Terahertz surface plasmon polaritons on a conductive right circular cone: Analytical description and experimental verification

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We report on an analytical solution of Maxwell's equations for the propagation of surface plasmon polaritons on a right circular cone. The problem was solved for THz frequencies in real metals and was therefore derived using the Leontovich approximation, which is valid for media with small surface impedances. The solution also accounts for both surface plasmon polaritons that are axisymmetric and those that have an angular structure in a plane normal to the cone's axis. This was an important consideration since it is crucial for describing surface phenomena such as surface-enhanced absorption, fluorescence, and Raman scattering. Our findings predict a total reflection of surface plasmon polaritons at the cone's apex, which was experimentally verified by an absence of light emitted from a heated cone's tip into the far-field region.

I. INTRODUCTION

Surface plasmon polaritons (SPPs) are bound, nonradiative electromagnetic waves that are associated with charge-density oscillations and propagate along a metal-dielectric interface [1,2]. Propagation and localization of SPPs have been actively studied in recent years [3,4], because convergent geometries such as v grooves [5], wedges, cones, and other tapered structures [6] can allow nanoscale focusing of electromagnetic energy [7] due to their subwavelength mode volume. These strong localizations are also believed to promote surface-enhanced Raman scattering, absorption, nonlinear effects, and also lead to nanoscale coupling and guiding of surface electromagnetic waves. Recently, several approaches have been applied to describe the propagation of SPPs on tapered structures [7]. Among them, the cone geometry is of particular interest since its apex supports highly localized excitations. In contrast to the classical problem of wave diffraction on an ideal conductive surface of a cone [8], solutions for the diffraction of SPPs must consider a system with energy losses, where the cone surface impedance ζ is nonzero. So far, this has been derived by using the finite element method for the rounded apex geometry [9], quasiseparation of variables in conical geometry [10,11], and analytically, with the adiabatic approximation [12,13]. In the latter case the approximation is only valid when the radius of the cone does not change significantly with distances on the order of the SPP wavelength. Therefore, the solution obtained with the adiabatic approximation had to be joined to the numerical solution of Maxwell's equations in the vicinity of the rounded tip [14]. Furthermore, in the referred works, only axisymmetric solutions have been considered, which are independent on the azimuthal angle φ, which is of principal importance to describe phenomena such as surface-enhanced Raman scattering and the Purcell effect.

In the present paper we report on a full analytical solution for the propagation of SPPs on a conductive right circular cone. To accommodate the finite conductivity, the Leontovich approximation (LA) [15] was used since it is valid for small impedances. Furthermore, the solution is presented in dependence on impedance since it governs the optical properties of metals both in normal and anomalous skin-effect conditions. We found that our solution predicts a total reflection of SPPs at the cone's apex, which was experimentally verified by an absence of light, emitted from a heated cone's tip into the far-field region.

II. MAXWELL'S EQUATIONS AND THE LEONTOVICH APPROXIMATION

We began by deriving the wave equation in spherical coordinates from Maxwell's equations, applied the Leontovich boundary condition, and discussed the limitations of the LA. To this end, the wave equation for a magnetic field $\mathbf{B}$ outside the cone, e.g., in vacuum, was considered and can be written as

$$\Delta \mathbf{B} + k^2 \mathbf{B} = \mathbf{0}, \tag{1}$$

where $k = \omega/c$ is a wave number, ω is SPP frequency, and c is speed of light. Taking into account that SPPs are TM waves, and consequently, $B_\theta = 0$ in the considered geometry (Fig. 1), components of the electric field with a time-harmonic factor $\exp(-i\omega t)$ can be expressed through the solution of Eq. (1) in the spherical coordinate system (r,θ,φ) as

$$\begin{aligned} E_\theta &= \frac{i}{kr}\left[\frac{1}{\sin\theta}\frac{\partial B_r}{\partial\varphi} - \frac{\partial(rB_\varphi)}{\partial r}\right], \\ E_r &= \frac{i}{kr\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\, B_\varphi), \quad E_\varphi = -\frac{i}{kr}\frac{\partial B_r}{\partial\varphi}. \end{aligned} \tag{2}$$

Here we consider a conductive cone with a vertex angle 2β, which occupies the space $\alpha \leqslant \theta \leqslant \pi$, $0 \leqslant \varphi \leqslant 2\pi$, $\alpha = \pi - \beta > \pi/2$, as is schematically sketched in Fig. 1. If ε is the dielectric permittivity of the metal cone and its magnetic

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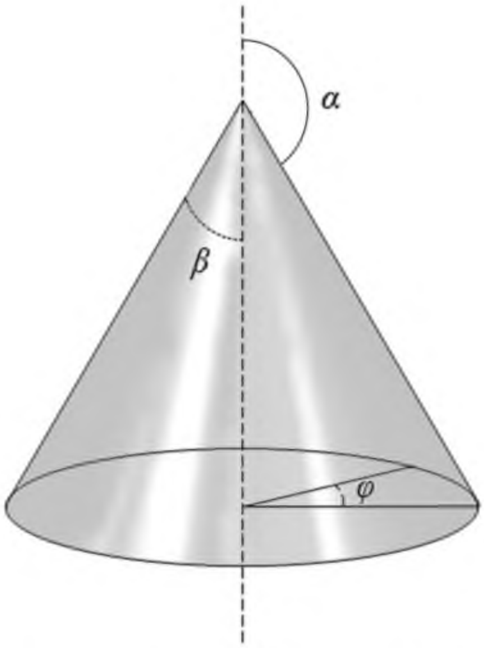

FIG. 1. Schematic representation of the cone. The half-angle at the cone's vertex is β, the angle between the cone's axis is α and its outer surface is ($\alpha = \pi - \beta$), and the azimuthal angle is φ.

permeability is unity, then for a good conductor in the THz (IR) and lower energy range

$$|\varepsilon| \gg 1, \tag{3}$$

and consequently, the impedance is small and therein

$$\zeta = 1/\sqrt{\varepsilon} \quad \text{and} \quad \zeta'' \equiv \operatorname{Im} \zeta < 0. \tag{4}$$

Thus, for the previously described case for Eqs. (1) and (2) we can use Leontovich's boundary condition

$$[\mathbf{n} \times \mathbf{E}] = -\zeta[\mathbf{n} \times [\mathbf{n} \times \mathbf{B}]], \tag{5}$$

where $\mathbf{n}$ is a normal to the cone's surface, directed inside the conductive medium. In the regarded geometry $\mathbf{n} = \mathbf{e}_\theta$, where $\mathbf{e}_\theta$ is a unit vector for the polar angle θ. We can rewrite Leontovich's boundary condition by substituting Eq. (2) into Eq. (5):

$$\left[\frac{\partial B_\varphi}{\partial \theta} + (\cot\theta - ikr\zeta)B_\varphi\right]_{\theta=\alpha} = 0, \qquad \left[\frac{\partial B_r}{\partial \theta} - ikr\zeta B_r\right]_{\theta=\alpha} = 0. \tag{6}$$

Therein the problem becomes closed when either boundary condition B_φ or B_r is applied to wave equation (1). Thus, there is no necessity to solve Maxwell's equations both inside and outside of the cone, and to consequently join the two solutions.

The accuracy of LA is determined by $\sim\zeta^3$ [16]. Here we should mention that LA breaks down for thin metal layers because of the necessity to account for not only the reflected field but also the field transmitted through the layer. Therefore, to use LA it is required that the skin depth δ of the metal is smaller than the thickness of the layer [15]. This means that the approximation is only valid when the condition

$$r \sin\beta > \delta \tag{7}$$

is met, and therein determines the minimum distance away from the cone's apex r where the LA can be applied. For example, for copper in the THz region, i.e., wavelengths $\simeq 10\ \mu$m, the calculated skin depth would be $\delta \simeq 10$ nm and condition (7) will only be met at a one wavelength distance away from the apex if $\beta > 0.1^\circ$. However, we found that most of the SPPs attenuate in the vicinity of the apex at distances as far as several wavelengths away from the taper. Both this case that can satisfy condition (7) and the SPP modes that do not will be discussed below.

III. RADIAL SURFACE PLASMON POLARITONS

In the following discussion we consider SPPs propagating along the cone generatrix (unit vector $\mathbf{e}_r$), and define them as *radial SPPs*. Radial SPPs have the only component of the magnetic-field vector directed along the tangent to the cone's surface (unit vector $\mathbf{e}_\varphi$). The magnitude of component B_φ outside of the cone (in vacuum) satisfies Eq. (1) and the first boundary condition from Eq. (6). As can be seen, the variables cannot be separated and the presence of a small parameter ζ does not simplify the problem since, as is well known, there are no regular methods to solve a boundary-value problem with a small parameter in boundary condition. Although in this particular case, the substitution

$$B_\varphi(r,\theta,\varphi) = \tilde{B}(r,\theta,\varphi)\exp[-ikr\zeta(\alpha - \theta)] \tag{8}$$

provides a possibility to exclude the dependence on r from the boundary condition obtaining

$$\left[\frac{\partial \tilde{B}}{\partial \theta} + \cot\theta\,\tilde{B}\right]_{\theta=\alpha} = 0, \tag{9}$$

therein also allowing the variables to be separated.

Substitution (8) can be physically explained as the SPPs localization at the interface. This is because, since $\operatorname{Im}\zeta < 0$ in Eq. (8), the exponent quickly decays as θ increases away from the cone's surface, which is determined by the angle α. This describes the decreasing behavior of both the magnetic and electric field of the SPPs at increasing distances away from the interface.

Substituting Eq. (8) into Eq. (1) leads to a rise of small terms $\sim\zeta$ in the wave equation for $\tilde{B}$. These small terms can, in principle, be considered by means of perturbation theory which is developed to solve these types of differential equations, e.g., [10,11]. In the present paper we do not account for these terms, but solve the wave equation for $\tilde{B}$ in the zeroth order by ζ. Thus, a nonzero ζ is only considered in the exponent in Eq. (8), which constitutes a localization of the SPPs at the interface of the metal cone. The group velocity of the SPPs coincides with the vacuum speed of light, although in a rigorous solution it varies by a factor of $\sim\zeta^2$.

In the frame of the formulated approximations, Eq. (1) can be rewritten for $\tilde{B}$ as follows:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial \tilde{B}}{\partial r}\right)+\frac{1}{r^2\,\sin\,\theta}\frac{\partial}{\partial \theta}\left(\sin\,\theta\frac{\partial \tilde{B}}{\partial \theta}\right) + \frac{1}{r^2\,\sin^2\,\theta}\frac{\partial^2 \tilde{B}}{\partial \varphi^2}+k^2\tilde{B}=0. \quad (10)$$

The separation of variables is possible in the boundary problem, which is defined by Eqs. (9) and (10). Therefore, the partial solution, which is a mode of a radial SPP, can be written as

$$\tilde{B}_{nm}(k;r,\theta,\varphi)=\frac{1}{\sqrt{kr}}J_{\nu_n+1/2}(kr)\mathcal{P}^{|m|}_{\nu_n}(\cos\,\theta)e^{im\varphi}, \quad (11)$$

where J is a Bessel function which has been chosen to be regular (when $r\to 0$) at the cone's apex. Therefore, SPPs form a standing wave on the cone's surface and attenuate at the apex. Here, $\mathcal{P}$ is a Legendre function of the first kind where its index ν_n is the nth positive root in incremental order of equation

$$\left[\frac{d\mathcal{P}^{|m|}_{\nu}}{d\theta}+\cot\ \theta\,\mathcal{P}^{|m|}_{\nu}\right]_{\theta=\alpha}=0, \quad (12)$$

which follows from the boundary condition (9). The functions $\mathcal{P}^{|m|}_{\nu_n}$ are mutually orthogonal and form a complete set in the interval $\theta\in[0,\alpha]$. We note that ordinary Legendre polynomials that are also functions of the first kind with an integer index are mutually orthogonal and form a complete set in the interval $\theta\in[0,\pi]$. The number m is analogous to the magnetic quantum number and defines the symmetry of the SPPs relative to the cone axis, i.e., $m=0$ corresponds to the monopolar (axisymmetric) SPPs, $m=1$ to the dipolar, etc. First and second radial SPP monopole, dipole, and quadruple modes for copper cones with a surface impedance $\zeta=-0.09i$ at 10 THz and with apex angles of 10° and 20° are presented in Figs. 2(a)–2(d).

IV. CIRCULAR SURFACE PLASMON POLARITONS

In the present section we consider *circular SPPs*, which are defined by the solution of Eq. (1) and the second boundary condition from Eq. (6). The same substitution defined in Eq. (8) leads to Eq. (10) with the boundary condition

$$\left.\frac{\partial \tilde{B}}{\partial \theta}\right|_{\theta=\alpha}=0. \quad (13)$$

The solution for circular SPPs has the same formal representation as defined in Eq. (11), although the indices ν_n are determined from

$$\left.\frac{d\mathcal{P}^{|m|}_{\nu}}{d\theta}\right|_{\theta=\alpha}=0. \quad (14)$$

Equation (14) has a root $\nu=0$, when $m=0$, since $\mathcal{P}_0=1$. This solution, if it exists, can be considered as *non-Leontovich* since it does not disappear in the vicinity of the cone's apex, and consequently does not satisfy condition (7). Furthermore, the roots of Eqs. (12) and (14) with $\nu=N$, $N<|m|$ (where N is a positive integer) should be omitted since this leads to the trivial solution $\tilde{B}\equiv 0$. Analogously to the case of radial SPPs, the first and second circular SPP monopole, dipole, and quadruple modes for a copper cone with a surface impedance of $\zeta=-0.09i$ at 10 THz are presented in Figs. 2(e)–2(h) for an apex angle of 10° and 20°.

V. ENERGY OF SURFACE PLASMON POLARITONS

In the following section we derive the energies for radial and circular SPP modes to determine their complete magnetic field. The magnetic field for both types of SPPs is determined by Eq. (11) up to a constant factor, which we denote as A_{mn}. To define this factor and to compare the fields produced by different SPP modes, we calculate their energy. If $\mathbf{B}^2/8\pi$ is the energy density of the SPPs, averaged over the field period,

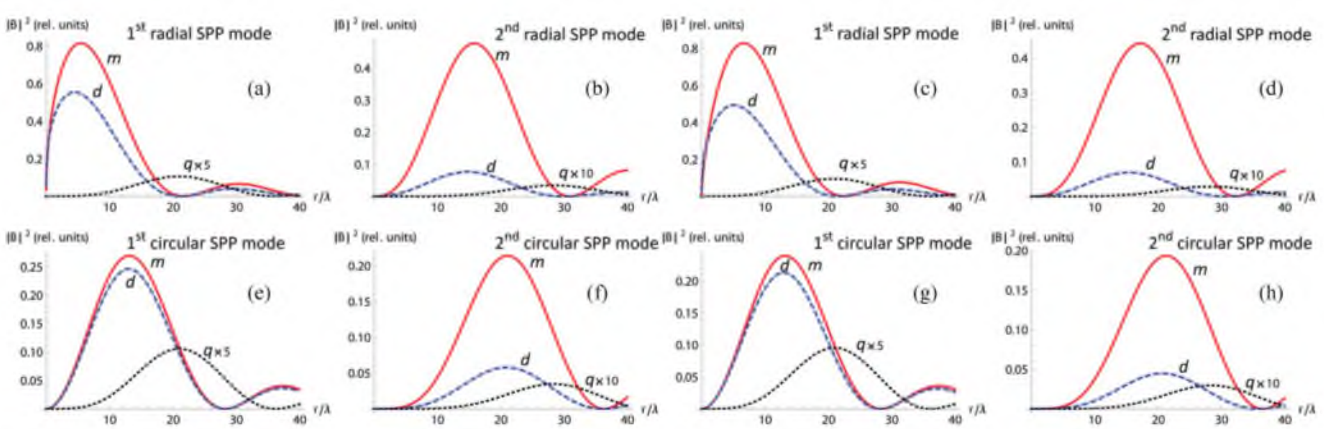

FIG. 2. (Color online) SPP modes on the surface of a copper cone with impedance $\zeta=-0.09i$. Solid red curves are monopole (m) SPP modes, dashed blue curves are dipole (d) SPP modes, and dotted black curves are quadruple (q) SPP modes for the first and second radial SPP modes on the cones with apex angles of 10° [(a), (b)] and of 20° [(c), (d)], and for the first and second circular SPP modes on the cones with apex angles of 10° [(e), (f)] and of 20° [(g), (h)]. All modes are normalized to the same total energy.

then the energy of each mode can be written as follows:

$$E_{nm} = \frac{A_{mn}^2}{4k}\int_0^\infty r\,dr\int_0^\alpha \left|\exp[-ikr\zeta(\alpha-\theta)]J_{\nu_n+1/2}(kr)\mathcal{P}_{\nu_n}^{|m|}(\cos\theta)\right|^2 \sin\theta\,d\theta$$
$$= \frac{A_{mn}^2}{4k}\int_0^\infty dr\int_0^\alpha \exp[-2k|\zeta''|r(\alpha-\theta)]\left[J_{\nu_n+1/2}(kr)\mathcal{P}_{\nu_n}^{|m|}(\cos\theta)\right]^2 r\,\sin\theta\,d\theta$$
$$= \frac{A_{mn}^2\Gamma(\nu_n+2)}{2\sqrt{\pi}\Gamma(\nu_n+3/2)k^3}\int_0^\alpha \frac{\sin\theta\left[\mathcal{P}_{\nu_n}^{|m|}(\cos\theta)\right]^2}{[2|\zeta''|(\alpha-\theta)]^{2\nu_n+3}}\,{}_2F_1\{\nu_n+1,\nu_n+2;2\nu_n+2;-[|\zeta''|(\alpha-\theta)]^{-2}\}d\theta, \qquad (15)$$

where ${}_2F_1$ is a hypergeometric function. The integrand in Eq. (15) has a singularity when $\theta \to \alpha$, and by exploiting its asymptotic behavior we can show that in its vicinity,

$$x^{-\nu-3/2}{}_2F_1(\nu+1,\nu+2;2\nu+2;-1/x) \simeq \frac{2^{2\nu+1}\Gamma(\nu+3/2)}{\Gamma(\nu+2)\sqrt{\pi x}} \quad \text{with} \quad x = [|\zeta''|(\alpha-\theta)]^2.$$

The logarithmic divergence of the integral that follows can be physically interpreted as the omittance of SPPs dissipation as they propagate along the cone's surface. The dissipation can be accounted for by the modes localized at the vicinity of the cone's apex with a substitution in Eq. (11): $J_{\nu_n+1/2}(kr) \to J_{\nu_n+1/2}(kr)\exp(-sr/2)$, where s is an attenuation constant which can be considered equal to the SPP attenuation constant on a plane surface. This assumption is valid since radial SPPs attenuate at a substantial distance from the cone's apex, which is also shown in the calculated results for $s = 10^{-4}k$ presented in Fig. 2. Therefore, Eq. (15) can be rewritten as

$$E_{nm} = \frac{A_{mn}^2\Gamma(\nu_n+2)}{2\sqrt{\pi}\Gamma(\nu_n+3/2)k^3}\int_0^\alpha \frac{\sin\theta\left[\mathcal{P}_{\nu_n}^{|m|}(\cos\theta)\right]^2 d\theta}{[2|\zeta''|(\alpha-\theta)+s/k]^{2\nu_n+3}}\,{}_2F_1(\nu_n+1,\nu_n+2;2\nu_n+2;-[|\zeta''|(\alpha-\theta)+s/2k]^{-2}). \qquad (16)$$

Here the integrand does not contain any singularities and hence can be treated numerically. Moreover, Eq. (16) should be considered as the definition for the constant factor A_{mn}, expressed in terms of energy E_{mn}, and thus determining the magnetic field of SPPs in a complete form.

VI. EXPERIMENTAL VERIFICATION

It is of particular interest to investigate the effect experimentally for a cone in a homogeneous isotropic medium such as air, since high conversion efficiency of SPPs have recently been experimentally observed by, using e.g., a butt-coupling configuration for a metallic wire and dielectric fiber [17]. Here, the expected result, which follows from the discussion above, is the absence of the SPPs conversion into photons at the cone's apex. To do so, one end of a bronze wire with a radius of 2 mm has been shaped as a cone with an apex angle of 20°. THz SPPs have been excited by heating up the specimen to 150 °C where most of the thermal radiation at this temperature corresponds to approximately 10 THz. To detect the radiation a ThermaCAM camera (FLIR Systems), equipped with a long-focusing objective with a spatial resolution of 100 μm, was used. The radiation intensity was converted into effective temperature and the resulting thermal picture is presented in Fig. 3(a), looking directly at the cones apex. As can be seen in Fig. 3(b), the radiation intensity is nearly constant across the tip, which is in agreement with the presented theory. If there was SPP conversion, the center pixels of the picture should show a much higher temperature. For example, the same setup was used for rectangular wedge geometry, and showed an over 100 °C higher temperature at the edges where SPP conversion took place [18]. We should, however, note that there is a small increase in intensity at the edges of the cone, where the cylinder (wire) and cone converge. Any theory about SPP conversion at the convergence of a cylinder and a cone is absent, at the moment, in contrast to the theory of SPP conversion at the edge of a wedge [19]. However, numerical calculations

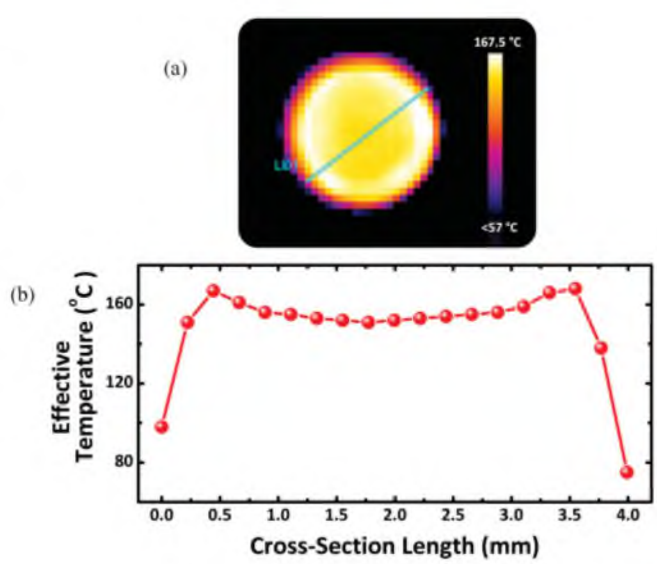

FIG. 3. (Color online) (a) Far-field THz image of a cone cross section in the plane which is normal to the cone axis. (b) Effective temperature profile, obtained from the data set along the blue line indicated in (a).

for a cylinder conjugated with a plane have already been reported [20].

VII. CONCLUDING REMARKS

In conclusion, we have presented a full analytical solution of Maxwell's equations for the propagation of SPPs on a conductive right circular cone. Our findings predict a total reflection of SPPs at the cone's apex with an accuracy in the order of magnitude of the surface impedance ζ. The solution has been derived for THz frequencies in real metals and was obtained using the Leontovich approximation, which is valid for the media with a small ζ. The solution accounts for both SPPs which are axisymmetric and those which have an angular structure in a plane normal to the cone's axis. The obtained results show that both radial and circular SPPs can be described with Bessel functions, and are consequently, standing waves. Furthermore, the position of the field maxima on the cone's tip for every SPP mode is determined by the first peak of the Bessel function. Finally, the total reflection of SPPs at the cone's apex was experimentally demonstrated for 10 THz SPPs as an absence of light emitted from a heated tip into the far-field region. We also observed the conversion of SPPs into photons at the convergence of the cone and the cylinder that was used to hold it into place.

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