Review article

Adam C. Overvig, Sajan Shrestha and Nanfang Yu*

Dimerized high contrast gratings

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Abstract: Metasurfaces and planar photonic crystals are two classes of subwavelength diffractive optical devices offering novel functionalities. The former employ independently operating subwavelength “meta-units” as their building blocks, while the latter exploit the collective response of many periodic building blocks. High contrast gratings (HCGs) are an example of one-dimensional (1D) planar photonic crystals with large refractive index contrast, exhibiting large in-plane scattering even with a limited number of grating periods. They are best known for their broadband features. Low contrast gratings (LCGs) are known for their control over sharp spectral features but require many periods due to small in-plane scattering. We explore a class of symmetry-broken HCGs called dimerized high contrast gratings (DHCGs), which have a period-doubling perturbation applied. DHCGs support modes accessible by free-space illumination with a long, controllable photon lifetime (inversely proportional to the magnitude of the perturbation) and reduced lateral energy divergence (confined by the high index contrast of the grating). We catalogue and clarify the resonant modes introduced by the dimerizing perturbation in 1D DHCGs and briefly explore the increased in-plane scattering present in two-dimensional (2D) DHCGs. We introduce an approach maximizing lateral localization by band structure engineering in the unperturbed HCG and using the dimerizing perturbation to generate sharp spectral features in devices with small footprint. We confirm the simultaneous control of photon lifetime and lateral localization with full-wave simulations of finite-sized DHCGs. We conclude by numerically demonstrating two compact devices (an optical modulator and a refractive index sensor) benefitting from the unique design freedoms of DHCGs.

1 Introduction

Enhancement of light-matter interactions is desirable for many nanophotonic devices. This is typically achieved with optical cavities, which trap photons for many optical cycles before the photons escape. This allows, for instance, a photon to interact with an active optical material for a longer time, which is advantageous for many applications. Increasing light-matter interactions allows optical modulators to be smaller and faster [1–6], nonlinear effects to be observed with a smaller volume of material [7, 8], lasers to emit with a weaker pump [9–12], optomechanical devices to be actuated with a smaller input optical power [13, 14], and enhanced quantum optical effects [15]. Enhanced optical lifetime also has the consequence of increasing the group delay of light passing through the optical cavity, corresponding to increasingly dispersive responses.

Recently, a class of flat optical devices called metasurfaces (and, in particular, metasurface lenses [16]) has been of interest in controlling both the phase and phase dispersion of the output wavefront [17–20]. This can be achieved by using sharp spectral features with varying photon lifetime [18–20]. However, the traditional metasurface approach assumes that the individual building blocks, or “meta-units”, operate independently [21]. This is starkly in contrast to the physical mechanism responsible for the high Q-factor resonances employed in these recent efforts, i.e. periodic effects, which are traditionally the purview of another class of flat optical devices called planar photonic crystals [22]. Yet the success of these metasurfaces suggests that there is room to explore a relaxation of the metasurface assumption and motivates study of long lifetime states in finite-size planar optical cavities. In other words, it suggests that design of dispersion-engineered metasurfaces may benefit from approaching the problem using diffractive optical elements on the boundary between traditional metasurfaces and planar photonic crystals.

The building blocks of such metasurfaces may be thought of as subwavelength photonic crystal slabs, which are known to act as planar optical cavities, trapping

*Corresponding author: Nanfang Yu, Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY 10027, USA, e-mail: ny2214@columbia.edu. <http://orcid.org/0000-0002-9462-4724>

Adam C. Overvig and Sajan Shrestha: Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY 10027, USA

light incident from out of plane before either reflecting, transmitting, or absorbing. As planar photonic crystals, they are commonly used for free-space optical devices requiring sharp spectral features [23–26]. First observed in metallic gratings and called “Wood’s anomalies” [27, 28], these resonances have a characteristic asymmetric line-shape, a feature of the well-known Fano resonance [29–31]. These resonances involve the interference of direct reflection from the metallic structure, or “bright” mode, with surface plasmon polaritons confined to the metallic grating, or “dark” mode.

Later work in dielectric gratings (of interest for the absence of optical losses) called these cavity modes “guided mode resonances” (GMR), referring to the coupling in and out of laterally travelling slab waveguide modes [23–26]. These are of considerable interest because the lifetime of the mode is easily controlled by the strength of the corrugation of the gratings: sharper spectral features are obtained for weaker corrugations. An inherent tradeoff in weakly corrugated gratings, however, is the total area required to observe the phenomenon: the larger the photon lifetime, the farther the waveguide modes travel laterally before being scattered out, and hence, the larger the planar footprint required for interference with the bright mode, in this case, the Fabry-Perot resonant mode in the slab.

This problem is solved by a class of subwavelength gratings with deep corrugation, called “high contrast gratings” (HCGs) [12, 32–34], in which the refractive index contrast between grating fingers and neighboring media is large and the lateral distance travelled by the guided modes is small due to in-plane Bragg reflection. Mostly utilized for their broad spectral features [32], HCGs are also known to support sharp spectral features [34, 35], a particular manifestation of the phenomenon referred to as a “bound state in the continuum” (BIC) [36–39]. These can be differentiated into two categories: BICs where coupling to free space at normal incidence is forbidden due to symmetry and BICs that can occur at any angle of incidence born of a mechanism unrelated to symmetry. The lifetimes of the latter type of BIC are a complex function of the angle of incidence and the height, index, duty cycle, and surrounding media of the gratings. From a design point of view then, the improvement of the performance (e.g. resonance visibility and Q-factor) for a finite-size grating comes at a cost of decreased ease of control of the sharp spectral features. We will show that this disadvantage can be avoided by purposefully accessing the symmetry-forbidden category of BICs.

We explore a class of subwavelength gratings (or planar photonic crystal slabs) we call “dimerized high

contrast gratings” (DHCGs), which employ symmetry breaking by a periodic perturbation to control the line-shape of sharp spectral features while inheriting the advantages of compact device footprint from their unperturbed counterparts (HCGs). We review the physics of symmetry breaking in one-dimensional (1D) and two-dimensional (2D) photonic crystals and explore the finite-size effects (i.e. the consequences of having a finite number of periods) in the DHCGs. We introduce a design approach that allows for maximizing the lateral confinement in the unperturbed structure and control of the sharp spectral feature with the perturbation. We perform full-wave simulations of finite-size devices illuminated by Gaussian beams to confirm the design approach. We conclude by numerically demonstrating a couple of device applications that benefit from this approach.

2 Symmetry breaking in planar photonic crystals

Symmetry breaking in planar photonic crystals results in a well-known phenomenon of introducing sharp Fano resonances excitable by free-space illumination [31, 40–46]. There are two requirements for such a feature to be observed at normal incidence: (1) a mode must exist in the band diagram at the center (“Gamma point”) of the First Brillouin Zone (FBZ) and (2) the mode must not be excluded by symmetry considerations. For instance, a normal incident planewave (which has even in-plane symmetry) cannot excite a mode with odd symmetry; this odd-even symmetry must be broken to satisfy requirement (2). A trivial version of symmetry breaking is excitation by a planewave incident at an angle slightly off the surface normal of the planar device, breaking the even symmetry of the incident light. Alternatively, the odd symmetry of the mode can be broken, allowing excitation at normal incidence, by breaking the mirror symmetry of the unit cell of the photonic crystal (e.g. skewed rather than rectangular grating fingers) [46–48]. In such approaches, a small perturbation can yield a sharp spectral feature with a linewidth controlled by the magnitude of the perturbation (i.e. the degree of symmetry breaking), a useful design tool analogous to changing the corrugation depth in low contrast gratings (LCGs).

We focus on periodic symmetry breaking [42–44, 46, 49, 50], wherein every other period is slightly perturbed. In a simple 1D grating, this can take two forms, which we call “gap perturbation” (every other grating finger is

displaced laterally) and “width perturbation” (every other grating finger is changed in size). The resulting structure (a DHCG) has two nearly identical grating fingers (a dimer) in each period: a dimerizing perturbation to an HCG. Figure 1 summarizes the differences in real space

and quasi-momentum space (“ k -space”) between LCGs, HCGs, and both versions of DHCGs and shows the resulting spectra due to transverse electric (TE) and transverse magnetic (TM) excitation of these subwavelength gratings at normal incidence.

Figure 1: Comparison of four subwavelength gratings.

Rows 1–4 depict the physics of, respectively, LCGs, unperturbed HCGs, width-perturbed dimerized HCGs (w-DHCGs), and gap-perturbed dimerized HCGs (g-DHCGs). Columns 1–4 depict, respectively, the typical geometry, band diagrams for $h=\infty$ calculated by a 1D plane-wave expansion method (where the white diamond represents the 0th-order domain), and spectral reflectance maps (calculated by rigorous coupled-wave analysis) with TE and TM incidence for different aspect ratios, h/a . LCGs can be seen to have very pointed bands near $k_x = k_0 \sin(\theta) = 0$ while having sharp spectral lines throughout the reflectance maps. HCGs have flat bands but primarily exhibit broad spectral features. DHCGs have flat bands but consistent sharp spectral features. Brillouin zone folding occurs upon doubling the period of a HCG, folding modes at the edge of the first Brillouin Zone (FBZ) (marked by closed and open circles for bonding and anti-bonding modes, respectively) onto the center of the FBZ in DHCGs. The band shapes are retained, but the modes are now accessible to free-space excitation with a coupling strength controlled by the magnitude of the perturbation. TE light excites the modes marked as red, and TM light excites modes marked as light blue.

A major departure from the abovementioned methods of symmetry breaking (e.g. oblique excitation, skewed grating fingers) is the impact on the band diagram (seen in Figure 1); because the period has been doubled in the DHCGs, the FBZ has been halved in size compared to the corresponding HCG. Modes previously at the edge of the FBZ now lie at the Gamma point, a phenomenon known as “Brillouin zone folding”. This causes the previously inaccessible modes (“bound” modes) to be above the light line and therefore excitable by free-space illumination. Figure 1 depicts the movement of two such modes by marking them in the HCG and DHCGs with open and closed circles. Importantly, in the gratings of Figure 1, these lowest two modes are also below the diffraction line, meaning that only one output diffractive order is allowed upon coupling

back into free space (useful for an optical device). We focus on these so-called 0th-order gratings, which operate in the white diamonds in the band diagrams in Figure 1.

Odd-even symmetry must be considered to properly understand DHCGs. This is starkly apparent upon comparison of the behaviors of TE and TM excitation of gap-perturbed and width-perturbed DHCGs (see the spectral maps in Figure 1, calculated by rigorous coupled wave analysis). TE light (polarized as E_z in Figure 2) couples into a mode at the top of the second band in the width-perturbed DHCG (w-DHCG) (red filled circles in Figure 1), but it couples into the bottom of the third band in the gap-perturbed DHCG (g-DHCG) (red open circles in Figure 1). The opposite is true for TM light (polarized as H_z), corresponding to the modes colored light blue in Figure 1.

Figure 2: Mode properties.

(A) Example mode profiles for w-DHCGs (left) and g-DHCGs (right). TE light (E_z component shown) excites bonding modes and TM light (E_y component shown) excites anti-bonding modes for w-DHCGs. Instead, TM light excites bonding modes and TE light excites anti-bonding modes for g-DHCGs. (B) Mode dispersion of TE excitation calculated by the scattering matrix method. Several distinct sets of modes are apparent and can be catalogued as bonding (B_{mn}) and anti-bonding (A_{mn}), where (m, n) are the number of lobes in the (x, y) directions in each grating finger. A similar plot can be constructed for TM. (C) The Q-factor, Q , extracted from FDTD simulations for a w-DHCG, where the perturbation δ is the difference in widths of each finger. The expected relation $Q = C/\delta^2$ holds with $C \cong 12 \text{ nm}^2$ at small perturbation but breaks down when the perturbation becomes large.

This can easily be understood by mirror symmetry of the mode profiles, depicted in Figure 2A, and can be shown to be a consequence of symmetry constraints on the first-order correction to the mode profile (see Supporting Information Section S.1). Considering TE polarization, we choose the high symmetry point of each DHCG (i.e. the center of a grating finger for a w-DHCG and the center of a gap for a g-DHCG) to be $x=0$, as shown in Figure 2A. By symmetry, E_z must have a node or an anti-node at $x=0$. For normal incidence, E_z of a leaky mode must have even symmetry in order to couple to free space, so E_z of the mode must have an anti-node at $x=0$. The resulting large overlap with grating fingers of the w-DHCG is analogous to a low-energy “bonding” states in atomic systems. In contrast, for the g-DHCG, E_z lies in the air gaps between adjacent fingers; the exclusion of the electric field from the center of a high index material is analogous to high-energy “anti-bonding” states in atomic systems. The same considerations apply to H_z in the case of TM light. However, as the electric field overlap with the material determines the energy level of the mode and as the magnetic field and electric field have opposite symmetries, for TM light, the bonding mode occurs in g-DHCGs and the anti-bonding mode in w-DHCGs.

It is evident from the spectral maps in Figure 1 that rather than single bonding or anti-bonding modes being excited, sets of similar modes are excited. These additional modes are due to the finite height of the grating allowing modes with several anti-nodes in the y -direction and are omitted (for clarity) in the band diagrams in Figure 1 by calculating an infinitely tall grating with a plane-wave expansion method. Also possible are modes with more anti-nodes in the x -direction (the grating direction), which correspond to, e.g. the 4th, 5th, and higher bands in the band diagrams. It is apparent from the spectral maps in Figure 1 that DHCGs contain all the broad and sharp spectral features of the unperturbed HCGs (especially in the region near $\lambda/a \sim 1-2$) but with many additional features due to Brillouin zone folding (especially in the region with $\lambda/a > 2$). In other words, a subset of the higher frequency modes of a DHCG is inherited from the unperturbed grating. The possible modes for a grating with a finite height can be calculated with the scattering matrix method or finite difference eigenvalue analysis (see Supporting Information Section S.2) and catalogued by their characteristics. Examples for TE excitation of gratings with varying heights and a fixed duty-cycle are given in Figure 2B. Bonding modes are denoted B_{mn} , where (m, n) correspond to the order in the x - and y -directions, respectively. Similarly, anti-bonding modes are denoted A_{mn} . Example mode profiles calculated with

the finite-difference time-domain (FDTD) method are shown for reference in Figure 2A. We note that the choice to label the modes by “bonding” and “anti-bonding” is a choice to emphasize eigenfrequency of the modes; an alternative classification scheme emphasizing symmetry by employing group theory [51] is supplied in the Supporting Information Section S.3.

Another feature of the spectral maps in Figure 1 is the varying linewidths for the two different methods of perturbation and two incident polarizations. Despite having the same magnitude of perturbation $\delta = 0.15a$ compared to the period, a , of the unperturbed HCG (where δ is the difference of gap widths in g-DHCGs and the difference of finger widths in w-DHCGs), some DHCGs primarily exhibit very sharp spectral features (e.g. TE excitation for w-DHCGs) and others primarily exhibit broad spectral features (e.g. TM excitation for g-DHCGs). In all cases, however, the relationship between the linewidth, $d\omega$, of a sharp spectral feature (parameterized by the quality factor, $Q = \omega/d\omega$) and the magnitude of the perturbation can be shown by a combination of perturbation theory and temporal coupled mode theory [52] (see Supporting Information Section S.4) to be as follows:

$$Q = \frac{C}{\delta^2}, \quad (1)$$

for small δ . The value of the constant C depends on the interactions between DHCG modes, the Fabry-Perot mode, and free-space waves mediated by evanescent waves at the output ports of the grating [34] and therefore differs substantially across different classes of gratings and excitation polarizations. If δ is too large, these complex interactions will change, and Equation (1) is invalidated by the dependence of C on δ . FDTD simulations (Figure 2C) confirm the $1/\delta^2$ behavior at low δ and show deviation from this curve when δ becomes large. Choosing δ to be smaller for the g-DHCGs with TM excitation can yield equally sharp resonances as the w-DHCGs with TE excitation; the value of C for the former case is simply much smaller. Note that when the perturbation vanishes, the Q -factor diverges according to Equation (1), corresponding to zero coupling strength to free space of the unperturbed grating, as expected of bound modes.

Similar spectra can be achieved by periodic symmetry breaking in 2D photonic crystals. Due to the greater number of degrees of freedom, there are many more symmetries to be considered compared to the simple 1D case. Figure 3 depicts a few examples of dimerizing perturbations in 2D photonic crystals. It is beyond the scope of this paper to catalogue periodic symmetry breaking in 2D photonic crystals

Figure 3: 2D DHCGs.

Three examples of 2D gratings are shown in real space (column 1, black dashed box representing the unit cell of the structure) and k -space (column 2, showing the first Brillouin zone (FBZ) and arrows tracing the path through k -space for band diagram calculations), and their band diagrams are calculated for an infinitely tall grating with the electric field pointed out of plane (column 3, light gray areas representing bound modes, dark gray areas representing modes with high diffractive orders, and closed/open markers denoting bonding/anti-bonding modes). The top row shows an unperturbed grating, with a few modes of interest marked for comparison with the two DHCGs in the second and third rows. The second row shows a dimerizing perturbation doubling the period in the x -direction; the FBZ has halved in the k_x direction. The blue portion of the unperturbed FBZ is translated into the new, perturbed FBZ by reciprocal lattice vector of the perturbed grating (indicated by the large dark arrow). Modes at the original M_x point (marked by red circles) have now moved to the new Γ point, making them accessible to free-space excitation. The modes at the original X point (marked by red squares) moved to the new M'_y point, still under the light line. The third row shows a dimerizing perturbation changing the period by $\sqrt{2}$ and rotating the unit cell by 45° . The original M_x point has now moved to the X'' point, and the original X point has moved to the Γ point. As the band near the original X point is very flat, the resulting modes at the new Γ point have very flat bands (particularly that marked with an open red square). Overlaid in the final panel is the spread of power in k -space of a Gaussian beam with frequency of the closed red square, with two different values of numerical aperture, $NA = \lambda/\pi w_0$, where w_0 is the e^{-2} waist radius of the Gaussian beam.

(which we note is not limited to just a dimerizing perturbation or to square lattices and allows many more types of perturbations than just width or gap perturbations). Interestingly, 2D photonic crystals can exhibit polarization-dependent (second row in Figure 3) or independent (third

row in Figure 3) resonances, unlike their 1D counterparts. Furthermore, in 2D photonic crystals, there is considerably more freedom to engineer the band structures before applying the perturbation; note in particular the very flat bands near the Gamma point in the third row of Figure 3.

As we will show, the band structure strongly impacts the performance of finite-size devices, suggesting 2D DHCGs as an excellent platform for compact, long photon lifetime planar optical devices.

3 Finite-size effects

To begin exploring the finite-size effects of planar photonic crystals, we review the physics of finite-size LCGs. In such devices, the resonance arises from the interference between the vertical, broadband Fabry-Perot resonances (the “bright” mode) with the laterally travelling waveguide mode (the “dark” mode). After many optical cycles, the waveguide mode may be scattered out, interfering with the Fabry-Perot mode at all output ports. This physical process is well-modeled by a coupled mode theory, and the bandwidth, $d\omega$, of the resulting line-shape is related to the photon lifetime of the guided mode, τ , in the canonical way: $d\omega\tau \sim 1$. This lifetime, τ , is naturally related to the scattering strength out of the LCG: the larger the scattering strength, the sooner the guided mode couples out, and thus, the shorter the lifetime. As a weaker corrugation corresponds to a decreased scattering strength of the guided mode, τ varies inversely to the degree of corrugation.

For a finite device to exhibit a sharp spectral feature, both the incident beam and the device must be larger than the lateral distance, D , that the guided mode travels before coupling out. Otherwise, the spatial overlap between the out-coupled wave and the Fabry-Perot mode will decrease, resulting in reduced interference. A simple model estimates the characteristic size needed to observe a spectral feature with lifetime τ . The group velocity of the travelling mode will be approximately equal to its phase velocity because the corrugation is weak (Bragg scattering is negligible). The characteristic lateral distance D that the mode

has travelled after a time τ is therefore $D = \frac{c}{n_{\text{group}}} \tau \equiv \frac{c}{n_{\text{phase}}} \tau$.

This can be written in a more suggestive form as follows:

$$D = Q\lambda_{\text{eff}}, \quad (2)$$

where $\lambda_{\text{eff}} = \frac{\lambda}{n_{\text{phase}}}$ is the effective wavelength of the guided mode. In other words, the device footprint scales (in linear dimension) proportionally to the quality factor of the spectral feature. For instance, for $Q=1000$ and $\lambda=1\text{ }\mu\text{m}$, the approximate size needed is of the order of millimeters; for $Q=10^6$, it is in meters.

In deeply corrugated gratings (HCGs and DHCGs), on the other hand, the group velocity can be much smaller

than the phase velocity due to strong in-plane Bragg scattering. Therefore, the distance required, $D = \frac{c}{n_{\text{group}}} \tau$, can

be much smaller than that in the weakly corrugated case. This is related to the set of phenomena known as “slow light” effects [53, 54] and corresponds to flat bands in the band diagram (i.e. where $\frac{d\omega}{dk}$ is small). In simple 1D HCGs, the flat bands typically used for slow light effects occur at the edge of the FBZ, which are under the light-line and inaccessible to free-space excitation (“bound” modes). In DHCGs, however, these modes are made accessible via the perturbation with little change to the shape of the band, meaning that the group velocity is retained. This suggests that the number of grating periods required to observe the sharp spectral features in Figure 1 will be much smaller than that required to observe equivalent features based on LCGs.

To better understand the impact of the band diagram on the number of grating periods required to observe a sharp spectral feature, we consider the incident light in k -space. A planewave has infinite extent in real-space ($\Delta x = \infty$) and correspondingly an infinitesimal extent in k -space $\Delta k = 1/\infty$. This means that an incident planewave will excite a single mode along a given band and, therefore, a single resonance frequency. A Gaussian beam, on the other hand, has a finite spread of both Δx and Δk and will excite a range of modes along the band, corresponding to a range of resonance frequencies $\Delta\omega$ (see the last panel in Figure 3 for reference). The resulting spectrum will consequently be a weighted combination of all the k components’ respective resonances, $\omega(k)$ (see Supporting Information Section S.5). Only if $\Delta\omega$ is smaller than the linewidth $d\omega$ of each resonance will the resonances at each (ω, k) spectrally overlap and $d\omega$ be observed. The more compact the Gaussian beam is, the larger Δk will be, and so the larger $\Delta\omega$ becomes. The band diagrams in Figure 1 show that LCGs have very sharp bands at the center of the FBZ, meaning that the allowed Δk is very small; the HCGs and DHCGs have very flat bands in comparison, suggesting that a much larger Δk is permissible.

The minimization of the finite-size effects in a 1D DHCG can thus be mapped to a problem of maximizing the flatness of the band in the unperturbed grating. As the first derivative $d\omega/dk$ is zero at the Gamma point upon periodic perturbation, the second derivative is needed to characterize the shape of the band. The spread of resonance frequencies can be approximated by a Taylor expansion as $\Delta\omega \equiv \frac{d^2\omega}{dk^2} (\Delta k)^2$, which suggests that minimizing $\frac{d^2\omega}{dk^2}$ will obtain a grating with minimal required footprint. Figure 4A depicts the impact of duty cycle, w/a , and aspect ratio,

h/a , of a silicon grating (surrounded by air, for simplicity) on the value of $\frac{d^2\omega}{dk^2}$ (calculated by plane-wave expansion and extracted by fitting to a polynomial) at the edge of the FBZ in the unperturbed HCG. Different combinations of duty cycle and aspect ratio will have different amounts of silicon and therefore exhibit different resonance frequencies. Contours of constant resonance frequency are overlaid in Figure 4A for reference. The white circle shows the minimal value possible for TE light and, therefore, the optimal device parameters to use.

A set of FDTD simulations is performed with varying device sizes from $30\text{ }\mu\text{m}$ to $250\text{ }\mu\text{m}$ (a is set to $1\text{ }\mu\text{m}$ for concreteness) and proportionally varying Gaussian beam radii (fixed to be $1/4$ th the device size in order to fully fit the

beam within the simulation boundaries), and the results are reported in Figure 4B. Figure 4C compares an example device with a size of $100\text{ }\mu\text{m}$ to an infinite device, confirming a great reduction in size compared to that predicted by Equation (2) for LCGs, which is roughly $D \cong 5000 \times 2\text{ }\mu\text{m} = 10\text{ mm}$. This corresponds to a reduction of linear dimension of 100. The slightly reduced Q-factor and resonance visibility seen in Figure 4C for the finite-size device can be explained by the incomplete flatness of the band near the Gamma point; there is a small spread of resonance frequencies excited, slightly smearing the resulting spectral peak. This effect increases as the number of periods decreases, resulting in changing Q , peak reflectance (resonance visibility), and amount of power leaked out of the sides of the finite-size device (Figure 4D). Evidently, the value of Q converges at

Figure 4: Finite-size effects in DHCGs.

(A) Magnitude of the curvature of the band associated with the $B_{1,1}$ mode of a w-DHCG for a range of aspect ratios, h/a , and duty cycles, w/a . The white circle highlights the optimal choice (minimal band curvature), and colored contours represent curves of constant resonance frequencies. (B) Finite-difference time-domain (FDTD) simulations of the grating chosen (A) for various finite lengths, D , of the device. (C) Comparison of a selected device with $D = 100\text{ }\mu\text{m}$ (blue curve) to an infinitely periodic grating (black curve). Power leaked out the sides of the finite-size device (red curve) is shown for comparison. The inset shows the field profiles of the finite-size device at the two peaks seen in the blue curve. (D) Peak values of the reflection peak and side leakage, and Q-factor as a function of D .

a device size of $D=150\text{ }\mu\text{m}$, where the side leakage reaches a negligible value. However, until roughly $D=250\text{ }\mu\text{m}$, a secondary peak is apparent in the spectra in Figure 4B. The inset of Figure 4C shows that this secondary peak has an envelope showing both a Gaussian and sinusoidal feature; it is a supermode of the finite grating [16] and correspondingly shifts in frequency as a function of D . FDTD simulations (omitted here) placing a dipole at the center of a finite-size grating show that higher order sinusoidal envelopes are possible, with decreasing strength at higher orders. The supermodes can be understood to be due to large $\pm k_x$ components of the incident beam forming a standing wave at a frequency lower than the primary peak, consistent with the concavity of the band for bonding modes. Simulations of anti-bonding modes (corresponding band concave up) in finite-size DHCGs show secondary peaks at higher frequencies compared with the primary peak. The primary peak can be thought of as the first order of these supermodes and is the only one of significance as the device becomes sufficiently large.

In an experimental device, the dimension along the grating finger direction must also be taken into account. As 1D gratings have no corrugation in this direction (the z -direction in Figure 1), they have no controllable lateral localization in that direction. Computational constraints make studying these effects in full-wave simulations difficult, but the physics confirmed by simulations of 1D gratings suggests that using 2D gratings (wherein both $\frac{d^2\omega}{dk_x^2}$ and $\frac{d^2\omega}{dk_y^2}$ in Figure 3 can be minimized) can properly confine the resonant mode. For instance, the second row of Figure 3 shows a 2D grating with a band corresponding to bonding modes of similar concavity in the k_x direction to the 1D grating studied in Figure 4 but with much flatter bands in the k_y direction. This implies that the required number of periods in the y -direction will be less than that demonstrated in Figure 4 for the x -direction. The third row of Figure 3 shows a 2D grating with a very flat band in both the k_a and k_b directions, implying an even further reduction of device size. Future work could explore optimizing the flatness of the band of such a 2D DHCG (for instance, by computational methods [55, 56]) for extremely compact planar photonic devices, including meta-units for constructing metasurfaces.

4 Applications of DHCGs

To demonstrate the utility of DHCGs, we present a brief numerical study of two applications of engineering sharp

spectral features with compact DHCGs. First, we explore multiphysics simulations of a CMOS-compatible optical modulator operating in the near-infrared. By incorporating a vertical p - i - n junction in a Silicon grating, the free-carrier dispersion effect can be employed to change the refractive index. The magnitude of the change in refractive indices is very small at near-infrared wavelengths and therefore requires increasing light-matter interactions to achieve appreciable modulation. Speed considerations, on the other hand, demand the device have a small footprint, which makes LCGs incompatible. As DHCGs are a platform in which sharp resonances can be controlled in a compact total size, they offer an excellent solution to a planar optical modulator with fast switching speeds using CMOS-compatible fabrication processes. We note that a similar approach with experimental verification has been achieved but by utilizing an adiabatic photonic crystal cavity to reduce the device's lateral size [49].

Figure 5A depicts a schematic of a DHCG modulator based on commercially available silicon-on-insulator (SOI) substrates. As depicted in Figure 5B, the device layer is 250 nm and the buried oxide layer is 3 μm . Leaving an n + doped, 50-nm-thick layer of silicon at the bottom of the etched trenches and doping the top of the fingers p + allows for injection of carriers vertically into the intrinsic region. The carrier distributions are calculated by solving the drift-diffusion equations on a finite-element grid with applied voltages of 0 and 1 V (Figure 5C). The TE $B_{1,1}$ bonding mode of a w-DHCGs is chosen because of its excellent overlap with this intrinsic region. Figure 5D shows that a modulator of the size 50 μm provides appreciable intensity modulation around the telecommunications band. The results demonstrate the utility of DHCGs for easy design of a compact planar optical modulator with controllable bandwidth.

Second, we utilize the excellent overlap with the air in the anti-bonding mode of TE-excited g-DHCGs (Figure 5E) to numerically demonstrate sensing of refractive indices of surrounding media. Figure 5F shows the spectra resulting from having air (refractive index of 1.0002) and carbon dioxide (refractive index of 1.001) surrounding the grating. This is generalizable to refractive index sensing of anything placed in the air gaps, such as for use in biosensors [57, 58].

5 Concluding remarks

We conclude with a discussion on the utility of the physics of DHCGs for the field of metasurfaces. Metasurfaces

Figure 5: Applications of DHCGs.

(A) Schematic of an optical modulator based on a corrugated w-DHCG incorporating *p*-type doping (purple) at the top of the fingers and *n*-type doping (green) at the bottom of the etched trenches, leaving intrinsically doped (gray) centers of the fingers. Electrodes (gold) allow for forward biasing of the resulting *p-i-n* junction, injecting carriers into the intrinsic region. (B) Geometrical parameters of a period of the modulator portrayed in (A). (C) Solutions to the drift-diffusion equations on a finite element grid, showing hole (*p*) and electron (*n*) concentrations (cm⁻³) on a log scale for applied voltages of 0 V and 1 V. (D) Transmission spectra near the B_{1,1} mode of a device 50 μm in size, with $Q \approx 1,500$ for applied voltages of 0 V and 1 V. The spectra are calculated using FDTD and a free-carrier model for the complex refractive indices based on the distributions of holes and electrons in (C). This simulation fully takes into account material losses as well as finite-size effects in the *x*-direction. The corrugation of the fingers in the *z*-direction is expected to localize the mode along the grating fingers. (E) A_{1,1} mode of a silicon DHCG on oxide showing excellent field overlap with an external gas when TM (*x*-polarized) light is incident from above. (F) Reflectance peaks ($Q \approx 3500$) near the mode in (E) with surrounding refractive indices of 1.0002 (air) and 1.001 (CO₂).

(such as gradient metasurfaces or metalenses) can be thought of as diffractive optical devices controlling the 0th diffraction order with minimal energy lost to the other, undesired diffraction orders. Traditionally, such a feat is achieved by engineering the form-factor (or shape) of the subwavelength meta-units composing a metasurface (e.g. the cross-sectional shape of a dielectric pillar) for a given subwavelength meta-unit spacing. This contrasts with the focus of traditional planar photonic crystals, which is principally to engineer the array factor (periodic arrangement) of subwavelength diffractive elements. It is becoming increasingly clear [59, 60] that metasurfaces with optimal performance (especially those based on dielectric meta-units, chosen to minimize optical losses) will benefit greatly from incorporate engineering of both form factor and array factor. Metasurface design will therefore benefit from an understanding of the finite-size effects in periodic arrangements of dielectric structures, as well as a robust method to tune photon lifetimes.

We note a number of advantages offered by DHCGs over unperturbed HCGs operating near bound states in the continuum. First, the sharp spectral features of DHCGs are substantially more robust to deviations in height, duty cycle, and index of refraction of the grating and angle of incidence (see Supporting Information Section S.5) than those of HCGs, which require specific combinations thereof for sharp spectral features to arise. Second, DHCGs allow ease and flexibility of design not present in HCGs due to the constraints of these geometrical parameters; there is no requirement on any geometric parameter except perturbation in a DHCG to get a desired Q-factor, allowing the remaining parameters to be used for other design purposes. For example, the design process of the modulator in Figure 5 tailored the duty cycle and grating period (given a fixed height and index of refraction of a commercial SOI wafer) to align the background Fabry-Perot resonance with the sharp spectral feature, maximizing resonance visibility. Third, the strong dependence of Q-factor on angle of incidence in HCGs deteriorates resonance visibility when

the waist of the incident Gaussian beam is too small (the in-plane wavevector spreading is too large). This occurs at a smaller beam waist for DHCGs due to the independence of Q-factor on angle of incidence (see Supporting Information Section S.5), allowing a smaller device footprint for the same resonance visibility. Finally, for a given set of geometrical parameters (notably, duty cycle), the TE $B_{1,1}$ mode supported by a w-DHCG (as used in the modulator in Figure 5) has the lowest eigenfrequency and correspondingly the maximal overlap with the grating fingers (in the case of the modulator, the active material) of any leaky mode. This implies that it is the optimal choice for enhancing light-matter interactions required for such an active device operating on free-space light.

We believe the physical principles reviewed here, along with the approach presented to control lateral localization simultaneously with photon lifetime, are fundamental to the proper design of metasurfaces. For instance, future dispersion-engineered metasurfaces may do well to incorporate band structure engineering to control the finite number of elements required to reliably reproduce the optical response calculated by infinitely periodic simulations. In addition, symmetry breaking is an excellent tool for controlling sharp resonances required by dispersion-engineered metasurfaces. Achieving a perfectly flat band for a wide range of the FBZ (such as in the third row of Figure 3) represents a significant blurring of device classification; device design may truly require the language of both metasurfaces and planar photonic crystals.

DHCGs offer a promising platform for engineering sharp spectral features in compact 1D and 2D devices. We demonstrated that DHCGs combine the benefits of LCGs (which allow for easy tuning of the sharp spectral features through the corrugation depth) and HCGs (which allow for compact devices due to strong in-plane Bragg scattering) by performing full-wave simulations on infinite and finite gratings. We introduced a simple design approach that maximizes the lateral localization in the unperturbed grating and controls the sharp spectral features via a period-doubling perturbation. We catalogued and clarified the possible resonant modes in 1D DHCGs and pointed to the utility of expanding this effort to 2D DHCGs. We numerically demonstrated two applications as examples of a class of compact, planar optical devices with enhanced light-matter interactions.

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