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## A Trade-off between Propagation Length and Light Confinement in Cylindrical Metal-Dielectric Waveguides \*

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We theoretically investigate the hybrid plasmonic modes of cylindrical nanocables with gold nanocore and two dielectric nanolayers (SiO<sub>2</sub> and BN). By solving a complete set of Maxwell's equations, the propagation constants and effective radii depending on geometrical parameters are numerically calculated. By declining a trade-off between propagation length and light confinement, high quality hybrid modes which can travel a long range of  $120-200\lambda$  with a subwavelength effective radius are obtained at the optical wavelength. These modes in one-dimensional cylindrical waveguides should have potential applications in nanoscale optical device designs.

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Surface plasmon polaritons (SPPs) are light waves coupled to free electron oscillations in metal-dielectric interfaces. These waves are evanescent near surfaces, which makes it possible to localize and guide light in a subwavelength scale.<sup>[1,2]</sup> To guide SPPs, researchers have explored many plasmonic waveguide structures such as thin metal films, [3-5] metal stripes, [6-8] two dimensional metal-dielectric multilayers,<sup>[9,10]</sup> subwavelength metal grooves, [11-13] nanoparticle chains, [14]and cylindrical waveguides.<sup>[15–20]</sup> Although the optical energy is well confined, the propagation length will be greatly reduced because of the Ohmic loss in metals. In fact, there is a trade-off between light confinement and propagation length in all kinds of SPP waveguides. To solve this problem, a hybrid waveguide combining the advantages of both SPP modes and dielectric waveguide modes is suggested. With the coupling of plasmonic and dielectric waveguides, hybrid modes can be improved to achieve a long propagating length while keeping moderate light confinement in a 'capacitor-like' structure.<sup>[21,22]</sup>

SPPs in one-dimensional (1D) metallic cylindrical waveguides have been extensively studied. In the 1970s, the first experiment using light scattering to excite SPP modes in 50 µm metallic cylinders was performed<sup>[15]</sup> and also explained by means of the virtual radiative modes with a complex frequency.<sup>[16]</sup> Then, a clear mode classification in two-layer cylindrical waveguide structures was thoroughly investigated where only negative real dielectric constant was considered.<sup>[17]</sup> The SPP modes in a lossy cylindrical metallic nanotube with a dielectric core were used to model light propagation of a scanning near field optical microscope (SNOM).<sup>[18,19]</sup> Mode coupling and transformation of SPPs in a lossy metallic cylindrical nanocable were also studied.<sup>[20]</sup> However, in the above-mentioned works (Refs. [18-20]), instead of a clear distinction between pure propagating modes and evanescent modes, the SPP modes mediated between the propagating and evanescent modes and generally the evanescent part dominated. Due to the Ohmic loss, the propagation lengths of these nanoscale 1D metallic waveguides were decreased to a small range, which greatly limits the applications in nanoscale optical devices. The aim of this work is to find hybrid SPP modes with a long range propagation length and good light confinement in 1D metallic-dielectric waveguides.

In this work, a hybrid plasmonic waveguide composed of a gold nanocore and two dielectric nanolayers is proposed, as shown in Fig. 1. The inner dielectric layer SiO<sub>2</sub> has a low dielectric constant and the outer dielectric layer BN has a high dielectric constant. The whole system can be regarded as a gold nanocore nesting in a BN nanotube, so the SPP modes in a metallic nanowire can couple to the waveguide modes in a nanotube, leading to some hybrid SPP modes. By adjusting thicknesses of the layers, the high quality hybrid modes which can travel a long range of  $120-200\lambda$  and have a subwavelength effective radius can be achieved at the optical wavelength. These modes in 1D cylindrical waveguides should have potential applications in nanoscale optical device designs.

The solution of Maxwell's equations in a cylindrical structure is well documented in the textbook.<sup>[23]</sup> Electromagnetic fields of the eigenmodes in the cylindrical coordinates  $(r, \theta, z)$  can be expressed as

$$\begin{split} E_r &= \Big[\frac{ik_z}{\gamma_j} f_n^{j\prime}(\gamma_j r) - \frac{\mu_j \omega n}{\gamma_j^2 r c} g_n^j(\gamma_j r)\Big]S_n, \\ E_\phi &= \Big[-\frac{nk_z}{\gamma_j^2 r} f_n^j(\gamma_j r) - \frac{i\mu_j \omega}{\gamma_j^2 c} g_n^{j\prime}(\gamma_j r)\Big]S_n, \\ E_z &= f_n^j(\gamma_j r)S_n, \\ H_r &= \Big[\frac{n\varepsilon_j \omega}{\gamma_j^2 r c} f_n^j(\gamma_j r) + \frac{ik_z}{\gamma_j} g_n^{j\prime}(\gamma_j r)\Big]S_n, \\ H_\phi &= \Big[\frac{i\varepsilon_j \omega}{\gamma_j c} f_n^{j\prime}(\gamma_j r) - \frac{nk_z}{\gamma_j^2 r} g_n^j(\gamma_j r)\Big]S_n, \end{split}$$

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$$H_z = g_n^j(\gamma_j r) S_n,\tag{1}$$

where *i* is the imaginary unit, *n* is an integer  $(n = 0, 1, 2, \dots)$ ,  $k_z$  is the propagation constant along the *z* direction (the cylinder axis) and here it is complex due to the loss of metal,  $\varepsilon_j$  is the dielectric constant of the medium *j* and *c* is the speed of light in vacuum. As we are not dealing with magnetic materials, the magnetic permeability  $\mu$  is set as unity.  $S_n$  is the exponential factor,

$$S_n = \exp(in\phi + ik_z z - i\omega t), \qquad (2)$$

 $\gamma_j$  is the transverse wave number in the *j*th medium,

$$\gamma_j^2 = \mu_j \varepsilon_j (\omega/c)^2 - k_z^2, \qquad (3)$$

and  $f_n^j$ ,  $g_n^j$  are the superposition of Bessel functions.



Fig. 1. The schematic diagram of a hybrid cylindrical metal-dielectric waveguide.

By applying the boundary conditions that the tangential components of  $\boldsymbol{E}$  and bmH must be continuous at the interface, a homogeneous system of linear equations for the expansion coefficients of  $f_n^j$  and  $g_n^j$  is obtained. The existence of the nontrivial solutions is guaranteed by letting the determinant of the system vanish. Then we obtain the transcendental equation  $det[M(k_z)] = 0$  for the complex propagation constant  $k_z$ . Using a numerical method,<sup>[20]</sup> we can solve the value of  $k_z$  for a specific mode. With the propagation constant, all the information of this mode can be obtained, including the EM fields, propagation length and Poynting vector.

Propagation length is defined as the length  $L_m = (2 \text{Im}(k_z))^{-1}$  after which the intensity of SPPs decreases to  $1/e^{[1]}$  Light confinement in the radial direction is described by the effective radius  $R_{\text{eff}}$ , defined as a hypothetic radius inside which 86.5% of the power is confined,

$$\frac{\int_{0}^{R_{\rm eff}} S_z dA}{\int_{0}^{\infty} S_z dA} = 86.5\%,$$
(4)

where  $S_z$  is the Poynting vector in the axis direction  $S_z = (E_r * H_{\phi} - E_{\phi} * H_r).^{[25]}$ 

In a gold nanowire embedded in a dielectric host, low-permittivity dielectric tends to guide a long-range SPP mode but with a large effective radius, while high-permittivity dielectric tends to channel a short SPP mode but with a small effective radius. As an example, we consider the n = 1 mode in the gold nanowire of  $r_0 = 40$  nm. The gold dielectric permittivity of  $\varepsilon_m = -11.75 + 1.25i$  at the wavelength of  $\lambda = 632.8$  nm is taken from Ref. [24]. With infinite SiO<sub>2</sub> cladding of  $\varepsilon_1 = 2.25$ , it has a long propagation length of  $L_m = 45.8$  µm and a large effective radius of  $R_{\rm eff} = 467.6$  nm; while with BN cladding of  $\varepsilon_2 = 4.41$ , it has a short length of  $L_m = 1.66$  µm and good confinement of  $R_{\rm eff} = 100$  nm (the calculations related to this part are not shown). To overcome this dilemma that the SPP mode in nanowire has either a long range with bad confinement or good confinement with a short traveling length, we set the gold nanowire in a high-permittivity dielectric nanotube, forming a metallic-dielectric nanocable as shown in Fig. 1. The waveguide modes of the nanotube will pull the electromagnetic energy of the SPP mode of the nanowire into the low-permittivity middle layer, leading to some hybrid SPP modes. Then, by carefully choosing the geometric parameters, compared to the SPP modes in nanowires, higher quality hybrid modes with both long propagation lengths and small effective radii are achieved.



Fig. 2. Dispersion relations of nanocable versus the thickness  $d_1$  of the SiO<sub>2</sub> middle layer. Here the gold nanocore is in size  $r_0 = 40$  nm and the BN outer layer is in thickness  $d_2 = 40$  nm.



Fig. 3. Field distribution at  $r_0 = 40$  nm,  $d_1 = 260$  nm,  $d_2 = 40$  nm. (a) HE<sub>11</sub> mode, (b) HE<sub>12</sub> mode, (c) EH<sub>11</sub> mode, (d) HE<sub>13</sub> mode.

In the following, the three-layer nanocable has a gold core of  $r_0 = 40$  nm, a varying SiO<sub>2</sub> middle layer of  $d_1 = 50{-}400$  nm and an outer BN layer of  $d_2 = 30{-}$ 

60 nm. We first explore the dispersion relations of the nanocable for n = 1 modes by varying  $d_1$  in Fig. 2. The corresponding field distribution is shown in Fig. 3. Then we choose the best quality hybrid mode HE<sub>13</sub> by comparing their propagation lengths and effective radii, as shown in Fig. 4. Finally, in Figs. 5 and 6, a trade-off between propagation length and effective radius with varying geometrical and material parameters are clearly shown.



**Fig. 4.** Propagation length and effective radius of the  $HE_{13}$  mode versus the thickness  $d_1$  of the SiO<sub>2</sub> layer.

Figure 2 displays the dispersion relations of the hybrid modes gold nanocable as a function of the middle layer thickness  $d_1$ . Here  $d_2 = 40$  nm. For comparison, the dispersion relations of a gold nanowire with infinite  $SiO_2$  and BN cladding are also shown. For a multi-interface cylindrical waveguide structure, such as nanotube or nanocable, there are no rigorous definitions about EH and HE modes. The classification of modes can refer to Ref. [17]. By comparing the amplitudes of  $E_z$  and  $H_z$ , if  $|E_z| > |H_z|$ , the mode is regarded as TM-like and designated as an EH mode; in the contrast, if  $|E_z| < |H_z|$ , this mode is TE-like and an HE mode. The adoption of this designation is only for the convenience of modes citing and it is somewhat arbitrary. Here TM modes for n = 0, which also exist in the nanocable, are not considered. Due to the coupling of the SPP mode of the gold nanowire and waveguide modes of the BN nanotube, four modes are obtained. Each hybrid mode has a distinct propagation constant, which corresponds to its field distribution (Fig. 3). The feature of the field distribution for each mode is also responsible for the variation trend of the propagation constant. Among all the four modes, the field of the  $HE_{13}$  mode has a distinguished distribution pattern compared to the other three modes. For the  $HE_{13}$  mode, the distribution in the  $SiO_2$  layer has a pattern similar to that of a waveguide mode, which means that more energy locates in the  $SiO_2$ layer and the loss will thereby decrease. By varying  $d_1$ , the imaginary parts of propagation constants of  $HE_{11}$ ,  $HE_{12}$  and  $EH_{11}$  lie between that of two nanowires with

 $SiO_2$  and BN claddings, which means that they do not have a longer-range propagation length than that in gold nanowires. Only the imaginary part of the  $HE_{13}$  mode is less than that in the nanowire with  $SiO_2$ cladding. We note that this mode appears when  $d_1$  is larger than 260 nm. It is a hybridizing result of the SPP modes in the gold nanocore and the waveguide mode in BN nanocladding, where the high quality in the propagation length and effective radius is further proved in Fig. 4.



**Fig. 5.** (a) Propagation length and (b) effective radius of  $HE_{13}$  mode with varying the thickness  $d_2$  of the BN outer layer.



**Fig. 6.** (a) Propagation length and (b) effective radius of the  $\text{HE}_{13}$  mode with varying the permittivities  $\varepsilon_1$  and  $\varepsilon_2$ .

In Fig. 4, we can see that the qualities of modes  $\text{HE}_{11}$ ,  $\text{HE}_{12}$  and  $\text{EH}_{11}$  are not substantially improved. However, mode  $\text{HE}_{13}$  overcomes the trade-off between the propagation length and effective radius in some degree. It can travel 80–130 µm or 120–200 $\lambda$  with an effective radius of only 500–600 nm. Especially, when  $d_1 = 400$  nm, it has a propagation length of 128 µm and an effective radius of 497 nm. The propagation length has been increased to more than two times of the original value compared to that in the nanowire with SiO<sub>2</sub> cladding, at a sacrifice of a little increase of the effective radius. It demonstrates the combination of the advantages of both the SPP mode and the waveguide mode in the hybrid mode HE<sub>13</sub>.

Figure 5 shows the details of the property of hybrid mode HE<sub>13</sub>. We can see that with an increment of  $d_2$ , both the propagation length and the effective radius decreases, showing a clear trade-off between them. For the same  $d_2$ , with a change of  $d_1$ , however there exists a minimum in the curves of propagation length. Especially, when  $d_1$  is larger than the value at the minimum point, the effective radius of the mode stays in a relative constant value as the propagation length increases. This means that the trade-off between the propagation length and the effective radius in this region is overcome. This improvement can be attributed to the advantage of the coupling between SPP modes and the waveguide modes.

Finally, we explore the effect of different permittivities of dielectric layers on the propagation length and effective radius. As shown in Fig. 6, we change  $\varepsilon_1$ from 2.0 to 4.0, with which the material can be easily selected in optical frequencies. Here  $\varepsilon_2$  is set as 4.41 (BN), 6.0 (BaTiO<sub>3</sub> or  $SrTiO_3$ ) and 8.0 (Sb<sub>2</sub>O<sub>3</sub> and  $\mathrm{SiO}_2$ ).<sup>[26]</sup> Generally speaking, when  $\varepsilon_1$  and  $\varepsilon_2$  are increased, both propagation length and effect radius are decreasing, which can be correspondingly explained as a decrease of optical propagation length with an increment of dielectric permittivity. When  $\varepsilon_1$  (or  $\varepsilon_2$ ) is fixed, with increasing  $\varepsilon_2$  (or  $\varepsilon_1$ ), both its propagation length and effective radius are decreased. In this situation, a trade-off between them is still seen. Thus this permittivity contraction can also effectively control the propagation properties of this hybrid SPP waveguide. Generally, for a specialized plasmonic waveguide structure, by releasing some propagation length we can reach good light confinement and vice versa.

In summary, by the coupling of SPP modes and waveguide modes, we have theoretically found a hybrid plasmonic mode with a long propagation length and good light confinement in a cylindrical metal-dielectric waveguide. At the optical wavelength of  $\lambda = 632.8 \text{ nm}$ , in a nanocable with the gold nanocore of 40 nm, a SiO<sub>2</sub> middle layer of 260–400 nm and a BN outer layer of 40 nm, we obtain the long propaga-

tion length of  $120-200\lambda$  and a small effective radius of subwavelength scale. It has also shown that the geometrical parameters as well as material permittivities can effectively adjust the propagation length and effective radius of the hybrid SPP mode. It should be confessed that the trade-off between the propagation length and effective radius still exists. However, with the combination of the mode coupling and the dielectric contrast effect, this hybrid mode method improves dramatically the properties of SPP modes in 1D cylindrical nanocables compared to that in nanowires with homogeneous dielectric cladding. With the development of fabrication technology, this hybrid waveguide structure can find applications in nanoscale optical devices such as SPP waveguides, spaser and SPP sensors.

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