

# Reflection Properties and Lasing Modes in the H-Polarization Case for an Infinite Chain of Dielectric and Silver Nanowires

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## ABSTRACT

We study the scattering of the H-polarized plane wave by a freestanding periodic grating that contains two circular cylinders on a single period, one made of silver and another dielectric. The reflection and transmission coefficients for such a grating demonstrate several types of resonances including plasmons and grating resonances. Besides, we analyze the associated eigenvalue problem where the dielectric cylinders are so-called quantum wires, i.e. have “negative-absorption” or “active” refractive index. The comparison of eigensolutions for the grating modes of two active chains, one with and another without silver elements shows that the thresholds of lasing are higher in the former case, apparently because of the losses in silver.

**Keywords:** gratings, scattering, plasmon, nanowires, lasing, threshold.

## 1. INTRODUCTION

Epitaxially grown layered semiconductor microcavities are ubiquitous elements of today’s advanced light-emitting devices. The existing technologies enable manufacturing the active regions in such cavities. These regions are shaped as cascaded quantum wells and, since recently, periodic arrays of quantum wires and can display, under the pumping, an inversed population of carriers. Therefore, it is interesting to investigate the possibility of non-attenuating in time emission of light from such laterally structured active cavities, i.e. the lasing. It is known that the lasing occurs on discrete frequencies associated with natural modes (a.k.a. eigenmodes) of the cavity if the pump power is above the threshold for the given modes. Therefore the lasing can be studied as an eigenvalue problem, modified for the presence of the active region [1,2] whose material is characterized using the concept of negative absorption (hence the term Lasing Eigenvalue Problem, LEP). Our goal is the accurate quantification of the lasing frequencies and thresholds of the natural modes of a periodic chain of circular wires made of various materials including active ones.

Here, the analysis of auxiliary problem of the light transmission and reflection by the infinite chain (or grating) of passive dielectric wires is important. This is because it reveals the resonances in the scattering characteristics and provides the initial-guess approximations for the numerical search of eigenvalues. Besides of the resonances associated with the wire shape (a.k.a. morphology resonances or internal ones) and with the grating periodicity (a.k.a. grating or external ones), there exist the so-called plasmon or material resonances, which are observed if the dielectric permittivity of the wires takes negative values. This is the case of the grating containing the noble-metal elements and the wavelength corresponding to the visible or infrared ranges.

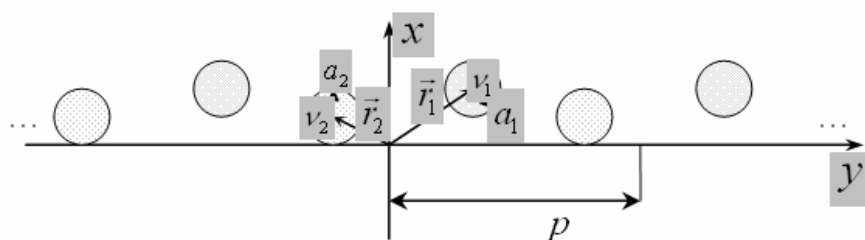


Figure 1. The sketch of infinite periodic chain containing silver and dielectric circular cylinders.

Although the publications studying classical transmission and reflection of plane waves by the gratings of passive dielectric and metallic wires of the circular cross-section are numerous (for instance, see [3-5]), the first direct mention of the so-called grating resonances close to the Rayleigh anomalies occurred in [4]. More recently, we have studied the associated problem of the lasing modes of the grating made of quantum wires [6]. It has revealed non-obvious effect the lowering of the lasing thresholds of the grating modes in the periodic structure if the wire radius decreases or, equivalently, the relative volume of the active media gets smaller. Additionally, the grating of quantum wires has lower thresholds of lasing of the grating modes in the H-polarization case that is explained by the non-magnetic nature of quantum wires.

For a grating of silver wires, the scattering problem analysis shows the interaction of the material caused plasmon resonances with the structure ones [7]. In particular, by tuning two resonances together one can significantly broaden the band of the intensive reflection from the grating.

Here we investigate new type of periodic resonator by putting silver and dielectric cylinders of nanoscale diameter in one period. For the silver nanowires, the values for refractive index of their material in the visible band are taken from [8] and interpolated using cubic splines. The eigenproblem is approached by adding a negative imaginary part (lasing threshold  $\gamma$ ) to the refractive index of the dielectric quantum wires and seeking it jointly with the lasing frequency  $\sigma$ . These values we call the LEP eigenpairs; they are discrete and each of them corresponds to specific mode. The modes can be classified by their nature such as those connected with electromagnetic field locked inside one cylinder in free space, interaction of two wires on the period, periodicity of the grating, and plasmonic nature of silver. To find the initial-guess values for LEP eigenpairs, we use the frequencies of almost total reflection in the auxiliary scattering problem where the refractive index of the dielectric cylinders remains a real value.

## 2. PROBLEM FORMULATION

Consider a grating made of the parallel to the  $z$ -axis and periodic along the  $x$ -axis circular cylinders (wires) in free space – see Fig. 1. The period is  $p$ , and two cylinders on the elementary period have the radii  $a_1$  and  $a_2$ , their centre locations, regarding to the local origin, have coordinates  $\vec{r}_1$  and  $\vec{r}_2$ , and their refractive indices are  $\nu_1$  and  $\nu_2$ , respectively. We suppose that the electromagnetic field is time-harmonic  $\sim \exp(-i\omega t)$  and does not vary along the  $z$ -axis, so the field analysis problem is two-dimensional. Aiming at the study of plasmon impact on the considered grating, we investigate the scattering of the H-polarized plane wave incident from the upper half-space (along the negative direction of the  $y$ -axis). The function  $U$ , denoting the  $Z_0 H_z$  component of the electromagnetic field, 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 cylinders' boundaries. The free space wavenumber is  $k = \omega / c = 2\pi / \lambda$ , where  $c$  is the free-space light velocity and  $\lambda$  is the wavelength, while inside the cylinders it is  $k\nu_i$ ; besides, in this paper we will also use the normalized by period frequency,  $\sigma = p / \lambda = kp / 2\pi$ .

As we consider the normal incidence, then according to the Floquet theorem the scattered field is a periodic function of  $x$  with period  $p$ :  $U(x, y) = U(x + p, y)$ . Thus, the same conditions are required on each pair of cylinders. In this case, we can investigate the field just within one cell of the grating and use the boundary conditions on each cylinder. The operator technique is applied, where construction of the composite T-matrix of two cylinders is performed similarly to [3]. Although the field in the cylinders' vicinity has the form of angular-exponent series with the cylindrical functions in coefficients (inside the cylinders the Bessel functions and outside the Hankel functions of the first kind), such series are not a convenient tool for large values of the space variable  $|y|$ . Therefore, the Poisson summation formula is applied to cast the series into the exponentially convergent series in terms of the Floquet harmonics. Then the field function in the upper and lower half-spaces  $|y| > d$ , where the lines  $|y| = d$  do not cross any of two cylinders, can be presented in the following way

$$\begin{aligned} U^+(x, y) &= \sum_{s=-\infty}^{+\infty} f_s^+ e^{ik(\pi_s x + \tau_s y)}, \quad y > d \\ U^-(x, y) &= \sum_{s=-\infty}^{+\infty} (\delta_0^s + f_s^-) e^{ik(\pi_s x - \tau_s y)}, \quad y < -d \end{aligned} \quad (1)$$

where

$$\begin{aligned} \pi_s &= s / \sigma \\ \tau_s &= \sqrt{1 - \pi_s^2} \end{aligned} \quad (2)$$

The matrix equation for determining the scattered-field coefficients can be cast to the following form:

$$(I - J^{-1} \cdot T \cdot L \cdot J) \cdot P = T \cdot J^{-1} \cdot p^{inc} \quad (3)$$

with

$$\begin{aligned} L &= [S_{m-n}(2\pi\sigma)] \\ p^{inc} &= [(-1)^m] \\ J &= [J_m(2\pi\sigma)\delta_n^m] \\ F^\pm &= [(-i\pi_n \pm \tau_n)^m] / (\pi\sigma) \\ f^\pm &= F^\pm \cdot J \cdot P \end{aligned} \quad (4)$$

Here the matrix  $L$  consists of the lattice sums, which provide rapid way of the summation of the slowly converging Hankel function series, for details look in [5]. This matrix reflects the periodic nature of the grating as it depends only on the value  $p/\lambda$ . The vector  $p^{inc}$  represents the incident field. The matrices  $F^\pm$  transform the expansions in terms of the Hankel functions to the ones in terms of the Floquet series. The matrix  $T$  defines the aggregate  $T$ -matrix of two cylinders in free space. The algorithm of its construction is similar to [9].

$$T = \beta_{0,1}\tilde{T}^1 + \beta_{0,2}\tilde{T}^2 \quad (5)$$

$$\tilde{T}^1 = (I - T^1\alpha_{1,2}T^2\alpha_{2,1})^{-1}T^1(\beta_{1,0} + \alpha_{1,2}T^2\alpha_{2,1}) \quad (6)$$

$$\tilde{T}^2 = (I - T^2\alpha_{2,1}T^1\alpha_{1,2})^{-1}T^2(\beta_{2,0} + \alpha_{2,1}T^1\alpha_{1,2})$$

$$T^i = \left[ -\frac{\nu_i^{-1}J_m(ka_i)J'_m(k\nu_i a_i) - J'_m(ka_i)J_m(k\nu_i a_i)}{\nu_i^{-1}H_m(ka_i)J'_m(k\nu_i a_i) - H'_m(ka_i)J_m(k\nu_i a_i)} \delta_n^m \right] \quad (7)$$

$$\alpha_{i,j} = [H_{n-m}(k|\vec{r}_i - \vec{r}_j|)e^{i(n-m)Arg(\vec{r}_i - \vec{r}_j)}]$$

$$\beta_{0,i} = [J_{n-m}(k|\vec{r}_i|)e^{-i(n-m)Arg(\vec{r}_i)}] \quad (8)$$

$$\beta_{i,0} = [J_{n-m}(k|\vec{r}_i|)e^{i(n-m)Arg(\vec{r}_i)}]$$

The matrices  $\tilde{T}^i$  ( $i=1,2$ ) represent the scattering matrices of each cylinder with account of the other's presence, and the diagonals  $\tilde{T}^i$  correspond to the scattering matrices of single cylinder in free space. Note that the refractive index  $\nu_i$  is involved only into the combination matrix  $T$ .

The matrix equation (3) differs from the one used in [3] by involvement of the diagonal matrix  $J$  that guarantees satisfaction of the Fredholm conditions. This allows us to yield steady results in both the scattering and the eigenvalue problems. The LEP eigenvalue pairs  $(k, \gamma)$  satisfy the following determinantal equation:

$$\det(I - J^{-1} \cdot T \cdot L \cdot J) = 0 \quad (9)$$

### 3. NUMERICAL RESULTS

The relief in Fig. 2(a) shows the variation of the reflectance of the dielectric-wire grating with  $p = 400$  nm on the wavelength and the wire radius, for the wires having the refractive index  $\nu_2 = 2.48$ . Here the dark ridges point the resonances of enhanced reflection; those with small values of the radius tend to the period multiple to the wavelength – these are the resonances on the grating modes.

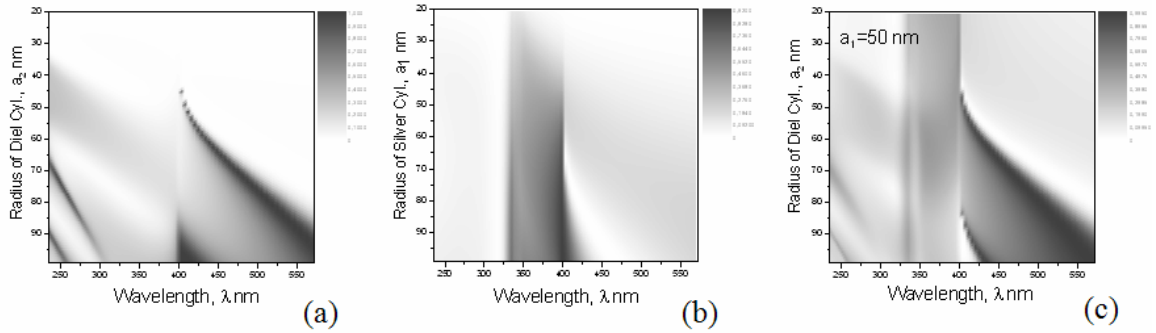


Figure 2. Reflectivity of the grating of dielectric cylinders with refractive index  $\nu_2 = 2.48$  and period 400 nm: (a) the same for the grating made of silver cylinders (b) the same for the mixed-cylinder grating (c) on the period, two cylinders are placed: the first is silver placed at the distance of 100 nm to the left from the origin and with a fixed radius of 50 nm; the second is dielectric symmetrically placed to the right from the origin, with the refractive index  $\nu_2 = 2.48$  and varying radius  $a_2$ .

In Fig. 2(b), we present the same relief as a function of two variables for the grating made of silver nanowires. One can see the interaction of two kinds of resonances. The first, observed near the wavelength of  $\lambda \approx 340$  nm, has plasmonic nature. Another appears at the wavelength slightly larger than the period,  $p$ . If merged together, they lead to a wide-band reflectance (more results on this effect, with a deeper discussion, can be found in [7]).

The most interesting relief is presented in Fig. 2(c). It shows the reflectivity of the mixed grating with two different cylinders on the period, as a function of the wavelength and the radius of the dielectric nanowire, with a

fixed radius of the silver nanowire. As such grating contains both the dielectric-material wires and the plasmon wires, one can see that the reflectivity behaviour inherits all mentioned before resonances.

In the eigenvalue problem with a “negative-absorption” refractive index assigned to the dielectric nanowires, we seek the LEP eigenpairs  $(k, \gamma)$  that satisfy the equation (9): the lasing frequency and the modal threshold or imaginary part of the refractive index. The initial-guess values are borrowed from the scattering problem by taking the frequency of the interested resonance and matching corresponding threshold. We have been interested in the low-threshold grating modes, which correspond to the darkest ridge in Fig. 2(a) for the dielectric-wire grating and its analogue in Fig. 2(c) for the mixed-wire grating. Fig. 3(a) shows that the lasing frequencies of the grating modes  $H_1^{g+}$  in the purely dielectric-wire and mixed-wire gratings have almost the same values hardly distinguishable from each other. This is unlike the thresholds of the same modes: for the dielectric-wire grating, they decay with shrinking of the wire radius (see [6]), however for the mixed grating they grow up. The explanation can be found in the fact that in the latter case the pumping of the active dielectric cylinders has to overcome the losses in the silver wires in addition to the radiative losses.

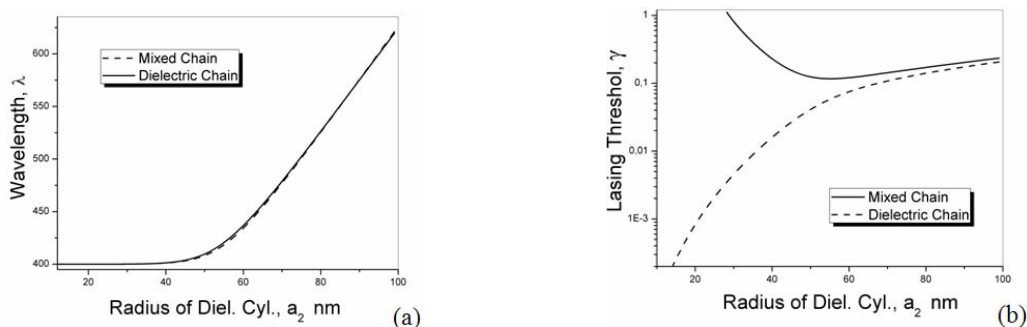


Figure 3. The LEP eigenpairs versus the quantum-wire radius: solid line corresponds to the mode  $H_1^{g+}$  for the grating with two cylinders per period, one active dielectric and other silver, where the first has the radius  $a_1$  varying from 100 nm to 15 nm and the centre 100 nm away from the origin and the silver with constant radius  $a_2 = 56.25$  nm and its centre is just symmetrically opposite from origin, the period is 400 nm. Dashed line shows the same for the grating without the silver wires.

#### 4. CONCLUSIONS

We have presented some preliminary results of the impact of the plasmon effects associated with the silver nanowires on the behaviour of the lasing frequencies and thresholds of the grating modes in the mixed grating built of the silver wires and dielectric quantum wires. They show that the thresholds become drastically higher if the radius of the quantum wires is smaller than a certain value depending on the quantum-wire refractive index and mode type.

#### ACKNOWLEDGEMENTS

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