

Improving Detection Sensitivity for Nanoscale Targets through Combined Photonic and Plasmonic Techniques

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Abstract: Photonic technique such as the whispering gallery mode (WGM) is often used for detection of small particles like bacteria and viruses. It offers good detection sensitivity and is advantageous over other detection techniques because the detection can be label free.¹ However, the detection sensitivity may not be sufficient when the size of the detection target is in nanoscale. To change this, in this study we use COMSOL to explore the combination of the WGM technique with plasmonic techniques such as Surface Plasmon Resonance (SPR) and Surface Enhanced Raman Scattering (SERS). Our simulation result shows that by designing the right setup and selecting the appropriate frequency, the three techniques can work in synergy and the detection sensitivity can be increased by three orders.

Keywords: WGM, SPR, SERS

1. Introduction

When a particle binds to a waveguide device (e.g., a cavity or a ring), part of the energy in the waveguide will enter the bound particle through evanescent wave, thus causing a shift in the resonance frequency of the waveguide device. The detection sensitivity of such a device depends on the energy distribution between the particle and the waveguide.

As shown in Figure 1, we developed a 2D model consisting of a straight optical waveguide and a ring waveguide with different refractive indexes using COMSOL.

In general, SPR often takes place at the surface of a thin flat metal layer. The amount of energy transmitted into and reflected from the metal layer varies with the frequency of the incident light. For given materials on both sides, there exists a small window of frequency in which the ratio of the transmitted to the reflected energy changes drastically, indicating the excitation of SPR.

Different from SPR, SERS takes place at rough surfaces by enhancing the local electromagnetic field

intensity. The enhancement varies with the nanostructures on the surface. In this study, the two plasmonic techniques (SPR and SERS) are incorporated into the WGM technique. To excite SPR and SERS, we place a sheet structure composed of either a flat gold surface or a nanostructured gold surface at a location outside the ring as shown in Figure 2.

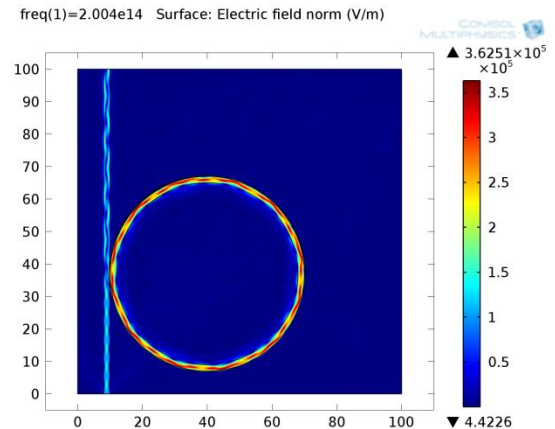


Figure 1. The resonance pattern of light in the ring at approximately 200×10^{12} Hz

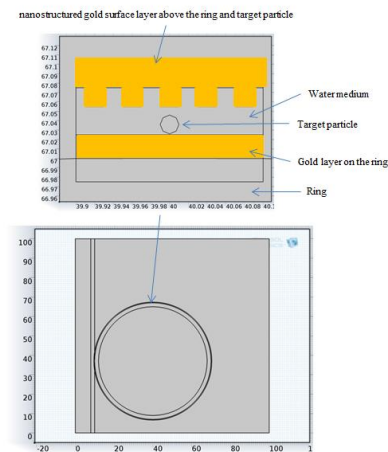


Figure 2. COMSOL model of a detection device built upon the combined photonic and plasmonic techniques

2. Governing Equation

Since both photonic and plasmonic phenomena are in essence electromagnetic waves, they are governed by the wave equation, thus we solved the problem using the Wave Equation in Frequency domain in COMSOL:

$$\nabla \times (\nabla \times E) - k_0^2 (\epsilon_r - \frac{j\sigma}{\omega\epsilon_0}) E = 0 \quad (1)$$

Here ϵ_r and σ are the permittivity and conductivity of medium where wave propagates respectively. ω is the angular frequency of wave and $k_0 = \frac{\omega}{c_0}$ where c_0 is the speed of light in vacuum.

3. Methods

The combined photonic and plasmonic device is composed of a straight bar-shape waveguide with width of 2 μm and a ring-shape waveguide with thickness of 2 μm and radius of 30 μm .² The distance between the bar and ring is adjustable and it is found that the device exhibits the highest performance when the gap distance is around 0.2 μm . Scattering boundary condition is applied to the sides of the bar waveguide. The incident light propagates along the bar waveguide from the lower end to the upper end. The energy at the upper end is calculated as the output.

A frequency sweeping analysis is performed to determine the resonant frequency at which most energy is locked in the ring. When a particle binds to the ring on the outside, the output energy will change depending on the physical and material properties of the particle.

4. Modeling Results

First, we considered the case of using the WGM technique alone. Figure 3 shows the frequency sweep result, exhibiting several resonant peaks of energy inside the ring waveguide. The full width half maximum is used as Q factor to estimate the response of the device.

For a particle with refractive index of 1.5 surrounded by water, the highest detection sensitivity is achieved when the particle has a size ranging from

5 nm to 10 nm. The slope of the regression curve between the output energy and particle size is determined as a measure of detection sensitivity as shown in Figure 4, where the sensitivity is determined to be $2 \times 10^{-11} \text{ J/m}^2 \cdot \mu\text{m}$.

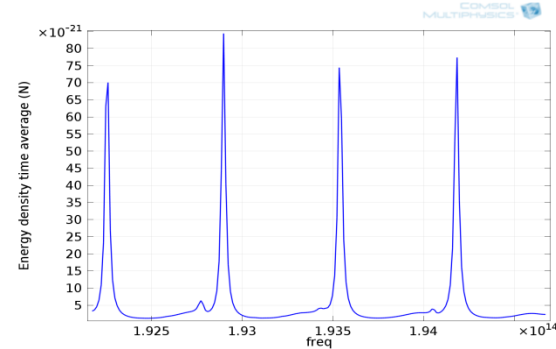


Figure 3. Resonance peak of energy in the ring waveguide

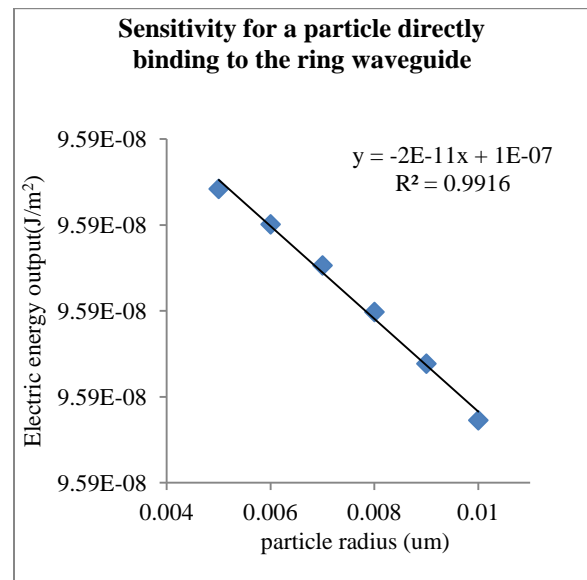


Figure 4. Energy output for particles of different sizes directly binding the ring waveguide

To excite the SPR phenomenon,³ we include a 25 nm long flat sheet (Figure 2). Figure 5 shows the frequency sweep result of the energy distribution between the outside and inside of the structure. Figure 6 shows that the energy distribution ratio varies drastically in this frequency range, indicating the excitation of SPR.

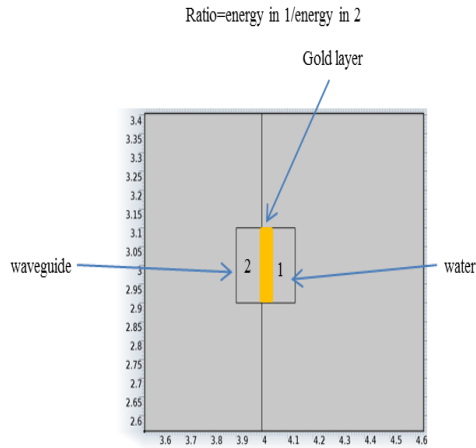


Figure 5. SPR setup for deciding energy distribution

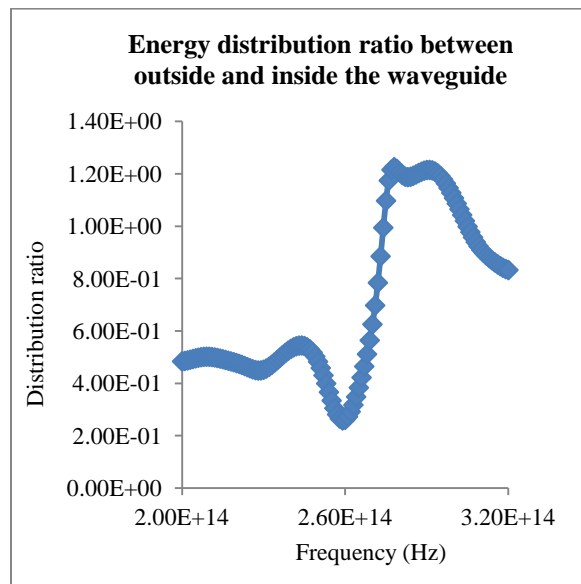


Figure 6. SPR behavior at the interface between waveguide and water

At a resonant frequency where the energy ratio peaks (see figure 6) the sensitivity value is expected to be high. Figure 7 shows at the resonant frequency of approximately 279×10^{12} Hz, the sensitivity is 9×10^{-9} J/m²*um, which is about 400 times better than the case without the SPR excitation sheet metal layer.

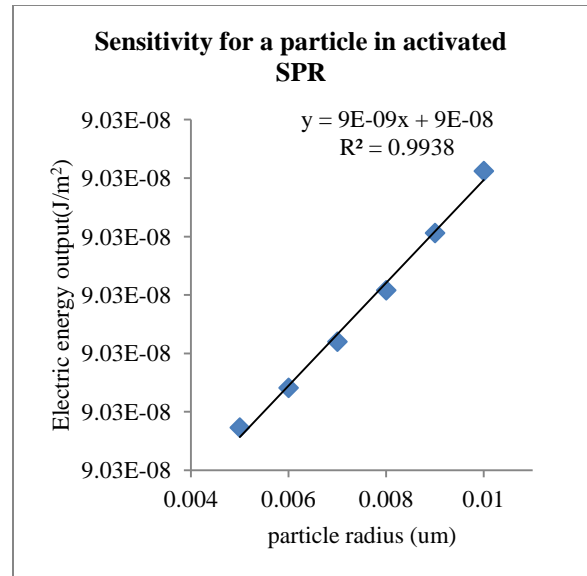
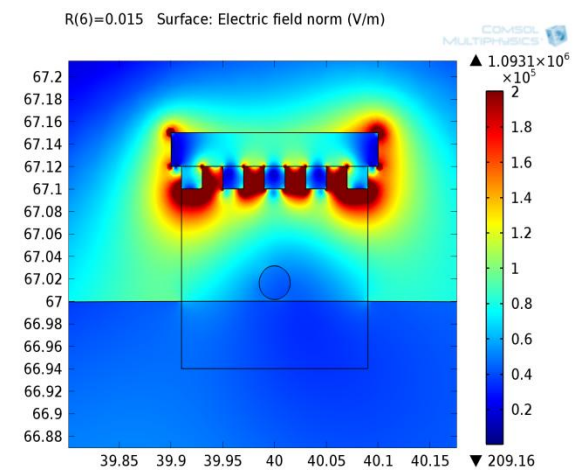
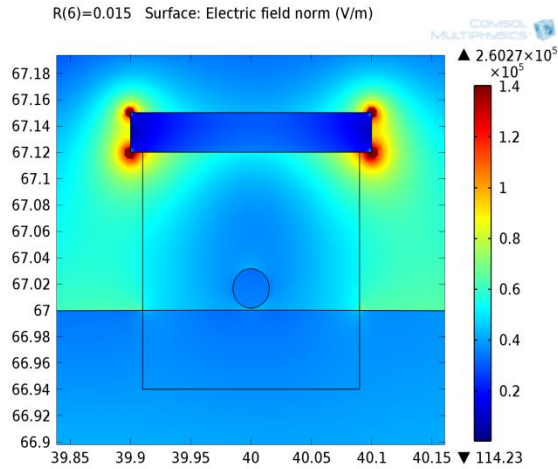


Figure 7. Energy output for particles of different sizes binding to the gold layer surface

To exciting SERS, a gold sheet layer with a rough surface is used.⁴ Figure 8 illustrates the difference in local electric fields when the sheet layer has a nanostructured surface (8a) or smooth surface (8b).



(a)



(b)

Figure 8. (a) A nanostructured surface generates strong local electric field (hot spots) through SERS activation. (b) A flat surface generates a much uniform electric field

When the distance between gold nanostructured sheet layer and ring waveguide is set at 50 nm to accommodate nanoscale particles (Figure 9), we obtained a sensitivity value about $5 \times 10^{-9} \text{ J/m}^2 \cdot \mu\text{m}$ (200 times improvement compared with direct binding without the nanostructured layer). In comparison, the case with the gap distance set at 70 nm (Figure 10(b)) has a sensitivity value of $4 \times 10^{-9} \text{ J/m}^2 \cdot \mu\text{m}$, indicating that as the nanostructured gold layer is moved farther away from the ring, the detection sensitivity will decrease.

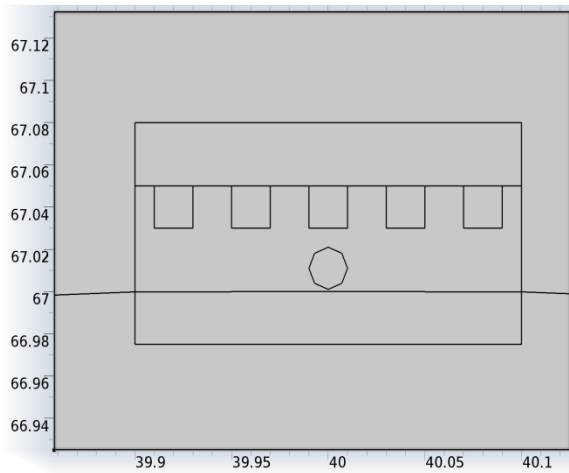
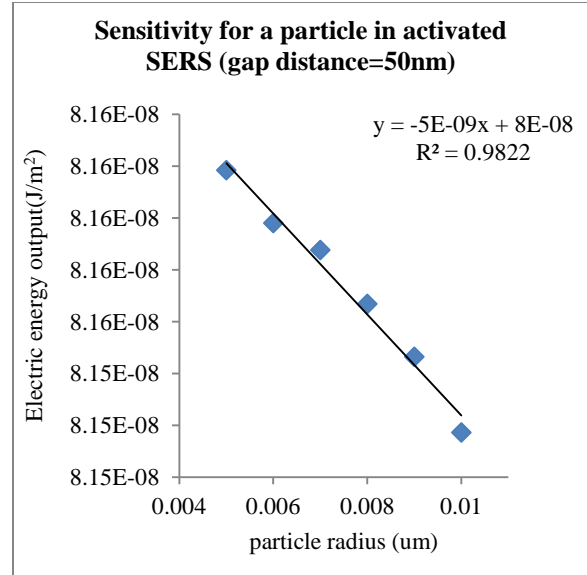


Figure 9. A nanostructured gold layer close to the ring waveguide for SERS activation



(a)

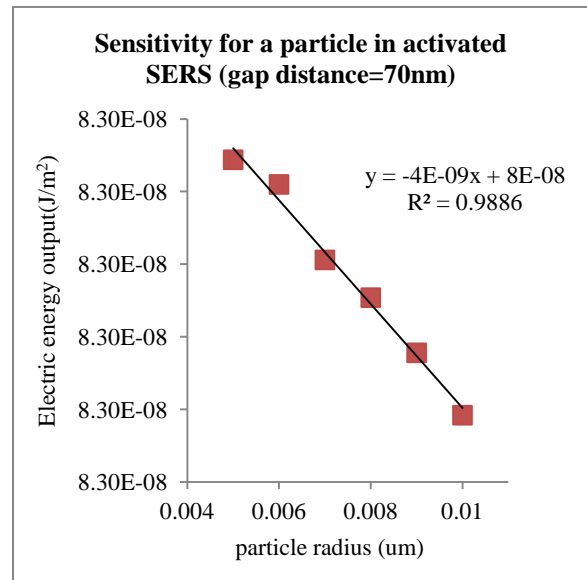


Figure 10. Energy output for particles of different sizes in field generated by SERS. (a) gap distance=50nm; (b) gap distance=70nm.

By combining SPR and SERS, we found that at the resonant frequency, the sensitivity value is drastically increased to $2 \times 10^{-7} \text{ J/m}^2 \cdot \mu\text{m}$ (10000 times improvement compared to direct binding) as shown in Figure 11.

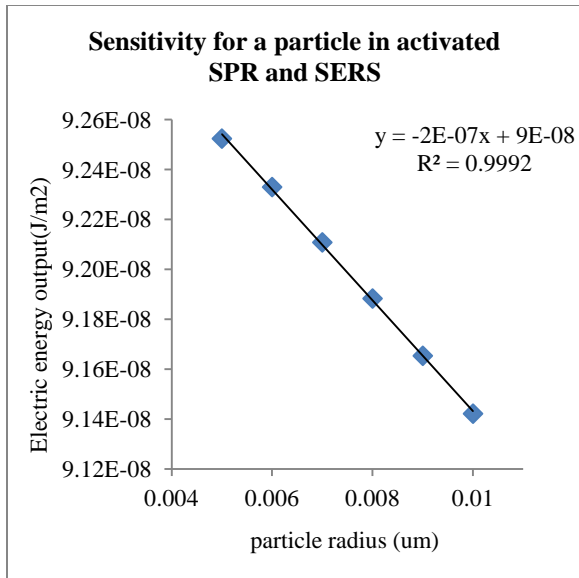


Figure 11. Energy output for particles of different sizes in field generated by activated SPR and SERS

We also found that when the dimensions of the nanostructure reduces (Figure 12), the detection sensitivity will decrease to $2 \times 10^{-8} \text{ J/m}^2 \cdot \mu\text{m}$ (1000 thousand times improvement compared to direct binding) as shown in Figure 13.

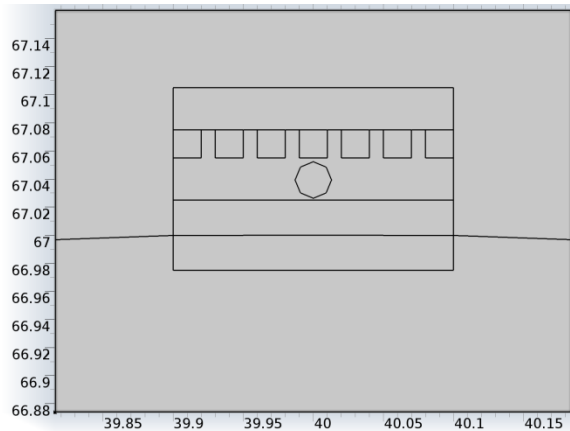


Figure 12. More compact nanostructured gold layer reduces detection sensitivity

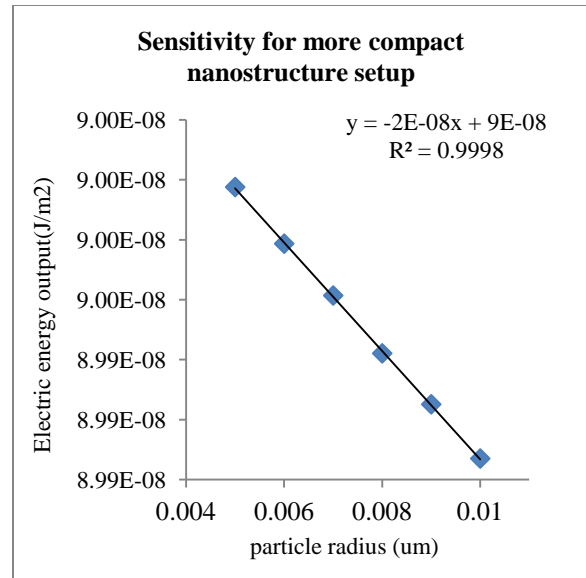
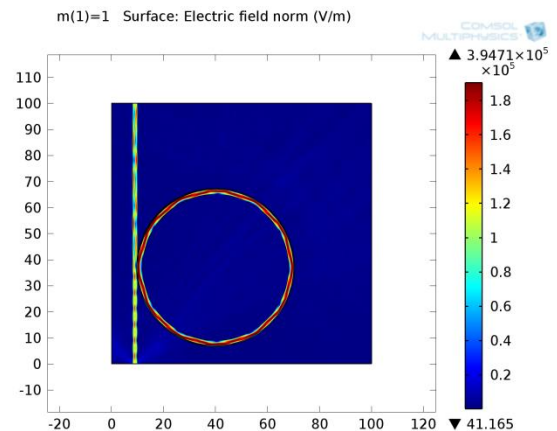
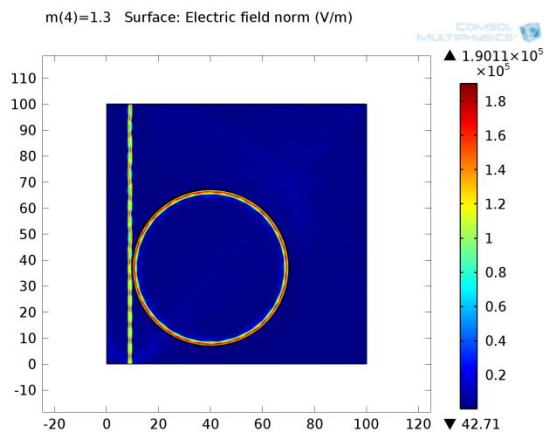


Figure 13. Energy output for particles of different sizes in field generated by more compact nanostructured surface

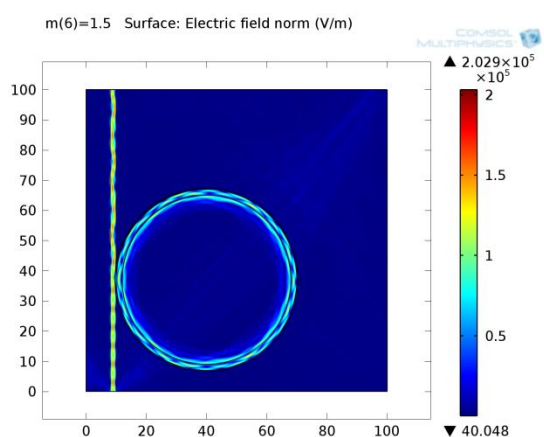
The refractive index of the material enclosed by the ring waveguide will also affect the detection sensitivity by altering the resonance pattern. Figure 14 shows that more energy will leak out of the ring when the refractive index of the enclosed space increases, leading to a decrease in detection sensitivity.



(a)



(b)



(c)

Figure 14. Refractive index of material enclosed by the ring affects the resonance pattern. Refractive index equals (a)1; (b) 1.3; (c)1.5

5. Conclusion

For the first time, we successfully combined WGM, SPR and SERS techniques in a single device by using COMSOL multiphysics modeling. The results show that the three techniques work in synergy and contribute to the improvement of detection sensitivity significantly. There is a good linear relationship between particle size and waveguide energy output, and this is true even when the particle is only several nanometers in size. This work provides new insight into how the distribution of energy in the photonic ring structure and the surrounding medium can affect the resonant behavior of a combined WGM/SPR/SERS detection device. By tuning a proper frequency we can significantly improve and optimize the detection sensitivity.

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