

Metals, and especially metallic nanoparticles are known to show so called plasmon resonance, i.e. collective electron oscillations inside and on the surface of a nanoparticle, with particular frequency due to the external dynamic electromagnetic field. Eigenfrequencies of these oscillations depend on the size, shape and the kind of metal that the particle is made off. On the other hand, in the case of surfaces of bulk materials, e.g. metal dielectric interfaces, nonlocalized propagating oscillations called surface plasmon polaritons are excited. Similar excitations can be created in nano-porous structures, and due to their complicated but extended surface both localized surface plasmons and nonlocalized propagating plasmon polaritons are excited. Because of the plasmon excitations, these materials show intriguing optical properties, including the ability to strongly locally enhance the electromagnetic field. This enables a lot of potential applications e.g. in sensors as substrates for surface enhanced Raman spectroscopy, in highly efficient white light sources of size of few hundred nanometres, and also in catalysis. In the recent years, methods of fabrication of nano-porous materials were greatly improved, and currently the size and density of pores can be controlled. In particular, materials with pores of sizes of few up to over a dozen of nanometres were prepared. These materials are especially interesting, because according to experimental observations in the case of homogeneous metallic nanoparticles of this size microscopic effects related to the inner electron dynamics in significant way change their macroscopic optical properties. The inner nano-porous structure in metallic or metallo-dielectric material may not only significantly influence its optical properties, but also make them more sensitive to the microscopic effects related to electrons dynamics. Among these effects are repulsive Coulomb interaction between the electrons, spilling out of the electrons outside of the metal boundary, and tunnelling. These effects are not included in the standard description used in the classical electrodynamics, which operates on the dielectric function. The dielectric function describes the response of the system to external electromagnetic field, and its form depends on microscopic nature of the material. Nevertheless, in the case of the materials in nanoscale the values of this function may significantly differ from the values for the bulk material. Therefore, it becomes necessary to use proper theoretical models of dielectric function accounting for the effects described above instead of the values measured experimentally. The aim of the project is to study the dependence between geometry and size of the inner structure of nanoporous metallic and metallo-dielectric materials and their fundamental optical properties. We want to understand whether and to what extent microscopic dynamics of the electrons manifests itself in macroscopic optical properties of these materials. We analyse such properties as light scattering and absorption spectra, density, distribution and size of the areas of strongly enhanced electromagnetic field and electron density distribution. Moreover, the study in the time domain makes it possible to analyse the mutual interaction between localized plasmons and nonlocalized plasmon polaritons.

In the scope of the project we are going to develop numerical models of the nano-porous materials differing by inner geometry of pores structure i.e. by average size, level of porosity, and pores distribution. The models will be described by finite element method (FEM) and density functional theory. Scope of application of FEM used to solve Maxwell equations (in classical systems) will be extended to cover also quantum effects significant in nanoscale of pores. Predictions of numerical models will be validated by measurements of fabricated plasmonic structures properties.

Integration of quantum effects description in FEM model is going to allow to calculate optical properties of systems of size up to few hundred of nanometers. This scale significantly exceeds current possibilities of quantum models based on density functional theory of sizes up to few nanometers.

In the next part of the project, numerical model will be used to optimize the structure with regard to the distribution and intensity of local electromagnetic field enhancement. The model can also be used to find novel functions of the material e.g. fabrication of a material sensitive to polarization of incident light (due to the manipulation of pores position). Depending on numerical results we plan to work on inventing of structures with the most promising properties. In particular, we intend to create structures optimized with regard to the strength of electromagnetic field enhancement and study their possibility to enhance Raman signal or fluorescence from selected molecules. We will investigate potential use of these structures as platforms for optical nanocavities enhancing the coupling strength with molecules.

Due to the wide range of application of nano-porous materials, the results of an accurate and systematic study of the dependence between their inner structure and their optical properties may significantly influence future research directions in this field. In particular, discovering an appropriate global parameters related to the macroscopic optical properties of the material may be very helpful in effective fabrication of novel materials having the desired properties. The knowledge gain in the project will also contribute to development of numerical simulation methods of porous layers, which frequently are a part of larger systems.