Rational Selection of Metal Subwavelength Apertures for Sensing Aerosol Nanoparticles

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***Abstract*—Metal subwavelength apertures have great potential for sensing nanoparticles in aerosols. This numerical study based on FDTD simulations compared various configurations of subwavelength apertures to investigate their key aerosol sensing performance characteristics, including sensitivity, signal variation, and fluidic resistance.**

Keywords—metal subwavelength aperture, plasmonics, finite-difference time-domain, particle sizing, ultrafine particle

I. Introduction

Airborne particles with diameters less than 100 nm are referred to as ultrafine particles (UFPs). The ability to measure ultrafine particles can be tremendously difficult due to their nanoscale size. One existing optical approach to measure airborne particles is the optical particle sizer (OPS). The OPS is based off monitoring the scattering of light from an incident laser beam caused by airborne particles in an aerosol stream. However, OPSs cannot reach into the ultrafine range due to weak signals caused by Rayleigh scattering. A promising solution to overcome this challenge is to implement a subwavelength aperture (SWA) in a metal film (Fig. 1a). A metal SWA can confine light into nanoscale dimensions and excite localized surface plasmons, both of which enhance optical signals induced by ultrafine particles traveling through the aperture. Our previous numerical modeling has revealed that the metal SWA can detect particles down to 15 nm [1].

Compared to existing sensing applications using SWAs, our work on aerosol sensing is different in at least the following aspects. Firstly, different configurations of SWAs have been studied extensively for biosensing and optical trapping in liquids, however, they have not been studied for sensing aerosol-based analytes [2]. The SWA is expected to be more sensitive for sensing nanoparticles in aerosols than in liquids due to the contrast in refractive index between the particle material and background. Secondly, in existing sensing applications, the analytes are either bounded to the metal surfaces via immobilized receptors or optically trapped into the strongest 'hot spots'. However, for aerosol sensing, the trajectories of airborne particles are highly variable due to Brownian diffusions, and the resultant optical signals can be significantly affected by the inhomogeneity of field enhancement. Therefore, the signal variation caused by different trajectories is much more pronounced in aerosol sensing and must be investigated. Lastly, the SWA for aerosol sensing also functions as a nano-fluidic channel for the flow of aerosol steam and the fluidic resistance of the channel plays a significant role in determining the aerosol sampling efficiency. From a simplistic view, the fluidic resistance will be inversely proportional to the channel's cross-sectional area.

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For aerosol sensing applications, the sensitivity, the signal variation (caused by random trajectories) and the fluidic resistance are all strongly dependent on the configuration of SWAs. This work investigated different configurations of SWAs, in particular, the circular aperture (Fig. 2a, 2b), the double nanohole (Fig. 2c, 2d), and the nanohole array (Fig. 2e, 2f) to compare their key aerosol sensing performances. These three configurations are most representative for SWAs. Both the circular aperture and double nanohole are single SWAs which are highly sensitive for individual nanoscale objects with high locality [2]. The double nanohole has an even stronger local field enhancement due to the gap plasmon mode at the tips, but the field enhancement profile is also highly non-uniform. The nanohole array relies on the coupling of surface plasmon polaritons to cause enhanced optical transmission, which is better suited for sensing ensembles of analytes [3].

II. Methods

The three different aperture configurations were simulated using Ansys Lumerical FDTD. Each simulation configuration was comprised of a 100 nm thick Gold (Au) film suspended in air. The particle material was silica. In each simulation, perfectly matched layers were used as simulation boundaries. For the single aperture simulations, a plane wave was launched using a total field scattered field source. For the nanohole array, a Gaussian source with a 1 $\mu\mu\mu\mu$ beam radius. A frequency domain power monitor and profile monitor were used to capture the transmission spectra and field enhancement profiles.

The simulated optical signal induced by a UFP is referred to as normalized transmission increment, ΔTT� $= \Delta TT/TT_0$, defined as the change in optical transmission ΔTT caused by the particle, normalized with the transmission of an empty aperture TT_0, as shown in Fig. 1b. In our previous theoretical work, we have found that ΔTT� is proportional to the field enhancement at the location of the particle inside the aperture, which is linked with the inhomogeneity of the field enhancement profile [1]. Sensitivity was simulated by introducing a 15 nm diameter silica UFP located at the center of the aperture. Signal variation

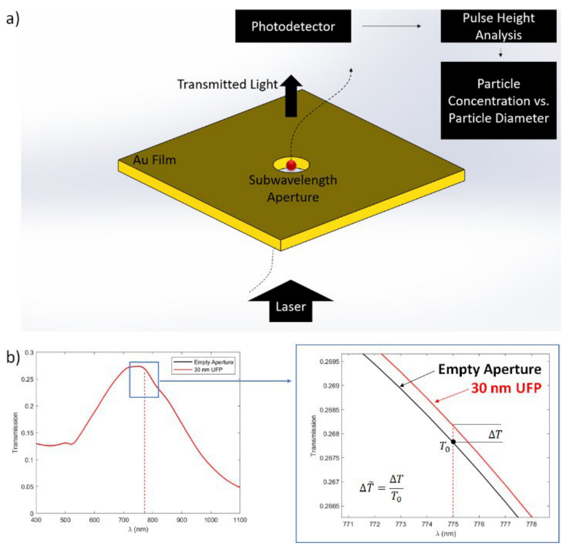

Fig. 1. (a) Schematic for sensing aerosol UFPs using a metal SWA. When a UFP travels through the aperture, a pulsatile increase in optical transmission of the laser beam will be detected by the photodetector. (b) Simulated transmission spectra showing the normalized transmission increment ΔTT� at the laser line.

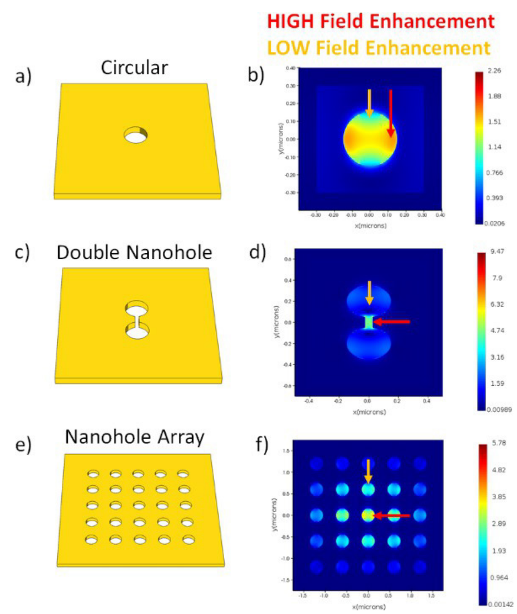

Fig. 2. Schematic and simulated electric field enhancment profile (horizontal plane) of circular aperture (d = 300 nm), double nanohole (d = 300 nm, gap = 50 × 100 nm), and nanohole array (d = 300 nm, pitch = 600 nm). The red and yellow arrow marks the location of 15 nm UFP for simulating the maximum and minimum signal, respectively.

TABLE I. SENSITIVITY, SIGNAL VARIATION, AND CROSS-SECTIONAL AREA OF VARIOUS CONFIGURATIONS.

	Circular	***Double Nanohole***	***Nanohole Array***
ΔTT� for 15 nm silica UFP at the center	1.62e-4	**14.8e-4**	0.2e-4
Signal variation	**18.5%**	98.9%	60.0%
Channel cross-sectional area	0.071 $\mu\mu\mu\mu^2$	0.146 $\mu\mu\mu\mu^2$	**1.767** $\mu\mu\mu\mu^2$

was calculated as the percent signal change between the maximum signal ΔTT�$_{mmmmmm}$ and the lowest signal ΔTT�$_{mmmmmm}$, given as (ΔTT�$_{mmmmmm}$ − ΔTT�$_{mmmmmm}$)/ΔTT�$_{mmmmmm}$. To find ΔTT�$_{mmmmmm}$, a 15 nm silica UFP was introduced at the highest field enhancement spot as indicated by the red arrows. While ΔTT�$_{mmmmmm}$ was simulated by the same UFP at the lowest field enhancement spot (yellow arrows).

III. Results and Discussion

The double nanohole aperture was found to be the most sensitive SWA, due to the gap plasmon mode. However, the signal can vary largely based on the UFP's location in the aperture, and the signal variation can reach more than 98%, which cannot deliver reliable and consistent readings for sensing UFPs in the aerosol.

The nanohole array has poor sensitivity due to a large mode volume, which, in this case, is limited by the size of the beam spot. The large mode volume causes weaker field confinement and therefore lower sensitivity. In addition, due to the effects of beam spot, the signal variation was also high, approximately 3 times larger than that of the circular aperture. In terms of fluidic properties, the nanohole array has a much larger cross-sectional area (*i.e.*, much lower fluidic resistance), which means it has the best aerosol sampling efficiency and allows larger volumes of aerosol to be sampled at a given duration. The high fluidic resistance is problematic for single SWAs, which limits their aerosol sampling efficiency. However, this negative effect can be compensated by introducing more single SWAs, separated by large distances, such that these individual SWAs can be simultaneously probed through a CCD device.

The circular aperture had a sensitivity lower than the double nanohole by one order of magnitude. However, the circular aperture was found to give the most consistent signal with the minimal signal variation among all configurations. For the applications concerned here, the main desire is to detect UFPs consitently, so the circular aperture is the best fit out of the three.

IV. Conclusion

Each metal SWA configuration has advantages and limitations. The circular aperture showed the best overall performance characteristics considering sensitivity to detect an ultrafine particle and minimal signal variation, although the aerosol sampling efficiency is low. This study advances the knowledge of how nanoplasmonic structures can be utilized in aerosol applications to sense nanoscale ultrafine particles.

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