Research article

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Monolithic high-contrast grating planar microcavities

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Abstract: Semiconductor planar microcavities significantly enhance the interaction between light and matter and are thus crucial as a fundamental research platform for investigations of quantum information processing, quantum dynamics, and exciton-polariton observations. Microcavities also serve as a very agile basis for modern resonant-cavity light-emitting and detecting devices now in large-scale production for applications in sensing and communication. The fabrication of microcavity devices composed of both common materials now used in photonics and uncommon or arbitrary materials that are new to photonics offers great freedom in the exploration of the functionalities of novel microcavity device concepts. Here we propose and carefully investigate two unique microcavity designs. The first design uses a monolithic high-index-contrast grating (MHCG) and a distributed Bragg reflector (DBR) as the microcavity mirrors. The second design uses two MHCGs as the microcavity mirrors. We demonstrate by numerical analysis that MHCG-DBR and MHCG-MHCG microcavities, whose lateral radial dimension is 16 μm , reach very large quality factors at the level of 10^4 and nearly 10^6 , as well as purposely designed wavelength tuning ranges of 8 and 60 nm in both

configurations, respectively. Our MHCG-MHCG microcavities with a very small size of 600 nm in the vertical dimension show extremely large quality factors, which can be explained by treating the optical modes as quasi-bound states in a continuum (BICs). Moreover, we verify our theoretical analysis and calibrate our simulation parameters by comparing to the experimental characteristics of an electrically injected MHCG-DBR microcavity vertical-cavity surface-emitting laser (VCSEL) emitting at a peak wavelength of about 980 nm. We use the calibrated parameters to simulate the emission characteristics of electrically injected VCSELs in various MHCG-DBR and MHCG-MHCG microcavity configurations to illustrate the influence of microcavity designs and their quality factors on the predicted lasing properties of the devices.

Keywords: planar microcavities; vertical-cavity surface-emitting lasers; subwavelength gratings; numerical simulations.

1 Introduction

Optoelectronic devices relying on high quality factor (Q -factor) optical microcavities are increasingly important research tools in science and technology. Numerous contemporary physics experiments use optical cavities for studies of the enhancement in detection sensitivity [1], nonlinear interactions [2], single-photon generation [3], observation of polariton-excitons [4], and quantum dynamics. A prominent example of the latter is the demonstration of Bose-Einstein condensation in photonic systems [5], which is observed along with the remarkable phenomena of coherent lasing below population inversion [6]. Moreover, numerous designs of commercial devices require the use of high Q -factor microcavities including vertical-cavity surface-emitting lasers (VCSELs) [7], resonant-cavity light-emitting diodes (RCLED) [8, 9], resonant-cavity solar cells with enhanced efficiency [10], wavelength-selective photodetectors [11], as well as Fabry-Pérot filters [12] and modulators [13].

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Microcavities can be realized in numerous geometries such as pillar microcavities based on distributed Bragg reflectors (DBRs) [14], photonic crystal slabs [15], ring and sphere resonators [16, 17], and Fano resonance periodic structures [18] and their plasmonic counterparts [19]. Achieving simultaneously a high cavity Q -factor, a small mode volume, and a nondivergent output is challenging. Perfecting one of these three properties typically results in the deterioration of the other two. However, microcavities that use DBR mirrors may achieve very close to optimum power reflectance properties, leading to high Q -factors and highly directed optical output powers at the cost of a relatively large mode volume. Recently, there have been many attempts to replace bulky (thick) DBRs and reduce the cavity mode volume by using high-index-contrast gratings (HCGs) [20] as mirrors in place of DBRs. HCGs can be as optically thin as half of the resonant wavelength while facilitating a further reduction of the mode volume. Microcavities with HCG mirrors may be 1/10 as thick in the vertical direction as the same microcavities with DBR mirrors [21]. Furthermore, the lateral parameters of the HCG enables engineering the light polarization, optical power reflectance spectra, phase of the reflected light, dispersion of cavity modes, output beam direction, resonant wavelength adjustment, and its dispersion without changing the thickness of the cavity [20, 22, 23]. The disadvantage of the HCG mirror lies in the fact that it either must be suspended in air or implemented on a layer of low refractive index that typically is a dielectric material, thus making the fabrication of HCGs fairly complex. Moreover, it is not possible to inject current through the HCG mirror in electrically driven devices since the air and/or the dielectric layers are nonconducting.

In our recent works, we have proposed a monolithic (formed in one single layer) HCG (MHCG) providing total optical power reflectance for refractive indices of the MHCG material larger than 1.75 [24] and inheriting the properties of HCGs together with the capability of reflected light phase control. MHCGs are robust and immune to mechanical failure (in contrast to membrane HCGs). They also do not require sophisticated critical point drying after selective wet-etching of the membrane for its release during processing. The MHCG parameters can be precisely controlled via electron beam lithography for research or via nanoimprint lithography [25] during mass production. A given MHCG may also cover an arbitrarily large area in contrast to a large-area suspended HCG, which would be at risk of collapse [26].

Our numerical findings were confirmed by experimental characterization of the power reflectance spectrum [27] of a stand-alone MHCG fabricated on a GaAs wafer and designed for a wavelength of 980 nm. Recently,

Kim et al. reported the first polariton laser constructed with an MHCG microcavity [28], and we showed the first electrically injected MHCG VCSEL [29]. Our VCSEL had a peak emission wavelength of 980 nm. Structures using the concepts of MHCG-DBR (M-D) and MHCG-MHCG (M-M) mirrors to form microcavities have been proposed by us earlier [30–32]; however, without an in-depth exploration of the microcavity mode behaviors, which is essential for controlling the properties of microcavities. This is the main topic of this paper.

One or two MHCG mirrors enable a significant simplification of a given microcavity structure by replacing one or both of the DBRs with a much thinner MHCG (see Figure 1). An MHCG as a top mirror provides easier access to the cavity than DBR for an optical beam in any arbitrary range of wavelengths incident from the free-space side [28]. An M-M microcavity can take the form of only one suspended layer, with a subwavelength grating implemented on both opposing surfaces. Embedding quantum structures inside the M-M microcavity (quantum wells, quantum dots, carrier confinement layers, etc.) enables the suspended M-M microcavity's functionality as an active device. An M-M microcavity can be realized in any material system used in modern photonics, eliminating the problematic monolithic growth of DBRs formed using, for example, GaN-, InP-, and ZnO-based materials.

The main goal of the analysis presented in this paper is to illustrate, via numerical modeling, the complex nature of planar MHCG microcavities with precise designs that facilitate very large Q -factor resonances and a broad range of resonant wavelengths induced by modification of only the MHCG parameters. In Section 2 and

Figure 1: Schematic cross-section of microcavities concerned in the analysis.

Schematic cross-sections of (A) a D-D microcavity, (B) an M-D microcavity, and (C) an M-M microcavity. Dark gray represents GaAs and light gray represents AlAs. All cavities are approximately 1λ thick optically and are marked by a white left-oriented curly bracket. The coordinate system used in all configurations is shown in (A).

in Supplementary Materials (S1) we present our numerical analysis method and microcavity designs. In Section 3 we consider optical phenomena occurring in the simplest designs of the MHCG microcavities, composed of monolithic material. This approach enables us to analyze microcavity structures with reduced complexity in M-D and M-M configurations, highlighting the optical phenomena and illustrating the pure impact of the MHCG on the properties of the planar microcavities. The calculations are carried out for a GaAs microcavity designed for a resonant wavelength of 980 nm; however, the general conclusions drawn in this section are applicable for structures based on different materials and resonant wavelengths. In Section 4 we consider a real-world example of M-D microcavities in the form of electrically injected M-D VCSELs. We analyze the M-D VCSELs' current versus power characteristics, taking into account the simulation parameters extracted from our experimental characteristics of GaAs-based D-D VCSELs with peak emission wavelengths of 980 nm. We thus validate our numerical model by comparing our simulated and experimental results for our electrically injected M-D VCSELs emitting at 980 nm.

2 Methods and microcavity designs

In optical calculations, to which owe most of our numerical results in this paper, we use an eigenvalue solver based on a fully vectorial plane wave admittance method (PWAM) [33]. Details on the PWAM algorithm can be found in S1. With this method we determine the complex wavenumbers ($k_0 = k_{\text{ore}} + ik_{\text{oim}}$) whose real parts (k_{ore}) correspond to the values of free-space wavevectors of the optical modes and whose imaginary parts (k_{oim}) are proportional to the optical losses of the modes. Mode's Q -factor is defined as $Q = -0.5 k_{\text{ore}} / k_{\text{oim}}$. In this section we analyze the fundamental mode of the smallest real part of k_0 , which is labeled HE_{11} . In our analysis, we consider the transverse electric (TE) polarization of the electromagnetic (EM) field. In this polarization, the sole electric field component, designated as E_x , is parallel to the grating stripes. This choice of polarization is arbitrary; the differences concern the parameters of the MHCGs for high power reflectance of TE and transverse-magnetic (TM) polarizations. Differences in the parameters of the MHCGs for TE and TM polarizations can also occur in the power reflectance spectrum and phase-shaping of the reflected light. However, we believe that any conclusions drawn from our microcavities with MHCGs realized in either the TE or the TM configuration would be the same.

3 Optical simulations of microcavities

In this section we analyze finite two-dimensional microcavities, as shown in Figure 1, with absorbing boundary conditions (ABCs) realized by perfectly matched layers (PMLs) [34]. We take the MHCG stripes to be infinite in the x -direction. We analyze the power reflectance of free-standing MHCGs in this section and assume that the MHCGs are infinite in the y -direction by taking into account a single MHCG period combined with periodic boundary conditions.

In this section we assume that the microcavities and the MHCGs are constructed of uniform GaAs. The DBRs are composed of 35 pairs of stacks of GaAs/AlAs quarter-wavelength layers whose refractive indices at 980 nm are 3.5211 and 2.9514, respectively. All the refractive indices used in the optical analysis presented in Section 3 are real numbers (with zero imaginary part), which means that there is no gain or internal absorption. The cavities in all the designs are approximately 1λ optically thick at 980 nm, corresponding to a physical thickness of 278 nm. The deviation of the cavity length from 1λ is induced by a phase change produced by the MHCG. The lateral size of the D-D microcavity is infinite to illustrate the maximum possible Q -factor that can be obtained for such a design and to emphasize the pure influence of the number of DBR pairs on the Q -factor. The Q -factor of a D-D microcavity pillar whose diameter is greater than $4\text{ }\mu\text{m}$ is very close to the value determined for an infinite D-D microcavity. More details on the simulation parameters can be found in S1.

We performed optimization of the parameters of the MHCG used in the M-D and M-M microcavities with respect to maximum power reflectance by simulating an infinite MHCG structure in the following way. We considered a single period of the MHCG with periodic boundary conditions, and assumed normal incidence of the incident wave and the following variable parameters: the MHCG grating period (L); the grating duty cycle (F); and the etching depth (h). This enabled the determination of the MHCG configurations that provide nearly 100% power reflectance (R) of the zeroth diffraction order (0-DO) at the wavelength (λ) of 980 nm. Although, unlike in HCGs, higher diffraction orders are always present in MHCGs, one can find the grating parameters that enable reflection predominantly into 0-DO, as discussed in [35]. From numerous R maxima in the domain of L , F , and h , we chose the R maxima with the smallest value of h , which yield the following parameters (labeled in this

paper as LFH_M): $L_M = 0.8171 \mu\text{m}$ (the period); $F_M = 0.3499$ (the duty cycle); and $h_M = 0.1639 \mu\text{m}$ (the etching depth). These parameters also provide the broadest reflection stop-band, which at the level of $R = 0.99$ reaches 60.9 nm .

3.1 M-D microcavity

Figure 2A shows the dependence of the Q -factor on the thickness of the cavity (d_c) for various numbers of MHCG stripes. By changing the thickness of the cavity, the resonance wavelength is modified accordingly. Hence, the figure contains a second, upper horizontal axis corresponding to the resonant wavelength of the fundamental mode. The resonant wavelength at 980 nm occurs for $d_c = 0.2762 \mu\text{m}$, which is optically equal to 0.992λ in the material of the cavity. The figure shows the increase in the Q -factor as the number of stripes increases, as to be expected since an increase in the lateral size of the optical aperture increases the optical length of the grating modes and their Q -factor [36].

The appearance of two local maxima of the Q -factor near $\lambda = 975 \text{ nm}$ and $\lambda = 980 \text{ nm}$ is induced by the coupling of the vertical mode to the mode propagating horizontally, whereby leakage of the vertical mode occurs. More detailed analysis of the phenomenon is discussed in S2.

Figure 2B presents the maxima of Q -factors from Figure 2A of the fundamental mode (black line) versus the number of MHCG stripes, revealing a monotonic increase in the Q -factor. Six consecutive higher order modes (numbered 1–6) follow the trend of the fundamental mode 0;

however, the ratio between the Q -factor of the zeroth- and first-order modes remains constant and higher than the ratio between consecutive adjacent modes. Resonant wavelengths of the modes as a function of the number of MHCG periods and distributions of the modes are discussed in S3. The blue curve in Figure 2B relate to a conventional D-D microcavity, providing a comparison of Q -factors of D-D and M-D microcavities and relating the numbers of MHCG stripes and top DBR periods.

The mechanism of Q -factor increase with increase in the number of MHCG periods is related to the elimination of the reflection into higher diffraction orders. The LFH_M parameters are found by assuming an infinitely periodic MHCG mirror and normal incidence of the incoming wave. In this configuration, higher diffraction orders are eliminated [35]. In the case of an M-D microcavity with a finite MHCG, the cavity modes contain propagating wavevectors with nonzero lateral components. One can expect that the smaller the width of the MHCG or the higher the order of the mode, the stronger will be the lateral components. In those cases, the reflection into higher diffraction orders can be observed, which contributes to a deterioration of the microcavity Q -factor. This mechanism is confirmed by Figure 3, which shows M-D microcavities of three different sizes of the MHCG composed of, respectively, 20, 60, and 100 periods. In the case of the microcavity of 20 periods, the zeroth-diffraction-order vertical emission, lateral emission, and the number of rays reflected by MHCG and propagating outside the microcavity can be observed (the white dashed arrows). The rays propagate in directions not parallel to the optical axis and hence can be transmitted

Figure 2: Q -factor of M-D microcavities as the function of cavity thickness for different number of MHCG periods in (A) and Q -factor of successive lowest order lateral modes in (B).

(A) Q -factor of an M-D microcavity for an MHCG with the LFH_M parameters and for different number of MHCG periods from 20 to 100 in steps of eight periods as a function of the cavity thickness (d_c) and resonant wavelength (λ) of the fundamental lateral mode. The blue dots represent the maxima of the Q -factor for a given number of MHCG periods. (B) Q -factor of an M-D cavity for seven lowest order modes (numbered from 0 to 6) as a function of the number of MHCG periods (color lines, bottom axis) and Q -factor of a D-D cavity as a function of the number of top and bottom DBR periods (blue line, top axis).

Figure 3: Cross-section in the yz -plane of a distribution of the normalized fundamental mode optical field intensity in M-D microcavities with (A) 20, (B) 60, and (C) 100 MHCG stripes.

The positions of the MHCG, microcavity, and DBR are indicated. The parameters of the MHCG design are $L_M = 817.1$ nm (period), $F_M = 0.3499$ (duty cycle), and $h_M = 163.9$ nm (etching depth). The white dashed arrows illustrate the propagation of the higher diffraction orders.

through the bottom DBR, contributing to optical losses. In the microcavity composed of 60 MHCG periods, leakage effects are significantly reduced (Figure 3B), and they are nearly eliminated for 100 MHCG periods. This mechanism is also responsible for the large difference between the Q -factors of the modes 0 and 1. The ratio of these Q -factors is independent of the number of MHCG periods, as can be seen in Figure 2B.

Our further analysis concerns the impact of L and F on the microcavity properties, which is highly demanding with respect to computational time and was therefore carried out for microcavities with MHCGs consisting of 20 stripes only. The results presented in this section can be extrapolated, however, for larger numbers of MHCG stripes based on the dependence of the cavity Q -factor displayed in Figure 2B. For example, a 10-fold increase in the Q -factor is possible by increasing the number of MHCG stripes to 80. Figure 4A presents a Q -factor map in the domain of L and F for $Q > 3000$, which reveals a relatively close correspondence to the map of the 0-DO power reflectance in Figure 4C.

Changes in L and F induce a modification of the reflected radiation phase, which is manifested by a variation in the resonant wavelength of the M-D microcavity, as shown in Figure 4B. Assuming an example Q -factor of

around 3000, manipulation of L and F enables the resonant wavelengths to be obtained in a range 976–982 nm.

In Figure 5 we compare the dependence of the Q -factor versus the zeroth diffraction order (0-DO) power reflectance (R_0) of the coupling mirror in the case of M-D (color points) and D-D (black line) microcavities. The output coupling mirror in the first case is the MHCG, while in the second case it is the DBR with a different number of periods. Both structures are identical in the number of DBR periods in the bottom outcoupling mirror. The results for the M-D microcavity are the combination of the results presented in Figure 4, where the pixel colors identify the resonant wavelengths of the M-D microcavity. The figure illustrates more clearly that the relationship between the MHCG 0-DO power reflectance and the Q -factor of the M-D microcavity is significantly different from that for the D-D microcavity. For example, MHCGs of $R_0 = 0.99$ result in microcavities of Q -factor ranging from 3000 to 5000. We attribute the variation in the Q -factor mainly to reduced reflection in the case of a finite MHCG structure, which can be different for various MHCG configurations. An increase in the infinite MHCG R_0 above 0.999 results in no further increase in the Q -factor for a finite microcavity. This asymptotic behavior is related to a certain level of lateral leakage and reflection into higher diffraction orders,

Figure 4: (A) Q -factor and (B) resonant wavelength of M-D microcavity and (C) power reflectance of MHCG mirror.

(A) Q -factor values, (B) resonant wavelength (λ), and (C) power reflectance (R_0) for 0-DO in the domain of the MHCG period (L) and duty cycle (F) for the M-D microcavity cavity when $h_M = 164$ nm.

Figure 5: Q -factor of a D-D microcavity as function of the 0-DO power reflectance (R_0) of the DBR (black line) and the M-D microcavity as function of the 0-DO power reflectance (R_0) of a free-standing infinite MHCG (points). The color points represent the resonant wavelengths of the M-D microcavities.

contributing to the reduced reflection that, together with emission, make up the total cavity losses.

3.2 M-M microcavity

Figure 6A shows the Q -factor of an M-M microcavity with different numbers of MHCG stripes versus the microcavity thickness. As in the previous case, the wavelengths of the fundamental modes are proportional to the thicknesses of the microcavities. Two horizontal x -axis scales are therefore displayed in Figure 6A. A resonant wavelength

of 980 nm occurs for $d_c = 0.273 \mu\text{m}$, which corresponds to an optical thickness of 0.982λ . Also, in this case, the deviation of the optical microcavity thickness from exactly 1λ corresponds to the phase shift sum produced by both the MHCG mirrors.

Increasing the number of MHCG stripes contributes to an increase of the Q -factor, as shown in Figure 6A. In the case of an MHCG consisting of a large number of stripes (>60), the resonant wavelength that gives the maximum Q -factor is close to 979.5 nm. In the case of a smaller number of stripes (<60), resonances appear around $\lambda = 980$ nm; however, their precise wavelengths vary irregularly in the range 979–982 nm with changes in the number of stripes.

The maximum values of the Q -factors as a function of the number of MHCG stripes are shown with a black line in Figure 6B, together with six consecutive lateral modes. The zeroth- and first-order modes' Q -factors become very similar for higher numbers of the MHCG periods, which is related to the very similar distributions of the optical field in these modes in M-M microcavities. The Q -factors of the modes generally increase with increasing number of MHCG periods. This behavior, however, is not strictly monotonic because of the nonmonotonic variation in the lateral light leakage determined by the width of the MHCG. Higher order modes follow the Q -factor trend of the fundamental mode; however, their Q -factors are noticeably smaller. A detailed analysis of the mode distributions and the lateral leakage in the case of modes 0 and 1 is presented in S4. For comparison, the blue line in Figure 6B illustrates the Q -factor of the D-D microcavity

Figure 6: (A) Q -factor of the M-M microcavity when both of the MHCG mirrors have the same, variable number of stripes from 20 to 100 as a function of the microcavity thickness (d_c) and the resonant wavelength (λ) of the fundamental mode. The blue dots represent the maxima of the Q -factor for a given number of MHCG stripes. (B) Q -factor of the seven lowest order modes of the M-M microcavity as a function of the number of MHCG stripes (colored lines, bottom axis) and Q -factor of a D-D cavity as a function of the number of top and bottom DBR periods (blue line, top axis). The parameters of the MHCGs are our standard LFH_M values.

as a function of the number of DBR periods, where the top and bottom DBR have an equal and varying number of periods. As can be seen in Figure 6B, the M-M microcavity with 20 MHCG periods results in a Q -factor of 2×10 , which is as high as that for the D-D microcavity with two 28 DBR pairs.

Comparing the M-M microcavity results to those of the M-D microcavity (given in Figure 3), we conclude that even in the case of 20 MHCG stripes the fundamental mode distributions of the M-M design, shown in Figure 7, do not reveal emission of any higher diffraction orders but show rather very small lateral emission, although the M-D and M-M designs use the same MHCG parameters. An increase in the number of the MHCG stripes eliminates any noticeable optical emission, but modifications of the mode envelope are observed.

Figure 8A, B shows maps of the Q -factors and resonant wavelengths of the M-M microcavities in the domain of the MHCG period (L) and duty cycle (F). The main difference between the results and the analogous maps presented in Figure 4 concerns the much more extensive area of high Q -factor in the case of the M-M microcavity. This enables achieving cavities with $Q > 3 \times 10^3$ in which the resonant wavelengths are in the range 938–995 nm, and

those cavities differ only in the transverse dimensions of the MHCG stripes (L , F). Such high Q -factors are due to the existence of bound states in the continuum (BICs) [37], which were very recently observed in an M-M microcavity fabricated of a uniform polymer [38].

BICs are spatially localized states in infinite periodic structures and are characterized by preventing light leakage from the cavity due to the orthogonality of the leaky modes in the structure with respect to modes in free space or due to destructive interference of leaky modes in the far field [39]. The resonant angular frequency of these states is localized above the light line in the $k_0 - k_y$ space, where k_0 is the vacuum wavenumber and k_y is the lateral wavevector component. Taghizadeh and Chung [37] showed that BICs occurring in an infinitely periodic structure can turn into quasi-BICs with a very high Q -factor for a finite periodic structure, which also occurs in an M-M microcavity as we show in this section.

Figure 9A is an analogue of Figure 8A and shows a map of the Q -factors of infinitely periodic M-M microcavities. The high Q -factor region in Figure 9A is significantly more extended toward smaller L in its two branches and reaches very high values of Q -factors in the vicinity of $F = 0.32$ (as in Figure 8A) and $F = 0.22$ (unlike in Figure 8A).

Figure 7: Cross-sectional distributions of normalized light intensity of the fundamental mode in M-M microcavities in the yz -plane for MHCGs with the following numbers of stripes: (A) 20, (B) 60, and (C) 100. The positions of the MHCG and microcavity are indicated. The parameters of the MHCG are our standard LFH_M parameters given in the text, and $d_c = 273$ nm.

Figure 8: (A) Q -factor and (B) resonant wavelength of M-M microcavity and (C) power reflectance of MHCG mirror. (A) Q -factor, (B) resonant wavelength (λ), and (C) power reflectance (R_0) for the fundamental 0-DO mode and for the λ values from (B) in the domain of geometrical parameters L and F of the MHCG when $h_M = 163.9$ nm. All are for an M-M microcavity.

Figure 9: Q -factor of M-M microcavity for (A) vertical wavevector and (B) tilted wavevector. (C) Derivative of M-M microcavity wavenumber as the function of lateral component of wavevector.

(A) Q -factor represented by colors of an infinitely periodic M-M microcavity in the domain of the MHCG period (L) and duty cycle (F) when $h_m = 163.9$ nm. (B) Q -factor values represented by colors and (C) derivative of the wavenumber (k_0) with respect to the lateral component of the wavevector (k_y) in the domain of MHCG duty cycle (F) and lateral component of the wavevector. Each $F_{\max}$ represents the M-M microcavity of the largest Q -factor for a given F extracted from (A).

$F_{\max}$ in Figure 9B represents the points of maximum Q -factor for each F from Figure 9A (the points lie in the red-orange narrow region in Figure 9A). The map in Figure 9B shows two BICs for $k_y = 0$ at $F_{\max} = 0.32$ and at $F_{\max} = 0.22$. A modification of $F_{\max}$ (which induces a corresponding modification of L , see Figure 9A) transforms BICs into accidental BICs that occur at $k_y \neq 0$ and enable high Q -factor values at $k_y = 0$, although the power reflectance of the MHCG is too small to sustain such a high Q -factor due to the Fabry-Pérot resonance. In Figure 9C we analyze the dispersion of k_0 as a function of k_y for the infinite M-M microcavities selected in Figure 9B. The dispersion map of k_0 reveals a broad $F_{\max}$ region in which the k_0 dispersion is nearly flat (the yellow region in Figure 9C for $F_{\max} > 0.25$). Flat dispersion enables a reduction of the lateral optical losses of a finite periodic structure since the group velocity (v_g) with respect to the lateral component of wavevector is given by the formula

$$v_g = \frac{\partial \omega}{\partial k_y} = c \frac{\partial k_0}{\partial k_y}$$

The finite structures (see Figure 8A) show high Q -factors for $F > 0.25$, which coincides with small v_g values in Figure 9C and the occurrence of a BIC and an accidental BIC for $F_{\max} > 0.32$ in Figure 9B. Although the BIC and accidental BIC occur for $F_{\max}$ from 0.22 to 0.25, the v_g in this range changes quickly with k_y , causing strong lateral leakage; hence, the finite M-M microcavities do not reach as high Q values as in the range for $F_{\max} > 0.32$ where accidental BIC also occurs. More detailed analysis of BIC occurrence in M-M microcavity is presented in S5.

In Figure 10 we compare the dependence of the Q -factor versus 0-DO power reflectance of both mirrors in

Figure 10: Q -factor of a D-D microcavity versus the power reflectance (R_0) of the top DBR (black line) and Q -factor for an M-M microcavity versus the power reflectance (R_0) of the MHCGs (points) at various resonant wavelengths. The color points represent the resonant wavelengths of the M-M microcavities.

the case of the M-M (color points) and D-D microcavities (black line) in an analogous manner to Figure 5. The M-M microcavity's Q -factors are above the line corresponding to the D-D microcavity, which is opposite to the behavior shown in Figure 5. The result indicates that the M-M microcavity points adjacent to the line of the D-D microcavity are related to the Fabry-Pérot resonance in the M-M microcavity due to the 0-DO reflection. The points above the D-D microcavity line show the enhancement caused by the hybrid resonance of the Fabry-Pérot and quasi-BIC. For example, there are designs of M-M microcavities that allow obtaining a Q -factor of 10^5 for an R_0 as small as 0.7. A D-D microcavity with both mirrors for which $R_0 = 0.7$ enables achieving a Q -factor of 30. In addition, it should be noted

that such a high Q -factor above 10^5 is provided by an M-M microcavity of very small dimensions, which are 600 nm in the vertical direction and 16 μm in the lateral directions.

4 Example: emission characteristics of MHCG VCSELs

To support optical simulations presented in Section 3, we perform a numerical analysis on an electrically pumped VCSEL with an output-coupling top MHCG mirror and a bottom DBR mirror with nearly total power reflectance at the design wavelength (i.e. an M-D VCSEL) and a VCSEL with two MHCG mirrors (i.e. an M-M VCSEL). Prior to this analysis, we first present experimental verification of the lasing operation of an electrically injected M-D VCSEL and use the experimental emission characteristics to validate our model.

In this section we use a self-consistent model combining three-dimensional PWAM and two-dimensional thermal and electrical models based on finite element methods represented in cylindrical coordinates, together with diffusion and gain models that take into account numerous interactions as described with great detail in [40] and also described in S6. We already calibrated the parameters used in our numerical self-consistent model using the measured characteristics of electrically injected D-D VCSELs emitting at 980 nm as reported earlier [27, 29, 41–44]. The designs of microcavities of the M-D and M-M VCSELs are appropriately modified with respect to the simple structure described earlier to enable current injection and radiative recombination of carriers in the active region. Details of the designs of simulated and experimentally realized, electrically

injected M-D VCSEL as well as simulated M-M VCSEL can be found in S7.

The processing of the electrically injected M-D VCSELs emitting at the wavelength of ~ 980 nm involves processing procedures developed and used at the TU Berlin for modern D-D VCSEL research. Additionally, the processing of MHCGs included electron beam lithography (EBL) together with inductively coupled plasma reactive ion etching (ICP-RIE). The procedure of the M-D VCSEL fabrication is described in greater detail elsewhere [29].

Since the bottom DBR, cavity, and active region of D-D VCSEL used previously for model calibration are the same as in the M-D VCSEL, only the top MHCG mirror requires calibration in our model based on experimental characteristics. Adequate discussion is provided in S8. The facet (i.e. the output coupling) mirror of our experimental device, as well as the top mirror we simulated, is composed of an MHCG realized in TM configuration and includes a 5.5-period DBR between the optical cavity and the MHCG to avoid the influence of the MHCG cross-sectional shape on the phase of the reflected light and thus to achieve resonance at the fixed wavelength of 980 nm. The added 5.5-period DBR also facilitates current spreading from the top p-metal anode down through the oxide aperture into the quantum well (QW) active region. The oxide aperture serves as a current funnel to direct the injected current into a finite area just above the QWs, which is a common design feature for oxide aperture VCSELs.

The thicker black curve in Figure 11A illustrates a typical diode current-voltage (I - V) curve of a fabricated M-D VCSEL with an oxide optical aperture diameter of 8 μm . Light-current (L - I) curves show the current threshold and LI rollover at the currents of 1.8 and 14 mA, respectively. The maximum emitted power and differential

Figure 11: Emission characteristics of (A) measured and simulated M-D VCSELs in TM configuration, (B) simulated M-D VCSELs and (C) simulated M-M VCSELs.

Simulated emitted optical power versus injected current characteristics of (A) M-D VCSEL with an added 5.5-period DBR (blue curve) and M-D VCSEL in TM configuration (red curve), (B) M-D VCSELs, and (C) M-M VCSELs. The plot in (A) includes measured experimental L - I (black solid curve) and the corresponding I - V (black dashed curve) characteristics of a 980-nm M-D VCSEL (with 5.5 top DBR periods). The numbers in (B) and (C) refer to the designs specified in Table 1.

wall-plug efficiency taken at room temperature under continuous-wave operation reach 1.2 mW and 75%, respectively, revealing a 10-fold increase with respect to our first demonstration of an M-D VCSEL [29]. The enhancement of emission efficiency is attributed to improved periodicity and elimination of the etched wall roughness of the MHCG stripes (see Figure 12). Our numerical results correspond very well to the experimental curve near the threshold and for the LI rollover current. The emitted optical power calculated by the model (blue curve) is somewhat higher than the experimental characteristics. This we attribute to the lower electrical resistivity of the p-type contacts with respect to the simulated device [41, 42]. The red curve in Figure 11A illustrates the L - I characteristics of the same structure but without the added DBR, which emits 50% less peak optical output power with respect to the M-D VCSEL with the added 5.5-period top DBR. This reduced optical output power is mainly caused by strong heat crowding near the MHCG, which is a thin layer separating the QW active region from air, causing accumulation of heat, as shown in Figure 13A. The added 5.5-period DBR acts as a heat spreader (and a current spreader as previously mentioned), facilitating the lateral transport of the heat energy. As we have shown earlier [31], the thermal rollover of M-D

VCSELs is not caused by the thermal detuning between the cavity resonance wavelength and the MHCG power reflectance spectrum since both generally red-shift accordingly with increasing temperature. The LI rollover is induced by the detuning of the optical microcavity resonance with the gain spectrum as in conventional D-D VCSELs.

In further analysis, we use the same self-consistent model and parameters as used in the comparison with our experimental characteristics. However, we use LFH_M parameters previously described here with variable L to enable achieving different values of power reflectance and M-D VCSELs without residual DBRs. Table 1 collects our chosen values of L and the corresponding Q -factors of the MHCG cavities calculated with a 2D model used in our optical analysis as already presented in Section 3, as well as the Q -factors of the M-D and M-M VCSELs as calculated with our 3D optical model. Our simulations of optical phenomena with a 3D model take into account the lateral losses along the MHCG stripes, which decrease the Q -factor with respect to the 2D model by less than 20% and 10%, for M-D and M-M VCSELs, respectively, when the length of the grating stripes is $20L$. An increase of the length of the stripes reduces lateral losses along the MHCG stripes and causes the Q -factor to converge to the value calculated

Figure 12: SEM images of a 980-nm M-D VCSEL.

(A) Top-down view of the top p-metal ring and the emitting aperture showing also the MHCG stripes. (B) A focused ion beam (FIB) cross-section of two MHCG stripes. (C) Top-down surface view of two MHCG stripes.

Figure 13: Temperature distributions in (A) M-D VCSEL and (B) M-M VCSEL.

Temperature distribution generated in the device near rollover illustrated in the cross-sections of a half the structures.

(A) An M-D VCSEL and (B) an M-M VCSEL. The 0 on the y -axis refers to the optical axis of the VCSELs.

Table 1: Parameters of a reference 980-nm D-D VCSEL and several constructions of 980-nm M-D and M-M VCSELs with MHCGs of different parameters L , F , and h corresponding to our standard LFH_m values given in the text.

Design no	L (μm)	Q_{2D}	Q_{3D}	$g_{th,av}$ (cm^{-1})	I_{th} (mA)	η (W/A)	P_{max} (mW)
M-D VCSEL							
1	0.818	1.3×10^4	9.5×10^3	420	1.2	0.04	0.28
2	0.802	7.2×10^3	5.5×10^3	720	1.4	0.20	1.25
3	0.781	3.4×10^3	2.7×10^3	1450	2.1	0.52	2.07
4	0.768	2.3×10^3	1.8×10^3	2060	2.8	0.54	1.65
M-M VCSEL							
0	0.809	1.6×10^5	1.4×10^5	21	1.34	4×10^{-4}	8.5×10^{-4}
1	0.804	4.8×10^4	4.6×10^4	67	1.44	0.19	0.32
2	0.798	1.7×10^4	1.6×10^4	191	1.66	0.31	0.35
3	0.791	6.7×10^3	6.6×10^3	460	2.09	0.26	0.19
4	0.781	3.0×10^3	2.9×10^3	~ 1020	–	–	–

The terms Q_{2D} and Q_{3D} are quality factors calculated with the 2D and 3D optical models for structures without doping (without internal absorption). The terms $g_{th,av}$, I_{th} , η , and P_{max} are calculated with a self-consistent model including internal absorptions. The term “design no” is the design number that correlates the designs in this table to the results in Figure 11. $g_{th,av}$, the averaged threshold gain; I_{th} , threshold current; η , differential efficiency at threshold; P_{max} , the maximum emitted power.

with our 2D model. Figure 11B, C depicts the dependences of the emitted optical power as a function of the current injected into the M-D and M-M VCSELs.

The M-M VCSELs emit even lower optical power as a result of more severe heat crowding with respect to the M-D VCSELs (Figure 13B). The short cavity suspended in air prevents vertical heat transport, enabling lateral heat transport only. This deteriorated heat dissipation causes an early LI rollover at low forward bias currents and contributes to a $6\times$ smaller emitted optical power with respect to the M-D VCSELs. The no. 0 design of the M-M VCSEL is characterized by an extremely large Q -factor value, which enabled a very low threshold gain and a very weak optical output power emission. Such a design cannot be considered as an efficient laser but can be applicable as a microcavity that enables the observation of the subtle effects of electron-photon interactions. The no. 4 design of the M-M VCSEL does not reach lasing threshold because the threshold gain ($g_{th,av} \sim 1020 \text{ cm}^{-1}$) requires a bias current that induces temperatures exceeding 150 K above room temperature in the active region. Such a high temperature detunes the gain spectrum and the optical resonance. Hence, to achieve lasing threshold, cavities of higher Q -factor are required in the M-M VCSELs in comparison to the M-D VCSELs to compensate for the higher temperature that induces thermal detuning of the gain peak and the microcavity resonance.

5 Conclusions

In this paper, we have presented the results of an extensive numerical analysis of monolithic, MHCG microcavities.

Two microcavity configurations composed of GaAs and designed for a 980-nm resonant wavelength were considered: the first with an MHCG mirror and a DBR mirror (designated M-D), and the second with two MHCG mirrors (referred to as M-M). Both designs showed a range of possible construction parameters, enabling high Q -factor resonances and a range of possible resonant wavelengths. These could be achieved by modifying the lateral MHCG parameters without modification of either the MHCG etching depth or the cavity length. To numerically investigate both types of microcavities we used the fully vectorial plane-wave admittance method.

Our analysis of the M-D cavity properties revealed a monotonic increase in the Q -factor of the microcavity with the increase in the number of MHCG stripes. Modification of the MHCG parameters from their optimal configuration decreased the Q -factor of the microcavity and also modified the reflectivity phase of the MHCG mirror, which induced a change in the resonant wavelength. Modification of the lateral parameters of the MHCG, while still sustaining a high level of the Q -factor, enabled variation of the resonant wavelength in the range of 6 nm.

In the M-M configuration, increasing the number of MHCG stripes increased the cavity Q -factor, although the increase was not monotonic. Varying the number of MHCG stripes modified the fundamental optical field intensity mode envelope, affecting the Q -factor. By equal variations of the lateral parameters of two MHCG mirrors, resonant wavelength tuning in the 60-nm range was theoretically obtained. The M-M design of very small dimensions, i.e. 600 nm in the vertical direction and 16 μm in the lateral direction, enabled achieving very high Q -factors of

nearly 10^6 , which cannot be explained based on normal incidence power reflectance but rather can be explained by the influence of quasi-BICs.

We provided example experimental characteristics of real-world, GaAs-based, electrically injected M-D VCSELs emitting at the wavelength of ~ 980 nm and compared the measured results with the theoretical results from our self-consistent model of VCSEL operation with parameters extracted from the experimental characteristics of a D-D 980-nm VCSEL. The experimental and numerical results agreed sufficiently well, thus proving the validity of our numerical model.

To provide an example of a device that uses both schemes of microcavities, we investigated the influence of the Q -factor on the emission characteristics of M-D and M-M VCSEL designs inspired by the microcavity design of a real-world, GaAs-based VCSEL. The emitted optical powers of M-D and M-M VCSELs were theoretically determined for cavities whose Q -factors ranged from 2×10^3 to 1×10^4 for M-D VCSELs and from 6×10^3 to 1×10^5 for M-M VCSELs. The M-D and M-M VCSELs showed emitted optical power at the level of 40% and 7%, respectively, of the emitted optical power of D-D VCSELs with equivalent oxide aperture diameters. The lower emitted optical powers were due to the strong effect of heat crowding in the proximity of the active region, which contributed to LI rollover at low bias currents. Improvement of the thermal management of the M-M VCSEL is challenging since heat is transported laterally from the active region. Hence, pulsed current operation can be more optimal for these kinds of microcavity structures. The Q -factor values of 2×10^3 and 6×10^3 can be considered as the minimum levels of continuous-wave operation for the M-D and M-M VCSELs, respectively. The lower Q -factor for M-D VCSELs results from the better intrinsic heat dissipation management available in these devices, which allows achieving higher threshold gains. It is worth mentioning that the thermal management of both M-D and M-M VCSEL designs can be improved by increasing the cavity length.

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