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Near-field gap effects on small microcavity whispering-gallery mode resonators

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Abstract
The near-field gap effects are investigated in planar dielectric microdisc and waveguide coupling structures, emphasizing miniaturization of integrated sensor systems. The simulation results show that the resonance frequency is not obviously affected by the gap dimension when the gap between a microcavity and its coupler is larger than 300 nm. However, the resonance frequency shifts observably with a further decreasing gap to the nanometre level. This shift is generally larger than the cavity resonance linewidth in the 10 μm diameter microdisc system, but is comparable to the cavity resonance linewidth in the 2 μm diameter microdisc system. With increasing gap, the cavity Q increases exponentially until it is saturated at a limit Q factor. An optimal gap dimension exists for maximum light energy transfer and storage. The concept of optimum gap is introduced and defined at the gap dimension where half-maximum energy storage capability is achieved; meanwhile, the cavity Q is high and the resonance frequency remains stable.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Whispering-gallery mode (WGM) optical cavities are typically dielectric circular structures in which photons are confined by repeated total internal reflections (TIRs) at the curvilinear boundary such that the EM field can close on itself, giving rise to resonances. Due to high cavity Q factor and finesse or high sensitivity in a small mode volume, WGM microcavities [1] have recently attracted increasing attention in the studies of quantum electrodynamics [2], integrated electro-photonic micro-devices [3], miniature optical biosensors [4], etc.

An ideal cavity would confine light indefinitely and would have resonance frequencies at precise values. In practice, energy losses exist due to diffraction, material absorption or scattering as a result of surface roughness or material inhomogeneity [5]. The cavity Q factor is defined as 2π times the ratio of the stored energy to energy losses per cycle. It is proportional to the photon confinement time. In general, a WGM resonance spectrum has a Lorentzian lineshape, and the quality factor can be expressed as $Q = \omega_0/\Delta\omega$ (ω_0 is the resonance central frequency and $\Delta\omega$ is the linewidth). The intrinsic Q of a cavity is predominantly determined by the morphology of the cavity. The larger the cavity, the higher the achievable Q factor. $Q > 10^9$ has been observed at red and near-infrared wavelengths in fused-silica sub-millimetre in diameter spheres [6, 7].

Sensitivity is paramount in the design and applications of WGM-based sensors. Under a resonance, an enhanced radiation field exists inside the periphery of a microcavity. A very strong evanescent field arises along the peripheral surface. Its strength decays exponentially with increasing distance from the surface. This evanescent field will certainly interact with molecules adsorbed or covalently attached to the microcavity. The interaction could induce a change in the WGM resonant frequencies. In other words, a shift or broadening (narrowing) or intensity change in the resonance signifies an altered WGM microcavity environment [8].

High-Q WGMs are not accessible by free-space beams and require employment of near-field couplers that provide energy transfer to the resonant EM waves in the resonator through the evanescent field of a guided wave or a TIR spot. Numerous coupling devices, such as high-index prisms with frustrated TIR [9], side-polished fibre couplers [10], optical fibre-tapers [11, 12], and integrated waveguides [13, 14], have been considered. Gorodetsky and Ilchenko [9] pointed out that efficient coupling can be expected on fulfilment of two main conditions: phase synchronism and significant overlap of the two evanescent fields in the gap that separates a resonator and its coupler. Thus, this small gap between a resonator and a waveguide is crucial for the near-field photon tunnelling and energy coupling and may further affect the real cavity Q [14] and resonance frequency [15].

The ability to achieve near lossless coupling is fundamental to many basic studies as well as to practical applications of WGM devices. Spillane *et al* [2] described the nature of loss by ideality and showed that under appropriate conditions ideality in excess of 99.97% is possible using fibre-taper coupling to high-Q silica microspheres. Cai *et al* [16] observed critical coupling in a fibre-taper to a silica-microsphere WGM system. The coupled-mode theory [17] attempted to understand the power coupling from tapered fibres and half-blocks into microspheres.

A simple geometric optics analysis of photon orbiting around a circular resonator shows that the free spectrum range is inversely proportional to the diameter of the resonator. Thus, microscale cavities ensure that the resonant frequencies are more sparsely distributed throughout the cavity size-dependent resonance spectrum than they are in corresponding mesoscale cavities [1]. On the one hand, this will greatly facilitate WGM sensing applications using spectroscopy techniques. On the other hand, the extremely high-Q has to be sacrificed. At several recent workshops on identifying research priorities to ensure US national security, it has been concluded that chemical and biological sensors and sensing systems must become part of a fully integrated protection system responding to diverse scenarios of potential terrorist actions. Novel approaches to biochemical threat detection are needed that do not rely on large quantities of reagents, provide faster response and have greater sensitivity and selectivity.

The extraordinary demand for integrated techniques and miniaturization presents a major challenge to the sensor community. The present study will then focus on simulations of very small microcavity (2 or 10 μm in diameter) and waveguide integrated systems. In small microcavity systems, the near-field gap effects are more significant because the shrinkage in cavity increases the curvature that will lead to increased diffraction loss as well as reduced cavity Q. In such a situation, efficient light energy transfer from a waveguide to the cavity is critical in order to achieve a high signal/noise ratio and to generate a high-Q resonance. Further, few prior studies have addressed the gap effects in such small microcavity systems.

Recent advances in the technology of nanofabrication offer the possibility of manufacturing new optical devices with unprecedented control. However, experimental manipulation of very small systems and precisely nanoscale gap control are still a challenge. To this end, computer-based simulation is more flexible in terms of precise gap variation, continuity of measurements and completeness of systematic studies. Moreover, simulation is more accurate in small systems because of refined meshes in reduced simulation domains.

2. Model

Consider an optical microdisc coupled with a light-delivery waveguide as shown in figure 1. A small air-gap separates the microcavity from the waveguide. The EM field in the microcavity and waveguide coupling structure is governed by time-dependent Maxwell's equations. By introducing time-harmonic waves, Maxwell's equations can be reduced to Helmholtz equations as follows:

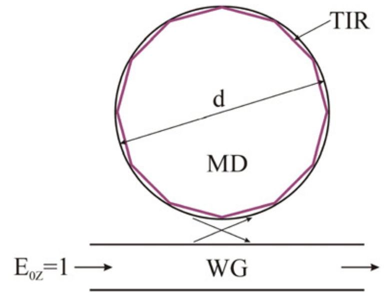

Figure 1. Sketch of a microdisc coupled with a waveguide.

$$\frac{1}{\mu}\nabla^2\bar{E}+\omega^2\varepsilon_c\bar{E}=0,$$
$$\frac{1}{\mu}\nabla^2\bar{H}+\omega^2\varepsilon_c\bar{H}=0, \quad (1)$$

where $\bar{E}$ and $\bar{H}$ are the electric and magnetic field vectors, respectively, and $\omega = 2\pi c/\lambda$. The complex permittivity is $\varepsilon_c = \varepsilon_{cr}\varepsilon_0 = \varepsilon - i(\sigma/\omega)$, where ε_{cr} is the complex relative permittivity and ε_0 is the permittivity in vacuum. If the complex index of refraction, $m = n - ik$, is given, the complex relative permittivity can be obtained through the relationship $\varepsilon_{cr} = m^2 = n^2 - k^2 - i2nk$. The absorption index k for a dielectric medium is extremely small and negligible.

WGM resonance inside the planar microdisc is typically an equatorial brilliant ring, and this ring is located on the same plane as the waveguide. So it is feasible to use a two-dimensional theoretical model. In the present calculations we apply in-plane TE waves, where the electric field vector has only a z-component and it propagates in the x–y plane. At the interface and physical boundaries, we used the natural continuity condition for the tangential component of the magnetic field. For the outside boundaries, the low-reflecting boundary condition is adopted. The low-reflecting means that only a small part of the wave is reflected and that the wave propagates through the boundary almost as if it were not present.

A laser beam is assumed to enter into the waveguide with a uniform electric field distribution. The laser wavelength is tunable. In the simulations, an index of refraction of 2.01 is assumed for both the microdisc and the waveguide, corresponding to the dielectric material Ni_3O_4 against the excitation wavelengths. The authors [8, 14] have successfully adopted the finite element method for solving the Helmholtz equations. The convergence and accuracy of the simulations were satisfactory. Details of the solution scheme are then not repeated here.

Two sets of the planar microdisc and waveguide coupling configuration are considered as follows: (1) a microdisc 2 μm in diameter is coupled with a 0.5 μm wide waveguide and (2) a microdisc of 10 μm in diameter is coupled with a 2 μm wide waveguide. The waveguides are straight. The gap dimension is defined by the smallest distance between a microcavity and

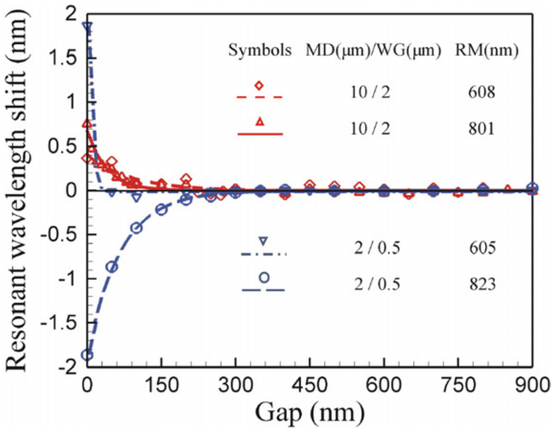

Figure 2. Resonance wavelength shift versus gap dimension.

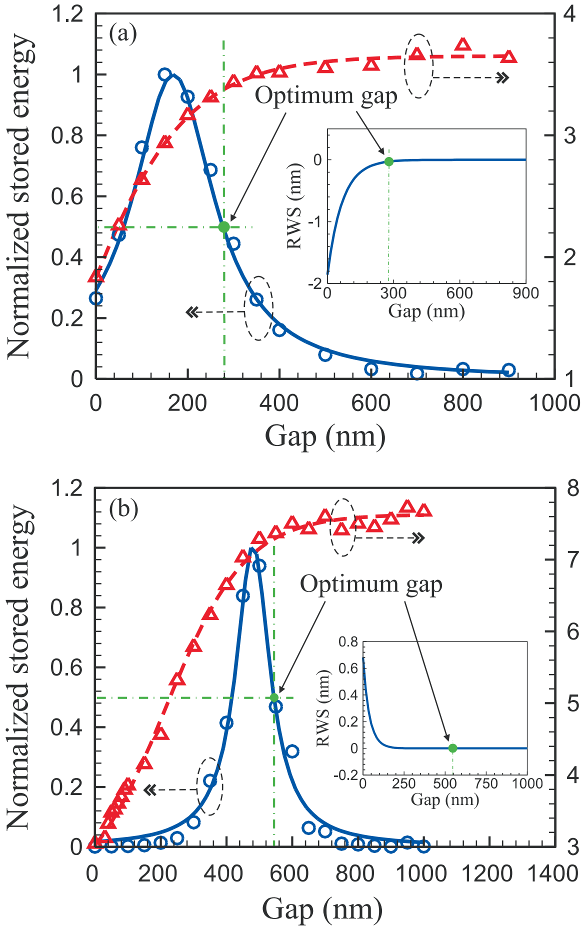

Figure 3. Gap effects on energy storage and resonance quality and the introduction of optimum gap concept: (*a*) a 2 μm diameter microdisc coupled with a 0.5 μm wide waveguide working on the 823 nm resonance mode and (*b*) a 10 μm diameter microdisc coupled with a 2 μm wide waveguide working on the 801 nm resonance mode.

its waveguide and varies between zero (in close contact) and 1000 nm. The incident light is in the near-infrared range. Thus, a gap larger than 1000 nm is not practical.

3. Results and discussion

Figure 2 shows the resonance wavelength shift (RWS) against the gap dimension (the shift is defined by $\lambda_g - \lambda_\infty$, where λ_g is the resonance wavelength at a given gap dimension and λ_∞ is the reference resonance wavelength at a very large gap width (1000 nm) in which the gap effect vanishes and the resonance wavelength is the intrinsic one of the microcavity). When the gap dimension is larger than 300 nm, it is observed that $(\lambda_g - \lambda_\infty)$ converges to zero for all the four considered resonance modes (two for each microdisc system); i.e. the resonance wavelength is very stable and little affected by the gap dimension. This is very useful for designing practical sensors based on the principle of resonance frequency shift. For narrow gaps (<300 nm), however, the resonance wavelength (frequency) is very sensitive to the gap dimension. The resonance wavelength shift is very appreciable when a zero gap (in close contact) is used. This is consistent with the experimental observation in a 430 μm diameter silica sphere [15]. The resonance wavelength may shift downwards or upwards depending on the microcavity/waveguide configuration and the resonance mode.

The stored energy and the Q factor versus the gap dimension are plotted in figures 3(*a*) and (*b*) for the 2 μm diameter microdisc system (resonance mode is at 823 nm) and the 10 μm diameter microdisc system (resonance mode is at 801 nm), respectively. The stored energy is normalized by the maximum value, respectively. It is seen that the energy storage is maximum at a gap dimension of about 180 nm for the 2 μm diameter microdisc system and of about 480 nm for the 10 μm diameter microdisc system. The existence of an optimal gap dimension for maximum energy transfer and storage inside a microcavity is due to the bi-directional photon tunnelling in the near-field gap. At this point, the scattering radiation intensity from the microcavity is the strongest, while the waveguide transmission is at minimum, leading to the deepest dip in its transmission spectrum. It is worth mentioning that the maximum energy transfer and storage is different from the critical coupling concept used in the literature. Critical coupling is a condition in which internal resonator loss and waveguide coupling loss are equal for a matched resonator-waveguide system, at which point the resulting transmission at the output of the waveguide goes to zero on resonance [9, 16]. The maximum energy storage condition at the 2 μm diameter microdisc system is not a critical coupling condition because only 65% of the input laser power is stored in the microcavity and the rest 35% outputs from the waveguide. Thus, critical coupling is not possible for the small 2 μm diameter microdisc system at the considered resonance mode. However, there still exists a maximum of energy storage and transfer. On further inspection of the 10 μm diameter microdisc system, we found that the critical coupling condition is achieved at its optimal gap dimension in which more than 99% of the input laser power is stored in the microcavity and less than 1% goes to the waveguide transmission.

The Q variation against the gap dimension is monotonic. With increasing gap the cavity Q initially increases exponentially and finally reaches to an asymptotic limit (limit Q factor) when the gap approaches the optical wavelength of interest. This limit Q factor is the maximum cavity Q in theory for a given microcavity configuration. It is predominantly determined by the cavity size and falls rapidly as the cavity size shrinks. In order to obtain a high-Q value, however, the gap dimension should also be wisely selected. Although the Q factor is the greatest when the gap dimension is close to one optical wavelength of interest, the energy stored in the microcavity is low (or the transmission in the waveguide is very high) so that the strength of collected signals, either through scattering in the microcavity or via waveguide transmission, is bad. For many applications (such as in sensors) and fundamental studies using WGM resonators, a compromise should be taken into account between signal intensity, signal/noise ratio, Q factor and resonance frequency stability. To this end, the concept of optimum gap is introduced (as shown in figure 3), and it is defined as the gap dimension at the half-maximum energy storage point to the large gap side. At the optimum gap, both the Q factor and the energy transfer are high and the resonance wavelength is stable.

The linewidth of a resonance is inversely proportional to the cavity Q. From figure 3, it is seen that the cavity Q at the optimum gap dimension is 4×10^3 for the 2 μm diameter microdisc system, corresponding to a linewidth of 0.2 nm. Generally the linewidth for the 2 μm diameter microdisc system is comparable to the RWS in figure 2. Thus, the frequency shift due to gap variation in this system may not be critical. The resolution in frequency shift sensing [4] is determined by the loaded cavity Q. The signal intensity is determined by the energy storage in the cavity. For the 10 μm diameter microdisc system, the cavity Q at its optimum gap dimension is 2×10^7, corresponding to a linewidth of 4×10^{-5} nm. The general linewidth for the 10 μm diameter microdisc system is smaller than the uncertainty of RWS in figure 2. Therefore, the resolution of measurement will be degraded by the RWS due to gap variation. The gap should be designed at a dimension where both the Q factor and the energy transfer are high and the resonance wavelength is relatively stable.

In summary, the concept of optimum gap is introduced and defined for efficient energy transfer from waveguide to microcavity or energy storage in microcavity, while at the same time maintaining high cavity Q and stable resonance frequency. This optimum gap is of great importance in design and applications of WGM-based devices, particularly in sensing applications where both signal intensity and linewidth are important and stability of resonance frequency is essential. This study also characterizes small optical microcavities. It is found that the Q factor depends not only on the morphology of a microcavity (as generally recognized in the field) but also on the gap dimension separating the microcavity and its coupler. With increasing gap, the Q factor increases exponentially before it reaches to an asymptotic limit. A limit Q factor can be achieved when the gap is designed to be the size of the optical wavelength of interest. It is also found that the resonance frequency does not obviously vary with the gap dimension when the gap dimension is larger than 300 nm. At small gaps ($<$300 nm), however, the resonance frequency shifts with varying gap dimension.

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