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Based on the Mie scattering theory, we study optical resonances with whispering gallery modes (WGMs) in tubular microcavities. Rigorous formulas are present to obtain resonant wavelengths and Q factors for the WGM resonances. It is found that the Q factors of microtubes can be dramatically increased by increasing the dielectric constants in tube walls. For common SiO/SiO_2 based microtubes, Q factors can be improved by one order when the microtubes are coated with thin high-index HfO_2 layers ($n = 1.95$, thickness = 10 nm). The results could be useful for designing better optical devices based on tubular microcavities. © *2011 American Institute of Physics*. [doi:10.1063/1.3664110]

In recent years, optical microcavities have received much attention due to their applications in optoelectronics and integrated optics.[1] In particular, using repetitive total internal reflections, light can be confined in circular microcavities for a long time.[2] Examples include microcylinders,[3] microrings,[4] microdisks,[5] and microspheres.[6] Recently, another kind of microcavities with such whispering gallery modes (WGMs), microtubes, has been fabricated by rolling up prestressed solid thin films.[7–9] Unlike other microcavities with WGMs, such tubular microcavities have subwavelength wall thicknesses and thus possess resonances that are very sensitive to ambient refractive index.[10] As a result, microtubes can act as optical sensors for identifying different liquids, promising high potential for lab-on-a-chip applications.[11,12]

Currently, WGM resonances in microtubes have been explored mainly by a waveguide approximation and finite-difference time-domain (FDTD) simulation.[7–9,13] However, the two methods cannot present quality (Q) factors of microtubes efficiently, especially for high-Q cases. Hence, a thorough study of WGM resonances in microtubes is absent.

In this paper, we apply a Mie scattering method to study the WGM resonances in microtubes. Rigorous formulas are derived to calculate the resonant wavelengths and the results agree well with those from the waveguide method. Our formulas can also present the Q factors of microtubes efficiently. It is found that the Q factors can be dramatically improved with increasing the refractive index n in tube walls. For common SiO/SiO_2 based microtubes, the Q factors can be improved by one order by coating mirotubes with thin high-index HfO_2 layers ($n = 1.95$, thickness $\delta = 10$ nm).

The microtube under study has an N-layered cylindrical structure as shown in Figs. 1(a) and 1(b). The layer indices i of the core and background are 1 and $N+1$, respectively. The ith layer has an outer radius of r_i and dielectric constant of $\varepsilon_i \equiv n_i^2$. The microtube is along the z direction. We consider transverse-magnetic/transverse-electric (TM/TE) waves that are propagating in the x-y plane and have electric/magnetic field along the z direction.

The wall of the microtube is a film with $N-1$ layers. When this film is flat, it can support waveguide modes with propagating constants β satisfying

$$2t - (1 - t^2)\tan(q_f\Delta) = 0, \quad (1)$$

where $t = \frac{q_b}{q_f}$ $\left(\frac{\varepsilon_f q_b}{\varepsilon_b q_f}\right)$ for waves with $E//z$ ($H//z$) [see Fig. 1(c)],[12] $q_b^2 = \beta^2 - \varepsilon_b k_0^2$, $q_f^2 = \varepsilon_f k_0^2 - \beta^2$, $k_0 = 2\pi/\lambda$, λ is the wavelength in vacuum, ε_b is the dielectric constant of background, and ε_f is the average dielectric constant of the film.[14] Thus, WGM resonances occur in the microtube when

$$\beta L = 2\pi m, \quad (2)$$

where $L = \pi(r_1 + r_N)$ and the integer m is the order of resonance.

Although the above waveguide method can be used to estimate the resonant wavelengths of microtubes, it cannot present Q factors. Here, we apply a Mie scattering method to obtain the Q factors of microtubes. When TM (TE) waves are incident on a microtube, the electric field $E_z(r, \phi)$ (magnetic field $H_z(r, \phi)$) in the ith layer can be expressed as $\sum_m [a_{i,m} J_m(k_i r) + b_{i,m} H_m^{(1)}(k_i r)] e^{im\phi}$, where $k_i = \sqrt{\varepsilon_i} k_0$, the origin of cylindrical coordinates (r, ϕ) is at the center of microtube, and the Bessel function J_m and the Hankel function $H_m^{(1)}$ of the first kind stand for incident and scattering waves, respectively.[15] Using continuities of E_z (H_z) and $\frac{\partial E_z}{\partial r}$ $\left(\frac{1}{\varepsilon}\frac{\partial H_z}{\partial r}\right)$ for TM (TE) waves, we have

$$\frac{J_m'(u) + D_{i+1,m} H_m^{(1)\prime}(u)}{J_m(u) + D_{i+1,m} H_m^{(1)}(u)} = \frac{\alpha_i}{\alpha_{i+1}} \frac{J_m'(v) + D_{i,m} H_m^{(1)\prime}(v)}{J_m(v) + D_{i,m} H_m^{(1)}(v)}, \quad (3)$$

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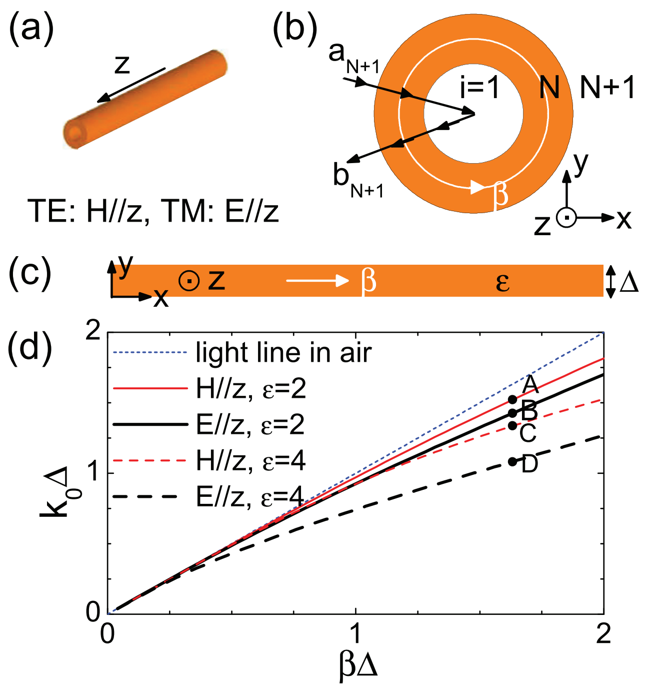

FIG. 1. (Color online) Schematic diagrams of (a) and (b) an N-layered cylindrical structure [$N=2$ is shown] and (c) a flat dielectric film with dielectric constant ϵ and thickness Δ in air. (a) and (b) are 3D and cross-section views, respectively. (d) Dispersion relationship of optical guiding modes for the film shown in (c). The modes A-D have $\beta\Delta = 1.633$ which is obtained from Eq. (2), $L=\pi(d-\Delta)$, and $\Delta = 0.02\,d$.

where $u=k_{i+1}r_{i+1}$, $v=k_i r_{i+1}$, $D_{i,m}\equiv \frac{b_{i,m}}{a_{i,m}}$, and $\alpha_i = k_i\ (k_i/\varepsilon_i)$ for TM (TE) waves. Using $D_{1,m}=0$ and Eq. (3), we can obtain the scattering coefficient $D_{N+1,m}$ of the microtube. The total scattering cross section of the microtube can then be obtained[15]

$$C_s \equiv \sum_m C_{s,m} = \sum_m \frac{2\lambda}{\pi}|D_{N+1,m}|^2. \tag{4}$$

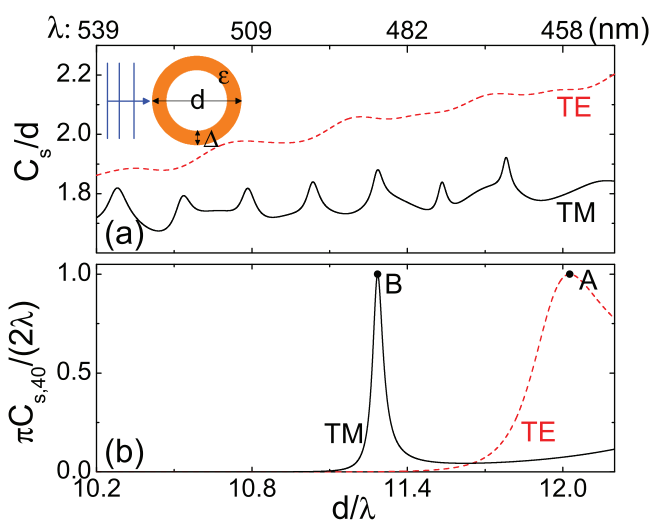

FIG. 2. (Color online) (a) Total and (b) $m=40$ partial scattering cross sections for a hollow microtube in air. The tube has an outer diameter d, and a dielectric constant of $\epsilon=2$ and thickness of $\Delta=0.02\,d$ in the wall. For $d=5.5\,\mu$m, the scale of wavelength λ is shown on the top of (a). The modes A and B in (b) are related to the modes A and B in Fig. 1(d), respectively.

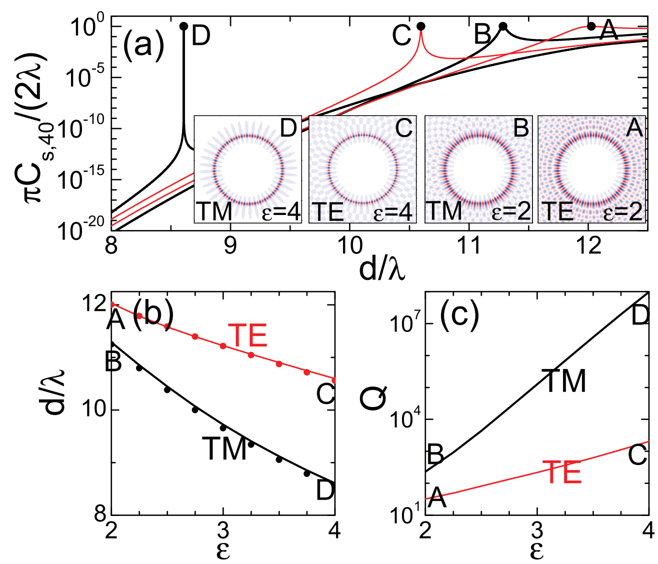

FIG. 3. (Color online) (a) Partial scattering cross sections of $m=40$, and (b) wavelengths λ and (c) Q factors of the $m=40$ resonant modes for the microtube with $\Delta=0.02\,d$ shown in Fig. 2(a). The insets to (a) show Re(E_z)/Re(H_z) for TM/TE resonances. The modes A-D are related to the modes A-D in Fig. 1(d), respectively. The lines and dots in (b) are obtained from (a) and from Eq. (2), respectively.

Near the resonant wavelength λ_m, the partial scattering cross section has a Lorentz line shape, $C_{s,m}=4k_0^{-1}\gamma_m^2/[(k_0-k_m)^2+\gamma_m^2]$, where $k_m=2\pi/\lambda_m$ and γ_m is the damping rate. The Q factor of the mth-order resonance can then be obtained by $Q=k_m/(2\gamma_m)$.[13,16]

We first study a hollow microtube with outer radius of d in air. The tube wall is a single layered film with dielectric constant $\varepsilon=2$ and thickness $\Delta=0.02\,d$. These parameters are close to those of SiO/SiO_2 based microtubes fabricated in experiments. Figure 2 shows the total and partial scattering cross sections of the microtube. From $C_{s,40}$ in Fig. 2(b), we can easily obtain the resonant wavelengths for the WGM resonances with $m=40$ and the results agree well with those by the waveguide method [Fig. 3(b)]. The WGM resonances come from the guiding modes in the tube wall. Compared with the guiding mode of TE resonance, the guiding mode of TM resonance is farther away from the light line in air and thus has larger decay (q_b) in air [Fig. 1(d)]. Hence, the Q factor of TM resonance is larger than that of TE [$Q=231/32$ for TM/TE, $\Delta=0.02\,d$, and $\varepsilon=2$]. We note that this result explains why TE resonances of microtubes are more difficult to be observed than TM in photoluminescent experiments.[7,12]

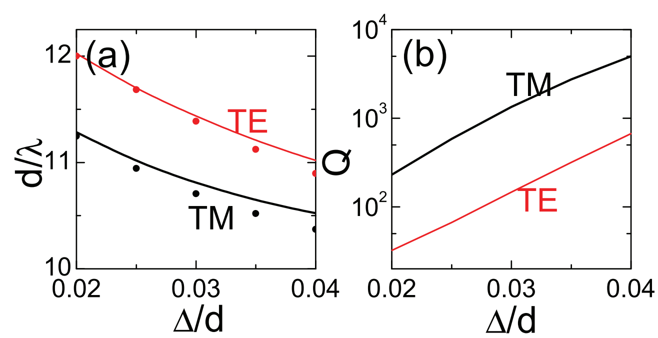

FIG. 4. (Color online) (a) and (b) The same as Figs. 3(b) and 3(c), respectively, but for microtubes with $\epsilon=2$.

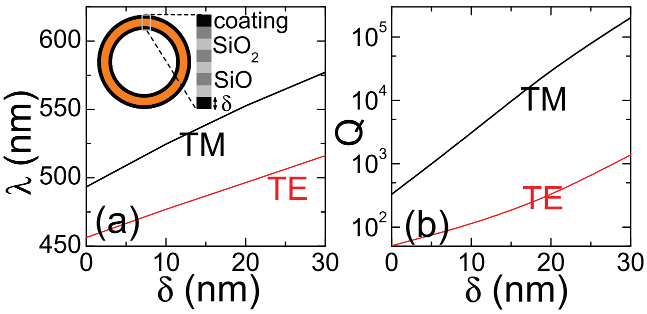

FIG. 5. (Color online) (a) Wavelengths and (b) Q factors of $m=40$ resonances for a hollow microtube in air. The tube has eight layers in wall, where the SiO/SiO_2/coating layer has a thickness of 6/2027/δ nm and dielectric constant of 2.1/2.4/3.8. The outer diameter d is 5.5 μm for a tube without HfO_2 coating layers.

Figure 3 shows the resonances with $m=40$ for microtubes with different ε in walls. For a constant of wall thickness $\Delta = 0.02\,d$, the Q factors are found to increase rapidly with increasing ε. Compared with the guiding modes with $\varepsilon = 4$, the guiding modes with $\varepsilon = 2$ are farther away from the light line in air [Fig. 1(d)]. Hence, the Q factors of microtubes with $\varepsilon = 4$ are higher in orders than those of $\varepsilon = 2$ [$Q = 9.8 \times 10^7/2034$ for TM/TE, $\Delta = 0.02\,d$, and $\varepsilon = 4$].

Figure 4 illustrates the dependence of the resonances with $m=40$ on the wall thickness Δ. From Fig. 4(a), we can see that for microtubes with thicker walls, the resonant wavelengths from the waveguide method deviate more from accurate results. For microtubes with $\varepsilon = 2$, the Q factors are found to increase with increasing Δ. However, the increasing of Q by doubling Δ is smaller than that by doubling ε [$\Delta dQ/d\Delta < \varepsilon\, dQ/d\varepsilon$; $Q = 4993/669$ for TM/TE, $\Delta = 0.04\,d$, and $\varepsilon = 2$].

SiO/SiO_2 based microtubes are interesting optical microcavities.[9] Such microtubes have no toxicity and exhibit photoluminescent effects, and thus can serve as label-free bio-sensors.[10,12] However, Since SiO/SiO_2 based microtubes have small thicknesses ($\Delta = 100$ nm) and small refractive indices ($n = 1.5$), they possess moderate Q factors ($\sim$100) and thus small resolution for sensing.[9] In Fig. 5, we show that when the microtubes are coated with thin high-index HfO_2 layers of $n = 1.95$ and thickness $\delta = 10$ nm, the Q factors can be highly improved [$Q = 329/3092$ before/after coating for TM]. These results could be useful to improve the performance of microtube sensors.

Above studies deal with ideal microtubes with Q factors of Q_i. We note that for real microtubes,[7–9] $Q = (Q_i^{-1} + Q_s^{-1})^{-1}$ where Q_s is related to the loss from surface imperfection and cone effects. Hence, when $Q_i < Q_s$, the tendencies for the Q-factor changes shown here should remain valid for rolled-up microtubes (where $Q_s \sim 5000$).

In summary, WGM resonances in microtubes have been systematically studied based on the Mie scattering method. Rigorous formulas were present to calculate the resonant wavelengths and Q factors of microtubes. It is found that comparing with increasing the wall thicknesses, increasing the refractive indices of tube walls can more efficiently enhance the Q factors of microtubes. For common SiO/SiO_2 based microtubes, the Q factors can be improved by one order with coating thin HfO_2 layers. Our results could be useful to design high-performance optical devices based on microtube cavities.

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[13]$Q \equiv \frac{k_m}{2\gamma_m}$ can also be obtained from $C_{s,m}(k_m + i\gamma_m) = \infty$ (which is equivalent to the exact approach used by Kipp[7]). But the calculation is more time-consuming than ours.
[14]Equation (1) is valid when $\Delta \ll \lambda$ or $N = 2$. For waves with $E//z$ or $H//z$, $\varepsilon_f = \sum \varepsilon_i \Delta_i / \Delta$ or $\Delta / \sum \varepsilon_i^{-1} \Delta_i$ with Δ_i being the thickness of the ith layer in the film.
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[16]k_m and γ_m can be extracted from two $C_{s,m}(k_0)$ points near k_m.