Electronic Supplementary Material (ESI) for Nanoscale.

Supporting information for:

A classical description of subnanometer resolution by atomic features in metallic structures

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Formalism of the FEM calculation

The 3D FEM calculation of our model system was built using Comsol Multiphysics 4.4 (v.248) software, utilizing the wave optics module for electromagnetic waves. This module enables calculating the full electric field E, under stationary conditions:

$$\nabla \times \frac{1}{\mu_r}(\nabla \times E) - k_0^2\left(\epsilon_r - \frac{i\sigma}{\omega\epsilon_0}\right)E = 0$$

where ϵ is the permittivity, σ the conductivity, μ_r the relative permeability, ω the angular frequency and k the wave vector.

By using the constitutive relation for linear materials ($\sigma = 0,\ \mu_r = 1$) the formula can be simplified to the Helmholtz equation:

$$\nabla^2 E - k_0^2\epsilon_r E = 0$$

used in our FEM implementation.

The basic model system consists of a cubic layered boundary with a lateral size $w = Z_{layer} + Z_{air} + Z_{sub}$ (Fig. 1). The thickness of the air (Z_{air}) or substrate (Z_{sub}) domain was varied according to the incident wavelength ($Z_{air/sub} = 2 \cdot \lambda_i \cdot \cos(\phi)$) to ensure identical phase conditions at the particle position. The incident field is originated from the bottom port boundary trough the physical domain. The angle of incidence (ϕ) was set to 60° for all the situations considered.

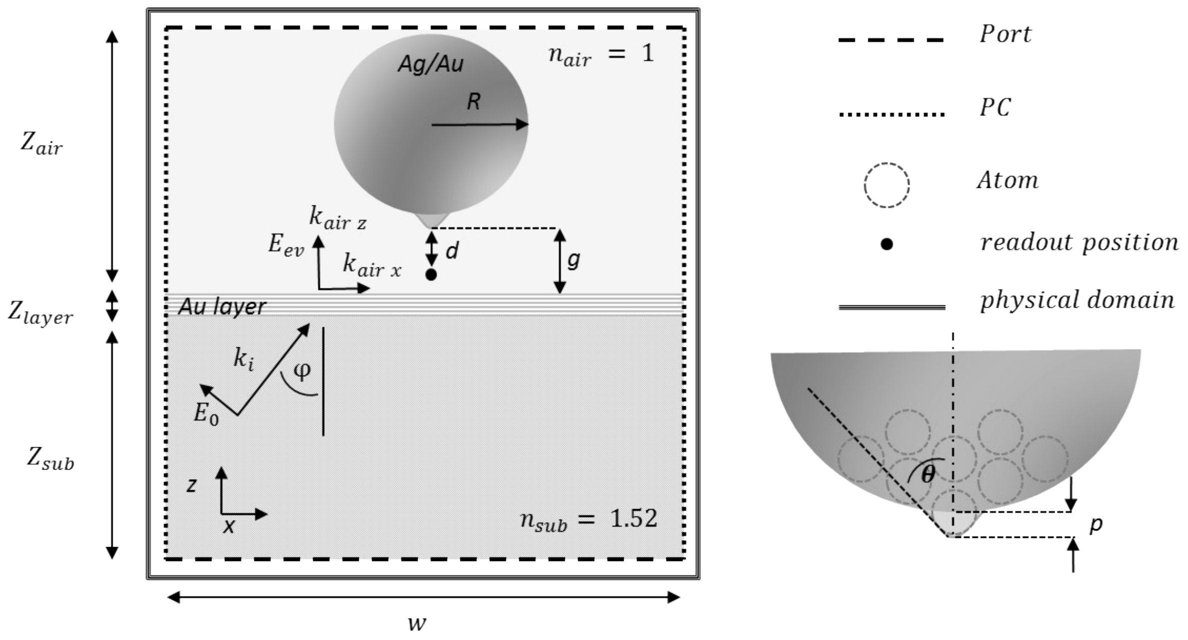

Figure 1. General scheme of the system considered for the 3D FEM calculations including all boundary conditions.

The incident power (P) for the bottom port was calculated according to:

$$P = I_0 w^2 \cos(\phi)$$

with the incident Intensity (I_0) set to $E_{ev} = 1\,V/m$ at the air/substrate interface according to:

$$I_0 = \frac{E_0^2 \cdot n_{air} \cdot c_0 \epsilon_0}{2}$$

where E_0 is the incident field, c_0 is the speed of light in vacuum and ϵ_0 the vacuum permittivity.

On the side walls, periodic conditions (PC) were used with a Floquet-periodicity to ensure a perfect planewave at the boundaries. Here also, a large distance between the scattering particle and the side walls was used to avoid numeric instabilities at the boundaries. For calculating the outgoing field at the port boundary on top, the following propagation constant (β) was necessary.

$$\beta = \left| k_{air} \sqrt{1 - \frac{\sin(\phi)^2 n_{sub}^2}{n_{air}^2}} \right|,$$

where k_{air} represents the k-vector in air, while n_{air} and n_{sub} are the refractive index of air (n = 1) and substrate (n = 1.52), respectively.

Depending on the configuration required for each case (specified in the main text), either a Au or Ag nanoparticle was used, or an additional 20 nm Au layer was introduced. The radius of the basic nanoparticle (R = 10 nm) and the gap distance from the surface (g = 1 nm) were kept constant for all simulations. Only the protrusion (p) or the angle (θ) were changed.

The enhancement factor and FWHM (lateral resolution) were calculated for several particle distances (d) at the readout position (black dot in Fig. 1). 100 readout positions in z ($\Delta z = 1\,nm$) and ± 500 positions in x ($\Delta x = 50\,nm$) were evaluated from the center position.

The minimum tetrahedral element mesh size was 0.09 nm for a virtual sphere of 100 nm around the nanoparticle. All other domains had a minimum tetrahedral mesh size of 5 nm to reduce the calculation time.

Finally, the stationary direct solver (MUMPS) was used to solve the system of equations. It proved to be effective and numerically robust for this implementation of our model system.