Shape-dependent field enhancement and plasmon resonance of Au, Al and Al/Al_2O_3 core/shell nanoparticles on Si surface

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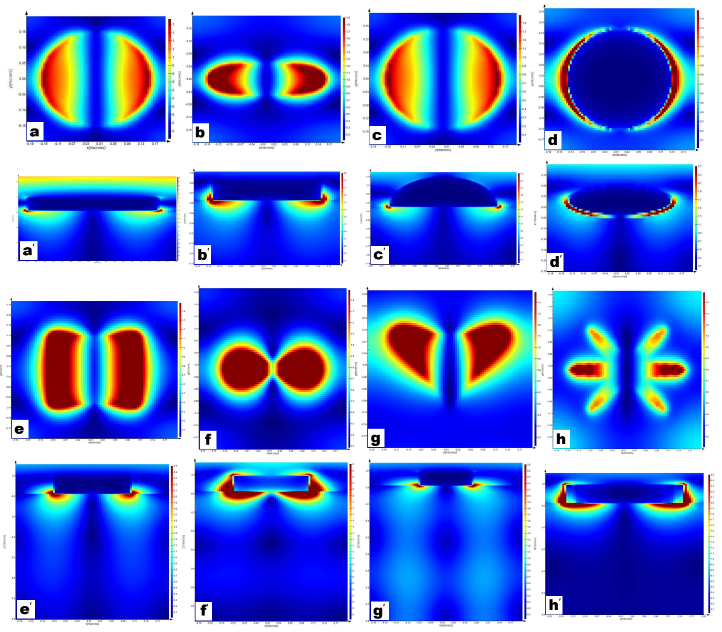
Abstract

Metallic nanostructures can manipulate light-matter interactions to induce absorption, scattering, and local field enhancement through their localized surface plasmon resonances (LSPR). Those method of improving silicon near infrared luminescence efficiency remain to be very promising. In recent years, significant attention is paid to plasmonic effects of metal nanoparticles (NPs) formed in volume or on a surface of semiconductors. The present work is devoted to a computation study of the effects of shape, size, and orientation of nanoparticles deposited on Si substrates as well as the effects of NP material (Au, Al and Al/Al_2O_3 core/shell) on the LSPR absorption of the structures.

Motivation

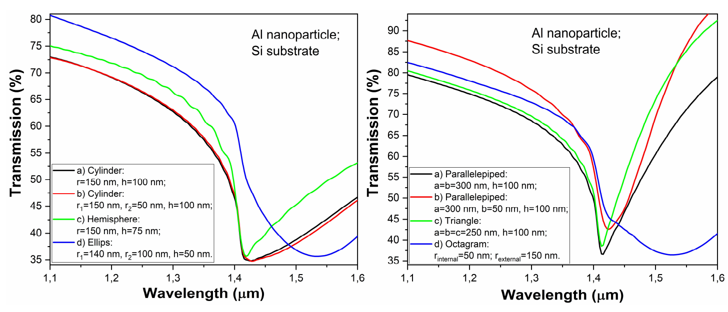
Silicon-based light-emitting structures (LES) are very promising light sources for optical communication technologies [1]. However, their development are slowdowning by low efficiencies of radiative recombination. Efforts to improve the limitations of the LESs efficiency have, among others, made use of plasmonic nanostructures. Large efficiency enhancement of luminescence was achieved by placing metal nanoparticles close to light emitters [2]. This has attracted intense research interests devoted to demonstrating such an enhancement in various media. Metallic nanostructures can manipulate light-matter interactions to induce absorption, scattering, and local field enhancement through their localized surface plasmon resonances. Field enhancement, especially near features with high curvature, is essential in many applications of plasmonic metal nanostructures, yet the potential of localised surface plasmon resonance for IR luminescence in Si crystals remains unknown. Here, we use the FDTD method (Lumerical FDTD Solution) to understand the dependence of field enhancement on size, shape, and metal type of the NP. In our simulation Au, Al and Al/Al_2O_3 core/shell NP with hemispherical, hemiellipsoidal, cylindrical, cubic, star like, etc. shape types were used.

FDTD simulation of plasmonic properties of single Al NPs of different shapes and orientation on Si substrate. The images below show the electric field intensity $|E|^2$ spatial distribution taken at the wavelength of maximum enhancement(In the table description of particles shape and size).

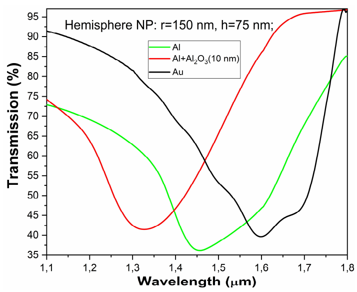


Symb	Shape	Description	Symb	Shape	Description
a, a'	Cylinder	r=150 nm; h=100 nm	e, e'	Parallelepiped	a=b=300 nm; h=100 nm
b, b'	Cylinder	r1=150 nm; r2=50 nm; h=100 nm	f, f'	Parallelepiped	a=300 nm; b=50 nm; h=100 nm
c, c'	Hemisphere	r=150 nm; h=75 nm	g, g'	Triangle	a=b=c=250 nm; h=100 nm
d, d'	Ellipse	r1=140 nm; r2=100 nm; h=50 nm	h, h'	Octagram	$r_{internal}$=50 nm; $r_{external}$=150 nm

FDTD simulation of transmission spectra of Al nanoparticles of different shapes, deposited on Silicon substrate.



Simulation of transmission spectra of Al, Au or Al covered with 10 nm of Al_2O_3 nanoparticles deposited on Si substrate.



Simulation of transmission spectra of Al nanoparticles with decreasing size (side perpendicular to light polarization), deposited on Silicon substrate.

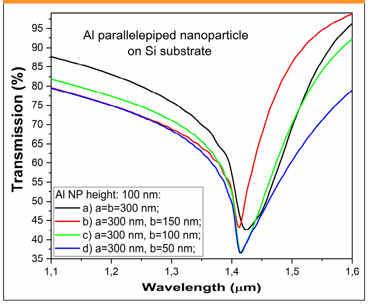


Table of LSPR field enhancement and its penetration depth estimated value obtained under excitation at 1,44 um for different shape of NP with roughly comparable volumes.

Shape	Max. intensity, E/E_0	Penetration depth, μm	Shape	Max. intensity, E/E_0	Penetration depth, μm
Circular cylinder	1,46	0,5	Square cuboid	3,26	0,8
Elliptical cylinder	4,65	0,85	Rectangular cuboid	7,35	0,75
Hemisphere	2,7	0,35	Equilateral triangle	4,17	1,25
Ellipse	3,34	0,45	Isosceles triangle	5,03	0,65
Coated (Al_2O_3) ellipse	2,91	0,75	Pentagram	3,98	0,85
Hemi-ellipse	2,45	1,1	Octagram	5,74	0,4

Conclusions

Metal nanostructures can be designed to have infrared resonance, this has required the use of complex shapes such as nanoellipse or nanoshells and large particles (radius > 150 nm), which has been a major bottleneck for the development of infrared plasmonics. Our calculations predict that they can offer substantial near field enhancement up to 20 times.

We found that the plasmonic response depended strongly on the morphology of the nanoparticle. For all Al or Al/Al_2O_3 core/shell NPs, the absorption spectrum showed a single broad band ascribed to the dipole plasmon, whereas for Au NPs the LSPR band were much stronger, wider and shifted toward lower energies. Also, the additional bands of Al NPs were assigned to the higher-order plasmon excitations were in the region of Si absorption. In addition, we showed that the near-field distribution was significantly perturbed and screened in the perturbed and concentrated in the presence of sharp angular NPs, like an elongated ellipsoid, triangular or star. This fact leads to an increase of penetration depth of nanoparticles LSPR. Finally, it is necessary to admit that star-like nanoparticles have the essential possibilities due to variety of plasmonic parameters and their LSPR peak maxima position.

References:

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