Optimizing bowtie structure parameters for specific incident light*

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We investigate optical properties of a bowtie-shaped aperture using the finite difference time domain method to optimize its geometric parameters for specific incident lights. The influence of the parameters on local field enhancement and resonant wavelength in the visible frequency range is numerically analysed. It is found that the major resonance of the spectrum is exponentially depended on the bowtie angle but independent of the whole aperture size. The simulation also demonstrates that increasing the aperture size raises the local field intensity on the exit plane due to an enlarged interaction area between the light and the metal medium. And the near-field spot size is closely related to the gap. Based on these results, the design rules of the bowtie structure can be optimized for specific wavelengths excited.

Keywords: bowtie aperture, localized surface plasmons, finite difference time domain method
PACC: 7320M, 5240D, 7360D

1. Introduction

Due to fascinating optical properties, interaction between lights and nanostructures has received great attentions, particularly in scanning near-field optical microscopy (SNOM),[1,2] nanolithography,[3,4] and surface-enhanced Raman scattering,[5,6] as well as concept designs of waveguides[7,8] and nano-optical devices[9,10] recently. Properly designed nanostructures are able to concentrate light into a small volume with high intensity. As high as three orders of magnitude on the field enhancement have been achieved when the light is passing through two-dimensional arrays of nanoholes[11−13] or a single aperture with periodic rings surrounded.[14,15] However, the near-field spot size in those cases is not far beyond the wavelength of incident light due to the structural periodicity.

Alternatively, modified single structures such as C-shape,[16] H-shape[17,18] L-shape[19] and bowtie apertures[20−26] have been proposed to both reduce the spot size and enhance the local field intensity. The focused tiny spot much smaller than the diffraction limit holds the promise for applications in nanolithography or high density data storage where a large amount of information is required. Among these researches, the bowtie aperture, for its extraordinary ability of light concentration and enhancement, has been widely studied numerically[20−22] and experimentally.[23−26] Recently, for example, a linewidth as narrow as 24 nm was written on a positive photoresist coated sample making use of a bowtie aperture modified on an atomic force microscope (AFM) probe.[2] The extraordinary light focusing and enhancement are attributed to the excitation of localized surface plasmons (LSPs), the collective oscillations of conductive electrons bounded by special geometry and confined on the surface. The LSP mode helps to efficiently deliver the photon energy from entrance to the exit side of the aperture. The local field intensity is therefore enhanced.

In fact, the response property of a nanostructure varies with its geometric shape. The optical resonance modes will be excited when the incident light is tuned to match the optical resonant wavelength of the structure. However, altering the exciting wavelength is inconvenient, particularly for certain lithography applications. Hence, the better way to obtain the maximal field intensity should be the option of the nanostructures, or in other words, optimisation of geometric parameters of a bowtie aperture. Nevertheless, detail analysis and optical property comparison for field en-

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hancement and mode resonance as a function of geometrical parameters have not been completely carried out. The aim of this work is to provide a guide for design and optimisation of a bowtie aperture for various applications.

The paper is organized as follows. In Section 2, the model and method applied are introduced briefly. In Section 3 we analyse the optical resonant characteristics of the bowtie aperture with various geometric parameters. The simulation results are discussed as well. Finally, a conclusion is presented in the last section.

2. Model and method

A bowtie aperture is composed of two open arms with a narrow gap in a free standing silver film. The geometry of the bowtie aperture is determined by two characteristic outline lengths, a and b, the gap S, the bowtie flare angle θ, and the film thickness t, as shown in Fig. 1. The effect of a dielectric substrate on such an aperture has already been studied.[27]

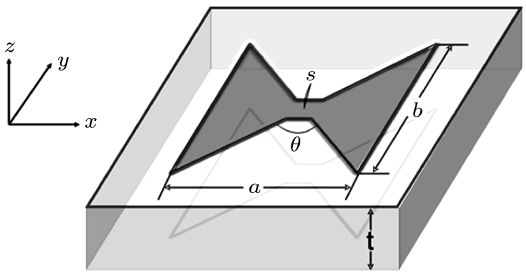


Fig. 1. Schematic view of the bowtie aperture in a free-standing metal (silver) film.

The dielectric constant of the metal (silver in this case) as a function of the incident exciting frequency ω, can be approximated by the Drude model

$$\hat{\varepsilon}(\omega) = \varepsilon_1 + \mathrm{i}\,\varepsilon_2 = 1 - \frac{\omega_\mathrm{p}^2}{\omega^2+\gamma^2} + \mathrm{i}\,\frac{\omega_\mathrm{p}^2\gamma^2}{\omega(\omega^2+\gamma^2)}, \quad (1)$$

where $\hat{\varepsilon}$, ω_p, γ represent the complex permittivity, plasma frequency, and damping rate of the metal respectively. At the visible regime, $\omega_\mathrm{p} = 3.8$ eV and $\gamma = 0.4$ eV have been applied, according to experimental data for silver.[28]

The finite difference time domain (FDTD) method is first benchmarked in comparison with Mie's theory on a spherical particle at the optical frequency and then applied to simulate the optical resonance characteristics of the aperture. A computational domain of 880 nm×880 nm×260 nm in x, y, z directions correspondingly is divided into small cells of 2 nm×2 nm×2 nm. For complete absorption of the waves, perfectly matched layers (PML) are applied on the boundary at all directions.

A modulated Gaussian plane wave with a central frequency of 3.75×10^{14} Hz is cast on the top of the silver film along the $-z$ direction. The incident field E_0 is linearly polarized across the narrow gap for exciting LSP modes in bowtie tips, crucially for the field enhancement. Due to its weak damping (small imaginary part of the permittivity), silver is adopted other than any metals else. Fast Fourier Transform (FFT) algorithm is employed for both the probe and the incident fields to effectively analyse the optical response of the bowtie aperture as light passes through. All apertures have a 60 nm thickness and the recorded dot is 5 nm below the centre of the exit plane.

3. Results and discussions

It is well known that geometry of a nanostructure strongly affects its optical property. Our numerical simulation is thus focused on the resonance properties in the visible regime. The near-field spectra with different bowtie angles of 60° and 90° are calculated. In the calculation, the outline length a varies in a range of 140 nm to 220 nm, in every 20 nm, while the bowtie gap is fixed as $S = 4$ nm×4 nm. The other length b is determined by S, θ, and corresponding a. There are then two resonance peaks found in the visible light frequency range and the major intensity peak can be as high as 650 times of the incident field as shown in Fig. 2. Each resonance is related to a specified mode in near-field while the major is a LSP mode bounded by the tips. For the same bowtie angle and gap, the position of the major resonant wavelength remains the same as the outline length a increasing, indicating this resonance is independent of the length a, i.e., the size of the aperture open. In addition, the calculated peak intensity increases with the outline length due to the fact that an enlarged light-metal interaction area can excite more electrons for the LSP mode near the metal tips.

The simulated near-field spectrum for the bowtie angle of 90° with various outline lengths shows a major resonance peak at a wavelength of 524 nm. At the resonance, the electric field intensity distribution in the plane 5 nm below the exit for different outline lengths a is recorded in Fig. 3. The LSP mode is localized near the gap between the two metal tips, producing a nanometer-sized light spot. The maximum intensities

confined for $a = 140$ and 220 nm are found to be 237 and 762 times higher than the incident light intensity respectively. In both cases, the measured near-field light spots have a full width half maximum (FWHM) of 10 nm and 14 nm in x and y directions respectively, well below the diffraction limit at a wavelength of 524 nm. The calculation also indicates that the resolution of the bowtie aperture is closely related to the gap rather than the global structure. Consequently enlarging the aperture size is an effective method to increase the field intensity with the focused light spot unexpanded.

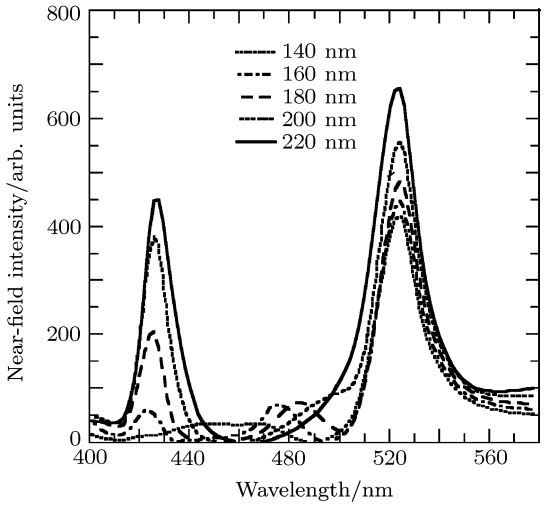


Fig. 2. The near-field intensity as a function of outline lengths a and incident wavelength. The outline length a varies from 140, 160, 180, 200, to 220 nm, as the gap and the bowtie angle are fixed at $S = 4$ nm×4 nm and $\theta = 90°$.

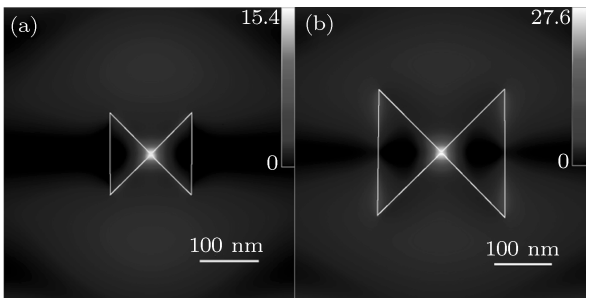


Fig. 3. The distribution of the electric field amplitude in a parallel plane 5 nm below the aperture exit with different outline lengths: (a) $a = 140$ nm; and (b) $a = 220$ nm.

The spectral position of the resonance remains unchanged for the same angle θ with various outline size. To further study the principle of the structure, we will concentrate on the other structural parameters hereafter. Figure 4 shows the near-field spectra for the apertures of various bowtie angles: 30°, 60°, 90° and 120° with a fixed outline length $b = 180$ nm. For decreased bowtie angle, the major resonance shows a red-shift from ∼ 500 nm to ∼ 610 nm. And stronger field enhancement can be achieved with larger angles owing to the enlarged light-metal tip interaction area. Notice that for the angle of $\theta = 60°$, the resonant wavelength is 550nm, in accordance with the resonance peak of the same angle for different outline lengths a (see, for example, Fig. 6(a) below), indicating that the resonance is closely related to the bowtie angle in the visible frequency.

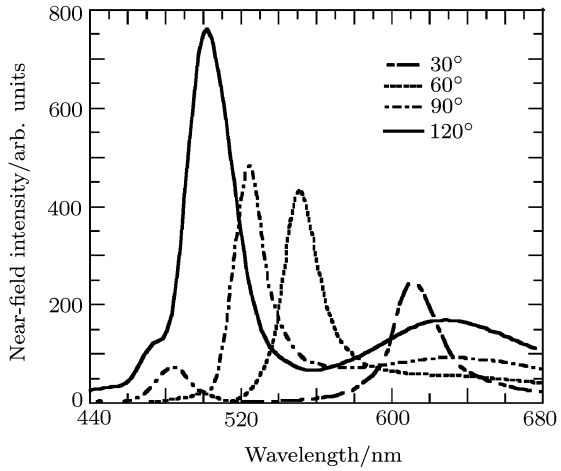


Fig. 4. The near-field spectra in various bowtie angles with a constant outline length $b = 180$ nm, while the gap is $S = 4$ nm×4 nm.

The gap S also plays an important role in the electric field enhancement. The near-field spectra with

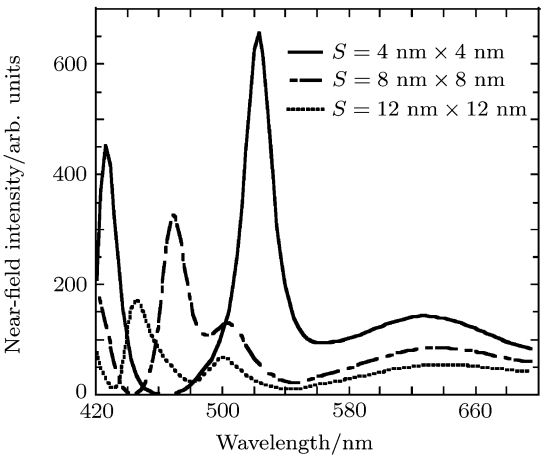


Fig. 5. The near- field spectra in various gaps S, while other parameters are fixed as $\theta = 90°$ and $a = 220$ nm.

different gaps of $S = 4$ nm×4 nm, 8 nm×8 nm, 12 nm×12 nm are illustrated in Fig. 5, while other parameters are kept constant except the outline length b. It is found that the smaller the gap is, the greater field enhancement will be due to stronger coupling of LSP modes between the neighbour tips. For decreased

gap width the strength between the two arms is enhanced and thus the resonant wavelength shows a red-shift just as experimentally observed by Rechberger *et al.*[29]

Near-field spectra with various bowtie angles for the same light throughout area of the apertures are shown in Fig. 6(a). The peak enhancement decays as the bowtie angle decrease, and the resonant wavelength has a red-shift. It is properly due to the fact that the metal tip is sharper for smaller bowtie angles, and thus the strength between the tips is enhanced. The phenomenon is already numerically demonstrated by Fischer and Martin[30] for dipole and bowtie antennas.

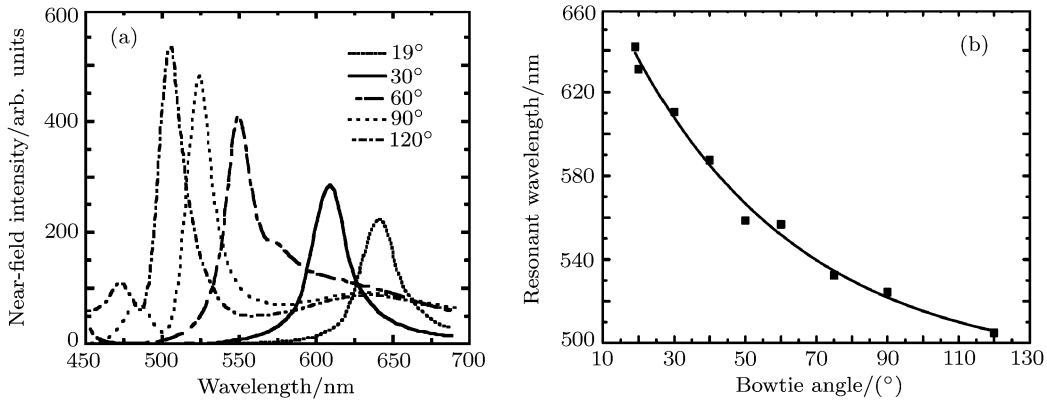


Fig. 6. (a) The near-field spectra in various bowtie angles θ with the same throughout area of the aperture, as well as $S = 4$ nm×4 nm, $a = 220$ nm; (b) the exponential dependence of the resonant wavelength on the bowtie angle.

Clearly, the resonance wavelength is strongly depended on the bowtie angle θ and the gap S, possibly due to the LSP modes confined near the tips being sensitive to the surrounding. Meanwhile, the aperture outline variation hardly either affects the LSP modes at the two tips or causes any shift in resonance.

We also find an exponentially dependence of the resonant wavelength on the bowtie angle θ as shown in Fig. 6(b). A resonant wavelength of 631 nm can be obtained with a bowtie angle of 20° for a He–Ne laser cast.

4. Conclusions

We have numerically investigated the mechanism of field enhancement and resonant wavelength of the bowtie aperture with various geometry parameters. Effects of the bowtie angles, outline lengths, and gaps on the mechanism have been analysed respectively.

We have found that:

High intensity spots can be generated below the aperture by increasing the outline length, because increased conductive electrons are excited in coupling to the LSP mode;

The main resonance is strongly depended on the bowtie angle and gap for the LSP mode being sensitive to the environment nearby;

Varying the outline length does not affect the LSP mode at the tips, so that the resonance wavelength remains unchanged also;

An exponentially blue-shifting relation between the resonant wavelength and the bowtie angle is also revealed for constant light throughout area;

Furthermore, a resonant wavelength of 631 nm can be realized for the He–Ne laser applied.

It is well known that various bowtie geometry structures can generate different LSP modes in helping to deliver energy from the entrance to the exit side of a bowtie aperture. As an LSP mode resonantly excited, enhanced electric field intensity is observed. Based on the simulation results, in the visible light range one can summarize the design basis for geometric parameters of bowtie apertures for particular applications in high resolution and field enhancement. First, the gap should be set small enough to reduce the spot size as well as to increase the coupling between the two tips of the bowtie. Then, by choosing a certain bowtie angle, the desired wavelength is obtained ranging from 500 nm to 650 nm. The range can also be enlarged further by adjusting the bowtie angles. On the other hand, if possible, the outline size of the aperture should be increased to improve the local field intensity.

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