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Plasmon resonance spectral peak shift due to morphing of gold nanoparticles for strain sensing

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ABSTRACT

The plasmon resonance spectral peak of a gold spherical nanoparticle (NP) will shift when the NP shape is changed from sphere to spheroid. This may be used as a novel strain detection method with gold NPs embedded in a medium of different refractive index (RI). Applying a strain to the external medium will cause a change in the shape of the NP from spherical to spheroidal. In our previous work, it was found that when the RI change of the medium surrounding the NPs is close to zero, the shape change induced plasmon resonance spectral peak shift will become important. In order to obtain only the wavelength shift values caused by the shape change of the NPs, the RI of medium surrounding the gold NPs is set at a constant of 1.45 and the RI of the gold NP is assumed unchanged. The T-matrix method is used to calculate the scattered light and light extinction by the NP morphing. The diameters of the gold NPs are set from 100 nm to 400 nm, with the size interval at 10 nm, to cover a wide size range for typical sizes of gold spherical NPs. The spectra of the light scattering and light extinction were calculated on the Delft University high performance computing cluster. The results show that the plasmon resonance spectral peak shift is related to the size of the NPs. Larger sizes of gold NPs have larger peak shift values, but there is an inflection point around 200 nm and the bandwidth of the resonance peak becomes larger which will cause a difficulty in precisely locating the peak.

Keywords: Strain sensing, gold nanoparticle, plasmon resonance, spectral shift

1. INTRODUCTION

One of the types of Structural Health Monitoring (SHM) for aerospace is strain based SHM¹ by evaluating strain or loading distribution. Developing novel strain sensing methods is important for SHM. Fibre optic sensors have the advantages of small size, low weight, immune to electromagnetic interference and capable for embedding into materials² that have been widely used as the sensors for SHM.³

Nanoparticle (NP) doped optical fibres have attracted the interest of some researchers^{4,5} and have been used for increasing the backscattered light for fibre optic sensors. Gold is one of the materials to dope into the optical fibre to increase the scattered light in infrared light range. Meanwhile, there are plasmon resonance spectral peaks generated by the extinction of the gold NPs in the visible light or near infrared light range which could be used for strain sensing if the intensity or the spectral peak shift is related to the shape change of the NPs.

In our previous work, it was found that the spectral peak may shift under axial strain. In addition, when the refractive index (RI) change of the medium surrounding the NPs is close to zero, the shape change induced plasmon resonance spectral peak shift will become important. Therefore, in order to obtain only the wavelength shift values caused by the shape change of the NPs, in this paper the RI of medium surrounding the gold NPs is set at a constant of 1.45 which is similar to the RI of fused silica in visible and near infrared light range and the RI of the gold NP is assumed unchanged. The T-matrix method⁶ is used to calculate the scattered light and light extinction by the NP morphing.

This paper includes four sections. The first section is the introduction. The methods for the simulation will be illustrated in the second section which is followed by the results section. The fourth section is conclusion.

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2. METHOD

Figure 1 is used to describe the conditions of a gold NP under strain change. The original gold NP is a spherical gold NP with a radius r . When the shape of the NP is deformed with axial strain in Z direction, the spherical gold NP changes its shape to spheroidal NP. One half axis of the spheroidal NP is defined as c and the other two half axes are defined as a . ϵ is the strain in Z direction. The Poisson's ratio γ is used to determine the transverse profile shape change as shown in Figure 1. The surrounding medium with the RI at 1.45 is assumed unchangeable under strain. Light is propagating from the left side of the NP to the right side of the NP along Z direction with X polarisation as shown in yellow arrow.

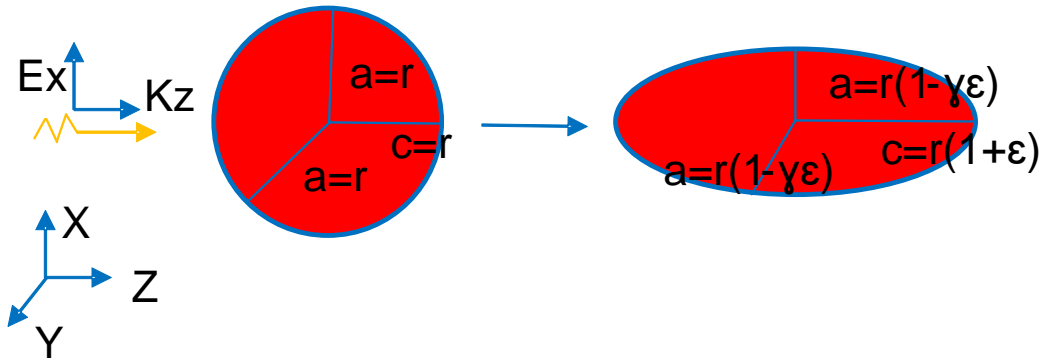


Figure 1: Shape change of gold NPs for simulation from spherical NPs to spheroidal NPs.

The RI of gold NP is assumed unchangeable under strain and the RI was calculated by the Scaffardi's RI model^{7,8} to calculate the RI of different size of spherical NPs (100 nm to 400 nm, with the size interval at 10 nm). The extinction of gold NPs was calculated by the T-matrix method.⁶ The peak wavelengths of the extinction spectra were obtained by finding the wavelengths corresponding to the maximum values of the peaks. The resolution of wavelength was set at 0.1 nm. The resolution of strain was set at 100 $\mu\epsilon$. The spectral peak shift at 0 strain was obtained by calculating the derivative at 0 of the 2-order polynomial fitting function of the peak wavelengths with strain values.

Because the T-matrix calculation is time-consuming, the Delft University high performance computing clusters (20 CPUs (Central Processing Units)) were used for the calculation for about 1 month. The simulated results will be shown in the next section.

3. RESULTS

The extinction spectra of the 100 nm, 150 nm, 200 nm, 250 nm, 300 nm, 350 nm, and 400 nm were evaluated respectively. Figures 2 to 8 show the simulated results.

Figures 2 (a) shows the extinction spectra of 100 nm size gold NP under strain with the spectra range from 300 nm to 2000 nm. There is a spectral peak (around 595 nm) in visible light range. Figures 2 (b) shows the spectral shift of the peak under strain. When the strain increases, the wavelength of the peak has a blue shift.

Figures 3 (a) shows the extinction spectra of 150 nm size gold NP. The wavelength of the spectral peak is around 680 nm at 0 strain. The bandwidth of the peak becomes broader than the results shown in Figures 2 (a). Figures 3 (b) shows the spectral shift of the peak under strain. The value of the spectral peak shift increases compared with the results shown in Figures 2 (b).

With the size of the NPs increase, more resonance spectral peak generated as shown from Figures 4 (a) to 8 (a). In order to compare the results with 100 nm and 150 nm size gold NPs. The higher order resonance spectral

peaks were not taken into comparison. The spectral peak shift increases and then decreases when the size of the NPs increases.

In order to show the exact values of the spectral peak shift under strain of different sizes of the NPs, the spectral peak shift results were listed in Table 1. In order to show the spectral peak shift change tendency of different sizes of NPs, Figure 9 was plotted. It can be seen from Figure 9 that there is an inflection point around 100 nm size of gold NP which has the most obvious spectral peak shift with in simulated size range.

The relationship between the spectral peak shift and the strain is not a linear function. Especially when the strain values are large for example near 0.1, the non-linearity is obvious.

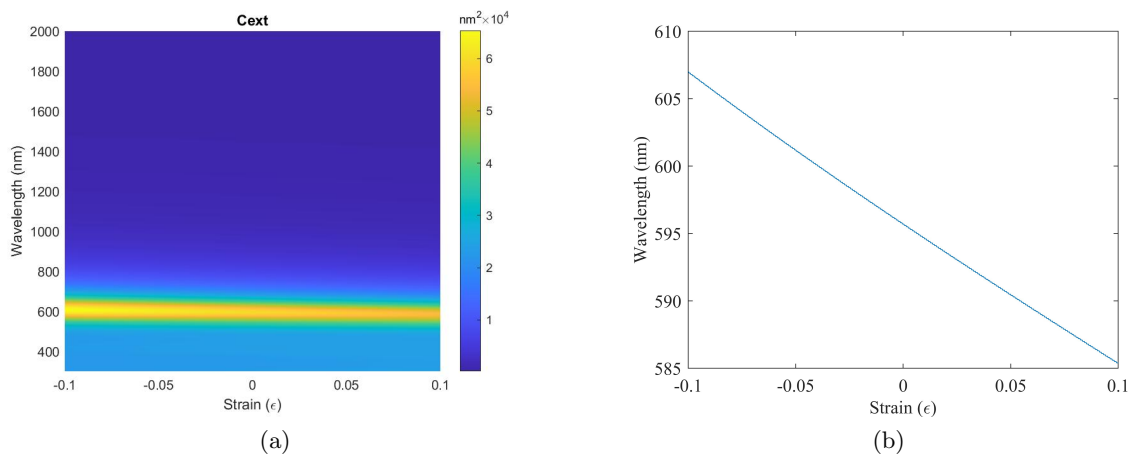


Figure 2: Extinction spectra and peak shift of 100 nm gold NP. (a) Extinction spectra; (b) Spectral peak shift.

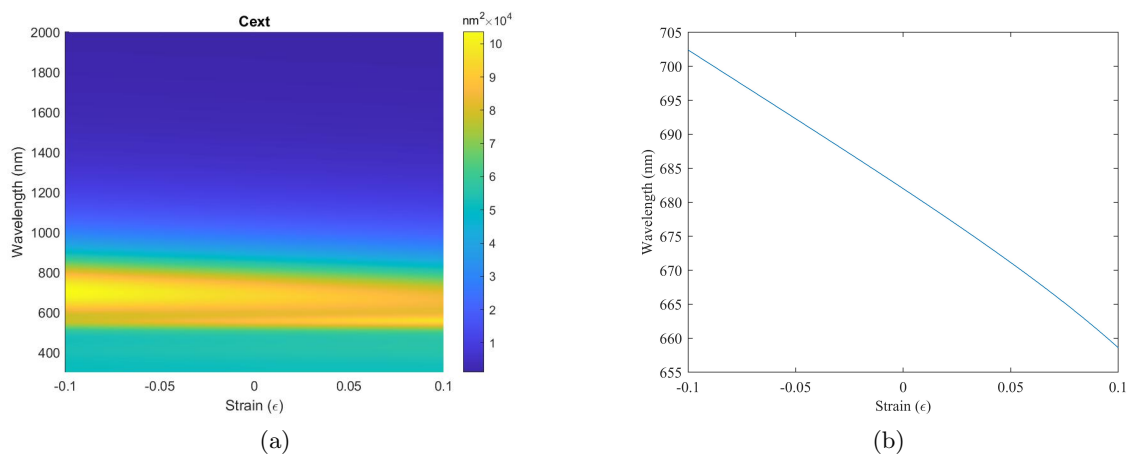


Figure 3: Extinction spectra and peak shift of 150 nm gold NP. (a) Extinction spectra; (b) Spectral peak shift.

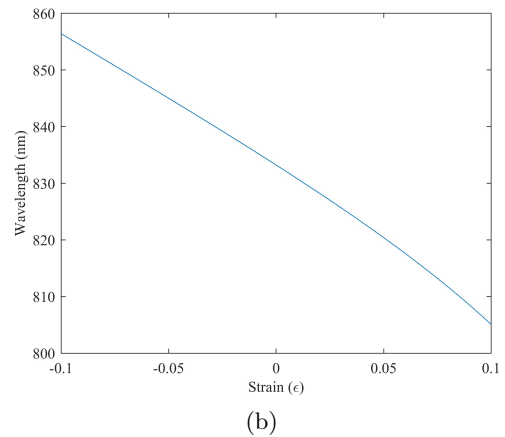
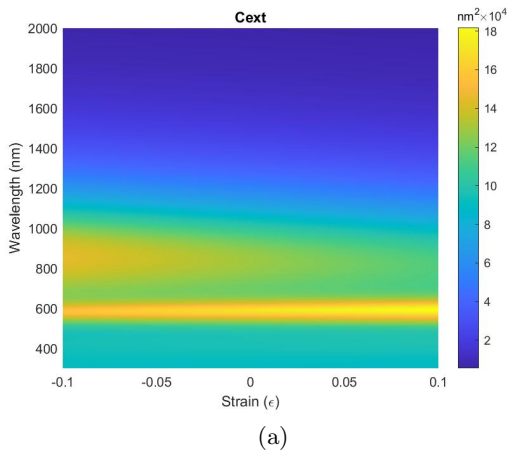


Figure 4: Extinction spectra and peak shift of 200 nm gold NP. (a) Extinction spectra; (b) Spectral peak shift.

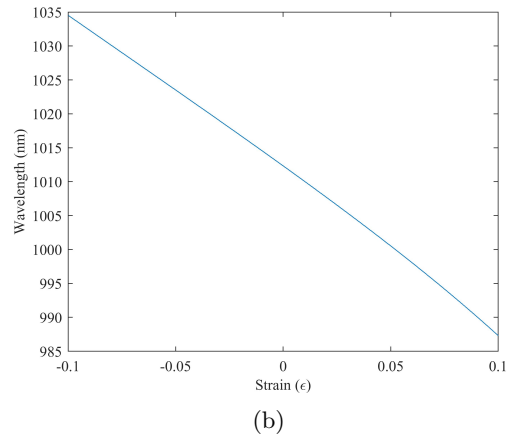
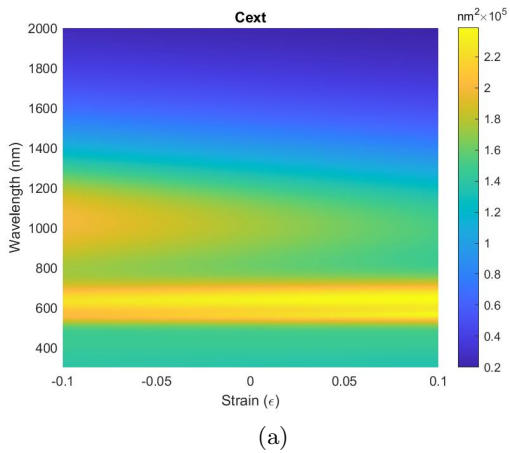


Figure 5: Extinction spectra and peak shift of 250 nm gold NP. (a) Extinction spectra; (b) Spectral peak shift.

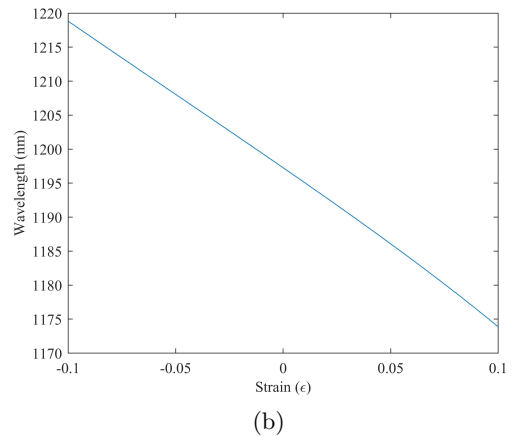
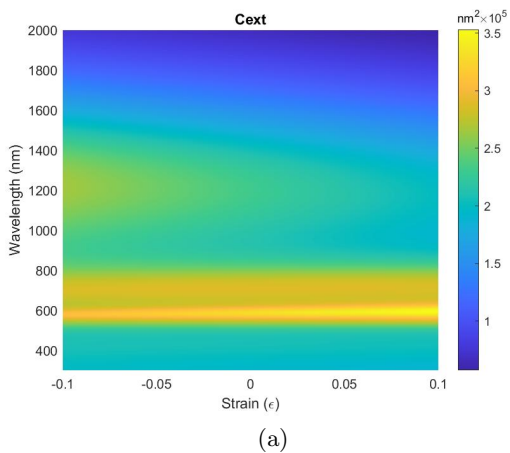


Figure 6: Extinction spectra and peak shift of 300 nm gold NP. (a) Extinction spectra; (b) Spectral peak shift.

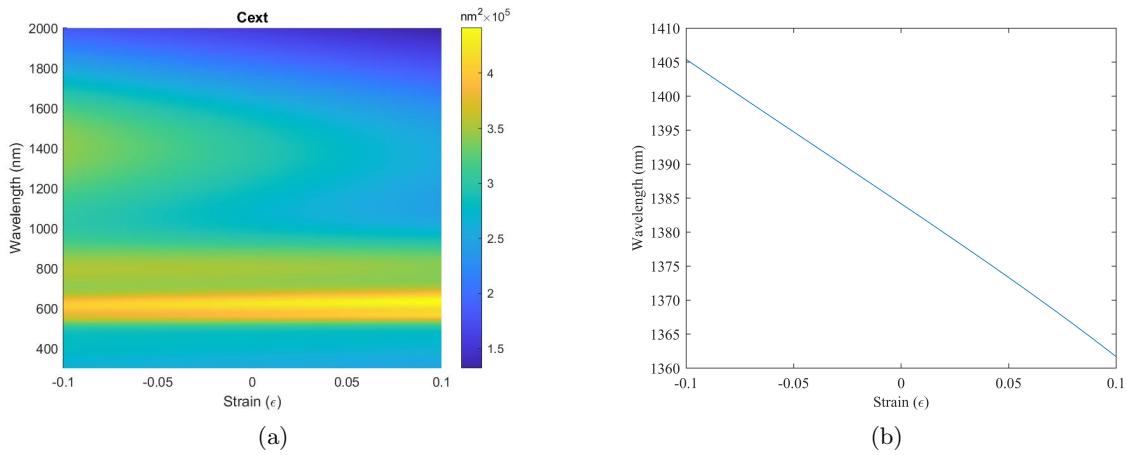


Figure 7: Extinction spectra and peak shift of 350 nm gold NP. (a) Extinction spectra; (b) Spectral peak shift.

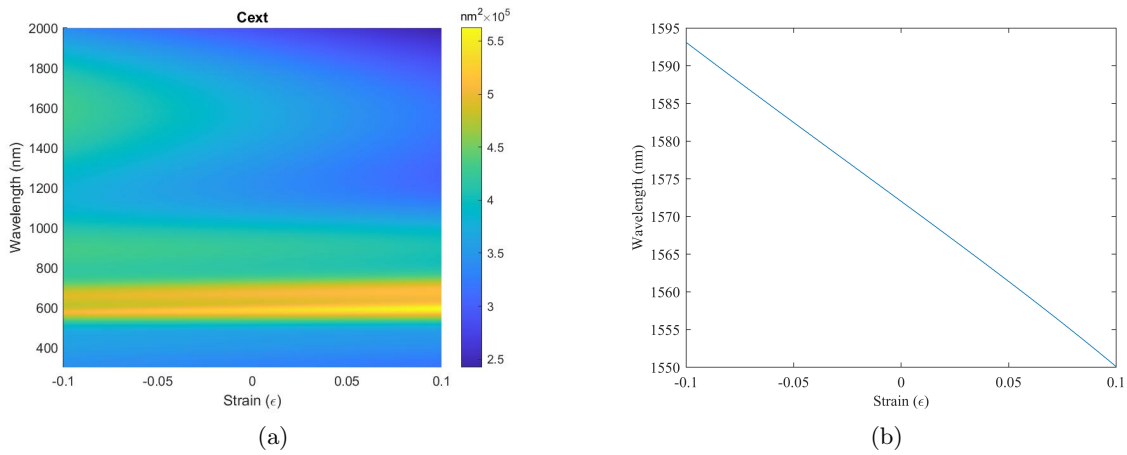


Figure 8: Extinction spectra and peak shift of 400 nm gold NP. (a) Extinction spectra; (b) Spectral peak shift.

Table 1: Spectral peak shift of gold NPs.

NP size	Spectral peak shift
100 nm	$-0.1077 \text{ pm}/\mu\epsilon$
150 nm	$-0.2148 \text{ pm}/\mu\epsilon$
200 nm	$-0.2509 \text{ pm}/\mu\epsilon$
250 nm	$-0.2328 \text{ pm}/\mu\epsilon$
300 nm	$-0.2222 \text{ pm}/\mu\epsilon$
350 nm	$-0.2163 \text{ pm}/\mu\epsilon$
400 nm	$-0.2129 \text{ pm}/\mu\epsilon$

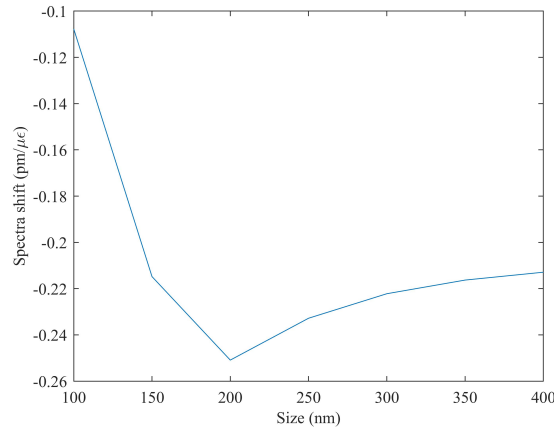


Figure 9: Spectra shift

4. CONCLUSION

Plasmon resonance spectral peak shift is related to the size of the NPs. Larger sizes of gold NPs have larger peak shift values, but there is an inflection point around 200 nm. The bandwidth of the resonance peak becomes larger when the size of gold NPs increases, which will cause a difficulty in precisely locating the peak. Although the spectral peak shift under strain is small, it may be an alternative method for strain detection.

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