# CONTROL OF MODES COUPLING, SELECTION AND ENHANCEMENT IN WAVELENGTH-SCALE OPTICAL MICROCAVITY STRUCTURES: APPLICATIONS TO MICROLASERS AND BIOSENSING

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***Abstract-*** Recent advances and remaining challenges in spectral engineering of wavelength-scale optical microcavity structures supporting modes with narrow linewidths, wide mode spacing, directional emission, and greatly enhanced sensitivity to the environmental changes will be reviewed. General recipes for efficient control and manipulation of modes coupling and selective enhancement in such structures will be discussed.

***Keywords*:** optical microcavities, photonic molecules, mode selection, frequency crossing (anti-crossing), whispering-gallery modes, low-threshold semiconductor microdisk lasers, bio(chemical) sensors, integral equations.

## INTRODUCTION

Dielectric and semiconductor optical microcavities have already proven to be among the most essential and versatile components of modern wavelength-division-multiplexed optoelectronic circuits that find use for light storage, frequency selection, filtering and switching [1-3]. Furthermore, their ability to confine light in small volumes and enhance light-matter interaction enables realization of novel miniatuarized light sources such as low-threshold microdisk lasers and light emitting diodes [1-5], and makes such cavities an indispensable tool for quantum electrodynamics experiments with single-photon emitters [6,7]. Finally, optical microcavities supporting high-Q modes have demonstrated potential in the development of inexpensive, ultra-compact, highly sensitive and robust bio- and chemical sensors for both mass and fluorescence sensing [8-10]. As compared to more traditional linear optical waveguide or fiber biosensors, microcavity-based devices benefit from much smaller size and higher sensitivity and show promise in detecting individual nanoparticles with the sizes below the diffraction limit, such as viral particles and proteins.

However, high-Q microdisk resonators suffer from inability to operate in single mode. This feature has prevented realizing thresholdless lasing in semiconductor microcavities, may compromise robust performance of microcavity-based sensors, and also complicates efficient numerical modeling of microcavity lasers. If more than one cavity mode frequency lies within the gain spectrum of the cavity material, it is not possible to accurately predict which mode will reach lasing threshold first only by knowing the eigenmode spectrum of a cold cavity found as a solution of the corresponding linear boundary-value problem. A fully nonlinear problem formulation will be necessary for the accurate description of actual stationary lasing states is such cavities making numerical modeling cumbersome and time-consuming [11,12].

This paper will discuss the ways to achieve new functionalities (e.g., quasi-single-mode operation on a high-Q mode) of optical microcavity structures for applications such as microlasers and biosensing platforms by making use of general design rules of selective modes suppression and enhancement [13-16].

## MODE SPECTRA AND COMPETITION IN MICROCAVITY LASERS

It has been known since 1946 that the spontaneous emission (SE) rate of emitters can be either inhibited or enhanced if the emitters are placed in a microcavity [17]. Throughout this paper, the term "microcavity structure" will be used in a broad meaning and will encompass individual thin-disk resonators, microposts, microspheres, photonic crystal (PhC) defect cavities, and photonic molecules composed of evanescently coupled cavities (Fig. 1). Microcavity structures enable light spatial confinement in a small volume and spectral confinement in a series of narrow wavelength bands (cavity modes). Scaling of microcavity structures to the dimensions comparable to the wavelength of the emitted light results in appearance of novel quantum phenomena and yields new functionalities of semiconductor light sources.

The spontaneous emission rate alteration relative to the bulk material, known as the Purcell effect, forms a basis for the development of low-threshold or thresholdless semiconductor microcavity lasers, light emitting diodes (LEDs), and devices for quantum information processing. A measure of the spontaneous emission rate enhancement is called the Purcell factor and is defined as: $F_P = 3Q(\lambda/n)^3 / (4\pi^2 V_{\text{eff}})$, where $\lambda$ is the mode wavelength, $Q$ is the mode quality factor, $V_{\text{eff}}$ is the effective mode volume, and $n$ is the refractive index of the material. For microlaser applications, the ratio $Q/V_{\text{eff}}$ is to be optimized for a reduction of lasing threshold [18-20].

However, this formula is only valid in the case when (i) only one microcavity mode overlaps the gain bandwidth, (ii) the emitter is located at the peak of the electric field, and (iii) the cavity resonant frequency equals the material gain peak frequency. Spectral, spatial and polarization mismatch between the cavity mode and cavity gain material results in significant decrease of the SE enhancement rate ($E$) from the value given by the Purcell factor. To account for this mismatch, the following formula can be used: $E = F_P \eta^2 \gamma_c (2\gamma_e + \gamma_c) / \left(4(1-\omega_c/\omega_e)^2 + (2\gamma_e + \gamma_c)^2\right) \left|\vec{E}(\vec{r})\right|^2 / \left|\vec{E}_{\max}\right|^2$, where $\omega_c$ and $\omega_e$ are the frequencies of the cavity mode and the material gain peak, $\gamma_c$ and $\gamma_e$ are the decay rates of the mode and the emitter, respectively, $\eta$ is the polarization mismatch factor, and $\vec{E}(\vec{r})$ is the electric field at the position of the emitter [21].

In most practical cases, however, the microcavity mode linewidths are much narrower than the material gain linewidth, and several mode frequencies can be observed within the material gain spectrum (Fig. 2a). Furthermore, the number of modes spectrally overlapping with the material gain increases with the increase of the cavity size. This tendency is demonstrated in Fig. 2b for the case of a microdisk cavity. It can be seen that while the Q-factors of whispering-gallery (WG) modes grow with the increase of the cavity radius, the cavity free spectral range (modes spectral spacing) shrinks. The WG modes are classified by two subscripts denoting the number of angular and radial field variations (see Fig. 2c). It should also be noted that all the WG modes in circular disks are double-degenerate. This degeneracy is often lifted because of microcavity shape imperfections thus doubling the number of available cavity modes. The presence of several competing modes results in decreasing the fraction of

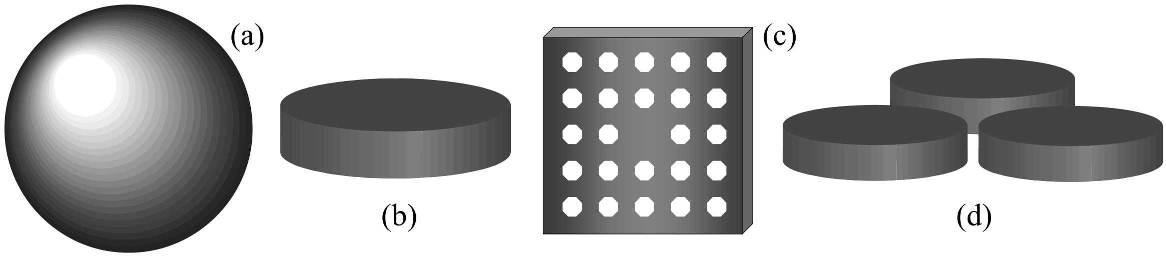


Figure 1 – Examples of microcavity structures: (a) microsphere, (b) microdisk resonator, (c) photonic crystal defect cavity, and (d) photonic molecule composed of side-coupled microdisks.

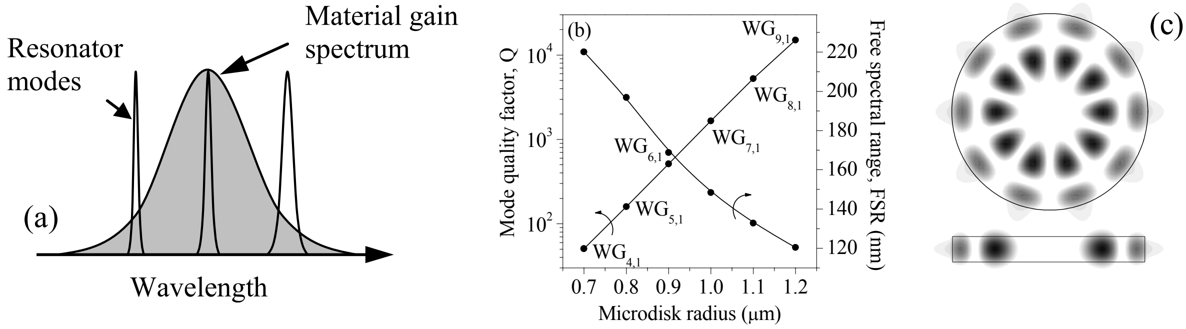


Figure 2 – (a) Schematic of a microcavity optical mode spectrum with a material gain spectrum in the background; (b) Q-factors and FSRs of circular microdisk WG-modes ($n_{disk}$ = 2.63, $n_e$ = 1.0) with resonant wavelengths around 1.55 μm versus the disk radius; (c) Magnetic field intensity distribution of the $WGE_{5,2}$ mode.

spontaneous emission going into each mode, and therefore in increasing the lasing threshold. Furthermore, two or more modes having close resonant frequencies can interact with each other through active cavity material causing mode locking [22].

To accurately study mode interactions and microcavity laser dynamics, a full nonlinear treatment of the corresponding boundary-value problem for a microcavity with gain is required. Recent developments in the non-linear analysis of microcavities have added to the theoretical understanding of their dynamical properties [11, 12]. However, nonlinear models yield cumbersome and time-consuming algorithms. Furthermore, for many applications, such as low-threshold lasers and single-photon sources, single-mode (or rather quasi-single mode) cavities are required. Here, we present and discuss a design strategy for the controlled manipulation of the cold-cavity spectrum with the aim to enhance one mode that has a resonant frequency within the material gain bandwidth and suppress all the other modes considered parasitic. Tuning of the cold-cavity spectrum can be performed by solving a linear boundary-value problem, which is done in this paper by using the Muller boundary integral equations (MBIEs) formalism [23]. Then, once a microcavity structure is optimized to support only one mode within a material gain spectrum, linearized models valid for single-mode lasing condition (such as e.g. linear stationary Maxwell-Bloch equations [12] or Laser Eigenvalue Problem formulation [24]) can be used to compute the stationary lasing states or modal thresholds.

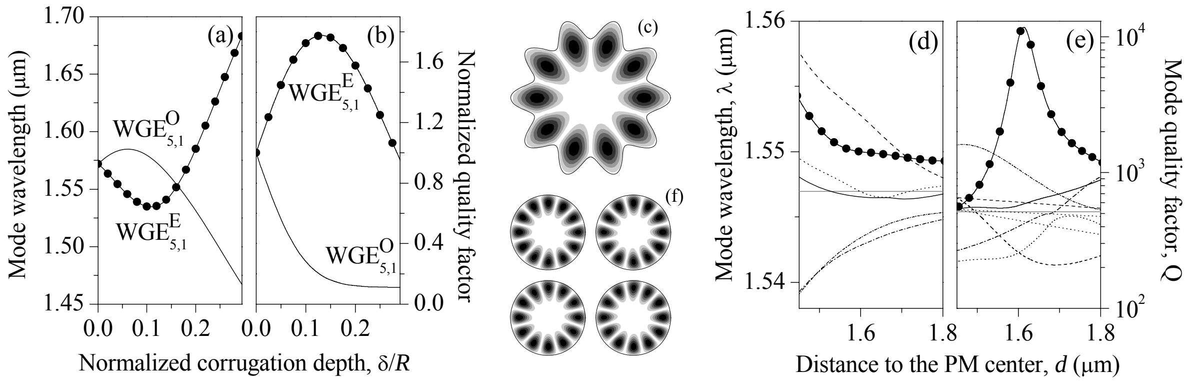


Figure 3 – (a) Wavelengths shift and (b) Q-factors change of $WGE_{5,1}$ modes of even and odd symmetry along the x-axis in a microgear cavity versus the microgear corrugation depth [14, 16] ($n_{disk}$ = 2.63, $r_{disk}$ = 0.8 μm); (c) Magnetic field intensity portrait of the enhanced $WGE_{5,1}$ mode in a microgear; (d) wavelengths shift and (e) Q-factors change of $WGE_{6,1}$ supermodes in a square PM composed of four identical microdisks ($n_{disk}$ = 2.63, $r_{disk}$ = 0.9 μm) versus the inter-cavity distance [28]; (f) Magnetic field intensity portrait of the enhanced $WGE_{6,1}$ mode in an optimally-tuned square PM ($d$ = 1.6125 μm).

## SELECTIVE MODE SUPPRESSION AND ENHANCEMENT

One of the ways to selectively enhance one of the modes in a microcavity is to introduce an artificial deformation of the cavity shape in such a way that this deformation if favorable for one mode and unfavorable for other closely located modes. Fig. 3 demonstrates an example of such a deformed cavity, termed microgear, which enables enhancement of one of the split WG-modes that form a degenerate pair in an ideal circular disk [13, 14, 25]. Splitting of the degenerate WG mode with the increase of the corrugation depth is shown in Fig. 3a; and it can be seen in Fig.3b that the enhanced mode (with the field portrait shown in Fig 3c) is the mode that is spatially matched to the contour corrugation. Other cavity shapes for controlled manipulation of WG modes include square resonators [14, 16], pierced microdisks [26, 27], notched microcavities [15], etc. It has also been demonstrated that symmetrical configurations of evanescently-coupled circular microdisks (so-called photonic molecules (PMs)) can also be tuned to achieve their quasi-single-mode operation [28]. Tuning of wavelengths and Q-factors of WG-supermodes supported by a square photonic molecule with the change of the inter-cavity distance is illustrated in Fig. 3 d and e, respectively. Clearly, for a certain value of this distance, one of the supermodes (with the field portrait shown in Fig. 3f) is significantly enhanced while all the other modes are suppressed.

Careful study of Figs. 3 a,b and d,e reveals that the Q-factor enhancement of one of the modes occurs due to mode coupling at a certain value of the external parameter that is changed to tune the microcavity system (at so-called exceptional points). Note that a term "microcavity mode" encompasses a complex value of the mode eigenfrequency and the corresponding eigenvector (i.e., modal spatial field distribution). It is known that the eigenvalues of matrices dependent on parameters can couple or decouple with crossing and avoided crossing scenarios under the change of these parameters [29, 30]. This phenomenon is of a general nature and can be observed in many physical systems. It enables mode enhancement because at the exceptional points, frequency anti-crossing (crossing) is accompanied by crossing (anti-crossing) of the corresponding widths of the resonance states.

Two more examples of parameter-tuning-induced mode coupling yielding selective mode enhancement are demonstrated in Fig. 4. Fig. 4a,b shows further enhancement of the high-Q first-radial-order WG-mode at the point where the corresponding mode frequency coincides with the frequency of the low-Q second-radial-order WG-mode [31]. In Fig. 4c, anti-crossing of WG-supermodes of a two-disk photonic molecule (composed of disk A and disk B of different radii) is observed if the radius of disk B is varied (also observed experimentally in [32]). Note that the Q-factor of the odd-even (OE) mode is enhanced at the point of the frequency anti-crossing when the disk radii are equal (see Fig. 4d for the field distributions of

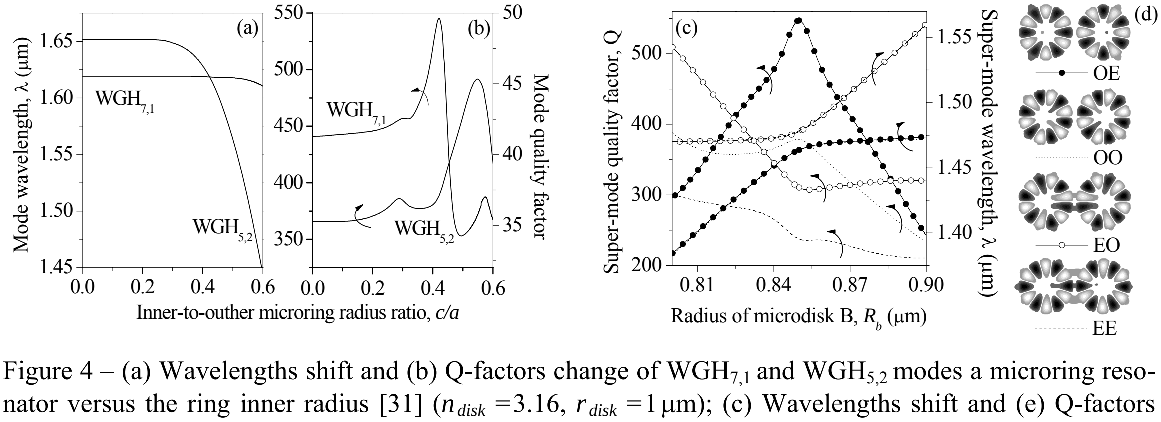


Figure 4 – (a) Wavelengths shift and (b) Q-factors change of $WGH_{7,1}$ and $WGH_{5,2}$ modes a microring resonator versus the ring inner radius [31] ($n_{disk} = 3.16$, $r_{disk} = 1$ μm); (c) Wavelengths shift and (e) Q-factors change of $WGE_{6,1}$ supermodes in a PM composed of two microdisks versus the radius of one of the disks ($n_{disk} = 2.63$); (d) Magnetic field portraits of the supermodes in a PM composed of identical disks.

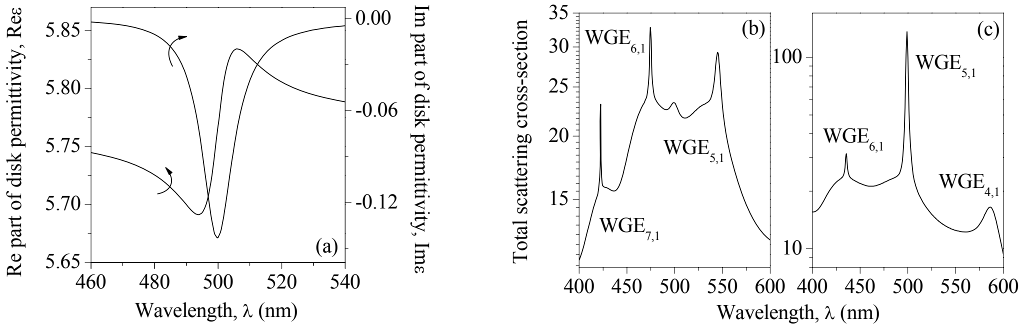


Figure 5 – (a) Values of the frequency-dependent real and imaginary parts of the dielectric constant inside the microdisk induced through population inversion; Plane-wave scattering spectra of microdisk resonators with radii of 300 nm (b) and 275 nm (c). $WGE_{5,1}$ mode in the 275 nm – radius microdisk is spectrally aligned with the material gain maximum.

the photonic molecule WG-supermodes of different symmetry). Recent publications also show the possibility of selective mode enhancement through mode coupling in disks-on-substrates [33] and pierced microdisk resonators [27].

Another way to reduce the threshold in a microcavity laser is to increase the fraction of spontaneous emission into the lasing mode by improving the spectral alignment between the material gain peak and the microcavity mode wavelength [34, 35]. Fig. 5 demonstrates selective enhancement of a WG-mode in a circular 2-D disk with a complex dielectric constant induced through population inversion. In Fig. 5a, the dielectric constant of the cavity with gain is shown as a function of wavelength. Material gain is introduced to the model by assuming a three-level laser material, and the following formula is used for calculation of the cavity complex dielectric constant: $\varepsilon(\lambda,\vec{r}) = \varepsilon_{cold}\left(1-\left(3\lambda^3/4\pi^2\right)\left(\gamma_{rad}^{1\to0}/\Delta\omega_a^{1\to0}\right)\Delta N_{01}(\vec{r})\Lambda(\omega,\Delta\omega_a^{1\to0})\right)$, where $\lambda$ is the wavelength, $\gamma_{rad}^{1\to0}$ is the decay rate from the exited to the ground level, $\Delta\omega_a^{1\to0}$ is the linewidth of the atomic transition from level 1 to the ground level, $\Delta N_{01}(\vec{r})$ is the population difference between level 1 and the ground state, and $\Lambda(\omega,\Delta\omega_a^{1\to0})$ is the Lorentzian line shape for the laser transition (see [35-38] for more detail). Fig. 5b presents a plane-wave microcavity scattering spectrum for the case when none of the cavity modes is aligned with the material gain peak (λ = 500 nm). Apart from an additional maximum appearing at λ = 500 nm, this spectrum does differ from the cold-cavity scattering spectrum (not shown). In Fig. 5c, the size of the cavity is tuned to achieve spectral alignment of the $WGE_{5,1}$ mode with the gain peak wavelength, and significant enhancement of this mode is observed.

## APPLICATIONS TO MASS & FLUORESCENCE SENSING AND EXTERNAL-GAIN LASERS

Single-high-Q-mode operation is also essential for high sensitivity of microdisk-based sensors [8-10], narrow wavelength-selective filters [2, 3], and evanescent-wave-coupled gain microcavity lasers [39, 40]. However, for these applications, the WG-mode interaction with analyte (or external gain medium) occurs only through the evanescent portion of the mode field. Herein lies the contradiction: as high-Q WG modes of microcavity sensors are very efficiently confined inside microcavities, they are not very sensitive to the small changes in the analyte dielectric constant. Similarly, in the evanescent-coupled-gain lasers the gain comes from the excited molecules in the evanescent-wave portion of the WG-mode field. Thus, it is proportional to the total number of the excited molecules in the evanescent-wave mode volume (note that this volume decreases with the increase of the mode Q-factor) [39].

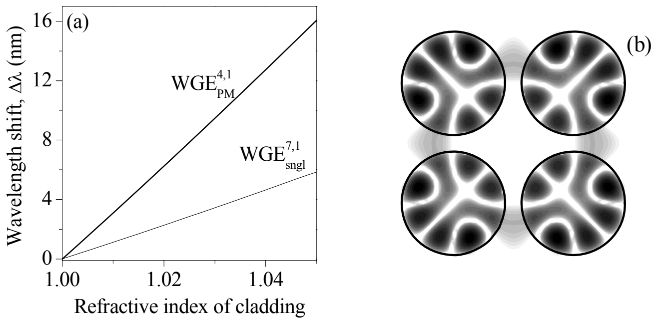


Figure 6 – (a) Comparison of the wavelength shifts as a function of the refractive index of the sensor cladding for a single 2 μm diameter microdisk operating on a $WG_{7,1}$ mode and for the square PM operating on the symmetry-enhanced $WG_{4,1}$ supermode ($n_{disk} = 2.63$, $r_{disk} = 0.67$ μm); (b) Magnetic field portrait of the enhanced $WGE_{4,1}$ mode in the optimally-tuned square PM.

To overcome this contradiction, photonic molecules supporting symmetry-enhanced supermodes with high Q-factors (such as shown in Fig. 3 d,e,f) can be used instead of individual microcavities [41]. As PM super-modes are collective multi-cavity resonances, they provide better overlap of the modal field with the analyte without degrading the mode Q factor. Such supermodes have been shown to be more sensitive to changes in the cavity environment than WG-modes of larger individual cavities with comparable values of Q-factors [41]. Fig. 6 demonstrates the performance improvement offered by the PM-based sensor for the detection of the changes in the dielectric constant of the sensor cladding over sensors based on individual microcavities with comparable Q-factors. A square optimally-tuned ($d$ = 1.101 μm) PM consisting of the air-clad 1.34 μm-diameter disks ($n$ = 2.63) is considered. This PM supports a symmetry-enhanced $WG_{4,1}$ supermode (with the field portrait shown in Fig. 3b). As illustrated in Fig. 6a, the resonant wavelength of the enhanced PM supermode systematically shifts to higher values with the increase of the refractive index of the cladding. This shift is noticeably greater than corresponding shift of individual microdisk WG-mode wavelength of higher radial index and comparable value of Q-factor.

Optimally-tuned photonic molecules are also expected to yield enhanced performance of biosensors based on the PMs immersed in a fluorophore solution and evanescent-coupled-gain lasers. For example, lasing in a microscopic cavity made of two nanoparticles acting as nano-mirrors in a homogeneous gain medium has recently been demonstrated [40].

## Conclusions

Basic design rules to tune spectral and threshold characteristics of micro-scale optical cavity structures by tailoring their geometry are formulated and discussed. The design strategy is based on MBIEs solution of corresponding linear boundary-value problems for cold cavities, which yields very efficient algorithms. The results of simulations provide leads to novel improved WG-mode microcavity designs for lowering thresholds of semiconductor microlasers and enhancing sensitivity of microcavity-based bio(chemical)sensors. Another emerging important application of high-Q (quasi)single-mode tunable microcavity structures is in the field of quantum information science for efficient generation of single photons or photon pairs, qubit storage and gate operation [6, 7].

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