Dependence of resonant wavelength on the width of subwavelength metallic slits: analysis and modulation

Xu-Sheng Lin¹,²*, Jun-Hu Yan¹, Yun-Bao Zheng¹, Li-Jun Wu², Sheng Lan²
¹School of Electronic and Information Engineering, Guangdong Polytechnic Normal University, Guangzhou 510665
²Laboratory of Photonic Information Technology, School for Information and Optoelectronic Science and Engineering, South China Normal University, Guangzhou 510006

E-mail: xslin64@yahoo.cn

Abstract The variation trend of the resonant wavelength of a subwavelength metallic slit with respect to its width has been investigated by using the Fabry-Perot model. It is determined by two antagonistic factors related to the effective refractive index and the phase of reflection. We show that the trend can be changed by directly modulating the dielectric constant of the structure. Our analysis is supported by the numerical simulation based on the finite-difference time-domain technique.

1. Introduction
Surface plasmon polaritons (SPPs) are electromagnetic waves coupled to the oscillation of the collective electrons at metal surfaces. As one of the SPP-based waveguides, metal-dielectric-metal (MDM) structures recently attract much attention due to their subwavelength characteristic, i.e., guiding of light below the diffraction limit that is essential for nanochip-scale circuits [1-4]. In such waveguides, the SPP modes are called “X-ray waves” with optical frequencies because of their much shorter wavelengths than those in vacuum. Keeping this unique property in mind, researchers are now interested in developing MDM waveguide-based devices for manipulating light on the nanoscale, such as optical couplers across the nano-micro interfaces [5, 6], ultra-compact waveguide bends and splitters [7, 8], high resolution tunable filters [9, 10], and subwavelength all-optical switchers [11-14].

It is noted that many of the above device structures are based on the truncated MDM waveguides, which are also called slit resonators. Due to the complicated optical properties of metals, it is difficult to express explicitly the relationship between the resonance properties (the resonant wavelength, the peak transmission, and the quality factor of resonance, etc.) and the geometric and material parameters of the structures. Thus, intuitive models that reflect or describe the properties of the resonators are very helpful. One of them is the Fabry-Perot model that is widely used and proved to be effective [15-24], especially the corrected version that adopts the effective refractive index and the phase of reflection [18, 19, 22-24]. Due to the drop of the effective refractive index, the resonant wavelength undergoes a blue-shift with the increase of the slit width. However, as the slit width increases further, it can turn to a red-shift, showing a V-shape dependence [17, 23]. Although many optical properties of single slit resonators have been investigated, this phenomenon is still not explained properly. As the variation pattern of resonant wavelength is an important aspect of the SPP resonator design, it is

* To whom any correspondence should be addressed.
worthy of being investigated in detail. Here, we show that the phenomenon can be explained by using the concepts of the effective refractive index and the phase of reflection. As the phase of reflection cannot be expressed in an intuitive way such as the direct use of Fresnel’s formula, people turn to rely on numerical calculations or simulations for better understanding [18, 22, 23]. We find that with the assistance of the results from the perfect electric conductor (PEC) cases, one can easily find out the influence of the phase of reflection and understand the variation pattern of the resonant wavelength.

2. Analysis and Simulation

The MDM resonator studied in this paper is shown in the inset of Fig. 1. It consists of a free-standing silver film with one isolated subwavelength slit that is filled with a dielectric. We use \( t \) and \( w \) to denote the thickness and width of the slit, while the permittivity of silver and the dielectric are represented by \( \varepsilon_{\text{Ag}} \) and \( \varepsilon_d \) respectively.

![Figure 1. Output transmission spectra of the Ag slit measured at 0nm, 50nm and 100nm above the outlet of the slit. Geometrical and material parameters are: \( t=100\text{nm}, w=20\text{nm}, \varepsilon_d=1 \). Inset is the structure of the slit resonator studied.](image)

Normally, both the surface plasmonic and conventional optical modes can be excited in MDM waveguides. However, when the slit width drops to deep subwavelength, only the fundamental SPP modes with even magnetic distribution can be accessed [3]. They are TM modes whose magnetic field parallel to y-axis. If we neglect the imaginary part of \( \varepsilon_{\text{Ag}} \), the dispersion of the fundamental SPP modes can be written as [3]

\[
\tan \left( k_{0} w \left( \frac{n_{\text{eff}}^2 - \varepsilon_d}{w} \right)^{1/2} \right) = \frac{\varepsilon_d}{-\varepsilon_{\text{Ag}}} \left( \frac{n_{\text{eff}}^2 - \varepsilon_{\text{Ag}}}{n_{\text{eff}}^2 - \varepsilon_d} \right)^{1/2} \tag{1}
\]

where \( k_{0} = \frac{2\pi}{\lambda_0} \) and \( \lambda_0 \) is the wavelength of light in vacuum, \( n_{\text{eff}} \) is the effective refractive index of the SPP mode. Once \( n_{\text{eff}} \) is obtained from Eq. 1 and Fabry-Perot resonant condition is fulfilled, we have

\[
\lambda_0 = \frac{2 n_{\text{eff}} t}{m - \delta} \tag{2}
\]

where \( m \) is the resonance order and \( \delta \) is the phase of reflection (unit: \( \pi \)) obtained at the slit entrance. It is noted that \( m \) is valid for physical sense. Although the width of slit, \( w \), does not appear in Eq. 2, it affects the location of \( \lambda_0 \) through \( n_{\text{eff}} \) and \( \delta \). To estimate the variation trend of \( \lambda_0 \) with respect to \( w \), it would be more convenient when the derivative of Eq. 2 is used. That is

\[
\frac{1}{\lambda_0} \cdot \frac{d\lambda_0}{dw} = \frac{1}{n_{\text{eff}}} \cdot \frac{dn_{\text{eff}}}{dw} + \frac{1}{1 - \delta} \cdot \frac{d\delta}{dw}. \tag{3}
\]
Here, we focus on the subwavelength resonators possessing only one resonance \((m=1)\). It is expected that \(\frac{dn_{ef}}{dw}<0\) and \(\frac{d}{dw}>0\), so the variation of \(\gamma\) with respect to \(w\) is decided by the “bout” of the two antagonistic factors, i.e., \(n_{ef}^{\gamma}\frac{dn_{ef}}{dw}\) and \((1-\gamma)^{\frac{d}{dw}}\). Thus, the balance of them leads to \(\frac{d}{dw}=0\). We consider it the reason why a maximum resonant frequency or a minimum resonant wavelength can be obtained \([17, 23]\).

To verify the above assumption, we carry out numerical simulations of Maxwell equations based on the finite-difference time-domain method. Since recent investigation has shown that the length of metallic slit has little influence on the resonant wavelength positions \([4]\), we simulate the two-dimensional slit structures instead of the three-dimensional ones for saving the computational time. The simulation domain is \(3\mu m \times 3\mu m\) surrounded by perfectly matched layers of \(0.2\mu m\) width. Spatial grid and temporal interval are set to be \(2\)nm and \((1/c)\)ns, respectively, where \(c\) is the speed of light in vacuum. As for the permittivity of Ag, we employ the Drude model plus two-pole Lorentzian form that shows a good description of empirical data over the wavelength range of 250nm to 1000nm \([8]\). Very short TM Gaussian pulse with centre wavelength at \(1\)\(\mu m\) is launched normally from the position of \(z=-0.1\mu m\) (below the slit). By setting monitors at the outlet of the slit, we can numerically measure the transmission spectrum and obtain the resonant wavelength of the metallic slit. One example in which \(t=100\)nm, \(w=20\)nm, and \(\lambda_{0}=1.00\) is shown in Fig. 1. The three spectra are measured at different positions (\(0\)nm, \(50\)nm and \(100\)nm) above the outlet. Since \(w\) is in deep subwavelength, only one resonant peak corresponding to the fundamental mode is excited. The peaks that correspond to the resonant wavelength appear at about \(0.565\mu m\), exhibiting weak dependence on the measuring position.

By repeating the above simulation for different slit widths, one can obtain the relationship between \(\gamma\) and \(w\) for a given thickness of slit. When the slit is filled with air, i.e., \(\epsilon_{s}=1.0\), the simulation results are depicted in Fig. 2 with solid circles. We can see that \(\gamma\) first drops and reaches its minimum at \(w=50\)nm. Then, it begins to rise when \(w\) increases further. The trend is the same as those shown in Refs. \([17, 23]\).

It has been suggested that two opposite factors are in action, as manifested in Eq. 3. Here we present a more detailed discussion. When the condition of \((k_{0}w) \cdot 0.5\) is fulfilled, which is valid for the case we study, one can easily derive the following relation from Eq. 1

\[
\frac{dn_{ef}}{dw} = -\frac{4}{\epsilon_{s}} \left(\frac{-\epsilon_{s}}{-\epsilon_{Ag}}\right)^{2}.
\]

Obviously, it shows that \(\frac{dn_{ef}}{dw}<0\) and \(\eta_{g}\) is very sensitive to \(w\) when \(w\) is small. One the other hand, in spite of the difficulty of deriving an analytical relation between \(\gamma\) and \(w\), we find it helpful to consider the perfect electric conductor (PEC) case, i.e., \(\eta_{g}=•••\). From Eq. 4, one finds \(\frac{dn_{ef}}{dw}=0\) for the PEC case. Thus, according to Eq. 3, we have

\[
\frac{d\delta}{dw} = \frac{2n_{ef}}{\lambda_{0}} \frac{d\lambda_{0}}{dw}.
\]

In Fig. 2, the relationship between \(\gamma\) and \(w\) obtained by FDTD simulation for the PEC case of \(\eta_{g}=1.0\) is depicted by dashed line. It shows that \(\gamma\) increases monotonously with \(w\). Actually, \(\gamma\) is almost proportional to \(w\), i.e., \(\frac{d}{dw}\) is a constant, which is in good agreement with the results given in Ref. \([19]\). Therefore, \(\frac{d}{dw}>0\) and \(\gamma\) shows weak dependence on \(w\) according to Eq. 5. We can conclude that \(\frac{dn_{ef}}{dw}\) plays a dominant role so \(\gamma\) decreases with \(w\) when \(w\) is very small. With increasing \(w\), \(\frac{dn_{ef}}{dw}\) begins to decrease and its action is balanced gradually by \(\frac{d}{dw}\). \(\frac{d}{dw}\) becomes dominant at larger \(w\) and as a result the dependence of \(\gamma\) on \(w\) is changed. In Fig. 2, it is true that the dependence of \(\gamma\) on \(w\) exhibits similar trend to the PEC case, implying that it is governed by the phase of reflection.
From the above discussion, we find that the dependence of $\lambda_0$ on $w$ can be engineered by modifying $d_\delta/dw$ and $dn_{\text{eff}}/dw$, which have completely different contributions. Two extreme cases are $\lambda_0$ increases or decreases monotonously with $w$. The former corresponds to the situation of large ($-\varepsilon_{\text{Ag}}$), similar to the PEC case shown in Fig. 2. The latter occurs for small $d_\delta/dw$. We find that one simple method to reduce $d_\delta/dw$ is to fill the slit with an insulator possessing a large refractive index. Fig. 3 shows the simulation results for $n_d=2.00$. Comparing with the case of $n_d=1.00$, $\lambda_0$ reaches its minimum at a larger $w(=100\text{nm})$ and it rises much more slowly after the minimum. This can be attributed to the smaller $d_\delta/dw$ caused by the larger $n_d$. Similarly, we can make a better understanding by comparing the PEC case, which is also depicted in Fig. 3. Apparently, $d_\delta/dw$ (thus $d_\delta/dw$) is much smaller than that in the case of $n_d=1.00$.

A further increase of $n_d$ to 3.45, which is the refractive index of GaAs or Silicon, makes the situation totally different. The results are shown in Fig. 4. The major difference between Fig. 4 and Fig. 3 is that $\lambda_0$ no longer increases with $w$. According to our simulation results, this trend does not change even when $w$ becomes much larger than 200nm (not shown here). It is suggested that the effect of the phase of reflection in this case is negligible. Actually, as can be seen from the PEC result in Fig. 4, $d_\delta/dw$ is very small and it reaches zero when $w$ is larger than 160nm.
Figure 4. Dependence of the resonant wavelength with the slit width of the Ag and PEC cases. It shows that the effect of the phase of reflection is negligible.

3. Summary
In conclusion, the effective refractive index and the phase of reflection have opposite effects on the variation trend of resonant wavelength with respect to the metallic slit width. Minimum resonant wavelength can be obtained when the two effects balance. Further more, the resonant wavelength can decrease monotonously with the slit width if the slit is filled with an insulator with a large refractive index.

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