

OPTICAL PHYSICS

Optical bound states in slotted high-contrast gratings

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This paper investigates the optical bound states in the continuum (BIC) supported by a slotted high-contrast grating (sHCG) structure. The sHCG structure consists of a periodic array of silicon ridges with a slot in each ridge. Given that the BICs are perfectly confined, their spectral locations are identified using a finite-element method formulated from a generalized eigenvalue problem. The real eigenvalues represent the wavelengths of BIC modes and the associated eigenvectors correspond to the electric field distributions. In the spectral and angular vicinity of the BICs, we studied the leaky waveguide modes using the rigorous coupled-wave analysis. The combination of the full-wave eigenvalue solver and the coupled-wave analysis provides an ideal setting to investigate the optical BICs of periodic structures for various applications. The simulation results show, for example, that the sHCG structures can support symmetry-protected bound states with a zero in-plane wave vector as well as high-quality-factor (high-Q) resonances for both TE and TM polarizations. By adjusting the slot, we can turn the BIC mode into high-Q modes and determine the linewidth of the mode by the degree of asymmetry. © 2016 Optical Society of America

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1. INTRODUCTION

Dielectric slabs with periodic sub-wavelength features, such as photonic crystal slabs, guided-mode resonance filters, and highcontrast gratings (HCG), have attracted considerable attention for their fascinating optical properties caused by the modulation and confinement of light [1-7]. Previous studies carried out on these devices have demonstrated numerous applications in highperformance optical filters [8–12], solid-state light sources [13,14], nonlinear optics [15–19], and biomolecule detection [20,21]. Among the grating-patterned slabs, the HCG structure, built upon a silicon-on-insulator substrate, is particularly interesting, owing to its extraordinary optical properties and compatibility with the complementary metal-oxide semiconductor process [22]. As reported by Mateus et al. [23] and Shokooh-Saremi and Magnusson [24], a HCG device allows broadband reflection with a reflectivity of more than 99% in the near-infrared wavelength regime. Following the demonstration of broadband reflection, recent studies have shown that a HCG device also exhibits Fano resonances with a high-quality factor (Q-factor). In 1929, von Neumann and Wigner first proposed the possibility of BICs based on potential engineering [25]. The possibility was also considered by Stillinger and Herrick [26]. More recently, Yoon et al. numerically investigated the TM-polarized optical bound states in the continuum (BIC) for a one-dimensional (1D) silicon grating [27].

The existence of a perfectly confined optical mode within the radiation continuum was shown using a parallel dielectric grating [28], 1D periodic array of dielectric rods and spheres [29,30], and a 2D photonic crystal slab [31–36] that supported a scattering resonance with a vanishing linewidth. A recent seminal work by Hsu et al. experimentally demonstrated the BICs of a 2D Si₃N₄ photonic crystal slab [37]. Later, layered sub-wavelength nanoparticles were numerically designed to achieve the BIC in three-dimensional open scattering systems [38]. For these devices, the optical bound states provide an ideal confinement of light in the continuum of the free-space light cone. Although the BICs do not radiate, the high-Q modes with quasi-embedded eigenvalues in the close vicinity of the BICs are particularly interesting, owing to their many potential applications in, e.g., optomechanics, nonlinear optics, cavity QED, and biomolecule detections. With regard to the HCG, the BICs play an important role in determining the characteristics of the radiative high-Q resonances. However, the relations between the broadband reflective modes, high-Q modes, and BICs have not yet been systematically studied.

This paper investigates the TE- and TM-polarized BICs and high-*Q* resonance modes of a silicon-based slotted HCG (sHCG). As shown in Fig. 1, the sHCG has a rectangular nanoslot cut into each ridge of the grating. The position of the slot in the ridge can determine the resonant characteristics of the device. Since the slot can be fabricated along with the HCG structure using a lithographic process, the proposed structure is ready to be manufactured. Although previous studies used rigorous coupled-wave analysis (RCWA) or a finite-difference time-domain method to identify BICs in an asymptotic manner [27], none of these studies directly calculated the eigenfrequency of the resonance modes that do not interact with the radiation continuum. Here, we employ a finite-element method (FEM) to solve the eigenvalue problems for the periodic structures, and consequently determine the resonance wavelengths (λ_r) and the associated mode distributions. The eigenvalue analysis shows that the BIC wavelengths increase proportionally with an increasing grating period and that the number of BICs increases with an increasing sHCG thickness. To more completely understand the phenomena associated with the BICs, we calculated the spectral and angular reflectance of 1D sHCG structures. Furthermore, we show that breaking the symmetry in the grating design produces the transition of a BIC mode to a high-Q mode.

This paper is organized in six sections. Section 2 specifies the sHCG structures and Section 3 describes the numerical methods used to analyze and simulate the phenomena of interest. Section 4 describes the bound states of the 1D sHCG device for two different polarizations. Section 5 demonstrates the possibility of forming asymmetric sHCG structures to turn BICs into high-*Q* resonances. Section 6 provides concluding remarks.

2. DEFINITIONS, PHENOMENOLOGY, AND CHARACTERIZATION TECHNIQUES

A. sHCG Structure and Physical Principles

The sHCG structure used in this study consists of a periodic pattern made of silicon and formed on a 3-µm-thick SiO₂ buffer layer. The main geometric parameters are the grating period (Λ_{1D}), grating width (w_g), slot width (w_s), nanoslot offset from the grating center (d_s) , grating-layer thickness (t_q) , and duty cycle ($\eta = w_{\sigma}/\Lambda$), as depicted in Fig. 1. For the symmetry protected structure, the slot stands at the middle of the ridge, which $d_s = 0$. The period of 1D arrays is smaller than the freespace wavelength λ . The thin device layer of silicon can be patterned by lithography, followed by a reactive-ion etching process [39]. Crystalline silicon is a suitable material to fabricate high-Q optical devices because it is transparent in the near-infrared regime, with a negligible extinction coefficient $\kappa < 0.001$ and a large refractive index n = 3.477. A planewave excitation beam is shone on the device from the grating side. As shown in the schematic view of the sHCG devices (Fig. 1), the incident angle θ_i is measured from the normal of the grating surface. Incident plane waves with their electric field polarized parallel or perpendicular to the grating bars are described as having transverse-electric (TE) or transversemagnetic (TM) polarizations, respectively.

Optical phenomena supported by HCGs and their underlying principles have been described previously [27,40-43]. Briefly, a HCG structure can be engineered to display strong broadband reflection and transmission, and narrowband high-Q resonances. The underlying principle of guided-mode resonance can be applied to understanding the resonances.



Fig. 1. Schematic of 1D sHCG structure on a SiO₂ substrate (not to scale). 1D SHCG consists of an array of slotted nano-ridges. Device is excited by a plane wave at an incidence angle of θ_i . TE- and TM-polarized modes correspond to the modes with the electric field component parallel and perpendicular to the grating lines, respectively.

For guided-mode resonance, incoming light is coupled to the in-plane waveguide mode via the grating modulation with the in-plane wavevector:

$$\mathbf{k}_{\parallel} = \hat{x}k_0 \sin \theta_i \pm \hat{x}G_x, \tag{1}$$

where $k_0 = 2\pi/\lambda$ is the free-space wavenumber and $G_x = 2m\pi/\Lambda$ with an integer *m*. The in-plane guided wave is scattered back into the continuum by the grating, and thus behaves as a leaky waveguide mode [44]. The constructive interference of the backward-scattered light with the zero-order reflection achieves a high-efficiency reflection. Meanwhile, the destructive interference of the forward-scattered light with the zero-order transmission produces a transmission minimum. The BIC characteristics can be simulated using electromagnetic simulations as discussed below.

B. Numerical Characterization Techniques

RCWA and the finite-difference time-domain method have previously been used to study HCG devices and photonic crystals [27]. These methods can simulate the optical phenomena that occur in a structure in response to excitation, and yield the reflectance, transmittance, and near-field distribution that can then be used to guide nanostructure design. Because these methods cannot find non-radiative BICs directly, we developed a generalized eigenvalue problem using an FEM-based solver to find all the BICs supported by the sHCG structure. The FEM simulation model included only one period of the sHCG structure. The periodic boundary condition in the *x*-direction, together with the perfectly matched layers in the *z*-direction, defined the simulation domain in the x-z plane. The simulation domain was discretized using a triangular mesh.

By basing the finite-element analysis on the electric-field discretization, the variational problem that is equivalent to the wave equation (source-free) led to a generalized eigenvalue problem [45]. By solving the generalized eigenvalue equation, the eigenvalue solver yielded the eigenvalues and eigenvectors, which represent the resonance wavelength and electric field, respectively. Only the real eigenvalues correspond to the bound states with a radiative coupling coefficient of zero ($\kappa = 0$). For the sHCG structure shown in Fig. 1(a), we used the eigenvalue

solver to determine the BICs for different device geometries. Appendix A provides the details and equations involved in the FEM analysis.

After finding the BICs, we used the RCWA method to study the BICs in an asymptotic manner. The RCWA algorithm is based on the Fourier expansions of the electromagnetic fields and the permittivity profiles $(\epsilon_r(x, y))$ in each layer of a periodic structure. The diffraction efficiencies for each harmonic in the Fourier expansion were calculated to determine the reflectance or transmittance. The analysis was carried out using a commercial RCWA software package (DiffractMOD, Synopsis). The RCWA simulation was set up to analyze a unit volume of the HCG structures, and periodic boundary conditions were applied to define the calculation domain, as labeled by the dashed box in Fig. 1. Twenty harmonics were used to expand the permittivity and fields along the *x*-direction. The dispersive and complex refractive indices of crystalline silicon, $n(\lambda) = n_{\rm si}(\lambda) + i\kappa_{\rm si}(\lambda)$, were taken from Palik's handbook [46], where $n_{si} = 3.486 + i0.001$ at $\lambda = 1550$ nm. The reflection and transmission spectra were calculated in the desired near-infrared wavelength range.

3. EIGENVALUE ANALYSIS OF SILICON-BASED sHCGs

The eigenvalue solver was applied to study how the geometric parameters of the silicon grating affect the BICs and illustrate the principles behind the sHCG-supported BICs. Material loss was neglected by assuming $\kappa_{si} = 0$, leaving out-of-plane scattering as the only loss mechanism. As a result, the real eigenvalue solutions correspond to the perfectly confined BICs and

(b)

2200

(a)

4000

those with an imaginary part are associated with the modes coupling with the radiation continuum. To characterize resonances supported by sHCGs with different grating periods, we considered sHCG structures with a thickness, duty cycle, slot width of $t_g = 500 \text{ nm}, \eta = 50\%$, and $w_s = 50 \text{ nm}$, respectively. As for the periodic boundary condition described in Eq. (A3), the phase shift was set to $\phi = 0$, representing the normal incidence case with $\theta_i = 0^\circ$. The grating period ranges from $\Lambda = 500$ to 1800 nm with the increment of 50 nm. Eigenvalues were solved for each grating period, but only the real eigenvalues are plotted in Fig. 2(a) as the BIC resonant wavelengths. The eigen-wavelengths can be grouped into three branches. The two branches shown in black represent the TE modes $(TE_{10} \text{ and } TE_{11})$ and the one shown in red is the TM_{10} mode. The modes are labeled as TE_{mn} (or TM_{mn}), where the integers m and n are determined by the distribution of the longitudinal component of the field along the x- and z-axes, respectively. The polarizations of these modes were determined by the electric-field components given by the eigenvectors. Here, the high refractive index grating-patterned silicon slab provides the inplane confinement. The Bragg condition gives the resonance wavelength,

$$\lambda = 2n_{\rm eff}\Lambda/m,\tag{2}$$

where n_{eff} is the effective waveguide index and *m* is a positive integer that denotes the order of diffraction. According to the Bragg condition, the resonance wavelength increases with the grating period, in agreement with the simulation results shown in Fig. 2(a).

Figure 2(b) shows the eigen-wavelengths calculated as functions of the grating thickness when the grating period and duty

(c)

2040

2020



Fig. 2. Eigen-wavelength calculated as a function of (a) the grating period, (b) the grating thickness, and (c) the slot width. (d) Eigenvectors of the TE₁₀, and TE₁₁ modes when $\Lambda = 880$ nm, $\eta = 50\%$, and $w_s = 50$ nm labeled by the blue line. For the TE modes, the E_y components at the corresponding wavelength 2012 nm and 1519 nm are plotted in the upper and lower panels, respectively. (e) Eigenvectors of the TM₁₀ mode. E_x and E_z components of the TM₁₀ mode are shown in the top and lower panels at $\lambda_r = 1459$ nm.

cycle are fixed at $\Lambda = 880$ nm and $\eta = 50\%$, respectively. The grating thickness increases from $t_g = 50$ to 1200 nm with the increment of 50 nm. The number of BIC modes can be estimated as $\#_{\text{BIC}} = \frac{2t_g}{\lambda} \sqrt{n_{\text{avg}}^2 - n_{\text{cladding}}^2}$, where n_{avg} can be estimated using the average refractive index of the patterned slab. As shown in Fig. 2(b), the number of BIC modes increases with the increasing grating thickness. Single-mode operation occurs when the grating thickness is less than 200 nm. For each mode, the BIC wavelength shifts to the red end as the grating thickness increases. Figure 2(c) shows the eigen-wavelengths calculated as a function of the slot width ranging from 10 to 100 nm. As shown in the figure, the BIC wavelength decreases when the slot widens for all three modes (TE_{00} , TE_{11} , and TM_{10}). The blueshift of the resonant wavelength can be attributed to the decrease of the averaged refractive index when the slot becomes wider.

Next, the field distributions of the BICs were studied using the eigenvectors associated with the real eigen-wavelengths. To this end, we considered a 1D sHCG device with grating period $\Lambda = 880$ nm, grating thickness $t_g = 500$ nm, and slot width 50 nm. This particular device supports three BICs at $\lambda_r = 1455.1, 1558.4, \text{ and } 2018.7 \text{ nm}, \text{ respectively. The modes}$ at $\lambda_r = 1455.1$ and 2018.7 nm are TE-polarized modes with only the E_{γ} components shown in the top and bottom panels of Fig. 2(d). The eigenvectors of the E_x and E_z components are trivial, and are therefore omitted from the figure. The mode at $\lambda_r = 1558.4$ nm is a TM-polarized mode with its E_x and E_z components shown in Fig. 2(e). Being a TM mode, its E_{γ} component is trivial compared to the E_x and E_z components. The resonant field distributions indicate that the order of Bragg diffraction is m = 2. We note that the distributions of the resonant fields are antisymmetric and these modes can be considered to be symmetry-protected bound states. The coupling to the continuum in the surface-normal direction is forbidden because of symmetry incompatibility with the external radiation, whose tangential field components are symmetric with respect to the mirror-symmetry axis at x = 0. The BIC mode is distinct from the resonance of distributed-feedback (DFB) cavities [47] because they reside inside the light cone of a photonic band diagram, which is shown in the following section. Moreover, we sought the real eigenvalues of the sHCG with the incident light at an oblique angle ($0^{\circ} < \theta_i < 90^{\circ}$). For the structure shown in Fig. 1(a), real eigenvalues are only present when $\theta_i = 0^\circ$.

4. BROADBAND, BIC, AND HIGH-Q MODES

The sHCG device can be designed to exhibit a single BIC mode when $t_g < 200$ nm. To illustrate the couplings between the broadband reflection, the high-Q mode, and the BIC, we selected a design that supports both TE and TM modes. The device consists of a grating with period $\Lambda = 880$ nm, thickness $t_g = 500$ nm, and slot width $w_s = 50$ nm. As shown in Figs. 2(a) and 2(b), there should be two TE modes and one TM mode. We first studied the TM mode. The calculated reflection spectra are plotted as functions of the incident angle in Fig. 3(a). The wavelength and incident angle range from 1200 to 2200 nm and from -15° to 15°, respectively. The



Fig. 3. TM-mode characteristics. (a) Calculated reflection spectra in the wavelength range 1200 to 2200 nm, for incident angles ranging from –15° to 15°. (b) Reflection spectra calculated for $\theta_i = 0^\circ, 0.5^\circ, 1^\circ,$ 2°, and 5°. The corresponding linewidths for each angle are plotted in the inset. (c) Near-field distributions of E_x , E_z , and H_y components for the high-Q resonance (Q-factor = 1.7×10^5) at $\lambda_r = 1458.3$ nm and $\theta_i = 0.01^\circ$.

TM-polarized resonances appear as reflection peaks. In contrast, the HCG structure without the slot exhibits the TMpolarized resonances as narrowband dips [48]. In Fig. 3(a), the region indicated by the red box contains the BIC and high-Q modes. To elaborate on these phenomena, the reflection spectra calculated for $\theta_i = 0^\circ$, 0.5°, 1°, 2°, and 5° are compared in Fig. 3(b). The resonant linewidth decreases significantly as the incidence angle approaches 0°. For example, when the incident angle is 1°, the resonance linewidth is 1.1 nm, which corresponds to a Q-factor of 1305. In comparison, the Q-factor increases to 4766.6 nm when θ_i is reduced to 0.5°. The vanishing of the linewidth at $\theta_i = 0^\circ$ implies the existence of BIC. As shown in Fig. 3(b), the BIC mode locates at $\lambda_r = 1458$ nm in the spectrum, in agreement with the eigenvalue analysis. Because the TM mode displays a weak reflection in the spectral range of interest, the high-Q resonance modes are displayed as peaks with a high reflectance at the resonant wavelength.

The near-field distribution of a representative high-Q mode is calculated using the RCWA simulation and shown in Fig. 3(c). Here, the near-field distributions of the E_x , E_z , and H_y components are associated with the high-Q resonance (Q-factor = 1.3×10^5) at $\lambda_r = 1458.3$ nm and $\theta_i = 0.01^\circ$. The color axis expresses the amplitudes of the electric and magnetic fields, normalized by that of the incident field. As seen from the field distributions, the maximum field enhancement factor is 1500. The enhancement factor of the field intensity is calculated by averaging the electric field intensities within the sHCG area $(-\Lambda/2 < x < \Lambda/2 \text{ and } 0 < z < t_g)$. As a result, the averaged enhancement factor of the field strength is approximately 1.7×10^5 . The distributions of the tangential components $(E_x \text{ and } H_y)$ are asymmetric. The mode can be excited because the asymmetric nature of the incident wave at $\theta_i = 0.01^\circ$.

Having characterized the TM mode, we used the same approach to study the TE-polarized modes. Figure 4(a) shows the



Fig. 4. Characteristics of the TE-mode. (a) Calculated reflection spectra in the wavelength range of 1200 nm to 2200 nm as a function of incident angles from -15° to 15°. (b) Reflection spectra calculated for $\theta_i = 0^\circ$, 0.5°, 1°, 2°, and 5° for the modes around 2012.9 nm. (c) Reflection spectra calculated for $\theta_i = 0^\circ$, 0.5°, 1°, 2°, and 5° for the modes around 1519.7 nm. Corresponding of linewidth for each small angle shown in inset. (d) Near field distributions of E_y , H_x , and H_z components with high-Q resonances (Q-factor = 4×10^7) at $\lambda_r = 2012.9$ nm and $\theta_i = 0.01^\circ$ for TE₁₀ (top) and TE₁₁ (bottom) mode, respectively.

reflection spectra of the TE modes plotted as a function of the incident angle, which ranges from -15° to 15°. As shown in Fig. 2(b), there are two TE-polarized BIC modes (TE₁₀ and TE_{11}) when the silicon grating thickness is 500 nm. In Fig. 4(a), the regions of the TE resonances are outlined by the black (TE₁₀ mode) and white boxes (TE₁₁ mode), respectively. Figures 4(b) and 4(c) summarize the reflection spectra for $\theta = 0^{\circ}$, 0.5°, 1°, 2°, and 5° for the TE₁₀ and TE₁₁ modes, respectively. Like the TM resonances, the TE modes also display as peaks in the reflection spectra. Also, the TE resonance linewidth decreases as the incidence angle approaches 0° and disappears at $\theta = 0^{\circ}$. This phenomenon indicates the existence of the BICs at $\lambda_r = 1519$ and 2012 nm. The near-field distributions of a representative high-Q mode for two TE modes are plotted, as obtained using the RCWA simulation. Figure 4(d) shows the amplitude distribution of the E_y , H_x , and H_z components that are associated with the high-Q resonance

at $\theta_i = 0.01^\circ$ for the TE₁₁ mode at $\lambda_r = 1519.7$ nm (top row) and the TE₁₀ mode at $\lambda_r = 2012.9$ nm (bottom row). The tangential components (E_y and H_x) of these mode are clearly asymmetric. The near fields of both TE modes are significantly enhanced relative to the incident wave.

5. ASYMMETRIC sHCGs

In the previous section, we showed that the transition from a BIC mode transit to a high-Q resonant mode when the sHCG is illuminated from an off-normal direction ($0^{\circ} < \theta < 1^{\circ}$). Recent research demonstrated an approach to transform the perfectly confined mode to high-Q resonances using nonequivalent sub-cells in one period of the grating [49]. Since the BIC mode with $k_x = 0$ is symmetry-protected, an asymmetric design of the sHCG can be exploited to eliminate the BIC and tune the high-Q resonant modes. This section demonstrates another approach that allows precise control of the resonance using the slot position. As shown in Fig. 5(a), we shift the slot from the center of the ridge to the right (or left) side with an offset of d_s . The shift of the slot results in an asymmetric sHCG structure. As a result, the symmetryprotected BIC mode disappears, and all the eigenvalues are complex. The resonant wavelength and the Q-factor are associated with the shift distance. Using the RCWA simulation, we studied the reflection characteristics of the asymmetric sHCG with the slot at off-center positions. Figure 5(b) shows the reflection spectra for $d_s = 1, 5, 10, 20$, and 40 nm, respectively, for the TM₁₀ mode. The incident angle is kept at $\theta_i = 0^\circ$, and the slot width is set as $w_s = 50$ nm. The resonant wavelength increases while the position of slot moves. It is clear that the resonant linewidth significantly increases as the slot approaches the edge of the ridge. The device with the d_s as small as 1 nm exhibits a linewidth of 0.004 nm and a Q-factor of 3.6×10^5 . Increasing d_s to 5 nm broadens the resonant linewidth to 1 nm (Q-factor of 1451). To elaborate how the resonance characteristics of the asymmetric sHCG resonator can be tuned, we summarized the Q-factor as a function of slot position in Fig. 5(c). As shown in the figure, the Q-factor decreases exponentially when the slot shifts toward the edge of the ridge.

We also used the eigenvalue solver to study the resonant wavelength and loss of the asymmetric sHCG devices. In the case of $d_s \neq 0$, all the eigenvalues are complex numbers. The real part of the complex number is the resonant wavelength of the asymmetry sHCG. Figure 6(a) shows the calculated eigen-wavelength as a function of the slot position. The resonant wavelengths of both TE₀₁ and TE₁₁ modes decrease the slot moves away from the center of the ridge. On the other hand, the resonant wavelength of the TM₁₀ mode increases while increasing the d_s . The breaking of device symmetry introduces radiation loss, which depends on the slot position. The radiation loss can be calculated using the imaginary part of the eigenvalues when $d_s \neq 0$. Figure 6(b) shows the change of radiative loss as a function of the slot position. For all three modes, the loss is strong when the sHCG has the highest degree of asymmetry, in which the center of the slot will be located at $w_{\sigma}/4 = 110$ nm. Thus, the loss is highest when d_s is approximately 85 nm. The BICs exist with zero radiative loss when the slot is located at the middle of the ridge $(d_s = 0)$ and the



Fig. 5. Asymmetric sHCG structure. (a) Schematics of sHCG, where the position of slot is shifted from the ridge center by a distance of d_s . (b) Reflection spectra for the asymmetric grating with $d_s = 1, 5, 10, 20$, and 40 nm. (c) The Q-factors are plotted as functions of d_s .



Fig. 6. Resonant characteristics of the asymmetric sHCG structure. (a) and (b) Resonant wavelength and loss as a function of slot position for TE_{10} , TE_{11} , and TM_{10} modes, respectively. (c) Reflection spectra for the asymmetric sHCG devices with $d_i = 80$, 120, and 140 nm, respectively.

boundary of the ridge ($d_s = 84.3$ nm). Figure 6(c) shows the reflection spectra when $d_s = 80$, 120, and 140 nm, respectively. When d_s increases beyond 80 nm, the resonant linewidth starts to decrease.

6. CONCLUSIONS

Optical bound states and the associated high-Q resonant modes supported by silicon-based sHCG structures were studied numerically. Special attention was given to the FEM eigenvalue solver, which is capable of finding the resonant wavelength and the near-field distributions of the BICs. Our results show that the number of bound states supported by a sHCG structure is determined by the thickness of the silicon slab. Using the calculated eigen-wavelengths, RCWA simulations were performed to characterize the resonant modes that are spectrally and angularly close to the BICs. The sHCG design investigated above displays one TM-polarized and two TE-polarized BICs. The TE- and TM-polarized resonances appear as narrowband peaks in the reflection spectra. Because the BICs are perfectly confined bound modes, they cannot be excited. The simulation of an asymmetric sHCG structure demonstrates that the BIC mode can be turned into a high-Q resonance, with the Q-factor being controlled by the degree of asymmetry.

The BIC and neighboring resonant modes of the sHCG structure can be applied to the construction of high-Q optical

resonators in the fields of optomechanics, nonlinear optics, and cavity QED with a tunable Q-factor by changing the coupling angle. They can also be used for refractive index-based biomolecule detection. The numerical techniques presented in this paper enable both source-excited and source-free assessments of BICs in slabs with a patterned grating. Understanding the phenomena above is an important step toward exploring more complex mechanisms involving the couplings between free-space fields, BICs, and high-Q modes.

APPENDIX A: GOVERNING EQUATIONS FOR THE FEM EIGENVALUE SOLVER

The electric field in the sHCG structure satisfies the secondorder wave equation

$$\nabla \times \mu_r^{-1}(\nabla \times \mathbf{E}) - k_0^2 \left(\epsilon_r + \frac{i\sigma}{\omega\epsilon_0}\right) \mathbf{E} = 0, \text{ in } \Omega,$$
 (A1)

and is subject to the following condition for a perfect electric conductor and floquet boundaries:

$$\hat{n} \times \mathbf{E} = 0$$
 on Γ_1 (A2)

$$\mathbf{E}_{F_{I}} = e^{i\phi} \mathbf{E}_{F_{r}} \quad \text{on } \Gamma_{2}, \tag{A3}$$

where Γ_1 and Γ_2 are the boundaries along the *z*- and *x*-axes, respectively. In (A1), the relative permeability $\mu_r = 1$, and

 σ and ϵ_r denote the relative permittivity and conductivity. In (A3) \mathbf{E}_{F_r} and \mathbf{E}_{F_l} are the fields at x = 0 and Λ , respectively, and the phase shift is given by $\phi = k_x \Lambda = k_0 \sin \theta_i \Lambda$. Perfect matching layers (PMLs) are applied along the *z*-direction to absorb the outgoing waves. In the PML regions, the anisotropic absorber model is used to create a reflection-free interface [50]. Then, by applying the variational principle, the solution to the problem defined by (A1)–(A3) is equivalent to

$$F(\mathbf{E}) = \frac{1}{2} \iint_{\Omega} [\mu_r^{-1}(\nabla \times \mathbf{E}) \cdot (\nabla \times \mathbf{E}) - k_0^2 \tilde{e}_r \mathbf{E} \cdot \mathbf{E}] \mathrm{d}\Omega.$$
 (A4)

To solve (A4), the electric field in the computation domain is discretized using the triangular elements

$$E_{t}^{e} = \sum_{i=1}^{n} e_{ti}^{e} N_{i}^{e}$$
 and $E_{z}^{e} = \sum_{i=1}^{n} e_{zi}^{e} \zeta_{i}^{e}$, (A5)

where $N_i^e(\zeta_i^e)$ and e_{ti}^e denote the vector expansion functions and the corresponding expansion coefficients. The final discretization of the variational problem (A4) amounts to a generalized eigenvalue problem

$$\begin{bmatrix} \mathbf{A}_{tt} & \mathbf{A}_{tz} \\ \mathbf{A}_{zt} & \mathbf{A}_{zz} \end{bmatrix} \begin{cases} e_t \\ e_z \end{cases} = k_0^2 \begin{bmatrix} \mathbf{B}_{tt} & \mathbf{B}_{tz} \\ \mathbf{B}_{zt} & \mathbf{B}_{zz} \end{bmatrix} \begin{cases} e_t \\ e_z \end{cases}, \quad (A6)$$

where A and B are complex matrices. Once the eigenvalues of (A6) are solved, the eigen-wavelengths are calculated as $\lambda_r = 2\pi/k_0$.

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