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Modeling of Localized Surface Plasmon Resonances in Silicon Nanostructures

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Abstract. *In this work, we consider numerical modeling of localized surface plasmon resonances (LSPR) in silicon nanoparticles doped with rare-earth elements (Eu, Er, Yb). Literature data on the complex dielectric function ε(ω) for crystalline Si and the corresponding silicides ($EuSi_2$, $ErSi_2$, $YbSi_2$) were used to construct models of spherical nanoparticles, including core–shell configurations with a SiO_2 oxide shell. Using Python-based software (implementation of Mie theory), absorption and scattering spectra were calculated and the position of the LSPR peak was determined. The influence of nanoparticle radius (≈10–100 nm), doping concentration, and the refractive index of the surrounding medium on the position and width of the plasmon peak as well as on local field enhancement was investigated. Based on the analysis of the obtained dependences, recommendations are formulated for selecting Si–RE nanostructure parameters to tune the resonance within the required spectral range (visible or infrared) for sensing and photonic applications.*

Keywords: *localized surface plasmon resonance, silicon nanoparticles, rare-earth elements, dielectric function, Mie theory, SiO_2 shell, plasmonics.*

INTRODUCTION

Modern advances in nanophotonics and plasmonics are directly related to our ability to control how light interacts with objects at the nanoscale. Of particular interest is the phenomenon of localized surface plasmon resonance (LSPR), which occurs in metallic and semiconductor nanoparticles. Under LSPR conditions, free electrons in a nanoparticle undergo collective oscillations driven by an external electromagnetic field. This results in a significant enhancement of the electromagnetic field in the immediate vicinity of the particle and the appearance of pronounced resonance peaks in optical absorption and scattering spectra.

Traditionally, plasmonic nanostructures are fabricated from noble metals such as gold (Au) and silver (Ag). However, given the technological importance of silicon, there is a growing demand for developing plasmonic effects based on silicon. One promising approach is heavy doping of silicon, including doping with rare-earth elements such as europium (Eu), erbium (Er), and ytterbium (Yb), and the formation of metallic silicide compounds capable of supporting plasmonic oscillations [1–3].

The main objective of this study is the development and investigation of a numerical model of LSPR in nanoparticles composed of silicon and rare-earth elements (Si–RE). This model enables us to determine how particle size, doping level, and the presence of a dielectric shell affect the spectral characteristics of the plasmon resonance.

RESEARCH OBJECTIVES AND METHODS

To achieve this goal, the following tasks were addressed:

- **Data collection and analysis:** Based on existing scientific literature, suitable models were selected to describe the complex dielectric function ε(ω) of crystalline silicon and rare-earth silicides ($EuSi_2$, $ErSi_2$, $YbSi_2$).
- **Geometry selection:** Two main nanostructure configurations were considered: simple spherical nanoparticles and core–shell particles, where the core consists of silicon or a silicide and the shell is silicon dioxide (SiO_2).
- **Development of a computational tool:** A Python-based algorithm was implemented to calculate absorption and scattering spectra using Mie theory and the selected ε(ω) dependencies.
- **Numerical simulations:** Calculations were performed for nanoparticles of various sizes (radii from 10 to 100 nm), with variation of doping levels (modeled via changes in the plasma contribution to ε(ω)) and different refractive indices of the surrounding medium.
- **Result analysis:** A detailed analysis was conducted to assess the influence of these parameters on the position, width of the LSPR peak, and the degree of local field enhancement.
- **Comparison with experiments:** The modeling results were compared with available experimental data from optical and Raman measurements of doped silicon nanostructures [4,5].

RESULTS AND DISCUSSION

Our numerical calculations demonstrate that even $EuSi_2$ nanoparticles with relatively small sizes (approximately 20–40 nm) exhibit a well-defined peak in the spectrum associated with surface plasmon oscillations. This peak is located in the near- and mid-infrared regions. As the particle size decreases, the resonance peak shifts toward shorter wavelengths and becomes narrower.

An increase in the free charge carrier concentration (which in our model corresponds to an increase in the plasma frequency) leads to a shift of the plasmon peak toward higher energies. For typical parameter values of rare-earth silicides, the position of the localized surface plasmon resonance can be tuned from several micrometers down to approximately 1–1.5 µm.

The addition of a dielectric SiO_2 shell and variations in the refractive index of the surrounding medium result in an expected red shift of the resonance peak and changes in its spectral shape. This confirms the high sensitivity of LSPR in silicon–rare-earth-based nanoparticles to the refractive index of the environment, which is a key feature for sensing applications.

A comparison of our results with available experimental data for heavily doped silicon nanoparticles and silicide films shows good qualitative agreement. Similar shifts and broadenings of plasmonic features in the spectra are observed with increasing carrier concentration and changes in the surrounding medium [6].

Mie scattering refers to the scattering of light or other electromagnetic radiation by particles whose sizes are comparable to the wavelength of light, such as dust in air, smoke, or fog.

CONCLUSIONS

In this work, a numerical model describing localized surface plasmon resonances in nanostructures composed of silicon doped with rare-earth elements has been developed. By applying Mie theory and performing calculations using Python software, we investigated how nanoparticle size, doping level, and the presence of a dielectric shell affect the position and characteristics of the LSPR peak.

The main conclusions are as follows:

- By varying the size of Si–RE nanoparticles within the range of 10–100 nm, it is possible to control the spectral position and width of the plasmon resonance.

- The choice of doping concentration and silicide phase allows the LSPR to be shifted into the desired region of the infrared spectrum.
- The presence of an oxide shell and changes in the refractive index of the surrounding medium provide additional tuning of the resonance, making such nanostructures promising for sensor applications.

The obtained results can serve as a basis for further experimental studies of Si–RE nanoparticles and for the development of silicon-based plasmonic elements compatible with existing photonic and optoelectronic technologies.

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