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**SCIENTIFIC REPORT ON SHORT VISIT
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in the framework of the ESF Network “Plasmon-Bionanosense”**

Topic:

**ACCURATE MODELING OF MICRO AND NANO RESONATORS AND LASERS ASSISTED
WITH PLASMONS AND PERIODICITY**

During the visits to DIPC and ENSC, I presented overview of my recent research activities and discussed potential collaborative efforts in this area with Dr. J. Aizpurua, and Dr. M. Lebental and Prof. J. Zyss, respectively. In particular, I have been seeking their advice for the possible applications of the advanced methods of simulation to the analysis and design of the arrays of micro and nanocavity lasers. This interaction will be important to my on-going and future research in computational electromagnetics and micro and nano-optics. It will also enable me to establish, in the case of DIPC, and strengthen, in the case of ENSC, collaboration with corresponding teams and apply for joint research projects.

I. SURFACE PLASMONS AND GRATING RESONANCES ON NANOSTRIP GRATINGS

In recent years, stand-alone noble-metal nanostrips have attracted remarkable attention due to easily tunable properties of the localized surface plasmon resonances (SPR) and potential applications in nanotechnology, optical devices and circuits, high-resolution near-field optical microscopy, and surface-enhanced Raman scattering. The finite periodic nanostrip gratings are even more interesting objects of research because of their specific properties induced by the periodicity, in addition to the existing SPR.

We have considered the H-polarized wave scattering by a finite flat grating of N silver nanostrips in free space in the context of co-existence of the SPRs and periodicity-induced resonance properties such as the grating resonances. The strips are of the same width d , thickness h and relative dielectric permittivity ϵ_r , and p is period. To characterize the complex dielectric permittivity of silver we took the experimental data of Johnson and Christi Assuming that strip thickness is considerably smaller than the light wavelength, the accurate numerical analysis is carried out using the combination of two-side generalized boundary conditions imposed on the strip median lines and Nystrom-type discretization of the resulting singular and hyper-singular integral equations. As follows from our analysis, the periodicity produces specific coupling and leads to the appearance of the grating resonances (GR) a.k.a. the lattice resonances near to $\lambda = p/m$, $m = 1, 2, \dots$ (at normal incidence). In turn, this causes large reflection, transmission, absorption, and near-field enhancement. We have also studied the interplay of the SPR and GR resonances if they approach each other and the optical response in dependence on the grating parameters, such as overall dimensions and number of strips.

II. LASING THRESHOLDS OF MODES OF PLASMON-ASSISTED NANOWIRE LASER

Recently, the demonstration of a truly nanoscale laser has been achieved in a random ensemble of plasmon-assisted gold nanospheres coated with dye-doped silica shells. Using the first-principle electromagnetic modeling of lasers as open resonators equipped with active regions, we have studied the modes of a nanowire laser made of a plasmon-assisted circular silver wire concentrically covered with an active coating. Such a coating is characterized with a complex-valued refractive index $\nu = \alpha - i\gamma$ where α is refractive index and $\gamma > 0$ is material gain. The field function in each region must satisfy the Helmholtz equation, the tangential-components continuity conditions across boundaries and the radiation condition at infinity. This electromagnetic field problem can be treated analytically using the separation of variables. We consider it as a lasing eigenvalue problem and look for the discrete pairs of real parameters (λ, γ) , where λ is mode emission wavelength and γ is threshold value of material gain necessary to bring the mode to lasing. Note that gain per unit length is $g = k\gamma$ [cm⁻¹].

We have investigated the lasing of sub-wavelength coated nanowire resonators in the visible-light range, at λ from 300 to 700 nm. Here, the silver is characterized by complex refractive index, which we interpolated using Akima splines from the data of Johnson and Christy. As known, bare silver nanowires

in the medium with index α demonstrate plasmon resonances near the wavelength where the silver dielectric function is $\varepsilon(\lambda) = \nu^2(\lambda) \approx -\alpha^2$. The lasing modes can be identified as plasmon modes and coating modes. It was expected to find a single plasmon mode (twice degenerated due to circular symmetry) in each azimuth family, however we have found three such modes in the studied range. Two of them are closely spaced in wavelength and have higher thresholds, and another one has a larger wavelength near to the expected value and a lower threshold. The explanation for the existence of such triplet can be seen in the specific dispersion of silver in the visible range. Besides of plasmon modes, the coating mode also exists in the deep violet however its threshold is much higher than for the plasmons.

III. ANALYSIS OF MICROCAVITY LASERS USING MULLER'S INTEGRAL EQUATIONS

We have investigated the modes of a thin flat microcavity laser in free space as solutions of 2D boundary-value problem for an open dielectric cavity made of gain material, with rigorous boundary conditions and radiation condition at infinity. To build an adequate model of microlaser, we apply the lasing eigenvalue problem (LEP) that enables one to find not only natural frequencies but also threshold gains. Mode frequencies and thresholds in a dielectric cavity continuously depend on the cavity shape and material. Besides of the mode threshold, the mode emission directionality is another most important characteristic of microlaser. A desire to achieve high directionality of light emission has lead to investigation of 2D microlasers of various shapes, from circle to polygon to spiral. In these studies, however, the thresholds have not been addressed directly; instead, the Q-factors were studied. Thus, our analysis with the aid of LEP is a step ahead in the adequate modeling of microcavity lasers.

Electromagnetic problems for arbitrary-shaped cavities can be efficiently analyzed based on integral equations. The LEP is equivalently reduced to the set of Muller's integral equations (IEs) of the Fredholm second kind. Further we use a Nystrom method for discretization of these IEs. In line with this method, the unknown functions are approximated with polynomials and the integrals are replaced with the sums according to appropriate quadrature rules. We choose quadrature rules taking into account the kernels' behavior to achieve the lowest possible error. Eigenvalues are found numerically as roots of correspondent determinantal equation. In the cavities with symmetry lines all modes break up to classes according to the symmetry properties of modal fields. The modes from different symmetry classes can be located closely to each other that create problems when finding them. Separation of the IEs to the independent sets for each class using field symmetry properties offers considerable advantages. It enables one to reduce the integration domain to a part of the contour and save computational time.

Some details of these studies and also the papers based on preceding research can be found at the website <http://www.ire.kharkov.ua/LMNO/publ.html>. Support of the ESF RNP "Plasmon-Bionanosense" will be acknowledged in the publications which will emerge due to the accomplished short visit.