Effects of shape of terminus on excitation of surface plasmon modes on metal nanowires*

Qiao Ya-Nan(乔雅楠) and Yang Shu(杨 树)†

Department of Physics, School of Sciences, Beijing University of Posts and Telecommunications, Beijing 100876, *China*

(Received 20 December 2013; revised manuscript received 18 March 2014; published online 20 August 2014)

The effects of the shape of a nanowire terminus on the excited surface plasmon polariton (SPP) modes are investigated. The conical terminus and terminus cut at a certain angle are studied. For the first time, the quantitative mode decompositions are carried out to derive the full information about excited SPP modes. It is demonstrated that tuning the shape of the terminus provides an effective method to control the composition of excited SPP modes on metal nanowires. It is especially found that some important patterns, such as the pure TM_0 mode and the superposition of TM_0 and HE_{+1} or HE_{-1} modes, can be generated by some specific shapes of the terminus, whereas there is no way to produce these patterns using flat-end nanowires.

Keywords: metal nanowire, shape of terminus, surface plasmon polariton modes, mode decomposition

PACS: 73.20.Mf, 42.82.Et, 81.07.Gf **DOI:** 10.1088/1674-1056/23/10/107305

1. Introduction

Constrained as they are by the diffraction limit, existing optical technologies face basic difficulties in integrated optical circuits and devices. Surface plasmon polaritons (SPPs) can be localized to sub-wavelength dimension and thus are regarded as a promising scenario to break through this limitation and also provide abundant applications.[1] Plasmonic waveguides, serving as a key element on which SPPs are excited, transmitted and transformed, have been extensively studied.[2–7] Among them, metal nanowires have drawn considerable attention due to their good performance and ease of fabrication and manipulation.[8–11] Especially, the further fabrication of nanoscale structures on normal metal nanowires has been recently recognized to be able to play important roles on the SPP's excitation and radiation properties. For example, it was demonstrated that by cascading nano-corrugation gratings with different periodicities on silver nanowires atop silicon, different colors can be spatially separated and chronologically released at different grating junctions.[12] Although nanowires with various cross sections can be generated by different fabricating methods,[13] the cylinder nanowire has been the most concerned and studied type until now. The plasmonic eigen modes on such nanowires can be analytically solved and have been well known.[14] How these modes can be excited on metal nanowires is a fundamental question in the relevant studies. The qualitative features and quantitative mode decomposition of optically excited SPP fields have been studied for flat-end nanowires.[15] However what the matter is for the nanowires with other shapes of terminus remains an open question, although it has been recognized that the shape of nanowire terminus may have a significant influence on the excitation of SPPs and may, consequently, notably affect the radiation properties.[16] In this paper, we will focus on this issue and aim to give a quantitative answer to this question, together with the corresponding physical explanations.

2. Numerical method, results, and discussion

The finite-difference time-domain (FDTD) method is used to simulate the excitation and propagation of SPPs on metallic nanowires. Since the effect of the shape of termination is the topic of the present study, the other model parameters are fixed in this paper. It is assumed that a semi-infinite-long silver nanowire of radius $R = 100$ nm is embedded in the dielectric background with permittivity $\varepsilon_d = 2$. A Gaussian beam with wavelength $\lambda = 590.4$ nm is used to illuminate the nanowire terminus to excite the SPPs. As is well known, for axisymmetric optical waveguides, such as normal optical fiber and other types of waveguides,[17,18] various confined modes may exist. For metal nanowires, it has been demonstrated that only transverse magnetic (TM) and TE-like hybrid (HE) modes can exist for zero and nonzero winding numbers, respectively.[14] For the presently adopted parameters, it has been shown that only the TM_0 and $HE_{\pm1}$ modes can be possibly excited.[15] The parallel and perpendicular polarizations of incident light are studied. In the FDTD simulation, in the propagating region the mesh sizes are set to be 2 nm and 10 nm transversely and longitudinally, respectively. For the excitation terminus part, a uniform mesh size of 2nm is adopted. The time step is chosen to be 200 fs. These parameters are testified to well satisfy the convergence. We perform the FDTD simulation and then carry out the mode decomposition of the obtained SPP fields to derive quantitative information about all

*Project supported by the National Basic Research Program of China (Grant No. 2010CB923202).

†Corresponding author. E-mail: syang@bupt.edu.cn

© 2014 Chinese Physical Society and IOP Publishing Ltd

of the excited modes.

Firstly we study a nanowire with a conical terminus, which can be regarded as a representative of cuspidal terminus with axial symmetry. The height of the cone, or alternatively the angle between conical surface and nanowire cross section θ, can be adjusted as shown in Fig. 1(a). Since the left–right symmetry that is kept for this structure is similar to a flat-end nanowire, the qualitative features of mode composition of the excited SPPs are expected to be the same as those of a flat-end nanowire. It is actually observed to be so. As described for flat-end nanowire,[15] for parallel polarization, the TM_0 and $HE_{\pm1}$ modes are all excited at the position where the $HE_{\pm1}$ modes are excited in equal amplitude, while their electric components E_r and E_z are in phase in the direction of light incidence. For perpendicular polarization, only the $HE_{\pm1}$ modes can be excited at the position where they also have the same amplitude, but their E_r and E_z are in phase in the vertical direction to the incident light on the cross-section plane. The amplitude distributions of electrical fields on the cross-section plane of the nanowire are shown in Fig. 1(b). Through mode decomposition, the amplitude and phase of each mode can be extracted. They are shown to change notably with angle θ. We use the amplitude of E_r to represent the strength of each mode. Figures 1(c) and 1(d) show the variations of amplitudes of E_r with θ for parallel and perpendicular polarizations, respectively. Here, and in all the following figures, the amplitudes are given 4 nm away from the edge of nanowire terminus in the incident direction. It is seen that the amplitude of TM_0 mode decreases significantly with increasing θ, while the amplitudes of $HE_{\pm1}$ modes display rather flat behaviors in both cases of parallel and perpendicular polarizations. These features can be explained as follows. Since the $HE_{\pm1}$ modes excited by the part with small radius on the conical surface are strongly suppressed by phase mismatching, they are mainly generated by the part near the terminus edge, so that the strength of the $HE_{\pm1}$ modes do not depend on θ sensitively. On the other hand, since small radius is favorable for the excitation of TM_0 mode, the total TM_0 mode must be regarded as the overall superposition of excitations from all parts of the conical surface. With increasing θ the phase differences among the excited fields from different parts of the cone are enlarged, so that these fields tend to cancel each other; therefore, the strength of TM_0 mode decreases significantly. It is seen that at $\theta = 60^\circ$ the amplitude of TM_0 mode is already quite small compared with that of $HE_{\pm1}$ modes, so that an approximate $HE_{\pm1}$ modes pattern is obtained.

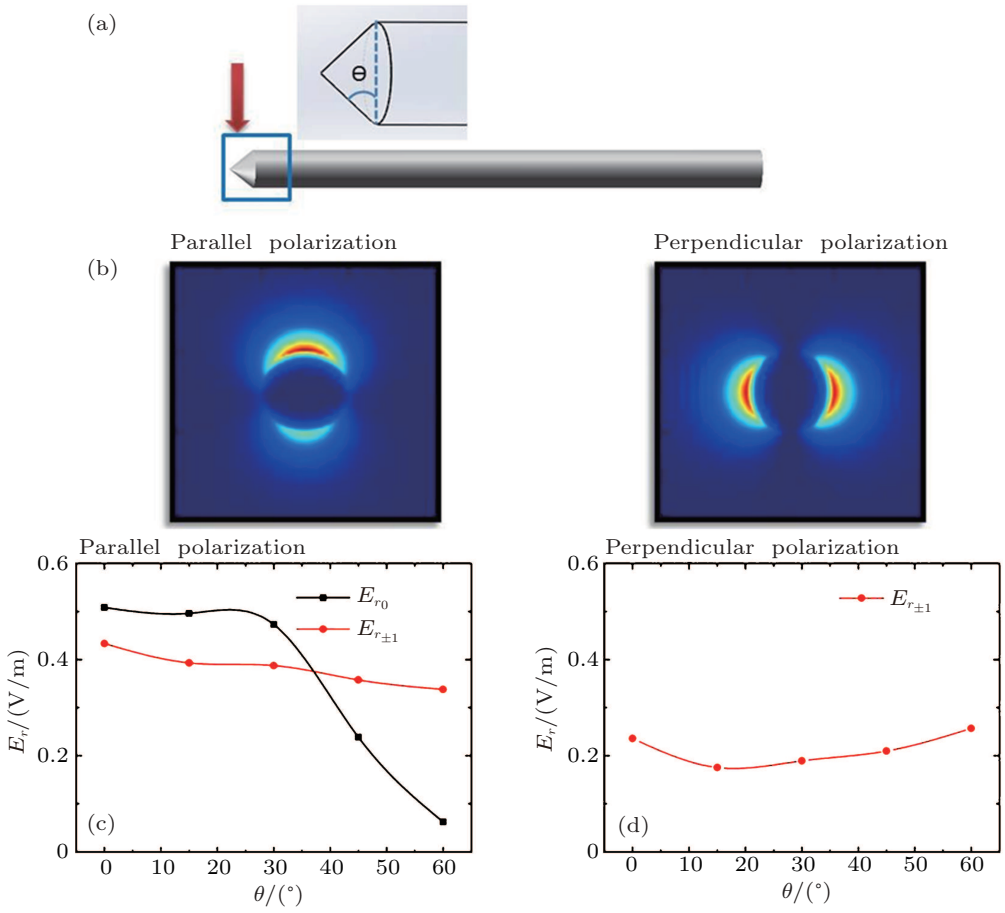


Fig. 1. (color online) (a) Schematic illustration of nanowire with conical terminus in homogeneous background. (b) Amplitude distributions of electrical fields on the cross-section plane of nanowire for the parallel and perpendicular polarizations. Amplitudes of E_r of excited modes as a function of θ for (c) parallel and (d) perpendicular polarizations.

The phase of each excited mode is another quantity of interest. While their significance and applications are to be further explored, here we focus on one thing, which is the phase difference between the $HE_{\pm1}$ modes excited by parallel and perpendicular polarizations. Here, the phases of $HE_{\pm1}$ modes refer to the phases for the positions with same radius but along incident direction and its vertical direction on the cross-section plane for parallel and perpendicular polarizations, respectively. This phase difference δ is found to change with θ notably, as shown in Fig. 2(a). It is noted that δ decreases from 108° to 84° as θ increases from 15° to 45°. The special point is $\theta = 30°$, where δ reaches a value of 90°. For this point it is easy to understand that, for an obliquely-polarized incident light that guarantees the same amplitudes of the $HE_{\pm1}$ modes excited, respectively, by the parallel and perpendicular components, one of the $HE_{\pm1}$ modes can be canceled completely, so that the TM_0 mode and a pure HE_{+1} or HE_{-1} mode remain. This pattern may be useful in some applications. It can only be generated for very specific wavelengths and nanowire radii,[15] and is not a general output, as claimed by another study[19] for flat-end nanowires. The adjustment of conical angle provides a practical way to generate such a pattern for arbitrary incident wavelength and nanowire radius. For example, figure 2(b) shows the cross-sectional distributions of the TM_0 and HE_{+1} pattern obtained at $\theta = 30°$. The rotating behavior with respect to propagating direction originates from the superposition of the two modes with different wave numbers.

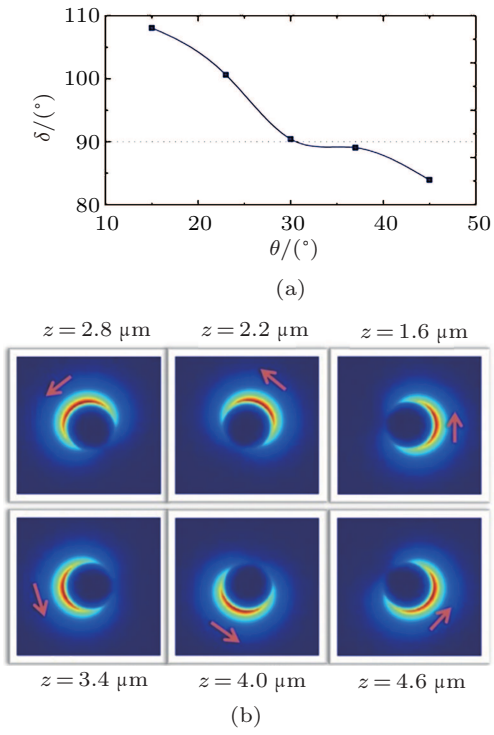


Fig. 2. (color online) (a) Phase difference δ between the $HE_{\pm1}$ modes under parallel and perpendicular polarizations as a function of θ. (b) Amplitude distributions of the superposition of TM_0 and HE_{+1} modes at different values of z, which are obtained at $\theta = 30°$.

Next, we consider a nanowire terminus that is cut at a certain angle. Although this structure may not exist realistically, it can be produced by a certain technique, such as ion beam etching. At the first step it is assumed that the incident light illuminates directly on the cutting surface, which can be upward or downward, as shown in Fig. 3(a). The cutting angle ψ is defined as being positive and negative for the upward and downward cases, respectively. Since the left–right symmetry is also kept in these cases, it is expected that the excited SPP pattern should also be similar to those excited by flat and conical ends. However, the amplitudes of excited modes are assumed to change with ψ significantly. We perform the simulations for different values of ψ, ranging from $-60°$ to 60°. The variations of mode amplitudes are shown in Figs. 3(b) and 3(c) for parallel and perpendicular polarizations, respectively. The variation behaviors are more complex than those for the conical-end nanowires. It is shown in Fig. 3(b) that the amplitude of E_r of TM_0 mode increases with increasing ψ and reaches a maximum at about $-40°$, it then starts to decrease. This behavior can be explained by the phase-matching between the excited fields and the TM_0 mode. Since the fields of TM_0 mode are axisymmetric, the most favorable situation for excitation occurs when the excited fields by different parts of nanowire terminus are in phase on the same cross section of nanowire. This condition can be satisfied for a certain cutting angle in the downward case. This angle can be calculated by equating the optical paths of excited fields reaching the same cross section through the medium and the nanowire. Noting that the medium and TM_0 plasmonic wavelengths are 417.5 nm and 344 nm respectively, the most favorable angle can be calculated to be $-39.5°$, which perfectly fits our numerical result, as shown in Fig. 3(b). When ψ deviates from this value, the phase-matching becomes increasingly worse, so that the amplitude of TM_0 mode decreases monotonically. As for the $HE_{\pm1}$ modes, the fields are in opposite phase on the upward and downward parts of the nanowire. The favorable angle is calculated to be $+2.1°$ (noting that the $HE_{\pm1}$ plasmonic wavelength is 380 nm), which happens to be very close to the flat-end case for our model parameters. It also fits perfectly with the numerical result.

When deviating from this angle, the amplitudes of $HE_{\pm1}$ modes decrease similarly due to the enlarged phase-mismatching, until the most unfavorable situation is reached for a certain negative value of ψ, where the excited fields by different parts of nanowire terminus are in phase. This unfavorable angle is calculated to be $-42.3°$. Around this point the $HE_{\pm1}$ modes are strongly suppressed. For example, the amplitude ratio of $E_{r_{\pm1}}$ and E_{r_0} is shown to be 1/18 at $\psi = -45°$. Thus, the $HE_{\pm1}$ modes can be well neglected and a highly approximate pure TM_0 mode is obtained. This mechanism indeed provides an effective and simple method to produce a highly approximate pure TM_0 mode, which has been an open

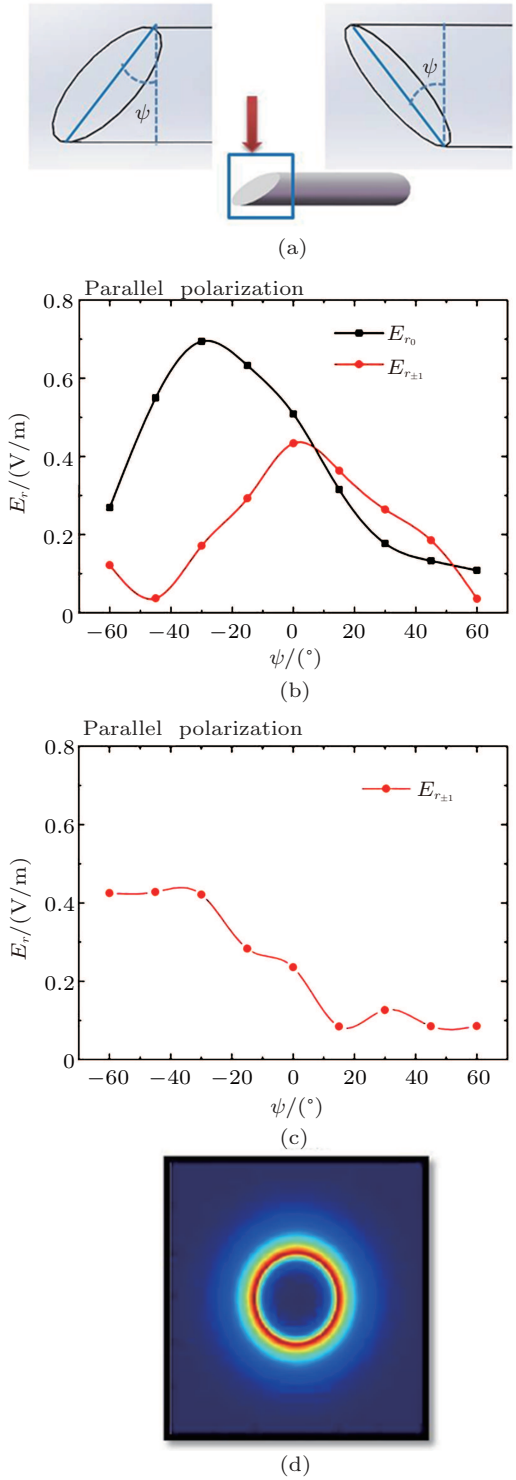


Fig. 3. (color online) (a) Schematic illustration of nanowire whose terminus is cut at angle ψ. ψ as defined as being positive and negative for upward and downward cases, respectively. (b) Amplitudes of E_r of excited modes as a function of ψ for (c) parallel and (b) perpendicular polarizations. (d) Amplitude distribution of highly approximate TM_0 mode which is obtained at $\psi = 45°$.

question up to now. Figure 3(d) shows the field distribution of the approximate TM_0 mode generated at $\psi = -45°$. Of course, for more negative ψ the amplitudes of $HE_{\pm1}$ modes would increase again. For perpendicular polarization, noting that the field distributions of $HE_{\pm1}$ modes are rotated 90° compared with those for parallel polarization, the most favorable situation for excitation of $HE_{\pm1}$ modes should occur when the optical paths to the same cross section are equal. This corresponds to the same angle, −42.3°. The decreasing behavior of amplitude with increasing ψ shown in Fig. 3(c) is in accordance with this expectation. The phases of the excited modes are also shown to vary notably with ψ. Their results are omitted here for concision. It should be mentioned that it is also feasible to generate a pattern like Fig. 2(b) by choosing a proper cutting angle ψ.

It is interesting to further study the case where the light is obliquely incident on the cutting surface. In this case the left–right symmetry is broken. The setup is illustrated in Fig. 4(a). γ is defined as the rotation angle of nanowire from the downward position of cutting surface. γ is positive (negative) when the rotation is clockwise (anti-clockwise). In this study, the cutting angle of the nanowire terminus is fixed to be 45°. We perform the simulations for different rotation angles. For example, the field distributions of $\gamma = \pm 90°$ for parallel and perpendicular polarizations are given in Figs. 4(b) and 4(c), respectively. In both cases, for non-zero γ it is found that the $HE_{\pm1}$ modes no longer have the same amplitudes, and the positions of E_r and E_z of $HE_{\pm1}$ modes being in phase are no longer in the same direction that is shown in the $\gamma = 0$ case. Also, it is observed that the TM_0 mode starts to emerge with the rotation for perpendicular polarization (noting that the TM_0 mode is forbidden for $\gamma = 0$). All these features are expected results due to the broken left–right symmetry. Figures 4(d) and 4(e) show the variations of amplitudes with γ in the cases of parallel and perpendicular polarizations, respectively. Similarly, the amplitude of each mode is determined by the degree of phase-matching between the mode field and the field excited by incident light. The detailed explanations are omitted here for concision. It should be noted that a strict symmetry is kept for the clockwise and anti-clockwise rotations. The sensitive dependence of mode amplitude on the rotation provides a simple method to tune the composition of different SPP modes, which could be useful in some applications and in studies of mode-dependent effects. The positions of E_r and E_z of $HE_{\pm1}$ modes being in phase are another characteristic quantity. The results are given in Figs. 4(f) and 4(g). β is defined as the rotation angle of this position with respect to the position in the case of $\gamma = 0$. It is noted that for parallel polarization this position rotates in the same direction as the rotation of nanowire and reaches ±68° when $\gamma = \pm 45°$, it then rotates back to the starting point when the nanowire is rotated ±180°; whereas, in the case of perpendicular polarization β beaches ±113° when $\gamma = \pm 90°$, and then rotates back. These features affect to a large degree the angular distribution of SPP fields on the cross section of nanowire and have an important influence on the angular distribution of radiation from the emitting end.

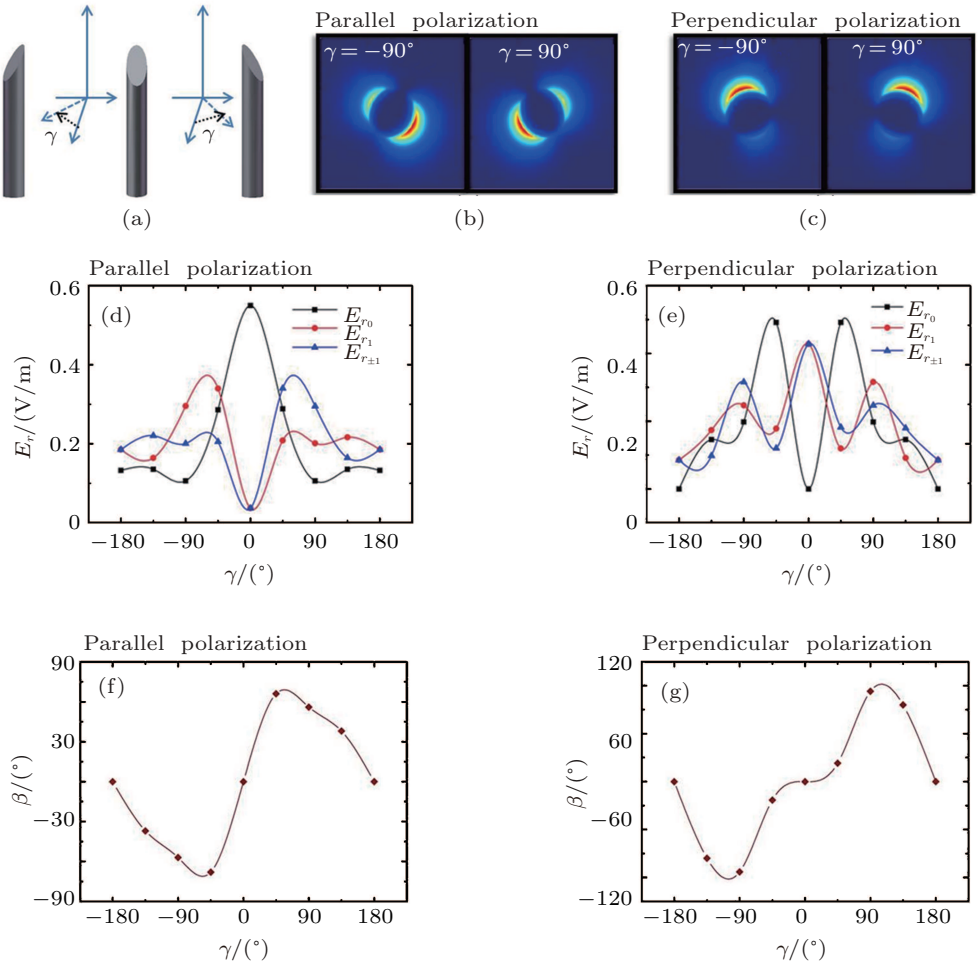


Fig. 4. (color online) (a) Illustration of rotation of the cut nanowire. γ is defined as being positive (negative) when the nanowire is rotated clockwise (anti-clockwise) against the propagating direction. (b) Amplitude distributions obtained at $\gamma = \pm 90°$ for (b) parallel and (c) perpendicular polarizations. Amplitudes of E_r of excited modes as a function of γ for (d) parallel and (e) perpendicular polarizations. The variations of rotation angle β of the position of the $HE_{\pm1}$ modes being in phase with γ for (f) parallel and (g) perpendicular polarizations.

3. Conclusions

In this paper we have quantitatively studied the effects of shape of nanowire terminus on the excitation of SPP modes. For the first time, quantitative mode decompositions are carried out to derive the full information about excited SPP modes. The excitation mechanisms of different modes are studied and explained. It is found that the SPP pattern excited by a conical terminus is qualitatively similar to that excited by a flat end. But the amplitudes and phases of excited modes vary notably with the conical angle. In particular, it is found that at a certain conical angle one of the $HE_{\pm1}$ modes can be in opposite phase for parallel and perpendicular polarizations; therefore, for a proper obliquely-polarized incident light this mode will be canceled out, and only the other $|m| = 1$ mode and TM_0 mode remain. On the other hand, it is found that the amplitudes of SPP modes excited by terminus cut at a certain angle exhibit a significant dependence on the cutting angle. It is especially demonstrated that, in the parallel-polarization case, at a certain negative angle the $HE_{\pm1}$ modes are strongly suppressed, so that a highly approximate pure TM_0 mode can be produced. Furthermore, it is shown that the rotation of the cutting surface breaks the left–right symmetry of the system. This leads to the asymmetrical $HE_{\pm1}$ modes for parallel and perpendicular polarizations, the emergence of TM_0 mode in the perpendicular-polarization case, and the rotation of cross-sectional field distribution. These new features are qualitatively different from those of the modes excited by flat end of nanowire and thus provide new dimensions of controlling the mode composition on metal nanowires. Although the different choices of model parameters can have a quantitative influence on the results, they are expected not to change the qualitative conclusions obtained here. The results in this paper provide a complete understanding of the effects of the studied shapes of terminus on the excited SPP modes on metal nanowires and may serve as a useful guide to the study of other types of shapes of terminus. The tuning of the shape of a nanowire terminus is demonstrated to be an effective method to control the composition of excited plasmonic modes and is at present a unique way to generate some special and important SPP patterns, which may lead to potential and important applications in nanowire-based optical circuits and devices.

References

[1] Maier S 2007 *Plasmonics Fundamentals and Applications* (Berlin: Springer) ed. Brongersma Mark L and Kik Pieter G 2007 *Surface Plasmon Nanophotonics* (Berlin: Springer)

[2] Pile D F P and Gramotnev D K 2004 *Opt. Lett.* **29** 1069

[3] Liu L, Han Z H and He S 2005 *Opt. Express* **13** 6645

[4] Feng N N, Brongersma M L and Negro L D 2007 *J. Quantum Electron.* **43** 479

[5] Wang B and Wang G P 2007 *Appl. Phys. Lett.* **90** 13114

[6] Kumar A and Srivastava T 2008 *Opt. Lett.* **33** 333

[7] Oulton R F, Sorger V, Genov D A, Pile D F P and Zhang X 2008 *Nat. Photon.* **2** 496

[8] Ditlbacher H, Hohenau A, Wagner D, Kreibig U, Rogers M, Hofer F, Aussenegg F R and Krenn J R 2005 *Phys. Rev. Lett.* **95** 257403

[9] Chang D E, Sørensen A S, Demler E A and Lukin M D 2007 *Nat. Phys.* **3** 807

[10] Akimov A V, Mukherjee A, Yu C L, Chang D E, Zibrov A S, Hemmer P R, Park H and Lukin M D 2007 *Nature* **450** 402

[11] Li Z P, Hao F, Huang Y Z, Fang Y R, Nordlander P and Xu H X 2009 *Nano Lett.* **9** 4383

[12] Hu Q, Xu D H, Zhou Y, Peng R W, Fan R H, Fang N X, Wang Q J, Huang X R and Wang M 2013 *Sci. Rep.* **3** 3095

[13] Xiong X, Zou C, Ren X, Liu A, Ye Y, Sun F and Guo G 2013 *Laser Photon. Rev.* **7** 1

[14] Chang D E, Sørensen A S, Hemmer P R and Lukin M D 2007 *Phys. Rev. B* **76** 035420

[15] Yang S and Pan C, Mode excitation of surface plasmon polaritons on metal nanowires, to be submitted.

[16] Li Z P, Bao K, Fang Y R, Huang Y Z, Nordlander P and Xu H X 2010 *Nano Lett.* **10** 1831

[17] Johnson S G, Ibanescu M, Skorobogatiy M, Weisberg O, Engeness T D, Soljačíc M, Jacobs S A, Joannopoulos J D and Fink Y 2001 *Opt. Express* **9** 748

[18] Hu Q, Zhao J Z, Peng R W, Gao F, Zhang R L and Wang M 2010 *Appl. Phys. Lett.* **96** 161101

[19] Zhang S, Wei H, Bao K, Håkanson U, Halas N J, Nordlander P and Xu H 2011 *Phys. Rev. Lett.* **107** 096801