Whispering-gallery mode micro-kylix resonators

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Owing to their ability to confine electromagnetic energy in ultrasmall dielectric volumes, micro-disk, ring and toroid resonators hold interest for both specific applications and fundamental investigations. Generally, contributions from various loss channels within these devices lead to limited spectral windows (Q-bands) where highest mode Q-factors manifest. Here we describe a strategy for tuning Q-bands using a new class of micro-resonators, named micro-kylix resonators, in which engineered stress within an initially flat disk results in either concave or convex devices. To shift the Q-band by 60nm towards short wavelengths in flat micro-disks a 50% diameter reduction is required, which causes severe radiative losses suppressing Q’s. With a micro-kylix, we achieve similar tuning and even higher Q’s by two orders of magnitude smaller diameter modification (0.4%). The phenomenon relies on geometry-induced smart interplay between modified dispersions of material absorption and radiative loss-related Q-factors. Micro-kylix devices can provide new functionalities and novel technological solutions for photonics and micro-resonator physics.

Recent technological advances in micro- and nanophotonics have boosted the realization and testing of extremely high Q-factor optical resonator systems. Much interest is focused on two-dimensional whispering-gallery mode (WGM) resonators [1, 2], such as micro-disks [3], rings [4] and toroids [5]; these are chip-integrable and offer a wide spectrum of possible applications ranging from microdisk (µ-disk) lasers [6, 7] to sensing [8]. Besides, WGM resonators are interesting for fundamental physics, such as cavity quantum electrodynamics [9], individual atom-photon quantum interactions [10] and for testing fascinating optical phenomena like radiation pressure forces [11].

The main figure of merit of a µ-disk is the Q-factor, which is a measure of the energy stored in the resonator versus the energy dissipated per round trip. Q-factor engineering is getting relevance since it improves significantly device performances. In addition, for active µ-disks high Q’s are desirable in spectral windows of maximum material gain; possible resonant mode competition can be overcome with an appropriate tuning of spectral positions of high-Q modes towards the gain band peak, without modifying the free-spectral range (FSR) of resonator modes. On the other hand, when WGM detection schemes are used in biosensing applications, analyte molecules spoil cavity Q-factor by binding to the resonator surface. In this case, an enhanced detection sensitivity would benefit from high-Q’s at shorter wavelengths, where analyte molecules possess stronger absorption. Basic schemes to shift high Q-factors from long to short wavelengths rely on achieving a stronger confinement of WGM modes within the resonator device; this is achieved either by increasing the µ-disk diameter or the thickness, both imposing larger device dimensions. As a consequence, these solutions cause unavoidable reduction of mode FSR and appearance of higher order mode families.

Here we report on a new class of µ-disk resonators, which we call micro-kylix (µ-kylix) resonators (Fig. 1(a)), in analogy with the Greek wine-drinking cup - κυλιξ, (inset photo, Fig. 1(a)) [12]. These present a bent µ-disk configuration, which, owing to an appropriate stress-engineering approach, can be realized both as a bent-up (cup-like, µ-kylix) or bent-down (umbrella-like, inverse µ-kylix) resonators. These devices support perfectly whispering-gallery modes and, at the same time, possess new and unexpected physical characteristics. The most striking of these, perhaps, is that their geometry induces a tuning of the Q-factor band of resonator modes towards the stronger material absorption range without degrading highest Q’s. Importantly, this tuning scheme does not require larger device sizes, but rather utilizes self-adjustment properties of originally stressed resonator core. Remarkably, the µ-kylix resonator benefits from unmodified FSR and cleaner WGM spectra due to the absence of higher order mode families.

We used a finite-difference time-domain (FDTD) tool to check if a µ-kylix acts as WGM resonator. Simulations have been performed using a freely-available FDTD software package [13], which exploits the azimuthal symmetry of micro-disk resonator to reduce the computational load. WGM resonances have been extracted using a harmonic inversion algorithm included in the software [13]. Starting with a 10 µm diameter flat micro-resonator, we first verified that it supports WGMs, and, then, we applied a bending to the flat disk in the z-direction (Fig. 1(b)). Indeed, the numerical simulation confirmed that the µ-kylix supports guided modes. As an example, Fig. 1(c) shows the electrical field distribution of a TM-polarized mode (azimuthal mode number $m = 47$, $\lambda = 829\ nm$) close to the edge of the µ-kylix resonator.
FIG. 1: The micro-kylix resonator. (a) Cross-sectional scanning electron micrograph (SEM) of a micro-kylix resonator. Inset: The Greek wine-drinking cup - κυλιξ, with a broad relatively shallow body raised on a stem from a foot [12]. (b) Three-dimensional view of an analytically calculated bent-up resonator using experimental dimensions (experimental bending radius of 47 µm). The extremes of the scale-bar represent the height difference between the edge and the center of a 200 nm-thick disk. (c) Electrical field distribution of the TM-polarized whispering-gallery mode shows a rather good confinement within the core of the µ-kylix resonator.

To realize the µ-kylix we used a combination of two materials, silicon-rich silicon oxide SiO$_{x}$ (SRO) and silicon nitride Si$_3$N$_4$. We take advantage of the fact that these two materials possesses different thermal expansion coefficients, which lead to unavoidable stresses at the end of the deposition process. The stress can be engineered by accurate control of the deposition temperature and the layer thickness. After disk definition and post formation to isolate the disk from the substrate, the accumulated stress gradients through the layer interfaces bend the micro-disk device Fig. 1(a)).

For µ-kylix we first deposit a 160 nm-thick SiO$_{x}$ layer on top of crystalline silicon wafers from a mixture of silane (SiH$_4$, 65 sccm) and nitrous oxide (N$_2$O, 973 sccm) gases using a parallel-plate plasma enhanced chemical vapor deposition (PECVD) chamber at T=300°C [19]. Si-nc were formed through a successive one hour annealing in an N$_2$ atmosphere at T=1100°C [17]. After the high-T treatment the SRO layer densifies down to 110 nm due to the release of hydrogen and micro-voids, present in the as-deposited layer. The residual compressive stress on SRO/bulk-Si interface was measured to be −100 MPa. In a next step, a similarly thick Si$_3$N$_4$ layer was deposited at 780°C using a low pressure chemical vapor deposition (LPCVD) technique (1.25 GPa tensile stress). A photolithographical patterning of disk arrays was followed by dry (anisotropic, disk formation) and wet etching (isotropic, post formation) steps.

In this way, µ-kylkes are obtained by engineering the stress in the bilayer structure. The simplicity of such a technological solution is combined to a large degree of freedom for not only the choice of materials, but also control of both the degree and the direction of disk reshaping. The degree of bend is strictly related to the thickness ratio of the two different materials, while the direction of bend (cup or umbrella) can be easily changed inverting the materials. An example of a µ-kylix is shown in the cross-sectional scanning electron micrograph of Fig. 1(b).

In our case we choose this set of materials for their interest in silicon photonics [15]. Optically active µ-kylix and µ-disk resonators are easily realized by annealing the SRO layer and, thus, inducing a phase separation of SiO$_2$ and silicon with the formation of Si nanocrystals (Si-nc) [16]. These show strong room-temperature emission in a wide spectral range (700-900 nm) [17], and a smooth increasing absorption band with a threshold at about 800 nm [18].

We measured the room-temperature micro-photoluminescence emission from single resonators in a free-space collection configuration (see Fig. 2(a,b)). In our experiments we excited individual micro-kylix

FIG. 2: WGM emission from µ-kylix and µ-disk resonators. (a) An SEM image of the µ-kylix array with a cross-sectioned µ-kylix resonator on the sample edge. The inset shows an optical image of µ-kylix array, with the bright spot corresponding to the Si-nc emission from a single device. (b) Micro-photoluminescence (PL) setup used for testing single devices. (c) Measured emission spectrum of the µ-kylix resonator, showing sharp whispering-gallery resonances of the lowest-order family raising out from the broad PL band of Si-nc. (d) Measured emission spectrum of the µ-disk resonator. The 2nd-order family modes manifest as broad and damped peaks next to intense 1st-order family resonances.
resonators focusing with a long-working distance objective the 488 nm line of a CW Argon laser and collected the emission of Si nanocrystals from the edge of the sample through a 25x objective. The signal was then spatially filtered to reduce the numerical aperture of the collecting set-up, selected by a polarizer and sent to a monochromator interfaced with a cooled silicon charge coupled device (CCD).

We observed sharp, sub-nanometer modal peaks arising from the wide emission band of Si-nc due to WGM. The measured spectrum (Fig. 2(c)), at first glance, is qualitatively similar to that observed from single-layer-SRO μ-disks [19], with the difference that the narrowest resonances here manifest at shorter wavelengths.

This observation led us to perform a second experiment. For this, we prepared a flat μ-disk, consisting of the same amount of SRO and SiN as in a μ-kylix resonator (Fig. 3(a)). In order to have the disk flat, we sandwiched the SRO layer between two 55 nm-thick SiN layers (Fig. 3(b)). This way the total thickness and the weighted-average refractive index of the μ-disk were similar to those of the μ-kylix.

We measured the WGM emission spectrum of the μ-disk (Fig. 3(d)) and compared with that of the μ-kylix. Lorentzian fit analysis of all appreciable peaks, plotted in Figure 3(d), evidences an important modification of Q-factors in μ-kylix. We observe that the Q-band maximum in the μ-kylix is blue-shifted by almost 60 nm with respect to that of the μ-disk. As a consequence, this shift results in higher Q-factors (roughly four-fold) at wavelengths (~760 nm), where our active material, SRO, has stronger absorption. Let us note that the reported values for the highest Q-factors are limited by the spectral resolution of our experimental setup; this does not interfere with the main results of this work.

Before explaining these observations and revealing the physical mechanisms behind, we first address the origin of spectral dispersion of Q-factors. In μ-disk resonators, the quality factors for a certain radial family of resonances form a band, owing to wavelength dispersions of Q’s related to various loss channels. In μ-disks of few micrometers in size, the total Q-factor dispersion is defined mainly by the interplay between the radiative and material Q’s, expressed as

\[ Q_{\text{total}}^{-1}(\lambda) \approx Q_{\text{rad}}^{-1}(\lambda) + Q_{\text{mat}}^{-1}(\lambda) + Q_{z}^{-1}, \]

with the semi-empirical term \( Q_{z}^{-1} \) accounting for losses due to nonideals in real devices. Moreover, in active micro-resonators the measured Q-band of WGM emission is limited to the spectral region of the active material luminescence band, in our case, that of Si-nc.

In our experiment, the possibility of having modified radiative losses is rather straightforward; stress-induced formation of μ-kylix resonators from nominally 10 μm flat disks, results in a slightly smaller (by ~50 nm) external diameter. For μ-disks, such a small modification of the diameter (by 0.4% only), is not expected to affect significantly \( Q_{\text{rad}} \). For 200 nm-thick passive flat devices of 10 μm and 9.96 μm of diameter, typical \( Q_{\text{rad}} \) values at \( \lambda = 800 \) nm are of the order of 10^8 and differ by only ~5% (Fig. 4(a)). Numerical simulations, however, show that in a μ-kylix resonator of 9.96 μm diameter \( Q_{\text{rad}} \) reduces by an order of magnitude with respect to the original μ-disk Fig. 4(a), down-triangled plot). A tenfold reduction in radiative Q associated to disk reshaping is an interesting result which has never been addressed. To model this, we introduce the concept of out-of-plane bending loss \( 1/Q_{\text{bend}}(z) \), which is a function of the bending degree, i.e. of the coordinate \( z \) of the out-of-plane lifting of the disk edge. Thus, the radiative Q for a μ-kylix can be modeled as

\[ Q_{\text{rad}}^{-1}(R, z) = Q_{\text{rad}}^{-1}(R) + Q_{\text{bend}}^{-1}(z), \]

FIG. 3: Tuning of quality factors in μ-kylix resonators. Scanning electron micrographs and corresponding shape sketches for (a) μ-kylix, (b) μ-disk and (c) inverse μ-kylix resonators, respectively. (d) Measured Q-factor bands for differently shaped resonators.

The change in \( Q_{\text{rad}}(R) \) leads to an important spectral blue-shift of the Q-band with an overall reduction of Q values. Since in experiment we only observe a shift but not a reduction of Q’s, we conclude that in a μ-kylix the \( Q_{\text{mat}} \) is also affected (increased). This scenario is surprising.
FIG. 4: Out-of-plane radiative losses and modified Q-dispersions. (a) Small reduction of the disk diameter by only 0.4% (from 10 µm to 9.96 µm) induces negligible change in radiative Q for µ-disks (• and ▲, respectively). Instead, bending the originally flat disk to an effective diameter of 9.96 µm (thus forming a µ-kylix) a tenfold attenuation of quality factor is observed. (b) Confinement factor dispersions, calculated for different resonator configurations. (c) (top panel) Numerical simulations of a non-absorbing µ-kylix show that due to a weaker mode confinement only 1st-order radial family manifests. Bottom panel shows that µ-disks support quite intense 2nd-order families. (d) Numerically calculated dispersions of radiative, material and total quality factors in a µ-disk and a µ-kylix according to Eq. 1.

The material quality factor is generally defined as $Q_{\text{mat}} = \frac{2\pi n_g}{(\Gamma \alpha \lambda)}$, where $n_g$ and $\Gamma$ are the group index and optical confinement factor of the mode in the active layer, respectively, and $\alpha$ is the material absorption at the wavelength $\lambda$. The material absorption has been measured by ellipsometry and was found to be the same for the different disk configurations (the stress does not affect the absorption of Si-nc’s). Possible modifications in $Q_{\text{mat}}$, therefore, should only result from differences in group indices and/or confinement factors. We performed further numerical simulations and reveal very similar $n_g$ for both µ-disk and µ-kylix ($n_g \approx 2.02$ and 2.12 at 800 nm, respectively). While slab-waveguide simulations for various layer sequences show almost identical $\Gamma$-values, in a disk geometry important differences are observed. Namely, the µ-kylix shows smaller $\Gamma$-values than the µ-disk ($\Gamma \approx 0.31$ and 0.4 at 800 nm, respectively) (Fig. 4(b)). Since $Q_{\text{mat}}$ is inversely proportional to $\Gamma$, a roughly 25% less confinement leads to an appreciable change in material Q’s. This, in its turn, modifies the Q-band, shifting it further to shorter wavelengths, but, more importantly, does not degrade highest Q values. Moreover, lower $\Gamma$ values explain why, on the contrary to µ-disks, the µ-kylix resonators do not support higher order mode families (Fig. 2(c,d)); the overall reduced confinement in µ-kylix alters guided mode propagation for higher order families (see Fig. 4(c)). Combining our numerical results for both modifications in $Q_{\text{rad}}$ and $Q_{\text{mat}}$, we reproduce qualitatively the experimentally observed Q-band tuning (Fig. 4(d)).

For a final confirmation that the disk geometry is responsible for the tuning of Q-factors, we performed a third experiment, in which inverse µ-kylixes were realized (Fig. 3(c)) and tested. The band shift for these devices is less pronounced (Fig. 3(d), blue empty circles), in accordance with the minor stress of the disk; much lower temperature of the SiOx/Si3N4 interface formation ($T = 300^\circ C$ in the PECVD deposition chamber) and eventual high-temperature annealing for Si-nc formation result in a reduced stress. Consequently, the inverse µ-kylix is characterized by a larger bending radius, $\approx 83\mu m$ (smaller $z$) and, hence, lower out-of-plane losses, $Q_{\text{bend}}^{-1}$.

It is important to note, that in conventional µ-disk resonators smaller diameters blue-shift the spectral range of highest Q-factors too. For example, a 60 nm shift of the Q-band is observed for µ-disk of twice smaller diameter (Fig. 5). In this case, the only modification in $Q_{\text{total}}$ arises from a severe attenuation of $Q_{\text{rad}}$'s, therefore, very
low values of highest $Q_{total}$ are observed. Moreover, the free spectral range in a 5 $\mu$m $\mu$-disk doubles with respect to a 10 $\mu$m one. We underline, that the $\mu$-kylix configuration provides the same amount of tuning of the Q-band with only a 0.4% of effective diameter modification, which also provides an almost unmodified FSR.

In conclusion, we have demonstrated a new class of bi-dimensional micro-resonators with out-of-plane bending, which perfectly support whispering-gallery modes. We refer to them as micro-kylixes. These resonators are chip-integrable and can be easily fabricated using standard microfabrication technology. Their particular geometry reveals new physics: tuning of the highest Q-factors towards shorter wavelengths, where the basic material has stronger absorption. This is achieved through a smart interplay between radiative and material quality factors. Our experimental results, validated by numerical simulations, indicate that this phenomenon could be exploited to obtain improved Q-factors in specific spectral windows (shorter wavelength) without modifying resonator’s physical size and the free spectral range. Micro-kylix resonators can offer novel technological solutions for micro-resonator physics and photonics research and may open the door to new functionalities of resonator devices, from sensing to optical amplification.

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