Chapter 5

Waveguide applications of localized surface plasmons associated with metallic nanocylinders

The surface plasmon polaritons [70, 71] provide high enhancement of electromagnetic field near the vicinity of metallic nanostructures. When two nanoparticles are brought together, interaction between individual surface plasmon modes generates additional resonances for the coupled system, provided the distance between the two nanoparticles is small enough in comparison with their size [72, 73]. Thus metallic nanoparticles can be implemented in application either by taking advantage of their local filed enhancement effect or by propagating the surface plasmon polariton modes over distances to build integrated optical waveguide circuits [74, 75]. The localized surface plasmon interactions between the individual nanoparticles are attributed to the signal transfer through periodic nanostructures. The guiding property of metallic nanoparticles to transport the electromagnetic energy below
diffraction limit has been studied intensively for a few decades [76, 77, 78, 79]. It has been observed that the local-field enhancement produced in the gap between nanoparticles could be applied to a waveguide for improving the transmission length of electromagnetic energy [80, 81, 82, 83, 84]. It is well understood that compared to single chain systems, pair chains increase the local field and hence reduce propagation losses [85, 86, 87, 88]. This chapter, discuss the plasmon guiding properties of a waveguide made up of nanocylinders. Electromagnetic energy propagation through dimer array is studied using FDTD method and it is discussed in section 1 of this chapter. Section 2 discuss the wave guiding properties of nanoshell cylinders having triangular geometry.

5.1 Dimer Array

Surface plasmon propagation along nanocylinder arrays are an alternative to dielectric waveguides in highly miniaturized integrated optical devices. The guiding principle in such structures relies on coupled plasmon modes set up by the near field dipole interactions. Finite difference time domain (FDTD) method is used for simulating dispersion of surface plasmon polaritons along silver nanocylinder arrays in anisotropic dielectric surroundings.

5.1.1 Simulation Model

Figure 5.1 shows the unit cell of infinitely long nano cylinder array in anisotropic medium. The silver cylinders in our inclusions are modeled using Drude plus two-pole Lorentzian form.

Here it is assumed that silver cylinders are embedded in anisotropic medium
with large permittivity ratios which can be obtained either by using photonic crystals or strained polymers [89].

![Diagram of 2-D FDTD computation domain](image)

Figure 5.1: The layout of the 2-D FDTD computation domain for calculating dispersion diagram for 1-D dimer periodic structures.

The anisotropic medium with principal dielectric constants $\varepsilon_x$, $\varepsilon_y$ and $\varepsilon_z$ can be expressed in tensor form as,

$$[\varepsilon_r] = \begin{pmatrix} \varepsilon_x & 0 & 0 \\ 0 & \varepsilon_y & 0 \\ 0 & 0 & \varepsilon_z \end{pmatrix}$$ (5.1)

FDTD method can be used to model periodic structures by applying Bloch’s boundary conditions (PBCs). Bloch theory is satisfied by field at any point in periodic structures, i.e,

$$E(d + a) = E(d) \exp(ika)$$ (5.2)
\[ H(d + a) = H(d) \exp(ika) \]  

(5.3)

where \( d \) is the distance vector of any location in computation domain, \( k \) is the wave vector and \( a \) is the lattice vector along the direction of periodicity. Proper absorbing boundary condition is used in FDTD method to truncate simulation domain without artificial reflections. In this work absorbing boundary conditions are handled using perfectly matched layers (PMLs), which is a fictitious absorbing material added around edges of the cell. In two dimensional simulation domain transverse electric modes with non zero \( E_x, E_y \) and \( H_z \) components are truncated using periodic boundary conditions in \( x \)-direction and perfectly matched layers of thickness 100 nm in \( y \)-direction. The radius of silver nano cylinders is 17 nm and lattice spacing is 54 nm. A line source parallel to the cylinder axes is considered to launch Gaussian waves, which is proportional to \( \exp(-i \omega t - (t - t_0)^2/2w^2) \) where \( \omega \) is the centre frequency, \( w \) is width of the Gaussian pulse and \( t_0 \) is the initial time.

5.1.2 Results and Discussion

Dispersion relation for infinite silver nano cylinder arrays embedded in anisotropic environment is numerically simulated. Figure 5.2 shows the optical propagation for three combinations of anisotropy with principal dielectric constants \( \varepsilon_x = 6, 7.5 \) and 9, \( \varepsilon_y = 2 \) and \( \varepsilon_z = 2 \). A red shift is observed as the anisotropy of the dielectric is increased. It is seen from the Figure 5.2 that dispersion can be modified by changing the anisotropy of the embedding medium.

The comparison of surface plasmon propagation along silver nano cylinders in anisotropic dielectric environment with equivalent isotropic environment is shown
Figure 5.2: Dispersion of plasmon modes in silver dimer nano cylinder arrays embedded in anisotropic medium.

In Figure 5.3, simulations are repeated for different combinations of anisotropy. It is seen that in each case the isotropic curve is red shifted from the corresponding anisotropic curve.
Figure 5.3: Dispersion diagram for two rows of periodic infinite-long (along z-axis) circular silver cylinders arranged in square lattice. Figure (3.a) (3.b) and (3.c) shows comparison of plasmon propagation in anisotropic medium with principal dielectric constants \{6, 2, 2\}, \{7.5, 2, 2\}, and \{9, 2, 2\} respectively with their equivalent isotropic values.

5.2 Trimer Array

The plasmon guiding properties of a waveguide made up of nanoshell cylinders whose basic unit cell is having a triangular geometry [90] is investigated. Nanoshell cylinders are considered instead of solid nanocylinders, since it is highly tunable
depending on the dimensions of the cylinder and material parameters. The propagation of plasmon modes through a realistic well defined finite structure which supports sub-wavelength wave propagation with reduced losses is studied, using Finite Element Method (FEM) using commercial software COMSOL and with Finite Difference Time Domain (FDTD) method using MEEP.

5.2.1 Simulation Model

The schematic diagram of the nanoshell cylinder array arranged in triangular geometry is shown in Fig. 5.4. The waveguide is illuminated with a transverse magnetic (TM) polarized plane wave in order to excite all resonance modes of the structure within UV, visible and IR region of the spectrum. The direction of the incident electric field $E$ is perpendicular to $k$ and parallel to the plane of incidence. The structure considered here consists of a total of forty nanoshell cylinders. The unit cell consists of infinitely long nanoshell cylinders arranged at the vertices of an equilateral triangle with the cylinder axis along Z direction. Each shell cylinders consists of a dielectric core cylinder surrounded by a metallic (silver) shell cylinder. The shell thickness of the cylinder shell is the difference between the particle radius ($R_1$) and the core radius ($R_2$). In this chapter, all the shell cylinders are considered to be identical. The plasmon resonances of nanocylinders with dimensions down to 2 nm can be studied using Maxwell’s theory \cite{91, 92}. The dimension of shell cylinders and the interparticle distance considered are well above the quantum regime. The scattering properties of particles having these dimensions are well explained by Maxwell’s theory. Throughout this study, the interparticle distance is fixed at 130 nm. The metal (silver) is modeled using the frequency dependent
complex refractive index data from Johnson and Christy (see Appendix).

The results are also calculated using FDTD. In FDTD simulation grid size is set as 1.6 nm. A Gaussian-pulse source roughly proportional to $\exp(-i\omega t - (t - t_0)^2/2w^2)$ (technically, the Gaussian sources considered are the (discrete-time) derivative of a Gaussian) is used to illuminate the structure. Here, $\omega$ is the incident angular frequency, $t$ time, $t_0$ the initial time and $w$ the width. The triangular arrangement of nanoshell cylinder array is illuminated by a gaussian plane wave source to excite all resonance modes of the structure. The silver nanocylinders are modeled using Drude plus two-pole Lorentzian form.

![Schematic diagram of the nanoshell cylinder array arranged in triangular geometry.](source)

Figure 5.4: Schematic diagram of the nanoshell cylinder array arranged in triangular geometry.

5.2.2 Results and Discussion

Propagation properties of the single chain, pair chain, and trimer chain arrays were compared. The transport of electromagnetic energy along chain of metal nanoshell cylinders relies on the near field interaction between shell cylinders that sets up
coupled dipole or higher order modes. This type coupling is similar to the process of resonant energy transfer observed in systems containing closely spaced optically excited atoms, molecules, or semiconductor nanocrystals [56]. Figure 5.5 compares the variation of power flow for the three geometries considered. The dimension of each nano shell cylinder is kept fixed with $R_1 = 50$ nm and $R_2 = 35$ nm. It is seen that the trimer array allows better power flow compared to dimer array and linear single chain.

![Figure 5.5: Variation of Normalized power flow with wavelength for single chain, pair chain, and trimer chain arrays.](image)

In order to understand the propagation characteristics of the three systems considered, the dispersion is obtained using FDTD for single chain, pair chain, and trimer chain arrays as shown in Fig. 5.6. The periodicity $a$ is set to be equal to 130nm. It can be seen from the figure that the maximum power flow obtained in Fig. 5.5 corresponds to the dipole resonance (shown in the inset) region of the infinite array. It also shows that the plasmon behavior in finite array waveguide
considered in this study resembles quite well to that of an infinite array.

![Graph of Dispersion Characteristics]

Figure 5.6: Dispersion characteristics of single chain, pair chain, and trimer chain arrays. Inset shows the dipole resonance mode which is excited.

The effect of the shell thickness on the light propagation in the waveguide is investigated. The outer shell radius is fixed at 50 nm and the inner core radius is varied. Figure 5.7 shows the variation of normalized power flow with the wavelength for different core thickness. It can be seen that guiding property is closely related to the near field coupling of the resonance modes in the unit cell [90].
Figure 5.7: Variation of Normalized power flow with wavelength for different inner core radius.

The effect of the material parameter of surrounding medium of the nanoshell on the guiding behavior of the structure was studied. As the permittivity of the embedding medium is increased, power flow shows a red shift (Fig 5.8(a)). This effect is due to the effective spatial shortening of the optical wavelength with the increase in the permittivity of the environment. As a result, the induced charges on the metal-dielectric outer interface decreases, resulting in a reduction of restoring forces acting on the polarized electrons. This increases the plasmon coupling strength, resulting in the red shift of power flow. The effect of permittivity of the surrounding medium on the dispersion behavior of the infinite array of trimer is studied using FDTD. From Fig. 5.8(b), it can be seen that with the increase in permittivity of surrounding medium, the dispersion curve shows the redshift as expected from the power flow curve.

Next, the effect of the material parameter of medium filling the core on the
guiding behavior of the structure was studied. The variation of normalized power flow with wavelength for different permittivity of the core dielectric is shown in Figures 5.9. The effect of the permittivity of the core medium is less compared to that of the surrounding medium, surface area of the boundary between the two media is less in comparison to latter case.
Figure 5.8: (a) Variation of Normalized power flow with wavelength for different permittivity of surrounding medium (b) Dispersion characteristics of trimer array embedded in different media.
Figure 5.9: Variation of Normalized power flow with wavelength for different permittivity of core.

Figure 5.10: Power flow through nanoshell cylinder array at wavelength 566 nm.

Power flow through nanoshell cylinder array at wavelength 566 nm is shown in Fig. 5.10. The outer radius of the cylinder is 50 nm and inner radius is 35 nm. From the figure, it can be seen that the entire power is confined within the structure. This is due to the large field enhancement between nanoshell cylinder structures which enhances the coupling of plasmon modes. The energy propagates without
much loss through the structure, thus nanoshell cylinder array can provide optical guidance confined in the region between the chains, which finds applications in various integrated nano-optical waveguide devices.

5.3 Conclusion

A plasmonic waveguide formed by an array of periodic infinite long silver cylinders at optical frequencies was modeled using FDTD method. It is shown that anisotropy of the surrounding medium can change the plasmon polariton propagation in silver nano cylinder arrays. This can have novel applications in the designs of waveguides, small antenna, and efficient absorbers.

The near field optical properties of an array of silver nano shell cylinders arranged in triangular geometry is also studied using Finite Element Method. By varying the surrounding dielectric environment, interparticle distance, radius of the nanocylinders, the plasmon resonance is tuned across the UV, visible and near infrared spectral range. Field propagation can be enhanced using a trimer array of nano shell cylinders compared to a pair array or linear single chain array. Surface plasmon resonance and field propagation can also be controlled by changing the permittivities of the inner core as well as surrounding medium.