Analysis and simulation of generating terahertz surface waves on a tapered field emission tip

Mark J. Hagmann, Gagan Kumar, Shashank Pandey, and Ajay Nahata

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Analysis and simulation of generating terahertz surface waves on a tapered field emission tip

Mark J. Hagmann\textsuperscript{a}
NewPath Research L.L.C., P.O. Box 3863, Salt Lake City, Utah 84110

Gagan Kumar, Shashank Pandey, and Ajay Nahata
Department of Electrical and Computer Engineering, University of Utah, Salt Lake City, Utah 84112-9206

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Finite difference-time domain simulations and analytical solutions show that terahertz transverse-magnetic surface waves are generated on a tapered field emitter tip by an oscillating terahertz current at the apex, where this current may be caused by photomixing with two lasers in laser-assisted field emission. The tip is modeled as a paraboloid so the analytical solution for the electromagnetic fields may be determined in paraboloidal coordinates using a basis of regular and irregular Coulomb wave functions. The simulations and analytical solutions show that there are quasistationary region and transitional region as the surface waves are generated by the oscillating current at the apex and then propagate on the tapered field emitter tip. © 2011 American Vacuum Society. [DOI: 10.1116/1.3560979]

I. INTRODUCTION

Photomixing (optical heterodyning) is used to generate terahertz radiation with semiconductors. In this method a dc bias is applied at the ends of an antenna and two lasers are focused on a semiconductor at the feed point to modulate the current through the antenna at the difference frequency of the two lasers to cause terahertz radiation.\textsuperscript{1} Photomixing in laser-assisted field emission offers promise as a new terahertz source because (1) the field emitter tip is much smaller than the wavelengths of the lasers so quasistatic conditions require that the electric field at the apex follows each cycle of the incident radiation; (2) the field emission current responds to changes in the electric field with a delay $\tau<2$ fs so the current should vary at frequencies of up to 500 THz (Refs. 2 and 3); and (3) the emitted current varies nonlinearly with the applied field so that terahertz mixing will occur.\textsuperscript{2} Furthermore, the output power at terahertz frequencies is increased by a resonance in the interaction of tunneling electrons with the laser radiation.\textsuperscript{2}

In the first microwave prototype, which is shown in Fig. 1, two tunable lasers are focused on the apex of a molybdenum field emitter tip which is mounted at the end of the horizontal wire to generate an output at the mixer frequency which may be tuned from 1 to 10 GHz.\textsuperscript{6} The output is taken from a SubMiniature Type A (SMA) coaxial feed through connector at the center of the metal end plate, and the dc voltage for field emission is applied to the small anode at the center of the glass end plate. The mixer current generates surface waves that propagate on the tip and then cause an axially symmetric transverse-magnetic (TM) Sommerfeld surface wave,\textsuperscript{7} with a characteristic impedance of approximately 50 $\Omega$, to propagate on the metal wire. The Sommerfeld wave is transformed to a coaxial output with a characteristic impedance of 50 $\Omega$ by the coaxial horn transition,\textsuperscript{8} which is mounted on the SMA connector. This device does generate microwave power which may be tuned from 1 to 10 GHz, but the dc field emission current is unstable so the output is in bursts of several seconds with an average power of only 100 pW. Generally, the field emission current is stabilized by heating the tip to 1000 °C or higher to remove contaminants before each usage,\textsuperscript{9} but the wire extension of the tip is too large for this to be practical. Other methods for cleaning may be used in later prototypes.\textsuperscript{9–11} This prototype has an overall length of 23 cm and a diameter of 10 cm. The techniques for design and fabrication have already been described with examples for proportionally smaller devices that could be tuned to operate from 10 GHz to 10 THz and 100 GHz to 100 THz, respectively.\textsuperscript{12}

Sommerfeld showed that the dominant mode for propagation of electromagnetic energy on a cylinder of metal with finite conductivity is an axially symmetric TM surface wave.\textsuperscript{7} Goubau showed by measurements and analyses that the radiation loss of the surface waves is reduced when the metal has a dielectric coating or corrugations.\textsuperscript{8} Simulations using the Drude model for the dielectric functions of metals at microwave and terahertz frequencies show that a wire may be used as a terahertz waveguide, with unique properties at terahertz frequencies,\textsuperscript{13} which was independently discovered later and attributed to surface plasmons/polaritons.\textsuperscript{14} Simulations of a conically tapered metal field emitter tip, with a current source at the apex to represent the mixer current which would be generated by photomixing, show that TM surface waves would propagate outward from the apex along the tip.\textsuperscript{15} For a given frequency and tip size there is an optimum value for the half-angle of the conical tip at which the power delivered to a 50 $\Omega$ load at the broad end of the tapered tip is maximum. The existence of this optimum is attributed to the combined effects of radiation loss, which is dominant with slower tapering, and reflection caused by the impedance mismatch, which is dominant with faster tapering.\textsuperscript{15}
Others are interested in the closely related problem for which terahertz TM surface waves propagate in the opposite directions on a tapered metal wire to concentrate the energy at the apex.\textsuperscript{16–24} Experiments and simulations show that the energy is confined to a size that is much smaller than a wavelength to provide greater resolution in terahertz microscopy and spectroscopy.\textsuperscript{16} However, it is difficult to interpret whether some of the phenomena which are seen in the measurements and simulations are quasistatic or caused by diffraction.\textsuperscript{\textsuperscript{17}} The cone\textsuperscript{19–23} and the paraboloid of revolution\textsuperscript{24} are two models of tapered objects where the directions on a tapered metal wire to concentrate the energy at the apex.\textsuperscript{16–24} Experiments and simulations show that the surface corresponds to a fixed value of one coordinate in an orthogonal system for which the wave equation is separable. Thus, the electromagnetic fields may be determined by using the method of separation of variables to obtain solutions which are the products of analytic functions of the separate coordinates. The cone is less appropriate because the radius of curvature is zero at the apex. Thus, the electric field is singular at this point whether the cone is made of a dielectric\textsuperscript{25} or a perfect conductor.\textsuperscript{26} The fields with a paraboloid have no singularity at the apex, but this model is more challenging because the exterior solution requires irregular Coulomb wave functions which are analytic but not orthogonal.\textsuperscript{27}

It is not appropriate to approximate a field emitter tip with a perfect conductor because at terahertz frequencies the depth of penetration for the fields is typically 10–100 times the radius of curvature at the apex. Furthermore, surface waves will not occur when the tip is perfectly conducting.\textsuperscript{28} The criteria for simplification with the Leontovich boundary conditions are also not satisfied.\textsuperscript{29} For a conical model, in spherical coordinates the radial part of the product solution for the fields in each mode is the spherical Bessel functions of the third kind or their derivatives.\textsuperscript{27} In the interior and exterior solutions the arguments of these functions are $k_C r$ and $k_0 r$, respectively, where $k_C$ and $k_0$ are the propagation constants in the two regions. For the Sommerfeld surface waves propagating on an infinite cylinder having finite conductivity the dependence of the fields upon the axial coordinate is the same in the interior and exterior solutions.\textsuperscript{6} However, it is not possible for the fields to have the same dependence on the radius inside and outside the cone except in the trivial case where $k_C = k_0$. More generally, it may be shown that for any tapered object the dependence of the fields on the coordinate parallel to the surface must be different in the interior and exterior solutions, so a superposition of modes is required to satisfy the boundary conditions.

Several groups have used analytical methods to study the focusing of terahertz radiation at the apex of a metal cone.\textsuperscript{19–23} For example, Sommerfeld’s solution for an infinite cylinder was used at each axial location on a slowly tapering cone\textsuperscript{19–22} with no correction for reflections caused by changes in the characteristic impedance.\textsuperscript{30} Others used the Eikonal method to approximate the effects of slow tapering in a cone,\textsuperscript{23} but none of these addressed the severity of their approximation at the end of the cone which is the region of interest. Kurihara et al.\textsuperscript{\textsuperscript{22,24}} presented a “zeroth-order analysis” for both the cone\textsuperscript{22} and the paraboloid,\textsuperscript{24} referring to first-order and higher-order analyses to be presented later, but none have yet written the electromagnetic fields for a conical model of the tapered metal waveguide as a modal expansion and determined the coefficients for this series by applying orthogonality in matching the boundary conditions.

Others have studied the scattering of electromagnetic radiation from the convex surface of a perfectly conducting paraboloid\textsuperscript{11,32} and the interior solution for a paraboloidal waveguide assuming a perfect conductor or using the approximation of the Leontovich boundary conditions.\textsuperscript{33} In the present work we consider an axial current source, representing a terahertz mixer current, at the apex of a metal paraboloid having finite conductivity as a model for a field emitter to study the generation and propagation of terahertz surface waves on a field emitter tip.

\section{II. ANALYSIS}

The paraboloid was chosen to model the field emitter tip because it has a smooth shape which tapers over an infinite length and it would also be a convenient model for the analysis of field emission because the Schrödinger equation, Laplace’s equation, and the wave equation are all separable in paraboloidal coordinates. Figure 2 shows the emitter, which is bounded by the surface $\eta = \eta_0$ in the paraboloidal coordinates $\xi$, $\eta$, and $\varphi$, where the positive and negative $z$-axes correspond to $\eta=0$ and $\xi=0$, respectively. Surfaces
with constant $\xi$ or $\eta$ are paraboloids of revolution with a common focus at the origin and open in the $+z$ or $-z$ directions, respectively. The angle $\varphi$ is directed on the $z$-axis. The paraboloidal coordinates are related to the Cartesian coordinates by $x = \xi \eta \cos \varphi$, $y = \xi \eta \sin \varphi$, and $z = \frac{1}{2}(\xi^2 - \eta^2)$.\(^6\)

The electromagnetic eigenmodes for an object are determined by solving the source-free Maxwell’s equations subject to the boundary conditions. For harmonic time dependence of $e^{i\omega t}$ in an isotropic homogeneous medium, for azimuthal symmetry in paraboloidal coordinates the system of equations for the fields separates into two sets for transverse-electric and TM modes. For the TM modes, which are consistent with an axial current and have the fields $H_\varphi$, $E_\xi$, and $E_\eta$ the set of equations is as follows:

\[
\frac{1}{\eta \sqrt{\xi^2 + \eta^2}} \frac{\partial}{\partial \eta} (\eta H_\varphi) = j \omega e E_\xi, \tag{1a}
\]

\[
\frac{1}{\xi \sqrt{\xi^2 + \eta^2}} \frac{\partial}{\partial \xi} (\xi H_\varphi) = - j \omega e E_\eta, \tag{1b}
\]

\[
\frac{1}{(\xi^2 + \eta^2)^{3/2}} \left( \frac{\partial}{\partial \xi} (\xi^2 + \eta^2 E_\varphi) - \frac{\partial}{\partial \eta} (\xi^2 + \eta^2 E_\xi) \right) = - j \omega \mu H_\varphi. \tag{1c}
\]

These three equations may be combined to give the following wave equation where the propagation constant $k = k_0 = \omega \sqrt{\varepsilon_0 \mu_0}$ for the exterior solution in the vacuum outside of the emitter ($\eta > \eta_0$) and $k = k_C = \omega \sqrt{\varepsilon_C \mu_0} = k_0 e_0$, where $e = e_0$ for the interior solution:

\[
\frac{\partial^2}{\partial \xi^2} \left[ \frac{1}{\xi} \frac{\partial}{\partial \xi} (\xi H_\varphi) \right] + \frac{\partial^2}{\partial \eta^2} (\eta H_\varphi) + k^2 (\xi^2 + \eta^2) H_\varphi = 0. \tag{2}
\]

The method of separation of variables may be used to solve Eq. (2) to determine $H_\varphi$, and then Eqs. (1a) and (1b) may be used to determine $E_\xi$ and $E_\eta$ to show that the fields are given by the following expressions:

\[
H_\varphi = \frac{1}{\xi \eta} C \left[ F_0 \left( d, \frac{k \xi^2}{2} \right) + a G_0 \left( d, \frac{k \xi^2}{2} \right) \right] F_0 \left( -d, \frac{k \eta^2}{2} \right) + b G_0 \left( -d, \frac{k \eta^2}{2} \right), \tag{3a}
\]

\[
E_\xi = \frac{-j}{\xi \sqrt{\xi^2 + \eta^2}} \sqrt{\frac{\mu}{\varepsilon}} C \left[ F_0 \left( d, \frac{k \xi^2}{2} \right) + a G_0 \left( d, \frac{k \xi^2}{2} \right) \right] F_0 \left( -d, \frac{k \eta^2}{2} \right) - d, \frac{k \eta^2}{2} + b G_0 \left( -d, \frac{k \eta^2}{2} \right), \tag{3b}
\]

\[
E_\eta = \frac{j}{\eta \sqrt{\xi^2 + \eta^2}} \sqrt{\frac{\mu}{\varepsilon}} C \left[ F_0 \left( d, \frac{k \xi^2}{2} \right) + a G_0 \left( d, \frac{k \xi^2}{2} \right) \right] F_0 \left( -d, \frac{k \eta^2}{2} \right) - d, \frac{k \eta^2}{2} + b G_0 \left( -d, \frac{k \eta^2}{2} \right). \tag{3c}
\]

Here, $F_0$ and $G_0$ are the regular and irregular Coulomb wave functions with index $0,3^7$ where the primes denote differentiation with respect to the second argument of each function, and the parameters $a$, $b$, $C$, and $d$ must be determined to satisfy the boundary conditions.

The irregular Coulomb wave function $G_0$ and its derivative $G'_0$ are singular when the second argument is zero which occurs $\eta = 0$ on the positive $z$-axis and when $\xi = 0$ on the negative $z$-axis. However, the irregular Coulomb wave function must be included in the exterior solution to have outward-going waves corresponding to those in the exterior solution for the Sommerfeld waves with an infinite cylinder.\(^6\) Thus, it is necessary to partition the space to have separate solutions in each of the following four regions: region I ($z < 0, \eta > \eta_0$): region II ($z > 0, \eta > \eta_0$): region III ($z < 0, \eta < \eta_0$); and region IV ($z > 0, \eta < \eta_0$). This partitioning is illustrated in Fig. 3.

In order for the fields to be nonsingular on the $z$-axis, it is necessary for the coefficient $a$ to be zero in regions I and III where $\xi = 0$ on the negative $z$-axis and $b$ to be zero in region IV where $\eta = 0$ on the positive $z$-axis. Furthermore, both $a$ and $b$ must be zero in regions III and IV to prevent a singularity at the origin. L’Hôpital’s rule may be used in Eqs. (3a)–(3c) to show that with these specifications all of the fields are finite at all points on the $z$-axis.

Next, requiring that there are only outgoing waves at infinity and that the fields are continuous at the III-IV boundary gives the following expressions for the fields in all four regions, where “34” denotes the combined regions III and IV:

\[
H_{34} = A \frac{F_0}{\xi \eta} \left( \frac{k_0 \xi^2}{2} \right) \left[ F_0 \left( -e, \frac{k_0 \eta^2}{2} \right) + j G_0 \left( -e, \frac{k_0 \eta^2}{2} \right) \right], \tag{4a}
\]
\( E_{\hat{\alpha}} = \frac{-jA}{\xi \sqrt{\xi^2 + \eta^2}} \sqrt{\frac{\mu_0}{\varepsilon_0}} F_0(e, k_0 \xi^2) \left[ F_0\left( e, -\frac{k_0 \eta^2}{2} \right) + jG_0\left( e, -\frac{k_0 \eta^2}{2} \right) \right] \), \quad (4b)

\( E_{\hat{\alpha}} = \frac{jA}{\eta \sqrt{\xi^2 + \eta^2}} \sqrt{\frac{\mu_0}{\varepsilon_0}} F_0(f, k_0 \xi^2) \left[ F_0\left( f, -\frac{k_0 \eta^2}{2} \right) + jG_0\left( f, -\frac{k_0 \eta^2}{2} \right) \right] \), \quad (4c)

\( H_{\hat{\alpha}1} = \frac{B}{\xi \eta} F_0\left( f, k_0 \xi^2 \right) + jG_0\left( f, k_0 \xi^2 \right) \left[ F_0\left( f, -\frac{k_0 \eta^2}{2} \right) + jG_0\left( f, -\frac{k_0 \eta^2}{2} \right) \right], \quad (5a) \)

\( H_{\hat{\alpha}1} = \frac{-jB}{\xi \sqrt{\xi^2 + \eta^2}} \sqrt{\frac{\mu_0}{\varepsilon_0}} F_0\left( f, k_0 \xi^2 \right) + jG_0\left( f, k_0 \xi^2 \right) \left[ F_0\left( f, -\frac{k_0 \eta^2}{2} \right) + jG_0\left( f, -\frac{k_0 \eta^2}{2} \right) \right], \quad (5b) \)

\( E_{\hat{\beta}} = \frac{jB}{\eta \sqrt{\xi^2 + \eta^2}} \sqrt{\frac{\mu_0}{\varepsilon_0}} F_0\left( f, k_0 \xi^2 \right) + jG_0\left( f, k_0 \xi^2 \right) \left[ F_0\left( f, -\frac{k_0 \eta^2}{2} \right) + jG_0\left( f, -\frac{k_0 \eta^2}{2} \right) \right], \quad (5c) \)

\( H_{\hat{\beta}34} = \frac{C}{\xi \eta} F_0\left( g, k_c \xi^2 \right) F_0\left( -g, k_c \xi^2 \right), \quad (6a) \)

\( E_{\hat{\beta}34} = \frac{-jC}{\xi \sqrt{\xi^2 + \eta^2}} \sqrt{\frac{\mu_0}{\varepsilon_0}} F_0\left( g, k_c \xi^2 \right) F_0\left( -g, k_c \xi^2 \right), \quad (6b) \)

\( E_{\hat{\beta}34} = \frac{jC}{\eta \sqrt{\xi^2 + \eta^2}} \sqrt{\frac{\mu_0}{\varepsilon_0}} F_0\left( g, k_c \xi^2 \right) F_0\left( -g, k_c \xi^2 \right), \quad (6c) \)

\( E_{\hat{\beta}34} = \frac{-jB}{\xi \sqrt{\xi^2 + \eta^2}} \sqrt{\frac{\mu_0}{\varepsilon_0}} F_0\left( f, k_0 \xi^2 \right) F_0\left( -f, k_0 \xi^2 \right), \quad (7a) \)

\( E_{\hat{\beta}34} = \frac{jB}{\xi \sqrt{\xi^2 + \eta^2}} \sqrt{\frac{\mu_0}{\varepsilon_0}} F_0\left( f, k_0 \xi^2 \right) F_0\left( -f, k_0 \xi^2 \right), \quad (7b) \)

\( H_{\hat{\beta}34} = \frac{1}{\xi \eta} \int_{-\infty}^{\infty} V(s) \left[ F_0\left( s, k_c \xi^2 \right) + jG_0\left( s, k_c \xi^2 \right) \right] F_0\left( -s, -\frac{k_c \eta^2}{2} \right) \left[ F_0\left( -s, -\frac{k_c \eta^2}{2} \right) + jG_0\left( -s, -\frac{k_c \eta^2}{2} \right) \right] ds, \quad (7c) \)

This set of nine simultaneous equations defines the fields for only one mode, but it has already been noted that a superposition of modes is required to satisfy the boundary conditions at the surface of a tapered object having finite conductivity, and this was demonstrated for the case of a cone. Thus, it is necessary to generalize these equations to integrals in which the coefficients \( A, B, \) and \( C \) are replaced by \( U(s), V(s), \) and \( W(s) \), where the continuous variable \( s \) replaces the parameters \( e, f, \) and \( g \). Therefore, the set of nine equations may be written as follows:

\( H_{\hat{\alpha}1} = \frac{1}{\xi \eta} \int_{-\infty}^{\infty} U(s) F_0\left( s, k_0 \xi^2 \right) F_0\left( -s, -\frac{k_0 \eta^2}{2} \right) + jG_0\left( -s, -\frac{k_0 \eta^2}{2} \right) ds, \quad (7a) \)

\( E_{\hat{\beta}34} = \frac{-jB}{\xi \sqrt{\xi^2 + \eta^2}} \sqrt{\frac{\mu_0}{\varepsilon_0}} \int_{-\infty}^{\infty} W(s) F_0\left( s, k_c \xi^2 \right) F_0\left( -s, -\frac{k_c \eta^2}{2} \right) ds, \quad (9a) \)

\( E_{\hat{\beta}34} = \frac{jB}{\eta \sqrt{\xi^2 + \eta^2}} \sqrt{\frac{\mu_0}{\varepsilon_0}} \int_{-\infty}^{\infty} W(s) F_0\left( s, k_c \xi^2 \right) F_0\left( -s, -\frac{k_c \eta^2}{2} \right) ds, \quad (9b) \)

\( E_{\hat{\beta}34} = \frac{-jC}{\xi \sqrt{\xi^2 + \eta^2}} \sqrt{\frac{\mu_0}{\varepsilon_0}} \int_{-\infty}^{\infty} W(s) F_0\left( s, k_c \xi^2 \right) F_0\left( -s, -\frac{k_c \eta^2}{2} \right) ds, \quad (9c) \)

It has already been noted that the irregular Coulomb functions are not orthogonal,\(^{27}\) so unlike the case for the cone, it is not possible to apply orthogonality to simplify determining the functions \( U(s), V(s), \) and \( W(s) \) in matching the boundary conditions. Thus, we use a numerical procedure in which a cost function is defined as the mean absolute fractional error
in satisfying the boundary conditions, averaged over each of the boundaries. Unconstrained derivative-free optimization must be used because the cost function is not smooth and it is computationally intensive to evaluate. However, as a first approximation at this time we test the possibility that a single mode may be sufficient when the wavelength is much smaller than the radius of curvature at the apex.

III. SIMULATIONS

The simulations were made with the finite difference-time domain (FDTD) software XFDTD using a $723 \times 250 \times 250$ grid of $2 \, \mu m$ Yee cells and a time step of $3.852 \, fs$. The source for these calculations was a point dipole represented by a single Yee cell at the apex, excited by a Gaussian derivative wave form having a peak power spectral density at $300 \, GHz$. In each case the model was on the long axis of the grid with the broad end of the paraboloid (opposite from the apex) adjacent to the absorbing wall at the rear boundary of the grid. Thus, when the results were examined in the time domain there were no significant effects of reflections from the broad end of the paraboloid so the results represent the modeled section of a paraboloid as part of a structure having infinite length.

The method of FDTD is widely used, unlike the new analytical method which is described in Sec. II, and FDTD has already been described elsewhere in considerable detail. This method may be used at virtually any frequency as long as there are a sufficient number of sample points per wavelength. Since high dielectric contrast was required in the examples, care was used to minimize the errors which can occur near the surface of the model due to stair casing of the Yee cells.

IV. RESULTS AND DISCUSSION

The value of $E'$, the total energy in the electric and magnetic fields per unit of axial length normalized relative to the value at the apex, was determined by integrating the sum of the electric and magnetic energy densities over a surface transverse to the direction of propagation with the analytical solution as well as with the simulations.

The objective was to make simulations at terahertz frequencies, generally defined as from 0.1 to 5 THz. However, using the first approximation of the analytical solution which consists of the single mode it was not possible to obtain convergence at frequencies above 1 GHz. Figure 4 shows $E'$ as a function of the distance from the apex at a frequency of 1 GHz for a paraboloid having a dielectric constant of 20, a conductivity $\sigma=1000 \, S/m$, a radius of curvature at the apex equal to 10 nm.

Figure 5 shows $E'$, the normalized energy per unit length, as a function of the distance from the apex at a frequency of 300 GHz, as determined by FDTD simulations with two different sets of dielectric properties. Each simulation used a paraboloid with a length of 1.4 mm and a radius of curvature of 260 nm at the apex as shown in Fig. 6. At the back end of the model the radius of the paraboloid is 38 $\mu m$ so the greatest value for the circumference is equal to 16% of the wave-length. This was necessary to avoid higher-order azimuthally dependent modes which occur when the circumference is greater than the wavelength. These two simulations were made for a perfect electrical conductor (PEC) as well as with the Drude model of tungsten metal at 300 GHz for which the conductivity $\sigma=1.77 \times 10^7 \, S/m$.

Two additional FDTD simulations were made using a cylindrical model in place of the paraboloid, but again at a frequency of 300 GHz with the dielectric properties for tungsten. Each model had a cylinder with a radius of 80 $\mu m$ and a length of 1.52 mm. In one model the source was a point dipole at the center of the flat end of the cylinder and in the other the point dipole was at the end of a hemispherical tungsten end cap attached to the cylinder. These two simulations also show a precipitous drop in $E'$ near the apex and they have similar values of $E'$ at the back end of the model: $7.5 \times 10^{-5}$ without the end cap and $1.90 \times 10^{-4}$ with the end cap. For comparison, the FDTD simulations for the parabo-
The lengths of the quasistationary and transition regions are reduced, which reduce the loss in this system.

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