Numerical analysis of the transmission efficiency of heat-drawn and chemically etched scanning near-field optical microscopes

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The scanning near-field optical microscope (SNOM) has been tested experimentally for a wide variety of applications, but, to date, there has been little work done on the numerical or analytical modeling of the optical field as it propagates throughout the SNOM probe. Therefore, the fabrication on the probes relies more on trial and error than on clear design principles. An algorithm has been developed for the study and optimization of the geometry of SNOM probes fabricated by the heat-drawn and the one-step chemically etched methods. The algorithm uses the finite-difference beam propagation method (FD-BPM) to model the field evolution throughout the SNOM structure. © 2000 Optical Society of America

1. Introduction

The scanning near-field optical microscope (SNOM) has proved to be a valuable tool in spectroscopy, lithography, and photonics. It also shows great promise for use in quantum dot research.

In this paper we address the important issue of the transmission efficiency (TE) of the SNOM probe in isolation; i.e., a generic algorithm is presented that permits the design and optimization of the fiber probe geometry in terms of its TE. The definition of TE depends on the mode of operation in which the SNOM probe is being used (refer to Fig. 1). When light is transmitted through the aperture (from left to right as shown in Fig. 1) the device is operating in transmission mode, and when light is collected through the aperture (from right to left as shown in Fig. 1) the device is operating in collection mode. The probe can also be used in a combination of transmission and collection modes. The main objective of operation in either mode is to maximize power transfer for processing and detection. In transmission mode, the TE is defined as the ratio of the power at the subwavelength aperture to the power launched into the untapered end of the probe. In collection mode, TE is defined as the ratio of the power contained in the fundamental mode at the untapered end of the probe (the SNOM probes studied here are fabricated from single-mode fiber) to the power launched into the subwavelength aperture.

The effects of the sample on transmission and on collection of power by the probe have been deliberately excluded. The emphasis here is on the optical properties of the probe in isolation. However, the technique presented herein could be extended to include the effects of the sample. The following sections describe both the physical model and the theoretical framework that we used to analyze the transmission properties of the SNOM fiber tip.

The technique described here uses the finite-difference beam propagation method (FD-BPM) in circular geometry to model the propagation of the optical signal into the fiber tip. This limits the illumination conditions to circular symmetry, in agreement with the normal usage of SNOM probes. The impetus for this study arose from the need to design a computer-aided design package that can be used as a guide to the design and optimization of SNOM probe geometries before device fabrication.

2. Fabrication Processes of SNOM Probes

In this paper we treat SNOM probes that are commonly fabricated from single-mode optical fiber by drawing [Fig. 2(a)], by single-step chemical etching [Fig. 2(b)].

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of metal
resultant probe profile is usually coated with a layer
SNOM probes fabricated by these techniques. The
characteristics. This is especially true for the draw-
Aperture diameter. The bulk of the power loss is
causen by the subwavelength aperture (approximately
50–200 nm). The smaller the size of the aperture,
the less throughput of optical power. Theoretical
calculations of optical transmission through a sub-
wavelength aperture have been studied by Bethe. In
his calculations Bethe considered a subwavelength
aperture of radius \(a\), \(a \ll \lambda\), in a perfectly conducting
screen. For normal incidence and transmission, the
throughput relation is proportional to \(a\) to the power
of 6. Consequently, as the radius becomes smaller,
the attenuation increases dramatically.
Metallic coating. The presence of a metal layer
ensures that the probe tip is optically opaque (except
for the subwavelength aperture) and focuses the
power contained in the fiber to maximize the amount
of power that passes through the aperture. The
drawback of having a metallic layer is that it is highly
absorbing at optical frequencies. For example, at
850 nm, aluminum has a refractive index with an
imaginary part of 7. For propagation in bulk media
this would correspond to an \(-60\,\text{dB}/\mu\text{m}\) loss. Any
interaction of the electric field with the metal coating
therefore will result in power loss. The degree of
loss that is due to the metal layer will depend to a
high degree on the probe geometry.
Taper length and cone half-angle. The cone half-
angle and the taper length are the main parameters
that determine the final geometry of the probe. Ac-

Fig. 2. Schematic of three probe geometries (not to scale): (a) heat-drawn, (b) one-step chemical etching, (c) hybrid drawn–etched.
Accordingly, these parameters have a significant effect on the overall performance of the device. The longer the taper region, the longer the interaction length between the electric field and the metallic coating. This interaction occurs at two prominent locations: first, where the evanescent part of the electric field starts to interact with the metallic coating because of the tapering of the probe, and second, at the probe tip where the electric field is tightly confined by the metallic layer. Intuitively, with a small cone half-angle the taper length will be relatively long. This will result in a greater length over which the evanescent field can interact with the metal coating. Also, the distance between the metallic waveguide cutoff points and the probe aperture will also increase, resulting in a greater power loss. With a large cone half-angle, the length of the probe taper will be short. Consequently the losses associated with the electric field's interaction with the metallic coating will be greatly reduced. As the cone angle increases (from a large cone half-angle) the fraction of incident electric field power at the probe aperture (compared with the total power of the initial electric field profile) decreases. This result is due to a decrease in the focusing effect of the metallic coating. The limiting case occurs when the cone half-angle is 90 deg; in this case there is no focusing by the metallic coating, and the only fraction of incident power that reaches the probe aperture is that which is contained within the area of the aperture. Hence there will be an optimal range of cone angles that will maximize the overall transmission efficiency of the probe.

Modal guidance of the metallic waveguide. With all SNOM devices the electric field is initially supported by an optical waveguiding structure (which usually has a core–cladding index profile). A point will be reached along the electric field's path to the tip where confinement will be due to the metallic dielectric waveguide. Of most concern with the application of the SNOM is that all modes of a metallic waveguide have cutoffs. Analytically this is the case when one is solving the Helmholtz equation for a cylindrical metallic waveguide and making the assumption that the metal is a perfect conductor (hence the electric field value at the metal–dielectric interface is zero). However, this assumption cannot be applied to the SNOM probe because of the dimensions and materials used within several micrometers of the probe tip. In this situation a modal analysis that takes into account the core–cladding–metal structure is required for better understanding of the waveguiding properties of the SNOM. Novotny and Hafner numerically analyzed such a structure, which included the effects of plasmons. This analysis concluded that the geometry of the probe should be designed to couple as much power as possible into the HE_{11} mode. The reasoning is that the HE_{11} mode, unlike the modes in standard metallic waveguides, does not become cut off. Results presented here are compared with those of Novotny et al. and are shown to be in good agreement.

Consequently, the TE of the probe depends on the final geometry in terms of its aperture size, length, index contrast, and taper shape and on the presence of the metal coating. Maximizing the TE of these probes is of great importance for the specific applications of lithography and quantum dot research.

4. Theory

The depth and degree of analysis for any optical device vary, depending on the information required. What level of accuracy is or is not acceptable with regard to the desired solutions? How precise do the results have to be? The answers can and will depend on a number of factors that will ultimately determine the depth of analysis undertaken.

Time, ease of use, fabrication tolerances, and the end use of the device are the major factors that lead to the use of the FD-BPM. The fabrication processes involved with SNOM probes have large tolerance margins associated with TE. Reproducibility in terms of the final probe geometry is significantly difficult. The process of pulling, etching, cleansing, and coating with a metal layer to produce an aperture of the order of 20–200 nm is extremely hard to achieve consistently.

One of the main aims of this research was to provide the end user with a software computer-aided design solution that can be used as a guide to the fabrication process in the design of SNOM probes. The point to make here is that, even if we go to the lengths of undertaking a full three-dimensional vectorial analysis, it is going to be nearly impossible to reproduce those results physically because of the wide tolerances associated with the fabrication process. Again, a full three-dimensionally vectorial analysis of SNOM probes is computationally intensive and extremely time consuming.

What is sought instead here is a computationally efficient means of obtaining the optimal geometry for a wide variety of SNOM probes. The FD-BPM is well known and is an ideal method to give the designer an idea of what type of probe geometry will be optimal before he or she fabricates the device. In this research we use a scalar version of the FD-BPM to study the optical behavior of SNOM devices. This is a fast and efficient method compared with a full vectorial analysis.

5. FD-BPM in Circular Geometry

Typical SNOM probes are made from standard telecom fibers, and consequently light propagation can be analyzed by the weak-guidance approximation. An important factor that simplifies implementation of the numerical algorithm is that the probe remains axisymmetric throughout its length. Mathematically, this means that there is no azimuthal field dependence because we assume that the tip is excited by use of the fundamental mode of the fiber and that this mode is axisymmetric. Furthermore, we can make the approximation that the field is mainly forward directed, and, consequently, we can apply the slowly varying approximation. Within this frame-
work, the field evolution is given by the well-known paraxial (or Fresnel) wave equation

\[ 2ikn_0 \frac{\partial \psi}{\partial z} = \frac{\partial^2 \psi}{\partial r^2} + \frac{1}{r} \frac{\partial \psi}{\partial r} + k^2[n^2(r, z) - n_0^2]\psi, \tag{1} \]

where \( \psi \) is the scalar field, \( r \) is the transverse coordinate, \( k = 2\pi/\lambda \) is the free-space wave number, \( n \) is the refractive-index distribution, \( n_0 \) is the reference background index, and \( \lambda \) is the wavelength of the monochromatic source. We implement the FD-BPM by replacing the partial derivatives in Eq. (1) by finite differences evaluated on a discretization grid. The resultant tridiagonal matrix is solved for the unknown electric field at longitudinal position \( z + \Delta z \). The boundary conditions used in this analysis were a combination of absorbing and transparent conditions.

6. Numerical Implementation

A. Transmission Mode

At the beginning of the simulation the input side of the fiber supports only the fundamental mode. Here the fundamental mode is solved for numerically according to the cross-sectional refractive-index profile of the fiber used in fabricating the SNOM. This modal solution is then used by the FD-BPM as the initial electric field profile to be launched into the input end of the probe. The input end of the probe is defined to be the place the tapering of the device begins. From this point on, the FD-BPM is used to propagate the electric field to the probe aperture.

B. Collection Mode

In collection mode, a Gaussian beam of unit power is launched into the subwavelength aperture. The FD-BPM is used to propagate the electric field to the untapered end of the probe. At the untapered end an overlap integral of the resultant electric field profile with the fundamental mode of the fiber is evaluated. We do this to calculate the ratio of power coupled into fundamental mode of the probe at the untapered end to the power launched into the probe’s aperture.

For both modes of operation the numerical grid’s discretization is changed dynamically to minimize errors associated with numerical accuracy. Information on field evolution, power within the probe, and the final electric field profile is stored to disk for data analysis.

C. SNOM Geometries

1. Heat-Drawn and Taffy-Pulled Techniques

We studied probes fabricated by the drawn technique for a number of cases to make a comparison between numerical and experimental data. Furthermore, fiber probes made by the drawn technique have well-known refractive-index profiles. With reference to Fig. 2(a), the relationship between the core and the cladding index profiles is \( \tan(\gamma) = (n/\gamma) C_{cl}/C_{co} \), where \( C_{co} \) is the core diameter and \( C_{cl} \) is the cladding diameter.

2. Chemically Etched Technique

In chemically etched probes the dimensions of the core and the cladding remain constant throughout the device. The final probe geometry is ultimately determined by the etching process used, which will define the cone half-angle of the SNOM probe after fabrication.

7. Results and Discussion

A. TE of Heat-Drawn or Taffy-Pulled SNOM’s

To assess the validity of the FD-BPM, we compared the numerical results obtained with the algorithm with experimental results from Valaskovic et al. The parameters used within the FD-BPM were set to be the same as, or as close as possible to, those used experimentally by Valaskovic et al. Initially, a probe of 1-mm length with an aperture diameter of 100 nm was injected with unit power. Figure 3 is a plot of the power contained within the probe versus distance from the probe tip. Because of the weak interaction between the guided field’s evanescent tail and the aluminum coating, little power is lost until within 40 \( \mu \)m of the probe tip. Two processes lead to the loss of power shown in Fig. 3. Within 40 \( \mu \)m of the probe tip, the optical field undergoes absorption, mainly as a result of the interaction of the evanescent field with the aluminum coating. Near 5 \( \mu \)m, the power exponentially decreases because the fundamental mode of the metallic waveguide is cut off. Figure 4 is a plot of TE versus aperture diameter. Here, experimental results obtained by Valaskovic et al. are plotted against numerical results obtained with the FD-BPM. Two lengths of taper were simulated (refer to the caption of Fig. 3). These results clearly show that a longer taper probe will incur greater losses. This result is due to the increased interaction length between the electric field and the metal layer. Also, there is a greater distance be-
between the probe tip and the cutoff points for the modes of the metallic waveguide.

B. TE Dependency on Cone Half-Angle

Figures 5 and 6 are plots of TE versus cone half-angle for transmission and collection modes, respectively. These plots were produced with the following simulation parameters:

- standard single-mode fiber with an 8-μm core diameter (refractive index of 1.450) and a 125-μm cladding diameter (refractive index of 1.447),
- wavelength of 850 nm,
- aluminum coating thickness of 50 nm (refractive index of 2 + i),
- aperture diameter of 200 nm.

We used these parameters to give the program predefined parameters from a known fiber type and then to determine what range of SNOM geometries would give the best performance in terms of TE.

The first point to note from Figs. 5 and 6 is that they have the same response. This is to be expected from the nature of the waveguiding structure itself; it is reciprocal in nature. There is also considerable difference in the TE plots between the two fabrication techniques, which is due to the tapering of the core profile in the heat-drawn probes especially at lower cone half-angles and results in a greater spreading of the spot size for the fundamental mode. Once the V value of the core goes below 2.0, the spot size of the fundamental mode begins to increase. This will result in a greater amount of power contained in the evanescent part of the electric field. Hence there will be more electric field power to interact with the lossy metallic coating, resulting in a higher loss than for the chemically etched case. For the chemically etched case the spot size of the fundamental mode will not spread because the core remains constant in diameter throughout the SNOM device. There will be less power contained in the evanescent field; hence there will be less power lost with the chemically etched probe.

The results show that the chemically etched probe has a narrow region of optimal TE between cone half-angles of 5 and 15 deg. These results should be compared with that when there is no real definitive optimal region of TE.

Common to both fabrication techniques is the oscillatory behavior of the power transmission that increases in both amplitude and period with increasing cone half-angle. This oscillation is due predominantly to the coupling of power between the two lowest-order modes supported by the structure. This phenomenon can be quantified by an adiabaticity criterion that was developed by Love et al. This will result in a greater amount of power contained in the evanescent part of the electric field. Hence there will be more electric field power to interact with the lossy metallic coating, resulting in a higher loss than for the chemically etched case. For the chemically etched case the spot size of the fundamental mode will not spread because the core remains constant in diameter throughout the SNOM device. There will be less power contained in the evanescent field; hence there will be less power lost with the chemically etched probe.

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ing increase in power exchange between the supported modes. This is seen in Figs. 5 and 6 as an increase in amplitude of the oscillations.

Novotny et al. defined the ideal range of cone half-angles for probe fabrication to be 15–25 deg. The differences between his results and those presented in this paper can be attributed to a number of factors: Novotny et al. used a numerical domain that included only the last portion of probe tip that would support the fundamental mode just before it is cut off (this part of the mode was used to excite the probe tip). This mode is the only source used for excitation of the probe tip under simulation. Modal evolution up to this point is disregarded, and the power contained in other modes is not taken into account (especially for the case of nonadiabatic probe geometry, which is applicable for the majority of probes fabricated). Accordingly, their study is a slightly idealized optimal case. In this paper, modal evolution is taken into account and consequently a more realistic and practical result is obtained.

C. Power Evolution throughout SNOM

Figures 7 and 8 show the power contained within the probe for the two fabrication techniques, Fig. 7 for a cone half-angle of 10 deg and Fig. 8 for a cone half-angle of 35 deg. For both cases it is evident that the heat-drawn fiber will undergo greater power loss. Again, this phenomenon is due to the greater spreading of the electric field in heat-drawn probes that was explained in Subsection 7.B.

Another important point to note is the greater power loss between the heat-drawn and the chemically etched cases for the smaller cone half-angle of 10 deg compared with that of the 35 deg. The extra loss is again attributed to the greater length over which the spot size of the fundamental mode can spread. With the 35-deg cone half-angle the spot size of the fundamental mode will not spread to the same extent as it does for the 10-deg half-angle because of the shorter probe length.

8. Conclusion

The algorithm presented here for the analysis of electromagnetic field evolution throughout SNOM probes has resulted in good agreement with experimental data for probes fabricated by the heat-drawn technique. The simplicity of the method used and its generality make it a perfect candidate for use in the design and optimization of SNOM probes. In particular, the FD-BPM permits the study of arbitrary probe tip geometry and refractive indices in a relatively straightforward way.

We have also reviewed the basic physics of SNOM probes and have shown how it results in a series of design rules that can help the designers of such probes. Of particular importance is the trade-off required between the two loss mechanisms involved to optimize the TE of these devices.

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