#### Volodymyr O. Byelobrov

## REPORT OF PROJECT WORK during the stay at the George Green Institute for Electromagnetics Research University of Nottingham, UK in February 2014– May 2014, the framework of the ESF Network "Plasmon-Bionanosence"

# Topic: Modeling of biosensors based on the periodic grating of silver nanoscale cylinders embedded in a dielectric slab from active medium.

During my stay at the University of Nottingham, I continued my Ph.D.-thesis study into the modeling of electromagnetic wave scattering by periodic reflectors in this particular project I investigated the model of an active dielectric slab with embedded silver slab Fig. 1. That model may be very beneficial for producing biosensors as this model offers the structure where the plasmon resonance may be influenced by surrounding area. The value of lasing threshold shows efficiency of such resonator.

According to the project plan, I investigated dielectric slab with periodic inclusions of silver



Fig.1 The cross-sectional geometry of a periodically structured dielectric slab

cylinders (wires). The inclusion period is p, the wire radius as a, and the slab refractive index is  $\alpha$ . We suppose that the field is time-harmonic with the wavelength  $\lambda$ . Although two alternative polarisations can be considered, based on my previous results the H-polarization is more efficient for 2-D periodic structures. Thus I concentrated on studying it and however I also made comparisons with the E-polarization. The function that represents the field z-component must satisfy the Helmholtz equation with appropriate wavenumber inside and outside of cylinders, the Sveshnikov radiation condition at infinity, the condition of local integrability of power, and the boundary conditions demanding continuity of the tangential field components at the slab and inclusions boundary. These conditions guarantee solution's uniqueness. Mathematical approach consists of derivation of infinite matrix equation for the field expansion coefficients by the method of variable separation similar to [1-3] with involvement of the specific lattice sums [4] the planar boundaries are considered using the T-matrix approach detailed in [3]. However, unlike [2,3] we emphasize that, to ensure convergence, this equation must be cast to the so-called Fredholm second kind form. Further, although certain basic features of the scattering, such as periodicity-caused resonances, are present irrespectively of the wavelength range, the visible range offers additional phenomena such as plasmon resonances if the wire material is a noble metal such as silver. Therefore I made computations for the visiblelight scattering by gratings containing silver wires. In [5] the interesting features of a active dielectric grating described using the approach of the active media [6]. Unlike active model of dielectric or silver grating surrounded by a lossless media, a grating in an active media demands investigation of the lattice sums of a complex argument. The approach of lattice sums was profoundly studied in [1] for a real argument. Further are given the necessary function for determination of the scattering angle (3), for it in [4] the following function was defined  $\tau(z) = \sqrt{1-z^2}$  which has two branch cuts in the complex domain (similar to cut branches of the scattering angle):  $(1,iy), y \ge 0$  and  $(-1,-iy), y \ge 0$ . Then introducing two auxiliary functions  $z-1 = r_{+}e^{i\theta_{+}} (-3\pi/2 < \theta_{+} < \pi/2)$  and  $z+1 = r_{-}e^{i\theta_{-}} (-\pi/2 < \theta_{-} < 3\pi/2)$  yields

$$\tau(z) = r_{+}r_{-}e^{i(\theta_{+}+\theta_{-})/2}.$$
(1)

Furthermore the Floquet coefficients are used:

$$\pi_l = l/\sigma, \quad \tau_l = \tau(\pi_l) \tag{2}$$

and the scattering angle valid for all complex values out of the cut brunches:

$$\phi_s = -i\ln(\pi_s - \tau_s) \tag{3}$$



Fig.2 Reliefs of absolute (a) and argument (b) value of the scattering angle (3).

The scattering angle is a key function in my study and its behaviour in the vicinity of the point z=1 satisfies correctness of calculating the lattice sums for values near the brunch point with strictly negative imaginary part.

Before investigating the modes of dielectric slab with silver periodic grating within, I studied the similar structure with inclusions filled with air on the silver grating places.

Firstly I investigate the scattering problem for the geometry proposed in Fig. 1. I consider a slab where the chain of inclusions placed in the slab centre, i.e.  $d_1 = d_2$ . The refractive index is  $\alpha = 1.4$ . The width of the slab is varied. On the reliefs shown in Fig.3 the series of wide flat ridges correspond to slab modes and Fig.3 (a) and (c) show they are similar for both polarizations. The other kind of resonances is aligned to the branch points  $\sigma = 1$  and  $\sigma = 2$ . The Hpolarization has higher Q-factor and so the periodic resonances are sharper in Fig.3 (a) comparing to in Fig. 3 (c). The ridge resonance frequencies investigated using the LEP are marked with black lines. The eigenvalues are calculated for the associated geometrical parameters, while the resonance frequency is taken as the initial value. On the upper plots of Fig.3 (b, c) one may see that the solutions for scattering and eigenvalue frequencies almost completely coincide.



Fig.3 Reliefs of reflectivity (a), (c) of a plane wave from a dielectric slab with  $\alpha = 1.4$ , p = 3.3333a and  $d_1 = d_2$  as a function of normalized frequency  $\sigma$  and the slab width *d*. Corresponding lasing threshold (lower plot) and lasing frequency (upper plot) compared to the resonance frequency for H-polarization (a), (b) and E-polarization (c),(d). The corresponding modes are indicated by the black lines.

At the same time the lasing threshold decays when the width of the slab becomes larger, dropping to around  $10^{-3}$ .

The influence of the slab period on the scattering properties and eigenvalues is also of interest.

In Fig.4 we investigate this for a structure consisting of a periodic grating with  $\alpha = 1.4 \text{ and } d_1 = d_2 = 2a$  i.e. width d = 6a. Reliefs of the reflectivity (scattering) shown in Fig. 4 (a) again show a background of slab modes that doesn't vary significantly with polarization. Fig. 3 (b) shows that the lasing threshold stays roughly the same. This is unlike the grating in free space where lasing thresholds decay as the period decreases [6]. However the lasing frequency slightly shifts from the scattering resonance frequency when the two (slab and periodical) modes interact.



Fig.4 Reliefs of reflectance (a) of a planar wave from a dielectric slab in the H-polarization with  $\alpha = 1.4$ ,  $d_1 = d_2 = 2$  depending on normalized frequency  $\sigma$  and the slab period *p*. Eigenvalues (b) on the upper plot there is comparison of the lasing frequency with resonance frequency from the scattering problem.

Further I investigated a dielectric slab with a silver grating with silver grating inside it. The reliefs of scattering from a dielectric grating with the refractive index  $\alpha = 1.2$ , of width d = 160nm with silver grating of radius a = 40nm that is placed from the upper and lower boundaries on distances  $d_1 = 20nm$  and  $d_2 = 60nm$ . Fig.5 shows presence of the plasmon resonance that stays roughly on the frequency  $\lambda \approx 348nm$ . Few grating resonance cross the plasmon one by periodical periodicity. The same structure investigated in the E-polarization shows similar periodic resonances but absence of the plasmon one.



Fig.5 Reliefs of reflectance (a) and absorbance (b) depending on the frequency(horizontal axis) and period (vertical axis) of a planar wave from a dielectric slab ( $\alpha = 1.2$ ) with an embedded silver grating (radius a = 40nm,  $d_1 = 20nm$ ,  $d_2 = 60nm$ ) the E-polarization depending on normalized frequency  $\sigma$  and the slab period *p*. Eigenvalues (b) on the upper plot there is comparison of the lasing frequency with resonance frequency from the scattering problem.



Fig.6 Reliefs of reflectance (a) and absorbance (b) of a planar wave from a dielectric slab of similar geometry as on Fig. 5 the Epolarization depending on normalized frequency  $\sigma$  and the slab period *p*. Eigenvalues (b) on the upper plot there is comparison of the lasing frequency with resonance frequency from the scattering problem.

Thanks to the ESF Exchange Travel Grant, I had a brilliant opportunity to have scientific meetings and discussions with Prof. Trevor Benson, Dr. Ana Vukovic and other academics and students of the George Green Institute for Electromagnetics Research, and had access to the library of the University of Nottingham.

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### Journal and conference papers related to the project and crediting ESF-Newfocus:

- 1. V.O. Byelobrov, T.M. Benson, A.I. Nosich, "*Natural modes of an active slab microcavity with air-filled periodic inclusions*" accepted by the international conference MIKON 2014, Gdansk, 2014.
- 2. V.O. Byelobrov, T.M. Benson, A.I. Nosich, "*Natural modes* of *periodic grating of silver nanoscale cylinders embedded in a dielectric slab from active medium*," submitted to the international conference MMET2014, Dnipropetrovsk, 2014.

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