Abstract

Research in plasmonics has primarily been done on individual noble metal nanoparticles such as gold (Au), silver (Ag), and copper (Cu), to study the effect of size, shape, surrounding medium, and interactions between the particles in their plasmonic response for several applications including plasmonic solar cells, photo-thermal, optical imaging, and sensing. However, each noble metal has its own advantages and disadvantages, for example, Ag and Au has good practical plasmonic behavior in the embedding medium, therefore, have attracted major attention as plasmonic materials. Au being expensive still has been used in many plasmonic applications, especially in biomedicines because of its better biocompatibility and chemical inertness. The nanoparticles of Ag have superior plasmonic intensity over Au and have relatively low cost. On the other hand, Cu nanoparticles show comparable plasmonic properties with Au at lowest cost, but its chemical instability limits its practical usefulness because of rapidly oxidized nature of Cu nanoparticles in the embedding medium.

Combining these metals to form alloys and coated nanostructures are the alternatives to use the benefits of individual noble metal nanoparticles with greater tunability in plasmonic properties. In this thesis, we mainly describe the plasmonic response of these combinations affected by the change of metal and its composition (Ag-Au, Ag-Cu, and Au-Cu), in addition to the other parameters such as shape, size, and surrounding medium. The effects of interactions between the alloy nanoparticles in one-dimensional array for various interparticle distance and number of nanoparticles have also been studied. In particular, it is aimed to optimize these parameters on the basis of tuning the localized surface plasmon resonance wavelength, its bandwidth, and absorption/scattering contribution in the total extinction towards cost-effective thin-film solar cells and biological applications. The formation of alloys significantly tune the
surface plasmon resonance and covers the broaden region of electromagnetic spectrum along with greater chemical stability and cost reduction for the desired applications. A linear relationship between the surface plasmon resonance and the metal composition are in good agreement with the available experimental results. Further, simulation results show that the sharp corner and edge shaped nanostructures such as cubes, rectangular, and bars have better to use for plasmonic application in comparison to their spherical counterparts such as sphere and prolate spheroid. The optimized size has been suggested for different shapes along with different metal composition towards their use in plasmonic solar cells and biomedical applications. We also investigated the optical absorption and scattering properties of cadmium based semiconductors coated with gold metal because of intense electric fields near the surface of gold nanoshells resulting from the surface plasmon resonance and with its better biocompatibility. The semiconductor core radius and metal shell thickness have been optimized for thin-film solar cells in the visible region and biomedical applications in the near infrared region.

The simulations performed using FORTRAN based Mie theory for isolated spherical alloys and Gans theory for prolate and oblate shape nanoparticles with the inclusion of surface scattering, radiation damping, and dynamic depolarization effects. Further, the code given by Bohren and Huffman for coated spheres has been used. A numerical technique called discrete dipole approximation (DDA) has been applied on the complex shape nanostructures and interactions between them in the form of arrays. This study may open up the ways for the experimentalists to synthesize the optimized configurations of nanostructures for a desired plasmonic application depending on the response of surface plasmons in the entire range of the electromagnetic spectrum with less effort, cost, and time.