|)$ defines the Green's function for two-dimensional Helmholtz equation, and the functions $v_j(\vec{r})$ and $w_j(\vec{r})$, $j=1,\ldots,N$ designate the unknown densities of electric and magnetic current, respectively, which are induced on the jth strip.

Performing the substitution of (7) in (3) and using the properties of the potentials of a simple and a double layers, as well as of their normal derivatives for the case of transition through the integration contour, the boundary problem (1)–(6) is equivalently reduced to a system of singular and hypersingular IE of the second kind

$$\mathrm{i}Qv_s(\vec{r}_0) + \sum_{j=1}^{N}\int_{L_j} w_j(\vec{r})\frac{\partial G(\vec{r},\vec{r}_0)}{\partial \vec{n}(\vec{r})}\mathrm{d}\vec{r} + k\sum_{j=1}^{N}\int_{L_j} v_j(\vec{r})G(\vec{r},\vec{r}_0)\mathrm{d}\vec{r} = -u_0(\vec{r}), \quad \vec{r}_0 \in L_s, \tag{8}$$

$$\mathrm{i}kRw_s(\vec{r}_0) + k\sum_{j=1}^{N}\int_{L_j} v_j(\vec{r})\frac{\partial G(\vec{r},\vec{r}_0)}{\partial \vec{n}(\vec{r}_0)}\mathrm{d}\vec{r} + \sum_{j=1}^{N}\int_{L_j} w_j(\vec{r})\frac{\partial^2 G(\vec{r},\vec{r}_0)}{\partial \vec{n}(\vec{r}_0)\partial \vec{n}(\vec{r})}\mathrm{d}\vec{r} = -\frac{\partial u_0(\vec{r}_0)}{\partial \vec{n}(\vec{r}_0)},$$

$$\vec{r}_0 \in L_s. \tag{9}$$

In the case of a planar grating one considers smooth parameterization of the form

$$x^j = x^j(t) = d(t+\eta_j)/2,$$

$$x_0^j = x_0^j(t_0) = d(t_0+\eta_j)/2,$$

where $\eta_j = (2j-1)+2(j-1)g/d$ and $\tilde{\rho}_{jl}(t,t_0) = k|x^j(t) - x_0^l(t_0)|$ for all $t, t_0 \in [-1,1]$.

As a result the system of IE (8), (9) degenerates into two independent IE systems in unknowns $w_j(\cdot)$ and $v_j(\cdot)$, respectively.

In turn, the parameterization of the following form is introduced for the blade grating

$$y^j = y^j(t) = d(t+1)/2, \quad x^j = (j-1)p,$$

$$y_0^s = d(t_0+1)/2, \quad x_0^s = (s-1)p,$$

where

$$\rho_{js}(t,t_0) = \sqrt{(x^j - x_0^s)^2 + [y^j(t) - y_0^s(t_0)]^2} = (d/2)\sqrt{(t-t_0)^2 + \sigma_{js}^2},$$

wherein $\sigma_{js} = 2p(j-s)/d$.

Consequently, after the substitution of variables the equation system (8), (9) can be rewritten in the general form for both gratings as follows:

$$4Q\kappa^{-1}v_s(t_0)+\sum_{j=1}^{N}\int_{-1}^{1}v_j(t)K_v^{js}(\kappa,t,t_0)\,\mathrm{d}t$$

$$+\sum_{j=1}^{N}\int_{-1}^{1}\tilde{w}_j(t)\sqrt{1-t^2}K_w^{js}(\kappa,t,t_0)\,\mathrm{d}t=f_v^s(\kappa,t_0),$$

$$s=1,\ldots,N, \tag{10}$$

$$4R\kappa^{-1}\tilde{w}_s(t_0)\sqrt{1-t_0^2}+\sum_{j=1}^{N}\int_{-1}^{1}\tilde{w}_j(t)\sqrt{1-t^2}M_w^{js}(\kappa,t,t_0)\,\mathrm{d}t$$

$$+\sum_{j=1}^{N}\int_{-1}^{1}v_j(t)M_v^{js}(\kappa,t,t_0)\,\mathrm{d}t=f_w^s(\kappa,t_0),$$

$$s=1,\ldots,N, \tag{11}$$

for all $t_0\in(-1,1)$ and $\kappa=\pi d/\lambda$.

It should be noted that the condition of local boundedness of energy (6) allows one to find unknown magnetic currents, which are induced by the jth tape as

$$w_j(t)=\tilde{w}_j(t)\sqrt{1-t^2},$$

where $\tilde{w}_j(t)$, $j=1,\ldots,N$ are new smooth functions, that must be determined on the whole interval [–1, 1].

In (10), (11) $K_w^{js}(\kappa,t,t_0)$, $K_v^{js}(\kappa,t,t_0)$, $M_v^{js}(\kappa,t,t_0)$, $M_w^{js}(\kappa,t,t_0)$ and $f_v^l(t_0)$, $f_w^l(t_0)$ for all $s,j=1,\ldots,N$ denote known smooth functions, which are determined according to the following formulas depending on the geometry of the grating:

– planar grating:

$$K_w^{js}(\kappa,t,t_0)=M_v^{js}(\kappa,t,t_0)\equiv 0,$$

$$K_v^{js}(\kappa,t,t_0)=\begin{cases}H_0^1(\kappa|t-t_0|), & j=s,\\ H_0^1(k\tilde{\rho}_{js}(t,t_0)), & j\neq s,\end{cases}$$

$$M_w^{js}(\kappa,t,t_0)=\begin{cases}\dfrac{H_1^{(1)}(\kappa|t-t_0|)}{\kappa|t-t_0|}, & j=s,\\[2ex] \dfrac{H_1^{(1)}(k\tilde{\rho}_{js}(t,t_0))}{\tilde{\rho}_{js}(t,t_0)}, & j\neq s,\end{cases}$$

$$f_v^s(\kappa,t_0)=4\mathrm{i}\kappa^{-1}\mathrm{e}^{-\mathrm{i}\kappa(t_0+\eta_s)\cos\beta},$$

$$f_w^s(\kappa,t_0)=4\kappa^{-1}\sin\beta\,\mathrm{e}^{-\mathrm{i}\kappa(t_0+\eta_s)\cos\beta};$$

– blade grating:

$$K_w^{js}(\kappa,t,t_0)=\begin{cases}0, & j=s,\\ \sigma_{sj}\dfrac{H_1^1(k\rho_{js}(t,t_0))}{\rho_{js}(t,t_0)}, & j\neq s,\end{cases}$$

$$K_v^{js}(\kappa,t,t_0)=\begin{cases}H_0^1(\kappa|t-t_0|), & j=s,\\ H_0^1(k\rho_{js}(t,t_0)), & j\neq s,\end{cases}$$

$$M_w^{js}(\kappa,t,t_0)=\begin{cases}\dfrac{H_1^{(1)}(\kappa|t-t_0|)}{\kappa|t-t_0|}, & j=s,\\ \sigma_{sj}^2\dfrac{H_0^{(1)}(k\rho_{js}(t,t_0))}{\rho_{js}(t,t_0)^2}+\dfrac{H_1^{(1)}(k\rho_{js}(t,t_0))}{k\rho_{js}(t,t_0)}\dfrac{(t-t_0)^2-\sigma_{sj}^2}{\rho_{js}(t,t_0)^2}, & j\neq s,\end{cases}$$

$$M_v^{js}(\kappa,t,t_0)=\begin{cases}0, & j=s,\\ \sigma_{sj}^2\dfrac{H_1^{(1)}(k\rho_{js}(t,t_0))}{\rho_{js}(t,t_0)^2}, & j\neq s,\end{cases}$$

$$f_v^s(\kappa,t_0)=\frac{4}{\kappa}\mathrm{i}e^{-\mathrm{i}\kappa(t_0+1)\sin\beta}e^{-2\mathrm{i}\kappa(s-1)\cos\beta/n_p},$$

$$f_w^s(\kappa,t_0)=\frac{4}{\kappa}\cos\beta e^{-\mathrm{i}\kappa(t_0+1)\sin\beta}e^{-2\mathrm{i}\kappa(s-1)\cos\beta/n_p},$$

where $\eta_s=(2s-1)+2(s-1)g/d$ and $n_p=d/p$.

Due to the asymptotic behavior of the Hankel functions the singular kernels of the obtained IE (10), (11) for the small values of the argument can be approximated as follows:

$$H_0^{(1)}(\kappa|t-t_0|)\sim(2\mathrm{i}/\pi)\ln|t-t_0|,\quad t\to t_0,$$

$$\frac{H_1^{(1)}(\kappa|t-t_0|)}{|t-t_0|}\sim\frac{\mathrm{i}\kappa}{\pi}\ln|t-t_0|-\frac{2i}{\pi\kappa|t-t_0|^2},\quad t\to t_0.$$

Hypersingular integrals are regarded in the sense of Hadamard finite part.

Note that the problem of wave scattering by strip grating in the case of E-polarization ($\vec{E}=(0,0,E_z)$, $\vec{H}=(H_x,H_y,0)$) is likewise reduced to the IE system, which is similar to (10), (11), with the difference consisting in the fact that the resistivities R and Q are interchanged.

4. DISCRETE MATHEMATICAL MODEL

Numerical solution of the IE (10), (11) we find in the form of interpolation polynomials with the further utilization of quadrature formulas of interpolation type with the highest algebraic accuracy. For the discretization of integrals with respect to the unknown functions $v_j(t)$, $j=1,\ldots,N$, one uses Gauss–Legendre quadrature formulas [11] of n_v order with nodes $\{\tau_k\}$ and corresponding collocation points $\{\tau_{0i}\}$ at the zeros of Legendre polynomials $\tau_k: P_{n_v}(\tau_k)=0, k=1,\ldots,n_v$, respectively.

In turn, for the discretization of integrals with hypersingular kernels with respect to the unknown functions $\widetilde{w}_j(t), j=1,\ldots,N$ one uses more efficient quadrature formulas (with weight function $\sqrt{1-t^2}$) of interpolation type with higher algebraic accuracy [10, 11] of n_w order with nodes $\{t_k\}$ and corresponding collocation points $\{t_{0i}\}$ at the zeros of Chebyshev polynomials of the second kind $t_k=\cos(\pi k/n_w)$: $T_{n_w}(t_j)=0,\ k=1,\ldots,n_w$. As the result of discretization of mentioned hereinabove IE, we obtain two independent systems of linear algebraic equations (SLAE) of order Nn_v and Nn_w with respect to for the unknown values $v_j(\tau_i),\ i=1,\ldots,n_v$ and $\widetilde{w}_j(t_k), k=1,\ldots,n_w$ (for all $j=1,\ldots,N$) for a planar grating and a coupled SLAE of the order $N(n_v+n_w)$ for a blade grating, respectively. It should be noted that in the case of the blade grating in order to solve the corresponding SLAE one must choose equal discretization orders $(n_v=n_w)$. Having solved the above-mentioned SLAE, we obtain an approximate solution of the initial IE (10), (11) in the form of interpolation polynomials.

Therefore, the developed mathematical model for the problem of light waves scattering by finite-sized gratings made of thin strips allows one to reduce the two-dimensional boundary problem to the systems of IE with singular or hypersingular kernels at the system of intervals. The developed numerical algorithm based on the Nystrom-type technique possesses guaranteed convergence (which is not worse than $1/n_v$ or $1/n_w$, respectively) [13]. Thus, the accuracy of the calculations is easily controlled by the interpolation order. In this case in order to provide computational error at the 10^{-4} level in the whole optical band it is enough to utilize $n_v=n_w=50$ [10, 11].

5. MAIN SCATTERING CHARACTERISTICS

Using the asymptotic representation of Hankel functions for large values of the argument, the scattered far field may be rewritten in the following form

$$U_{\text{sc}}(\varphi)\sim(2/\mathrm{i}\pi kr)^{1/2}\mathrm{e}^{\mathrm{i}kr}\Phi(\varphi),\quad r\to\infty,$$

where φ denotes the observation angle, $\Phi(\varphi)$ stands for the radiation pattern of the scattered far field, which for the planar grating equals

$$\Phi(\varphi)=\frac{\mathrm{i}k}{4}\sum_{j=1}^{N}\int_{S_j}[v_j(x)-\mathrm{i}\sin\varphi\, w_j(x)]\mathrm{e}^{-\mathrm{i}kx\cos\varphi}\mathrm{d}x,$$

and for the blade grating

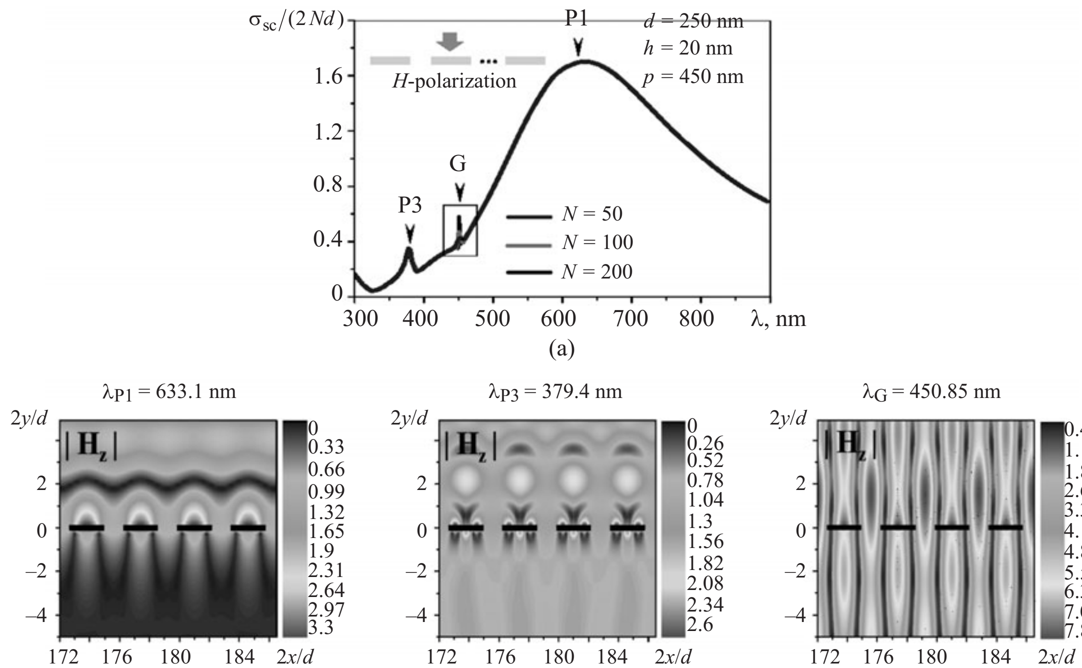
$$\Phi(\varphi)=\frac{\mathrm{i}k}{4}\sum_{j=1}^{N}\int_{S_j}v_j(y)\mathrm{e}^{-\mathrm{i}k(x_j\cos\varphi+y\sin\varphi)\cos\varphi}\mathrm{d}y-\mathrm{i}\cos\varphi\,\frac{\mathrm{i}k}{4}\sum_{j=1}^{N}\int_{S_j}w_j(y)\mathrm{e}^{-\mathrm{i}k(x_j\cos\varphi+y\sin\varphi)\cos\varphi}\mathrm{d}y.$$

Total scattering cross section is determined using the integration of normal component of the Poynting vector on a circle of large radius and it is represented in the form

$$\sigma_{\text{sc}}=\frac{2}{\pi k}\int_0^{2\pi}|\Phi(\varphi)|^2\,\mathrm{d}\varphi.$$

Absorption cross section is calculated as

$$\sigma_{\text{abs}}=\sum_{j=1}^{N}\int_{S_j}[\mathrm{Re}\,Q|v_j(x)|^2+\mathrm{Re}\,R|w_j(x)|^2]\mathrm{d}x.$$



(b)

Fig. 2.

6. NUMERICAL RESULTS

6.1. Planar grating

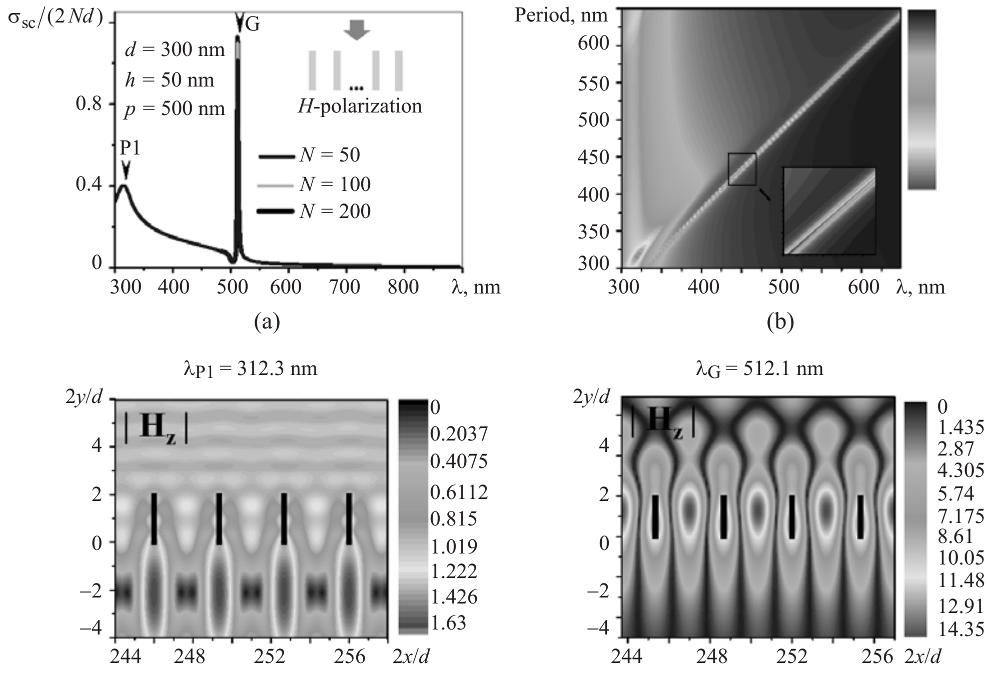
Strip gratings, which consist of a finite number of silver nanostrips, demonstrate characteristic resonances on the surface plasmons in the optical wavelength range in the case of scattering of *H*-polarized plane wave. Their intensity and wavelength depend mainly on the properties of material of the strips and of the surrounding medium, as well as on the width and the thickness of nanostrips. This allows one to tune the nanostrips for the effective interaction with the light.

In turn, the gratings, which consist of several tens or hundreds of nanostrips, in addition to the plasmon resonances also show novel effects associated with the periodicity of the scatterer. Fig. 2a presents a dimensionless (normalized to $2Nd$) cross section of total scattering, which has been calculated as a function of the wavelength for the gratings consisting of $N = 50$, 100, 200 strips with the parameters $d = 250$ nm, $h =$ 20 nm, $p = 450$ nm.

It is evident that in the entire visible range in the case of normal incidence of a plane wave ($\beta = \pi / 2$) two plasmon resonances are excited on the wavelengths: $\lambda_{P1} = 633.1$ nm, $\lambda_{P3} = 379.4$ nm, and an additional resonance on the wavelength $\lambda_G = 450.85$ nm. The latter one corresponds to the so-called grating mode (grating resonance), whose wavelength is located in the vicinity of the Rayleigh anomaly for an infinite grating $\lambda_{R.A.} = p(1+\cos\beta) / m$ for $m = 1$ [6]. In the general case the grating resonances have the form of asymmetric Fano-type resonances, whose wavelengths depend weakly on the shape and the size of grating's elements. In contrast to the plasmon resonances, which are explained by the collective oscillations of free electrons in the metal, the grating resonances are attributable to the collective oscillations of grating's elements (in this case of metal nanostrips).

Figure 2b presents the corresponding plots of $|H_z|$ function, i.e. of the absolute magnitude of the total magnetic near field for the grating made of $N = 100$ strips for two plasmon resonances λ_{P1}, λ_{P3}, as well as for the grating resonance λ_G (in the vicinity of four central strips Nos. 48–52). The plots, which correspond to the plasmons, demonstrate a high localization of the fields along each strip.

Note that these plasmon resonances correspond to Fabry–Perot modes, which are formed due to the reflection of its own surface plasmon waves of the corresponding metal layer from the edges of each strip of the grating. Therefore, at the resonances an integer number of half-wavelengths of the corresponding layer's eigenwave falls within each strip.



(c)
Fig. 3.

In contrast to the plasmons, in the case of grating resonance the magnetic field has the form of an intensive standing wave, that is formed by ±1-st Floquet harmonics, which propagate along the grating, i.e. by two quasi-plane waves. As one can see, this intensive field extends over several periods in the direction, which is normal relative to the grating.

6.2. Blade Grating

Similarly to the planar grating, Fig. 3a presents the plots of normalized to $2Nd$ scattering cross sections for the blade grating, which consists of $N = 50$, 100, 200 strips with the parameters $d = 300$ nm, $h = 50$ nm, $p = 500$ nm.

It should be noted that in the case of *H*-polarization the blade grating compared to a planar one has higher Q-factor grating resonances near the wavelengths, that are multiple of the period. This is caused by the fact that the geometry of a blade grating facilitates much stronger interaction between the adjacent strips, than it does in the case of the planar grating. It is apparent that the blade grating consisting of $N = 50$ strips demonstrates more narrow grating resonance than a similar planar grating consisting of $N = 200$ strips (Fig. 2a).

On the profile of the normalized cross section of total scattering (Fig. 3b) there is a sharp pronounced “ridge” along the line $\lambda = p$, which corresponds to the grating resonance, and an intense “hill” in the vicinity $\lambda = 330$ nm, that corresponds to the main plasmon resonance. In this case $d = 300$ nm and $h = 50$ nm are fixed ($\beta = \pi/2$).

Figure 3c shows the plots of the magnetic near-field for the plasmon resonance at $\lambda_{P1} = 312.3$ nm, as well as for the grating resonance at $\lambda_G = 512.1$ nm. Similarly to the planar grating, the location of the grating resonance for the blade grating depends on the grating’s period and on the angle of incidence, while its quality factor depends on the total dimensions of the grating, namely on the amount of strips, their width and thickness.

As is known, in the case of scattering of *E*-polarized plane wave (vector $\vec{E}$ is parallel to the plane of a strip) the excitation of surface plasmon waves and plasmon resonances is absent at the single thin strips made of precious metals, as well as at the finite gratings consisting of them (both planar and blade ones) [11, 14]. In this case the gratings made of silver strips do not demonstrate grating resonances generated by the presence of periodicity, which are clearly visible for *H*-polarization.

The explanation for this may be found from the analysis of the problem of diffraction of plane waves on an infinite grating [6]. In this problem one can successfully find the approximate complex eigenfrequencies for the grating modes and make sure that in the case of E-polarization their quality factor is $|\varepsilon_r(\lambda)|^2$ lower than for the H-polarization. Because of the absence of plasmons and resonances for the grating modes this paper does not present the results of calculations of the cross section of total scattering in the case of E-polarization.

A numerical experiment has been carried out. It consisted in the comparison of the spectra of cross sections of total scattering and of total absorption, as well as of far-field radiation patterns, which have been calculated using the presented hereinbefore model and the commercial simulation software FEM (Finite Elements Method) based on the finite elements method. The comparison results, which have been obatined by the two techniques, are practically the same over the whole visible frequency band except the narrow vicinities near the plasmon resonances, where the difference equals 1–7% depending on the strip thickness (the thinner the strip is, the less the differences are).

Note the significant advantage of the GBC technique, which consists in its fast performance and low insistence to the computer resources. Thus, to calculate the main characteristics of scattering and absorption for the H-polarized wave by a single silver strip with parameters d = 250 nm, h = 20 nm with the above-mentioned accuracy using GBC and further discretization of IE by Nystrom-type technique it took 8 seconds on a PC equipped with a processor Intel Centrino Duo 2.2 GHz and 1 GB of RAM. The calculation of the same quantities using the FEM software took approximately 4 hours, i.e. about 1800 times longer. The high efficiency of the suggested technique allows one to calculate quickly the scattering characteristics for gratings consisting of 200 and more such strips, i.e. for the composite object with the size of 200 and more wavelengths.

7. CONCLUSIONS

This paper suggests an efficient and rapidly convergent numerical algorithm for the investigation of scattering and absorption of light taking into account the resonance phenomena for the gratings consisting of a finite number of thin silver nanostrips (which are thinner than the wavelength in free space). The model, which is based on the approximate GBC, allows one to exclude from consideration the field within each strip. Because of this, it is possible to reduce the two-dimensional boundary problem to two independent or dependent IE systems (for a planar or a blade grating, respectively) with singular and hypersingular kernels.

The solution of IE is sought in the form of interpolation polynomials of some degree, whose coefficients satisfy the SLAE. The further utilization of quadrature formulas of interpolation type with the highest algebraic accuracy provides rapid convergence of approximate solutions to the exact ones.

With the aid of the developed numerical algorithm it is possible to predict the performance of optical nanoantennas, which consist of a finite number of thin nanostrips made of precious metals, with the accuracy sufficient for practical applications. The investigation of properties of the surface plasmon resonances, as well as of the grating resonances, which are generated by the periodicity, near the Rayleigh anomalies, allows one to design the grating scatterers and absorbers, that can more efficiently interact with the light.

REFERENCES

1. T. Søndergaard, S. J. Bozhevolnyi, "Strip and gap plasmon polariton optical resonators," Phys. Stat. Sol. (B) **245**, No. 1, 9 (2008), DOI: 10.1002/pssb.200743225.
2. D. M. Natarov, V. O. Byelobrov, R. Sauleau, T. M. Benson, A. I. Nosich, "Periodicity-induced effects in the scattering and absorption of light by infinite and finite gratings of circular silver nanowires," Optics Express **19**, No. 22, 22176 (2011), DOI: 10.1364/OE.19.022176.
3. D. M. Natarov, R. Sauleau, A. I. Nosich, "Periodicity-enhanced plasmon resonances in the scattering of light by sparse finite gratings of circular silver nanowires," IEEE Photonics Technol. Lett. **24**, No. 1, 43 (2012), DOI: 10.1109/ LPT.2011.2172203.
4. P. Ghenuche, G. Vincent, M. Laroche, N. Bardou, R. Haïdar, J.-L. Pelouard, S. Collin, "Optical extinction in a single layer of nanorods," Phys. Rev. Lett. **109**, 143903 (2012), DOI: 10.1103/ PhysRevLett.109.143903.
5. V. O. Byelobrov, T. M. Benson, A. I. Nosich, "Binary grating of subwavelength silver and quantum wires as a photonic-plasmonic lasing platform with nanoscale elements," IEEE J. Selected Topics Quantum Electron. **18**, No. 6, 1839 (2012), DOI: 10.1109/JSTQE.2012.2213586.
6. T. L. Zinenko, M. Marciniak, A. I. Nosich, "Accurate analysis of light scattering and absorption by an infinite flat grating of thin silver nanostrips in free space using the method of analytical regularization," IEEE J. Selected Topics Quantum Electron. **19**, No. 3 (2013), DOI: 10.1109/JSTQE.2012.2227685.

7. J. P. Kottmann, O. J. F. Martin, "Accurate solution of the volume integral equation for high-permittivity scatterers," IEEE Trans. Antennas Propag. **48**, No. 11, 1719 (Nov. 2000), DOI: 10.1109/8.900229.
8. V. Giannini, J. A. Sánchez-Gil, "Calculations of light scattering from isolated and interacting metallic nanowires of arbitrary cross section by means of Green's theorem surface integral equations in parametric form," JOSA A **24**, No. 9, 2822 (2007), DOI: 10.1364/JOSAA.24.002822.
9. E. Bleszynski, M. Bleszynski, T. Jaroszewicz, "Surface-integral equations for electromagnetic scattering from impenetrable and penetrable sheets," IEEE Antennas Propag. Magazine **35**, No. 6, 14 (Dec. 1993), DOI: 10.1109/74.248480.
10. O. V. Shapoval, R. Sauleau, A. I. Nosich, "Scattering and absorption of waves by flat material strips analyzed using generalized boundary conditions and Nystrom-type algorithm," IEEE Trans. Antennas Propag. **59**, No. 9, 3339 (Sept. 2011), DOI: 10.1109/TAP.2011.2161547.
11. M. V. Balaban, E. I. Smotrova, O. V. Shapoval, V. S. Bulygin, A. I. Nosich, "Nystrom-type techniques for solving electromagnetics integral equations with smooth and singular kernels," Int. J. Numer. Model.: Electronic Networks, Devices and Fields **25**, Nos. 5-6, 490 (2012), DOI: 10.1002/jnm.1827.
12. P. B. Johnson, R. W. Christy, "Optical constants of the noble metals," Phys. Rev. B **6**, No. 12, 4370 (1972), DOI: 10.1103/PhysRevB.6.4370.
13. Yu. V. Gandel', A. S. Kononenko, "Justification of the numerical solution of a hypersingular integral equation," Differential Equations **42**, No. 9, 1326 (2006), DOI: 10.1134/S0012266106090114.
14. I. O. Sukharevsky, O. V. Shapoval, A. I. Nosich, A. Altintas, "Validity and limitations of the median-line integral equation technique in the scattering by material strips of sub-wavelength thickness," IEEE Trans. Antennas and Propagation **62**, No. 7, 3623 (July 2014), DOI: 10.1109/TAP. 2014.2316295.