Single-mode guiding properties of subwavelength-diameter silica and silicon wire waveguides

Limin Tong
Division of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA
ltong@fas.harvard.edu

Centre for Optical and Electromagnetic Research, State Key Laboratory of Modern Optical Instrumentation, Zhejiang University, Hangzhou 310027, China
phytong@zju.edu.cn

Jingyi Lou
Department of Physics and State Key Laboratory of Silicon Materials, Zhejiang University, Hangzhou 310027, China

Eric Mazur
Department of Physics and Division of Engineering and Applied Sciences, Harvard University, Cambridge, MA 02138, USA
Mazur@deas.harvard.edu

http://www.mazur.harvard.edu

Abstract: Single-mode optical wave guiding properties of silica and silicon subwavelength-diameter wires are studied with exact solutions of Maxwell’s equations. Single mode conditions, modal fields, power distribution, group velocities and waveguide dispersions are studied. It shows that air-clad subwavelength-diameter wires have interesting properties such as tight-confinement ability, enhanced evanescent fields and large waveguide dispersions that are very promising for developing future microphotonic devices with subwavelength-width structures.

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References and links
1. Introduction

In the past 30 years, dielectric optical waveguides with widths or diameters from micrometers to millimeters have got successful applications in many fields such as optical communication, optical sensing and optical power delivery systems [1-3]. Photonic device applications benefit from minimizing the width of the waveguides, but fabricating low-loss optical waveguides with subwavelength diameters remains challenging because of high precision requirement. Recently, several types of dielectric submicrometer- and nanometer-diameter wires of optical qualities have been obtained [4-5]. These wires, with diameters smaller than a micrometer, are tens to thousands times thinner than the commonly used micrometer-diameter waveguides. They can be used as air-clad wire-waveguides with subwavelength-diameter cores, and building blocks in the future micro- and nano- photonic devices. However, in contrast to the well-studied optical waveguide with diameter larger than the wavelength, guiding property of subwavelength-diameter wire-waveguides has not been adequately studied. In this paper, based on exact solutions of Maxwell’s equations and numerical calculations, we study basic guiding properties of subwavelength-diameter wires. We choose fused silica (SiO$_2$) and single crystal silicon (Si) as typical dielectric materials for our simulation under the following considerations: (1) fused silica and single crystal silicon are among the most important photonic and optoelectronic materials within the visible and near-infrared ranges; (2) both silica and silicon wires with submicrometer- or nanometer- diameters have been successfully fabricated [5-7]; (3) their optical and physical properties are well studied, and they have typical values of moderate and high refractive indices (about 1.45 for silica and 3.5 for silicon).

2. Basic model

For basic consideration, we assume that the wire has a circular cross-section, an infinite air clad, and a step-index profile. The wire diameter ($D$) is not very small (e.g. $D>10$ nm) so that the statistic parameters — permittivity ($\varepsilon$) and permeability ($\mu$) — can be used to describe the responses of a dielectric medium to an incident electromagnetic field. The length of the wire is large enough (e.g. long than 10 $\mu$m) to establish the spatial steady state. We also assume that the wire is very uniform in diameter and smooth in sidewall, which has been shown achievable recently [5].

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The mathematic model of an air-clad dielectric wire is shown in Fig. 1. Assuming the refractive indices of the wire material and the air are \( n_1 \) and \( n_2 \) respectively, then the wire has the following index profile

\[
n(r) = \begin{cases} n_1, & 0 < r < a, \\ n_2, & a \leq r < \infty \end{cases}
\]

where \( a \) is the radius of the wire.

For microphotonic applications, usually a short length (e.g., tens to hundreds of micrometers) of the wire is long enough. Therefore we assume that the wire is non-dissipative and source free, which is true for most of the dielectric materials within their transparent ranges. With these assumptions, one can reduce Maxwell’s equations to the following Helmholtz equations

\[
\left\{ \nabla^2 + n^2 k^2 - \beta^2 \right\} \tilde{e} = 0,
\]

\[
\left\{ \nabla^2 + n^2 k^2 - \beta^2 \right\} \tilde{h} = 0
\]

where \( k = \frac{2\pi}{\lambda} \), and \( \beta \) is the propagation constant.

Exact solutions for this model can be found in Ref. [8]. The eigenvalue equations of Eq. (2) for various modes are as follows

for \( HE_{vm} \) and \( EH_{vm} \) modes:

\[
\left\{ \frac{J_v'(U)}{UJ_v(U)} + \frac{K_v'(W)}{WK_v(W)} \right\} \left\{ \frac{J_v'(U)}{UJ_v(U)} + \frac{n_2^2K_v'(W)}{n_1^2WK_v(W)} \right\} = \left( \frac{v\beta}{kn_1} \right)^2 \left( \frac{V}{UW} \right)^4
\]

(3)

for \( TE_{0m} \) modes:

\[
\frac{J_v(U)}{UJ_v(U)} + \frac{K_v(W)}{WK_v(W)} = 0
\]

(4)

for \( TM_{0m} \) modes:

\[
\frac{n_1^2J_v(U)}{UJ_v(U)} + \frac{n_2^2K_v(W)}{WK_v(W)} = 0
\]

(5)

where \( J_v \) is the Bessel function of the first kind, and \( K_v \) is the modified Bessel function of the second kind, \( U = D(k_0n_1^2\beta)^{1/2}/2 \), \( W = D(\beta^2 - k_0n_2^2)^{1/2}/2 \), \( V = k_0a(n_1^2 - n_2^2)^{1/2} \), and \( D = 2a \).

We assume that the index of the air \((n_2)\) is 1.0, and use the following Sellmeier-type dispersion formula (at room temperature) to obtain the refractive indices of the wire materials

\[
n_2 = 1.0 \text{(air)}
\]
for fused silica (SiO₂) [9]:

\[
\frac{n^2 - 1}{\lambda^2} = \frac{0.6961663\lambda^2}{\lambda^2 - (0.0684043)^2} + \frac{0.4079426\lambda^2}{\lambda^2 - (0.1162414)^2} + \frac{0.8974794\lambda^2}{\lambda^2 - (9.896161)^2}
\]

(6)

for single crystal silicon [10]:

\[
\frac{n^2 - 1}{\lambda^2} = \frac{0.939816\lambda^2}{\lambda^2} + \frac{0.00093358\lambda^2}{\lambda^2 - 1.22567}
\]

(7)

where the unit of \(\lambda\) is \(\mu m\).

Propagation constants (\(\beta\)) of these air-clad wire waveguides are obtained numerically. For example, shown in Fig. 2 and 3 are diameter-dependent \(\beta\) of silica and silicon wires at the wavelength of 633 nm and 1.5 \(\mu m\) respectively, where the wire diameter (\(D\)) is directly related to the V-number [\(V = k_0 D (n_1^2 - n_2^2)^{1/2}/2\)]. It is clear that, when the wire diameter reduced to a certain value (denoted as \(D_{\text{SM}}\), corresponding to \(V=2.405\)), only the \(HE_{11}\) mode exists, corresponding to the single mode operation. Several high-order modes are also plotted as dotted lines.

**3. Single-mode condition and fundamental modes**

The single mode condition of an air-clad wire-waveguide, as illustratively shown in Figs. 2-4 (where the dashed lines are dividing lines), can be obtained from Eqs. (4) and (5) as

\[
V = 2\pi \cdot \frac{a}{\lambda_0} \left(n_1^2 - n_2^2\right)^{1/2} = 2.405.
\]

(8)

Single mode conditions of the air-clad silica- and silicon-wire waveguides with respect to the wavelengths and wire diameters, are shown as solid lines in Fig. 4. The region beneath the solid line corresponds to the single-mode region. For comparison, wavelength of the propagating light inside the wire material (that is \(\lambda = \lambda_0/ n_1\)) is also plotted as dashed line. It shows that, a subwavelength-diameter silica wire is always single mode, while a subwavelength-diameter silicon wire is single mode only when its diameter lays below the solid line. For example, at the wavelength of 633 nm (He-Ne laser), a silica wire with a diameter less than 457 nm will always be a single-mode waveguide; and at the wavelength of 1.5 \(\mu m\), to be a single-mode waveguide, diameters of silica- and silicon-wires should be less than about 1.1 \(\mu m\) and 345 nm respectively. Taking into consideration that UV absorption...
edges are about 200 nm for silica [9] and 1200 nm for silicon [10], the minimum critical diameters \(D_{\text{crit}}\) for silica and silicon wires are about 129 nm and 272 nm at these edges respectively. Since the interest of this work is single-mode properties, we consider the fundamental mode in the following discussion.

For fundamental modes \((HE_{11})\) modes, Eq. (3) becomes

\[
\begin{bmatrix}
J'_1(U) + K'_1(W) \\
UJ'_1(U) + n_z^2 K'_1(W)
\end{bmatrix}
\begin{bmatrix}
J'_1(U) + n_z^2 K'_1(W) \\
UJ'_1(U) + n_z^2 W K'_1(W)
\end{bmatrix}
= \left(\frac{\beta}{kn_1}\right)^2 \left(\begin{array}{c}
V \\
U W
\end{array}\right)
\]

with numerical solutions of the propagation constant \(\beta\) of the \(HE_{11}\) modes for silica and silicon at some typical wavelengths shown in Fig. 2 and Fig. 3 (solid lines). When expressing the electromagnetic fields as

\[
\begin{array}{l}
\vec{E}(r,\phi,z) = (e_e \hat{r} + e_\phi \hat{\phi} + e_z \hat{z})e^{i\beta} e^{-ior}, \\
\vec{H}(r,\phi,z) = (h_e \hat{r} + h_\phi \hat{\phi} + h_z \hat{z})e^{i\beta} e^{-ior}
\end{array}
\]

electric fields of the fundamental modes are expressed as [8]

inside the core \((0 < r < a)\):

\[
e_e = \frac{-a_1 J_0(UR) + a_2 J_2(UR)}{J_1(U)} \cdot f_1(\phi),
\]

(11)

\[
e_\phi = \frac{-a_1 J_0(UR) - a_2 J_2(UR)}{J_1(U)} \cdot g_1(\phi),
\]

(12)

\[
e_z = \frac{-iU J_1(UR)}{a_2 J_1(U)} \cdot f_1(\phi)
\]

(13)

and outside the core \((a < r < \infty)\):

\[
e_e = \frac{-a_1 K_0(WR) - a_2 K_2(WR)}{K_1(W)} \cdot f_1(\phi),
\]

(14)
where \( f_1(\phi) = \sin(\phi) \), \( g_1(\phi) = \cos(\phi) \),

\[
\begin{align*}
\alpha_i &= \frac{F_i - 1}{2}, \quad \alpha_2 = \frac{F_i + 1}{2}, \quad \alpha_3 = \frac{F_i + 1}{2}, \quad \alpha_4 = \frac{F_i + 1 - 2\Delta}{2}, \\
F_1 &= \left( \frac{UW}{V} \right)^2 \left[ b_1^2 + (1 - 2\Delta)b_2 \right], \quad F_2 = \left( \frac{UW}{V} \right)^2 \left( \frac{1}{b_1} + b_2 \right), \\
b_1 &= \frac{1}{2U} \begin{bmatrix} J_0(U) \\ J_1(U) \end{bmatrix}, \quad b_2 = -\frac{1}{2W} \begin{bmatrix} K_0(W) + K_1(W) \\ K_0(W) + K_1(W) \end{bmatrix}.
\end{align*}
\]

The \( h \)-components can be obtained from \( e \)-components with some calculations and are not presented here.

Normalized electric components of the fundamental modes in cylindrical coordination for silica wires at 633-nm wavelength are shown in Fig. 5. For reference, Gaussian profiles (dashed line) are provided in the radial distributions, and the electric field of a wire with a critical diameter \( (D_{\text{crit}}) \) is also provided as a dotted line. Comparing with the Gaussian profile, air-clad silica wire shows much tighter field confinement within a certain diameter range (e.g., around 400 nm) due to the high index contrast between the air and silica. When the diameter reduces to a certain degree (e.g., 200 nm), the field begins to extend to a far distance with considerable amplitude, indicating that the majority of the field is no longer tightly confined inside or around the wire. Similar behaviors are obtained for silica and silicon wires at other wavelengths.

**Fig. 5.** Electric components of \( HE_{11} \) modes of silica wires at 633-nm wavelength with different diameters in cylindrical coordination. Normalizations are applied as: \( e_r(r=0)=1 \) and \( e_\phi(r=0)=1 \). Wire diameters are arrowed to each curve in unit of nm.

**4. Fraction of power inside the core and effective diameter**

In practical applications such as evanescent wave based optical sensing [11, 12], it is important to know the profile of the power distribution around the waveguide. For the wires considered here, the average energy flows in the radial \( (r) \) and azimuthal \( (\phi) \) directions are zero, so we only consider the energy flow in \( z \)-direction. The \( z \)-components of Poynting vectors are obtained as [8]

inside the core \( (0<r<a) \):
Profiles of Poynting vectors for 200- and 400-nm-diameter silica wires at 633-nm wavelength are shown in Fig. 6, in which the mesh-profile stands for propagating fields inside the wire, and the gradient profile stands for evanescent fields in air. As we can see, while a 400-nm-diameter wire confines major power inside the wire, a 200-nm-diameter wire leaves a large amount of light guided outside as evanescent waves.

To obtain more straightforward information of the power distribution in the radial direction, we calculate the fractional power inside the core ($\eta$) and the effective diameter of the light field ($D_{\text{eff}}$) defined as following:

$$
\eta = \frac{\int_{0}^{\infty} S_{z1} dA}{\int_{0}^{\infty} S_{z1} dA + \int_{a}^{\infty} S_{z2} dA}
$$

(19)

where $dA = a^2 R dR d\phi = r \cdot dr \cdot d\phi$, and $\eta$ represents the percentage of the confined light power inside the solid core. $D_{\text{eff}}$ is obtained from

$$
\left\{ \begin{array}{ll}
\frac{\int_{0}^{D_{\text{eff}}} S_{z1} dA}{\int_{0}^{a} S_{z1} dA + \int_{a}^{\infty} S_{z2} dA} &= 86.5\% , \quad (\text{if } D_{\text{eff}} \leq a) , \\
\frac{\int_{0}^{a} S_{z1} dA + \int_{D_{\text{eff}}}^{\infty} S_{z1} dA}{\int_{0}^{a} S_{z1} dA + \int_{a}^{\infty} S_{z2} dA} &= 86.5\% , \quad (\text{if } D_{\text{eff}} > a) .
\end{array} \right.
$$

(20)

where $D_{\text{eff}}$ is a hypothetic diameter inside which 86.5% (that is $1-e^2$) of the total power is included.
Calculated $\eta$ as a function of the wire diameter ($D$) is shown in Fig. 7 for silica wire (633-nm and 1.5-µm wavelengths) and silicon wire (1.5-µm wavelength). It shows that, at the critical diameter ($DSM$) (dashed line), $\eta$ is about 81% for silica wire (633-nm and 1.5-µm wavelength) and 89% for silicon wire (1.5-µm wavelength). The diameter for confining 90% energy inside the core of the fundamental mode is about 566 nm (silica wire at 633-nm wavelength), 1342 nm (silica wire at 1.5-µm wavelength) and 346 nm (silicon wire at 1.5-µm wavelength). Tight confinement is helpful for reducing the modal width and increasing the integrated density of the optical circuits with less cross-talk [8, 13], while weaker confinement will be beneficial for energy exchanging between wires within a short interaction length [14], as well as for improving the sensitivity of evanescent wave based sensors [15].

The effective diameters ($D_{eff}$) of the fundamental modes of silica and silicon wires are shown in Fig. 8. For comparison, the real diameters of the wires are provided as dotted lines. $D_{eff}$ is large when the wire diameter is very small, and it decreases quickly with the increasing of the wire diameter. The two curves intersect near the critical diameter (dashed line), and the real diameter exceeds the effective diameter thereafter. The intersection point represents the minimum usable wire diameter at the nominated wavelength when using an 86.5% confinement for estimation. It is clear that, a wire with a certain diameter (e.g., 450-nm-diameter silica wire at 633-nm wavelength) is able to confine the major power within a subwavelength width. In addition, $D_{eff}$ is very larger if the wire diameter is very small. For example, at 633-nm wavelength, for silica wire with a diameter of 200 nm, $D_{eff}$ is about 2.3 µm, which is over 10 times larger than the wire diameter. Maintaining a steady guiding field in such situation is difficult, any small deviation (such as surface contamination and micro-bends) from the ideal condition will lead to significant change in propagating fields. However, the high susceptibility of such a guiding wire may provide high sensitivity for optical sensing.
5. Group velocity and waveguide dispersion

Group velocity and dispersion of optical waveguides are important in many applications. Group velocity of the wire waveguide we discussed here is given as [8]

\[ v_g = \frac{c}{n_1^2} \left( \frac{\beta}{k} \frac{1}{1 - 2\Delta(1 - \eta)} \right). \]  

(21)

From which diameter-dependent group velocities of \( HE_{11} \) modes of air-clad silica and silicon wire are obtained and shown in Fig. 9. Results show that, when the wire diameter (\( D \)) is very small, \( v_g \) approaches the light speed (\( c \)) in vacuum since most of the light energy is propagated in air. When \( D \) increases, more and more energy enters the wire core, \( v_g \) decreases until it reaches a minimum value that is smaller than \( c/n_1 \). After this point, \( v_g \) increases with \( D \). When the \( D \) is large enough, \( v_g \) finally approaching \( c/n_1 \), the group velocity of a plane wave in the wire material.

From Eq. (21), wavelength-dependent group velocities are also obtained. As shown in Fig. 10, for a given wire diameter (\( D \)), \( v_g \) approaches \( c \) when the wavelength (\( \lambda \)) is very larger and \( c/n_1 \) when \( \lambda \) is very small, with a minimum value smaller than \( c/n_1 \).

With group velocity obtained above, waveguide dispersion (\( D_w \)) is obtained as [16]

\[ D_w = \frac{d(v_g^{-1})}{d\lambda}. \]  

(22)
Diameter- and wavelength-dependent waveguide dispersions of air-clad silica and silicon wires are shown in Fig. 11 and Fig. 12. For reference, in Fig. 12, material dispersions of fused silica and single crystal silicon calculated from Eqs. (6) and (7) are also provided. It shows that, waveguide dispersions ($D_w$) of these wire-waveguides can be very large comparing with those of weakly guiding fibers and material dispersions. For example, $D_w$ of an 800-nm-diameter silica wire at 1.5-µm wavelength is about -1400 ps/nm.km, which is about 70 times larger than that of the material dispersion. In contrast to those of ps/nm.km for weakly guided glass fibers [17], $D_w$ of silica and silicon wires can go ns/nm.km level. Results also show that, at a particular wavelength, the total dispersion (combined material and waveguide dispersions) of a wire-waveguide can be made zero, positive or considerably negative when a proper diameter is chosen. Controlling light propagation properties by tailoring waveguide dispersion is used in many fields such as optical communication and nonlinear optics [1, 18, 19], therefore, these wires present opportunities for achieving enhanced dispersions with reduced sizes.

6. Discussions and conclusions

So far we have studied the basic properties of air-clad subwavelength-diameter silica and silicon wires for optical wave guiding. We assume that the wires are ideally uniform in terms of the sidewall smoothness and diameter uniformity. In most cases, a real wire could not be ideally uniform. However, low-loss optical wave guiding places strict requirements on the
sidewall smoothness and diameter uniformity [20, 21], especially when the width or diameter of the waveguide is very small [22, 23]. Therefore, practically useful wire-waveguide should have excellent uniformities to achieve low optical loss. Meanwhile, fused silica and single crystal silicon are among the most important materials for photonics, optoelectronics and electronics. Many other dielectric or semiconductor materials have refractive indices that fall between that of silica and silicon. Therefore, our results are helpful for estimating the guiding properties of many other dielectric or semiconductor wire waveguides.

Comparing with large-diameter optical waveguides, air-clad subwavelength-diameter wires show interesting properties such as enhanced evanescent fields, tight light confinement and large waveguide dispersions, which may provide opportunities for developing a number of miniaturized, high-performance and novel types of photonic devices.

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