Design of Complex Metal-dielectric Diffraction Gratings

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Abstract— A Volume Integral Equation (VIE) Method was developed to simulate optical wave diffraction on metal-dielectric one and two dimensional diffraction gratings based on flat multilayered structures with regular inhomogeneity in each layer. Exact solution of the equation is obtained with the Galerkin method, taking into account complex dielectric permittivity of metals and semiconductors in optical range. The Method is applicable for s and p polarized waves. As objects to investigate we chose metal-dielectric photonic crystals and multilayer reflective dielectric-semiconductor diffraction gratings. Dispersion characteristics with windows of opacity are found out. The results are compared to the simulations done by commercial numerical software.

1. INTRODUCTION

Mathematical and computational methods in electromagnetic theory have been attracting an increasing attention of scientific community because of recent hi-tech progress. Implementation of photonic and plasmonic nanostructures significantly expends horizons of signal processing. The unique capabilities of plasmonic waveguides to manipulate light signals in volumes less than diffraction limit will allow us to increase device densities in integrated photonic circuits. Plasmonic based sensors and detectors have already been used in biomedicine and optical communications [1]. High power laser systems recently reached PetaWatt power [2], and their progress led to the development of multilayer dielectric (MLD) diffraction gratings. Nowadays MLD gratings with impressive performances and size have been designed and manufactured by several companies [3, 4]. Better understanding of light diffraction and propagation ensures effective design of nanolayered diffraction gratings and photonic crystals. To proof a design accuracy, the same object needs to be simulated by different methods.

The majority of mathematical methods for calculation of electromagnetic fields can be split in two groups. The first group, the methods based on direct solution of wave equations with defined boundary conditions, includes finite-difference time-domain, the finite element method, and the finite integration technique. In the second group of methods the boundary problem is reduced to the solution of integrals, the integra-differential, pairs of integrals, and pairs of sum equations. The advantage of the first group of methods is their versatility. Their disadvantages are high requirements for a computer processing power, long calculation time, the need to digitize not only the scattering object, but also the space around the scatterer, and difficulties with simulations of small-scale elements. In addition, there is a problem with satisfaction of boundary conditions for radiation to open space. For the second group of methods these problems do not exist. The choice of the integral equation (IE) type is defined by the structure of the object under investigation. Therefore, the methods based on the IE solution are not as universal as the methods in the first group, but computer programs based on them work several orders of magnitude faster.

The main goal of this paper is a development of new semi-analytical method to solve vector integral-differential equation, describing electromagnetic wave diffraction and propagation in twodimensional periodic all-dielectric and metal-dielectric structures. As the subjects of investigation we chose plane wave propagation in photonics crystals and laser pulse diffraction on multilayer dielectric diffraction gratings. Both objects are planar multilayer structures formatted of dielectric or metallic layers (number of layers is N_l) in N_s layers there are insertions. The insertions are periodical with period — d. Dielectric layers are parallel to the plane $z = 0$. The number of layers in a structure is arbitrary, top and bottom layers are half infinite and the layer numeration is from top to bottom. Plane electromagnetic wave of arbitrary polarization $\vec{E}^e(x, y, z)$ is incident on the first layer. Horizontal cross-section of the insertion has an elliptical shape, and the size of

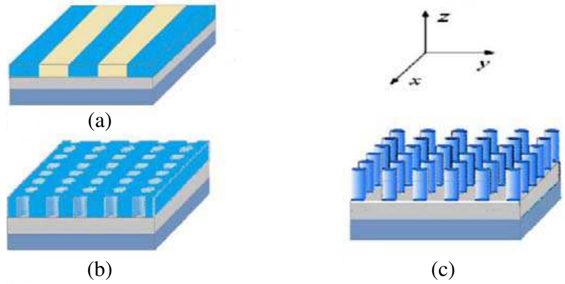

Figure 1: Structures under consideration.

the ellipse depends on the vertical coordinate z. The vertical cross-section is a trapezium. Because the number of insertions and their locations are arbitrary, we can simulate structures of absolutely arbitrary cross-section. Dielectric constants of the layers are complex, which gives us a possibility to simulate metal layers in optical wavelength range. The grating is periodical in x direction, and fields can be described by function $\exp(-ik_x x)$ where $(k_{1,x}, k_{1,y}, k_{1,z})$ are wave vector components of incident wave.

2. VOLUME INTEGRAL METHOD

In Lerer's paper [5] the problem of diffraction on a multilayer two-dimensional dielectric diffraction grating was reduced to the solution of a volume integral-differential equation (VIDE). VIDEs have several advantages: they are simpler than surface ones [6]; inhomogeneity and nonlinearity do not make simulations more complicated as it happens in the case of surface equations and also the method gives an electrical field inside of insertions as the equation solution.

One embodiment of this method was implemented in paper [7]. In this paper we propose another implementation of the method for more complex DR and an arbitrary direction of external electromagnetic wave propagation. Since the structure is periodic, the equation is solved only inside of the volume of one insertion with cross section S:

$$\frac{D_r(y,z)}{\tau} = E_r^e(y,z) + \frac{1}{d}\sum_{q=-\infty}^{\infty}\sum_{s=1}^{3}\int_S \exp[i\beta_q\bar{y}]\,\tilde{g}_{rs}(z,z')\,D_s(z')\,dy'dz', \quad r=1,2,3, \quad yz \in S \quad (1)$$

where $\bar{y} = y - y'$, $D_r(y,z) = E_r(y,z)\,\tau(yz)$, $\tau(y,z) = \varepsilon_b(yz)/\varepsilon_2 - \varepsilon_n(z)$, $\beta_q = \frac{2q\pi}{d} + k_{1,x}k_{1,y}k_{1,z}$, are projections of incident wave vector, $\varepsilon_n(z), \varepsilon_b(xyz)$ is dieletric permitivity of ambient layer at the point of observation and of insertion. The expressions for the elements of tensor Green function $\tilde{g}_{rs}$ for external field $\vec{E}^e(yz)$ were developed in [8]. $\vec{E}^e(yz)$ is the incident field plus the field scattered by the multilayer structure without inhomogeneity. If the plane of incidence is $y = 0$ the Equation (1) splits into two equations which describe either TE or TM waves.

The Equation (1) is bi-singular [5] and effective numerical simulation methods supposed to take this fact into account. A method to simulate optical metallic nano-vibrators based on semi-analytical IE solution was presented in papers [5] and [8]. The method is based on integral representation of Green Function. The VIDE kernel singularity shows itself in slow convergence in matrix elements of the set of linear algebraic equations obtained by the Galerkin Method. It is simpler to improve the convergence than to make integral kernel singularity regularization. This approach was used in this work. We seek a solution in the form

$$D_r(y',z') = \sum_{\mu=0}^{N_y-1}\sum_{v=1}^{N_z} X_{\mu\nu}^r V_{\mu\nu}(y',z')$$

where $X_{\mu\nu}^r$ are unknown coefficients, $V_{\mu\nu}(y'z')$ are basis functions, where $V_{\mu\nu}(y,z) = Y_{\mu\nu}(y)\,\sigma_\nu^{(1)}(z)$, $Y_{\mu\nu}(y) = C_{\mu\nu}P_\mu(\frac{y-\bar{y}_v}{l_v})$, where P_μ are Legendre polynomials, $\bar{y}_v$ are coordinates of inhomogeneity center, l_v is the inhomogeneity half-width at $z = z_v$, z_v is a knot of spline function $\sigma_\nu^{(1)}(z)$ and the constant $C_{\mu\nu}$ is chosen so that the Fourier transformation of $Y_{\mu\nu}(y)$ can be represented as $\tilde{Y}_{\mu\nu}(\beta_q) = (-i)^\mu \frac{J_{\mu+1/2}(\beta_q l_v)}{(\beta_q l_v)^{1/2}} \exp(-i\beta_q\bar{y}_v)$. For one dimensional grating the asymptotic series is summed analytically.

3. SIMULATION RESULTS

In this work we investigated two types of photonic crystals (PC). The first one is sieve-looking, made of several dielectric layers with round periodical halls in them. In particular, the structure consists of three layers of dielectric, placed on a dielectric substrate, as shown in the Fig. 2.

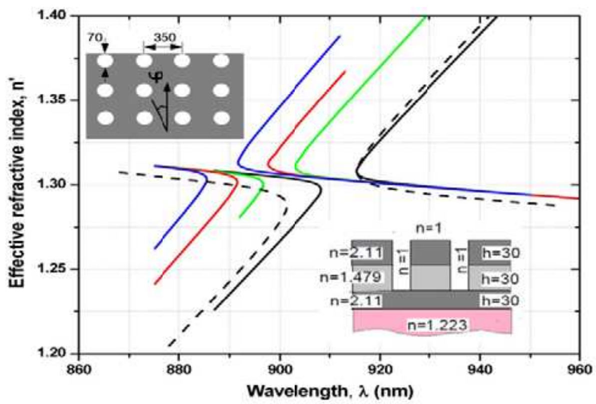

Figure 2: Dispersion characteristics of waves propagating at different angles to the axis x in all-dielectric PC [Fig. 1(b)]. Black solid curves correspond to $\varphi = 0°$, green to $\varphi = 10°$, red to $\varphi = 12°$, and blue to $\varphi = 14°$. The dashed curves depict the result for $\varphi = 0°$ obtained by Ansoft HFSS commercials oftware. All dimensions are in nanometers.

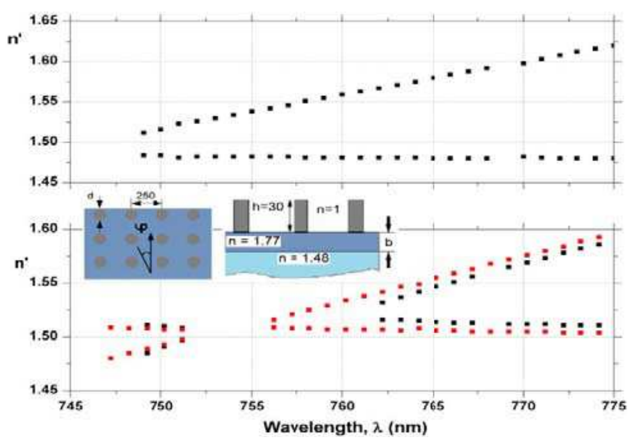

Figure 3: Dispersion characteristics for PC made of silver cylinders placed on a two-layer dielectric structure [Fig. 1(c)]. The dielectric layer thickness is $b = 100$ nm on the upper graph and $b = 150$ nm on the lower graph. The red symbols refer to cylinders of 70 nm diameter, black to 90 nm. A wave propagates at the angle $\varphi = 0°$.

Two-dimensional grating is perforated in two upper layers. As can be seen from the Fig. 2, the PC has a window of opacity. In the opacity window area the phase velocity of zero harmonic with a normal dispersion ($p = q = 0$, p, q are the numbers of spatial harmonics on x and y axes, respectively) and minus first harmonic with anomalous dispersion ($p = -1$, $q = 0$) become equal, and dispersion curves for both harmonics merge and make one wedge-looking curve. From the equality of phase speeds for these spatial harmonics it follows that wavelength in the middle of opacity window satisfies the condition

$$\frac{dn}{\lambda}\cos\varphi = 0.5, \tag{2}$$

where d is PC period. At this wavelength, waves reflected from neighboring insertions interfere in phase, and wave propagation in the PC becomes impossible. In the Fig. 2 we can see that opacity window moves toward shorter wavelength when the angle of propagation changes from 0° to 14°, what is consistent with the Equation (2). Also, from our calculations, we found that waves with wavelength longer than 665 nm cannot propagate in the structure on Fig. 2, if we remove reflecting heterogeneities in the form of air holes. This happens because the effective refractive index of such layered structure without holes becomes smaller than refractive index of the substrate and so the waves leak into the substrate. For comparison of VIE method with modern numerical methods, we simulated this structure by HFSS code, and placed the result in the Fig. 2 as a dashed curve.

In the Fig. 3, a plasmon wave propagates on the boundary of perforated silver layer and dielectric substrate. Losses at the edges of opacity window drastically increase, and in the framework of low-loss model we cannot close curves. For $\lambda \leq 776$ nm ERI is less than substrate refractive index, wave leaks into the substrate.

Following the needs of chirped pulse amplification lasers we designed a multilayer diffraction grating for pulse compression. The grating design is shown in the Fig. 4; a central wavelength 1053 nm, grating period of 1740 l/mm and the angle of incidence 72°. The grating reflective mirror consists of chirped stock of thirteen HfO2/SiO2 layers with all the structure planted on fused silica substrate. The thickness of the bi-layers is linearly increasing from corrugated layer to substrate. The grating has a wide reflective bandwidth: 98% of reflective efficiency into the −1st diffraction order for bandwidth 1030–1070 nm, and can be used in ultrafast lasers based on neodymium glass.

For the lasers with central wavelength 910 nm we used more sophisticated design of diffraction

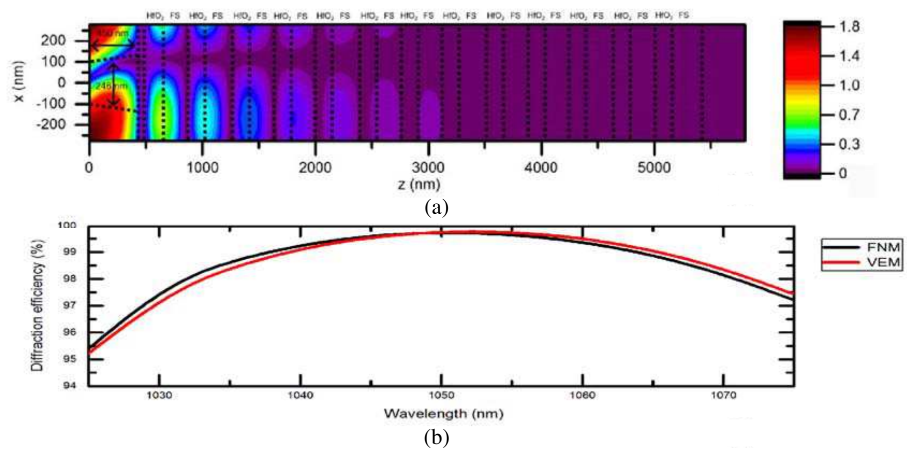

Figure 4: (a) MLD grating structure and the field reinforcement $|E/E_0|$ inside of the MLD structure, duty cycle 43 (100*the distance between grooves at half depth/grating constant) and trapezoidal angle 5.7°. All distances are in nm. (b) Diffraction efficiency vs wavelength simulated with commercial package LightTrans Virtual Lab by Fourier Modal Method and semi-analytical Volume Integral Method.

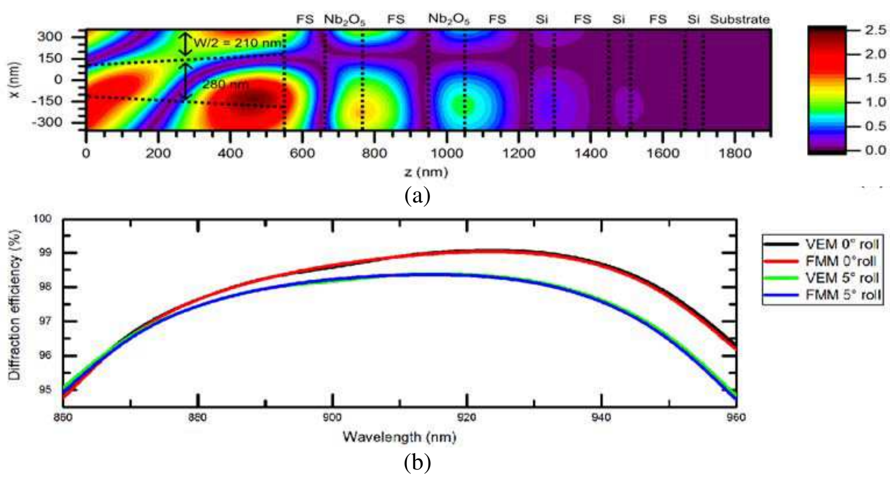

Figure 5: (a) MLD+semiconductor grating structure and the field reinforcement $|E/E_0|$ inside of the MLD structure. The presented MLD grating has a period 700 nm, groove depth 550 nm, duty cycle 0.4 and trapezoidal angle 7°, which is the angle between the side of trapezoidal groove and z-axis. (b) Comparison between semi-analytical Volume integral equation method (VEM) and Fourier Modal Method (FMM) in LightTrans Virtual Lab.

grating than for lasers with central length 1053 nm. Here we present Littrow-mounted semiconductor-dielectric reflective diffraction grating with efficiency higher than 96% over 100 nm. The corrugated layer is made of fused silica and two top bi-layers are made of hafnia/silica. At the bottom of the multilayer stack we incorporate three silicon/fused silica bi-layers. The idea to use silicon/silica bi-layers is based on low light absorption by silicon for wavelengths longer than 900 nm and on relatively big difference in refraction coefficients of silicon and silica [11]. The grating design, electric field distribution and diffraction efficiency are presented on Fig. 5.

4. CONCLUSION

A Volume Integral Equation (VIE) Method was developed to simulate optical wave diffraction on metal-dielectric one and two dimensional diffraction gratings based on flat multilayered structures with regular inhomogeneity in each layer. Exact solution of the equation is obtained with the Galerkin method, taking into account the complex dielectric permittivity of metals and semiconductors in optical range. As examples of photonic crystals we simulated sieve-looking diffraction grating placed on multilayer dielectric substrate and metal forest-looking grating placed on multilayer dielectric substrate. The results are compared to the simulations done by commercial numerical software Ansoft HFSS. Also, VIE Method was applied for a design of broad-band multilayer reflective diffraction gratings for compression of high-energy ultra-short laser pulses. Electric field distribution inside of the gratings is also numerically studied. The results were compared to the simulations by numerical Fourier Modal Method in LightTrans Virtual Lab. The methods show excellent agreement.

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