Supplementary Material

Double resonant plasmonic lattices for Raman studies

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The Fourier Modal Method (FMM) simulations depicted in Fig. A1 representing transmission (percentage intensity) through the structure as a function of the out of plane radiation angles and the wavelength in the Far-field.

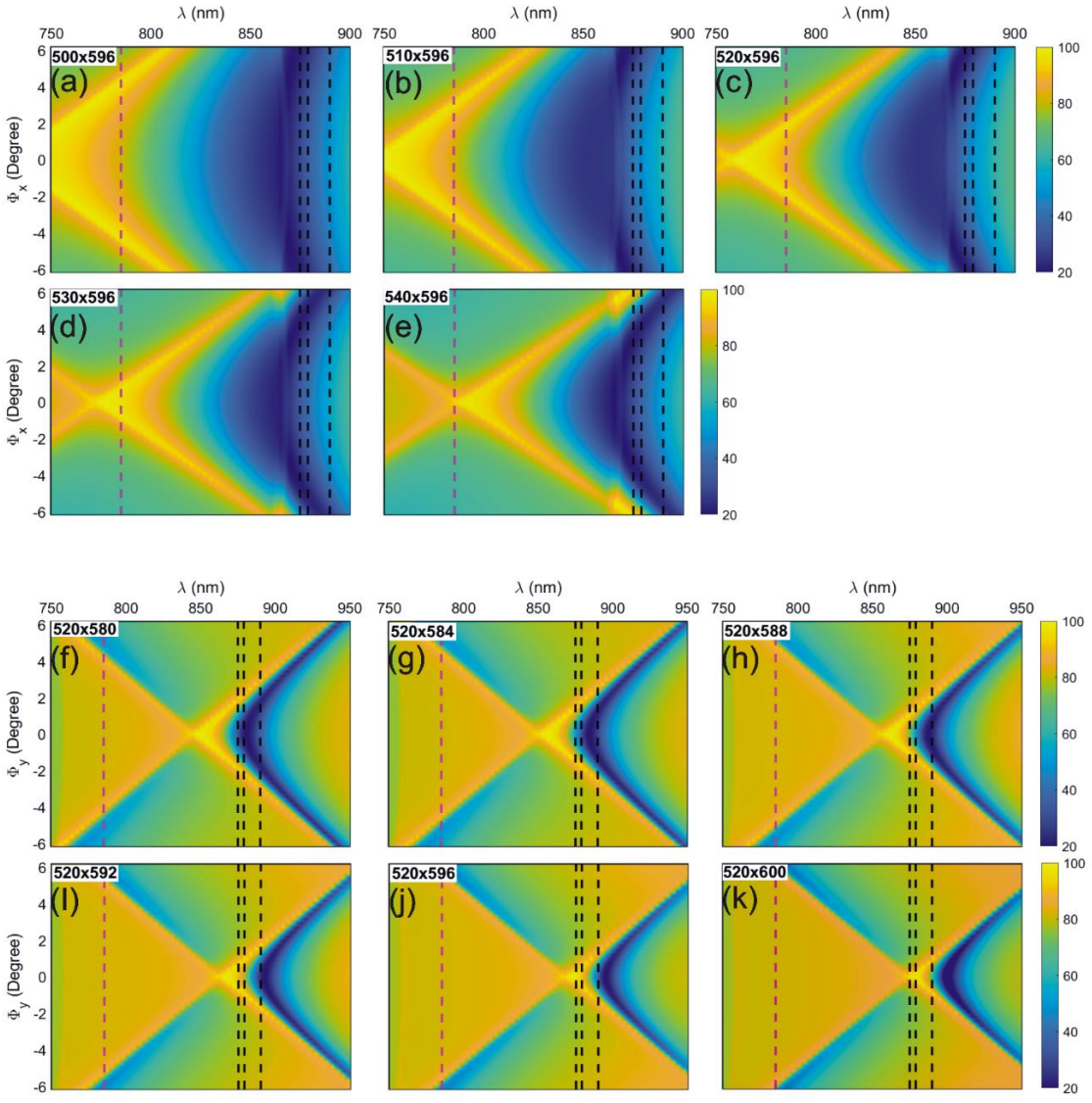

Fig. A1: Ordered arrays, (a - e) and (f – k) shows radiation coupling in x- and y- direction periodicity, respectively. The surface lattice resonance is slightly red-shifted as P_x increases from 500 nm to 540 nm at P_y = 596 nm fixed. On the other side, P_y is varied from 580 nm to 600 nm for P_x = 520 nm fixed. The red dotted line represent the Raman excitation wavelength, while the three black dotted lines represent the Raman transitions of the molecule (Rhodamine 6G).

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The FMM calculations were performed by taking into account our far-field transmission intensity measurement setup. In all cases, we considered that the light is incidence from the substrate side, which is SiO_2. The complex refractive index of silver was obtained against wavelengths by interpolating the Palik's data [1]. The medium among silver particles and the output region were considered as index matching oil, which has a refractive index of ~1.46. To achieve a converged result, ±7 diffraction orders were considered in the FMM analysis. For both P_x and P_y periodic structure, only TE mode was considered in the calculation, however, in the case of P_y, the considered structure was rotated by 90 degrees to make it consistent with the experimental setup. Finally, transmission amplitudes were calculated against the desired range of incidence angles and wavelengths for each P_x and P_y structure.

The finite-difference time-domain (FDTD) simulations were done using Lumerical's FDTD Solutions package. The nanoparticle size used in the simulation was 154 nm in diameter and 50 nm tall, placed in the middle of the simulation volume. Tabulated values for silver were used for the permittivity [1]. The background refractive index used for the simulation was 1.45. A 1 nm mesh size was used for the nanoparticle volume. Symmetric and anti-symmetric boundary conditions were used in x and y directions to create a periodic system with periods of 500x596 and 520x580, while reducing the computational load. A plane wave was used to excite the nanoparticle lattice from the top, and the field profiles were obtained in the x-y plane 10 nm above the nanoparticles.

Enhancement plots of integrated Raman intensities as a function of extinctions.

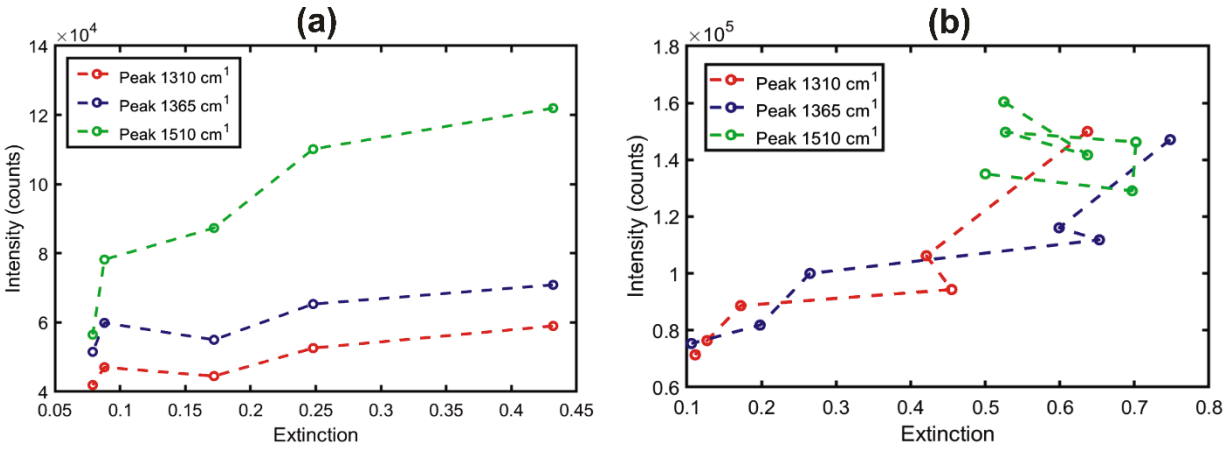

Fig. A2: The plot showing Raman peak intensities (a) for Px induced effect and their extinction at the Raman excitation wavelength and (b) refers to Py induced effect with the Raman peak intensities and their corresponding extinction at each Raman peak wavelength for all the samples.

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FDTD simulation for a 168 nm nanoparticle diameter and its extinction spectrum showing the variation of extinction values at different Raman transitions.

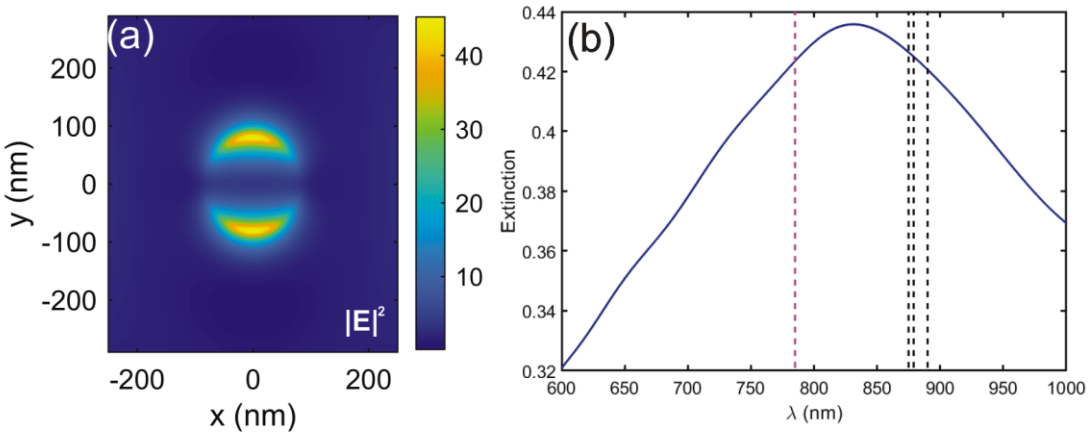

Fig A3: FDTD simulations for optimized particle diameter for random samples. (a) shows E_y at 785nm (Raman excitation wavelength), multiplied by the E_y at 879 nm (middle Raman peak wavelength). (b) shows the extinction spectrum together with the Raman excitation wavelength and three different Raman transitions (red and black dashed lines, respectively).

References

1. E. D. Palik, *Handbook of optical constants of solids*, Academic press, 1998.

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