

Electro-optic symmetry breaking of BIC modes for tunable infrared emissivity

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ABSTRACT

We present an electro-optic pathway to break symmetry to enable dynamic light-matter interaction in guided-mode resonance grating. Breaking of mirror symmetry allows accessing bound states in the continuum (BIC) that are otherwise inaccessible. We design an electrically tunable GaAs-based guided-mode resonance grating that exhibits infrared absorption peaks in the longwave IR. The grating consists of GaAs dielectric sandwiched between the top gold contacts and the bottom gold reflector. We analyze the dependence of Q-factors on the choice of the design. We show that by careful design of the structure, a substantial radiative coupling can be obtained with broken symmetry. Our simulations predict that due to the electro-optic properties of GaAs, the application of a voltage across the dielectric allows a change in the refractive index to break the symmetry of the structure and turns the emission peak ON. Reversible refractive index tuning restores symmetry and turns the emission OFF. The concept presents a novel route toward tunable directional absorption and emission.

1. Introduction

Naturally occurring thermal emission is incoherent and static [1]. In the past two decades, infrared metamaterials have emerged to control the thermal emission spectra [2]. More recently, the possibility of dynamic and tunable thermal emission has been gathering increased attention. Material platforms such as phase-change materials [3–6], quantum wells [7,8], microelectromechanical systems [9,10], graphene [11], and III-V semiconductors [12] have been investigated for this purpose. Control of thermal emission has potential applications in energy technology [13], sensing [14], radiative cooling [15], image encoding [16], and communication [17].

The design of metamaterials for dynamic modulation of thermal emissivity could provide fine control in the spectral domain. While temperature-driven phase-change materials have been investigated for this purpose [18,19] electro-optic switching provides a much faster response [20,21]. In this context, exploring the range of angle- and wavelength-dependent tuning that can be induced by an electro-optic shift of refractive index is of general interest. Previous work in the mid-wave and long-wave infrared regime have investigated active tuning of thermal emission spectra by electro-optics. The strategies to modulate the reflection/absorption of infrared light rely primarily on a change in refractive index that leads to a shift in resonance, and/or on

modulation of absorption. For example, a shift in refractive index upon carrier injection was utilized to electrically control the resonance frequencies [12,22]. Many other works take advantage of graphene for engineering such tunability of infrared light [11,20]. In another instance, tunable properties of ITO were utilized to demonstrate tunable reflectance that effectively turns the absorption ON and OFF [23].

The tunability of light-matter interactions can be enhanced if the interaction is highly sensitive to index perturbation. High sensitivity can be achieved by considering the effect of refractive index perturbation on the photonic resonance modes and band structures of the metamaterial. In our previous work, we demonstrated the use of refractive index tuning to achieve Brillouin-Zone folding. The resulting change in the photonic band structure results in sensitive, narrow linewidth switching at off-normal angles [24]. Here, we propose a new strategy for narrow linewidth emissivity switching that operates at normal incidence. The operating principle is based on using a small refractive index shift to break the symmetry of a bound state in the continuum (BIC). This enables selective ON-OFF switching of infrared emission at normal incidence.

Bound states in the continuum (BICs) are nonradiative states with an infinite lifetime [25]. Symmetry-protected BICs cannot radiatively couple to incoming or outgoing plane waves. BICs have been extensively studied due to their exciting properties, such as high energy confinement

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[26] and robustness [27]. Quasfi-BICs with very high Q-factors have been realized in photonic crystals [28], waveguide arrays [29], and gratings [30]. By perturbing the symmetry of the system, bound states become accessible to radiative coupling. Most previous studies have focused on static photonic structures, where the symmetry is perturbed via geometric variations in the structure [31–35].

Here we present a reversible, electro-optic pathway to break the symmetry of a BIC mode, tuning its coupling to outgoing radiation. We design a guided-mode resonance device in the infrared with the capability for electro-optic tuning. Guided-mode resonance devices [36,37] are periodic structures that provide strong localization of electric fields, resulting in high, narrow linewidth absorption [38] and emission [39]. We theoretically demonstrate a device geometry that allows the selective tuning of the refractive index of portions of the guided-mode resonance device, breaking the mirror symmetry within each unit cell. We study the effect of device geometry on radiative coupling. We show that by changing the geometry, one can design the structure to enhance the radiative coupling of the symmetry-broken resonance mode. We demonstrate that by careful choice of grating geometry, critical coupling required for strong absorption can be achieved. We explicitly model the voltage-dependent carrier concentrations and refractive index shifts within the semiconductor layer of the device, allowing us to numerically analyze the effect of symmetry breaking on thermal emission spectra in the long-wave infrared. We show that in a guided-mode-resonance grating based on GaAs and gold, reversible symmetry breaking can actively turn the emission ON and OFF. These results indicate exciting possibilities for achieving electrically tunable control over thermal emission spectra at normal incidence.

2. Theory

To illustrate the main idea presented in the paper, consider a guided mode resonance grating situated over a gold back reflector. The unit cell of the grating is shown in Fig. 1(a). The unit cell has two dielectric stripes (with refractive index $n = 3.3$) of equal heights, separated by a small gap. The gap between the stripes of a unit is smaller than the gap between the dielectric stripes of adjacent units. Such a symmetric structure supports both symmetric and anti-symmetric modes at normal incidence ($k_x = 0$) [40]. For a normally-incident plane wave with the electric field polarized out of the plane, modes with odd mirror symmetry ($E_z(x) = -E_z(-x)$) cannot couple with the incident wave. This leads to near-zero absorptivity. If the normal-incidence absorptivity is zero,

the emissivity at normal is also zero by Kirchhoff's Law.

A modal profile with odd mirror symmetry is shown in Fig. 1(b). The electric field excited by a normally incident plane wave at the resonance frequency is shown in Fig. 1(c). As expected, the mirror symmetry of the field is different than in Fig. 1(b), and $E_z(x) = E_z(-x)$. We do not observe excitation of the resonant mode.

We study the effect of index perturbations shown in Fig. 1(d). The left dielectric stripe has a reduced refractive index ($n = 3.2$), and the unit cell has no mirror symmetry. Fig. 1(e) shows the modal profile of the perturbed grating with broken symmetry. The profile appears slightly asymmetric. As shown in Fig. 1(f), the mode can now be excited by a normally incident plane wave at the resonance frequency. The corresponding field profile shown in Fig. 1(f) displays the excitation of the resonance. The fields resemble the mode in Fig. 1(e), and the magnitude is much larger than in the non-resonant case of Fig. 1(c). While perturbation of symmetry could also be achieved by changing the geometry, we focus on active, reversible breaking of symmetry by electro-optic tuning of the refractive index.

To achieve high absorptivity (or emissivity) on resonance, the radiative loss rate and absorptive loss rate of the resonance must be comparable. The radiative and absorptive quality factors are inversely proportional to the loss rates. The peak absorptivity amplitude of the grating approaches 100% when the quality factors are equal [39].

To understand the dependence of Q factors on perturbations, we calculate radiative and absorptive Q factors for the design geometries of interest. The total Q factor Q_{total} is obtained using eigenfrequency simulations in COMSOL. By setting the imaginary part of the permittivity to zero (and effectively turning off the losses), we obtain the radiative Q factor Q_{rad} . Thus, the absorptive Q can be obtained as $Q_{\text{abs}} = (1/Q_{\text{total}} - 1/Q_{\text{rad}})^{-1}$. The quality factors are plotted in Fig. 2(a). For the unperturbed grating, the Q_{rad} is infinite while Q_{abs} is small. As seen in Fig. 2(a), for the perturbation of 10^{-4} , Q_{rad} is about 2×10^9 while Q_{abs} is about 1100. As the index perturbation is introduced to break symmetry, Q_{rad} reduces while Q_{abs} remains relatively constant. More substantial perturbation brings Q_{rad} and Q_{abs} closer until they are equal. To characterize the dependency of Q_{rad} on perturbation, Koshelev et al. [35] introduced a metric called asymmetry parameter α . They studied various cases of geometric perturbation and observed that α depends on the structure. Here we define $\alpha = |\Delta n|/n$ and verify the inverse squared law [35] between Q_{rad} and α . It is shown by the dashed line in Fig. 2(a). Q_{abs} is primarily determined by material loss, whereas the modal profile and the geometry determine Q_{rad} . Therefore, we expect the intersection

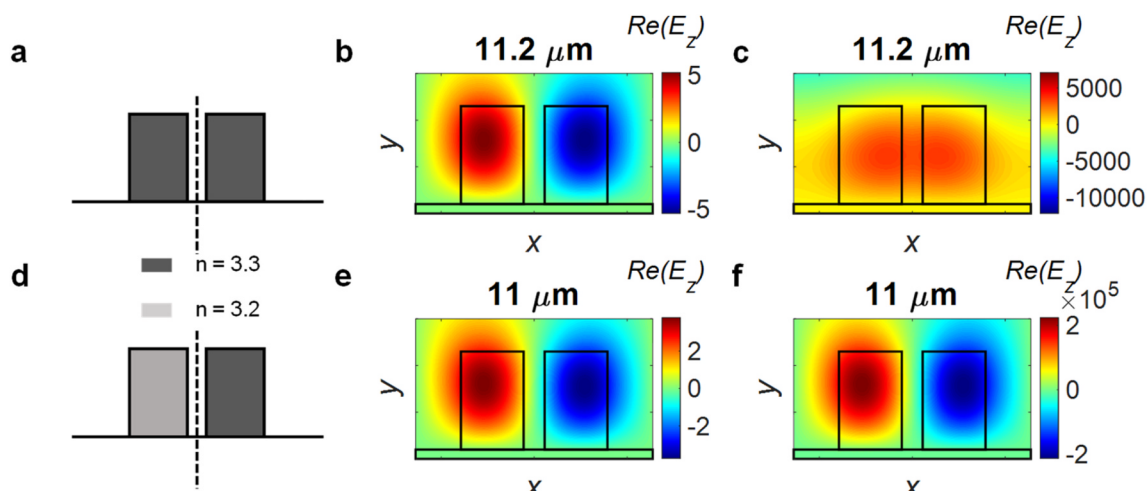


Fig. 1. (a) Unit cell of a grating with mirror symmetry. Dielectric stripes situated over a gold layer have a height of 2.1 μm and a width of 1.35 μm. The separation between them is 225 nm, while the periodicity of the structure is 5.1 μm. (b) The corresponding modal profile of a typical BIC mode with odd mirror symmetry $E_z(x) = -E_z(-x)$. (c) Field excitation of the BIC with normally incident plane wave shows weak coupling. (d) Unit cell of a grating with broken symmetry. (e) Modal profile for the corresponding perturbed grating with broken symmetry. (f) Excitation of the resonance with normally incident plane wave.

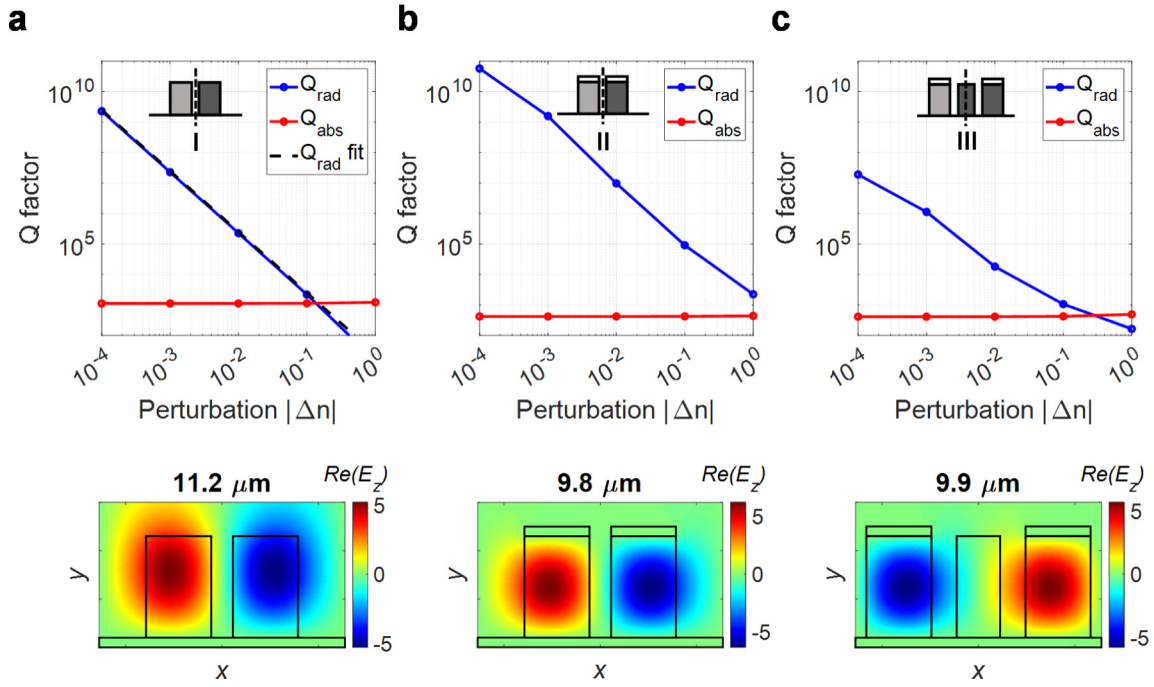


Fig. 2. Radiative and absorptive Q plotted vs. index perturbation for three different grating designs. The corresponding field profiles of BIC modes are shown below. (a) Design I: two dielectric stripes. (b) Design II: two dielectric stripes with metallic caps (200 nm thick). (c) Design III: three dielectric stripes with metallic caps on the left and right stripes. The center-to-center distance between the left and right stripes is $3.3 \mu\text{m}$. The center stripe is 900 nm wide.

point between the two curves to occur at a larger value of Δn if the material loss were higher (lower Q_{abs}).

Device I is an idealized structure; in general, electrical contacts must be added to provide index tuning. Device II (Fig. 2(b) inset) adds metallic caps to the grating to serve as electrical top contacts, while the metal back plane serves as a bottom contact. However, the addition of metallic caps changes the modal profile, affecting the response of the grating to perturbation. In Fig. 2(b), we plot the Q factors. We notice that Q_{rad} is now significantly higher, while Q_{abs} has reduced to ~ 400 . As seen from the field plot below Fig. 2(b), the field has an increased confinement in the dielectric, and the presence of the metallic caps appears to reduce the radiative coupling. The presence of lossy metal caps also explains the reduction in Q_{abs} . A substantial difference between Q_{rad} and Q_{abs} remains at significant index perturbation. It is thus not straightforward to achieve critical coupling ($Q_{\text{rad}} = Q_{\text{abs}}$) without the use of extremely high Δn values.

To ameliorate this problem, we introduce a modified design with improved performance. Design III has a unit cell with three dielectric stripes of equal heights, with the center stripe having a smaller width (Fig. 2(c) inset). The left and right stripes have metallic caps. Q factors for this design are plotted in Fig. 2(c). We notice that Q_{rad} is reduced by orders of magnitude with respect to Fig. 2(b). The addition of the center stripe may provide an access route for the radiative coupling to the external plane waves. Although Q_{rad} and Q_{abs} are not equal, they are comparable in magnitude for index perturbation of 0.1. Literature indicates that such a change in refractive index is achievable in the case of materials such as GaAs [22], InAs [41], and ITO [42] in the mid and long-IR regimes.

3. Results and discussion

Fig. 3 illustrates how the electro-optic tuning required for Design III may be achieved in practice. Fig. 3(a) shows the schematic, where the dashed line indicates one unit cell. Fig. 3(b) shows the unit cell dimensions in detail. Within each unit cell, the center stripe has a smaller width. The left and right stripes have 200 nm thick gold caps. The grating is situated over a reflecting gold substrate. GaAs was chosen

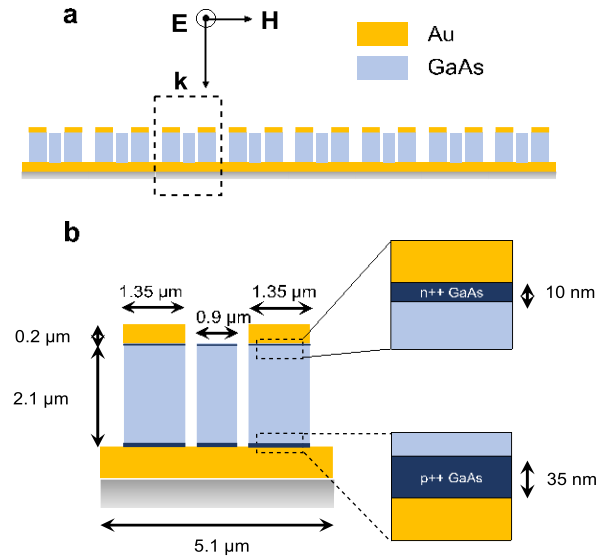


Fig. 3. (a) Guided-mode resonance grating consisting of a dielectric (GaAs) on a gold substrate with gold caps. (b) The unit cell of the grating has three dielectric stripes with equal heights. The center stripe has a smaller width. Only the left and right stripes have metallic caps. The top and bottom layers of the dielectric are heavily doped with n++ and p++, respectively.

because its refractive index is affected by carrier concentration. Top and bottom metal contacts can be used to inject charge carriers into the GaAs layer. To allow the injection of carriers into the intrinsic GaAs layer, a small portion of the layer near the metal contacts is heavily doped. Such heavily doped layers are typically used to avoid the formation of large depletion regions [43]. As schematically shown in Fig. 3(b), we assume that the 10 nm layer of GaAs near the top contact is n++ doped ($5 \times 10^{18} \text{ cm}^{-3}$) and the 35 nm thick layer of GaAs near the bottom contact is p++ doped ($5 \times 10^{18} \text{ cm}^{-3}$). Together with the contacts, the layers form a p-i-n junction electro-optic modulator. Although only the left GaAs

stripe will be subjected to carrier injection, both the right and the left stripes have gold caps and all stripes have heavily doped layers so that the original structure is symmetric. In our simulations, we confine ourselves to transverse electric polarization (H_x, H_y, E_z). The dimensions of the unit cell were chosen to have resonance around 10 μm , which is approximately the thermal wavelength at room temperature. The dimensions shown in Fig. 3(b) were optimized for maximum susceptibility to index perturbation by trial and error.

Fig. 4(a) shows the configuration to allow index perturbation by applying a voltage across the dielectric stripe. Only the left stripe within each unit cell will undergo a change in carrier concentration and refractive index. We simulate the effect of voltage on carrier concentration in GaAs using Lumerical CHARGE. We use steady state boundary conditions with the gold cap as a contact at 0 V and the bottom gold layer as a contact with varying voltage from 0.5 to 2 V.

The simulated carrier concentration of electrons (n) in the GaAs layer at 0 V and 1.4 V is shown in Fig. 4(b) and (c), respectively. The application of voltage significantly changes the carrier concentration across the majority of the GaAs layer. The carrier concentration of electrons (n) at the center of the GaAs layer is plotted as a function of applied voltage in Fig. 4(d). The highlighted data points correspond to 0 V ($1.76 \times 10^6 \text{ cm}^{-3}$) and 1.4 V ($6.48 \times 10^{17} \text{ cm}^{-3}$). These values are used to estimate refractive indices of the tunable GaAs layer.

Predicted values of refractive index (n) and extinction coefficients (κ) for various concentration levels are plotted in Fig. 4(e) and (f), respectively. Refractive index values are obtained from the GaAs Drude model that accounts for the change in plasma frequency as a function of carrier concentration, and fit is given by [44].

$$\epsilon = \epsilon_\infty - \frac{\omega_p^2}{\omega^2 + i\omega\Gamma} \quad (1)$$

Here ϵ_∞ , ω , ω_p and Γ are flow-frequency permittivity, angular frequency, plasma frequency, and damping constant, respectively. The plasma frequency of doped GaAs is carrier-dependent and is given by

$$\omega_p = \frac{N_d e^2}{\epsilon_0 \epsilon_\infty m^*} \quad (2)$$

Here, ϵ_0 , e , N_d and m^* are free-space permittivity, elementary charge, doping concentration, and effective electron mass, respectively. m^* is assumed to be $0.52 m_0$ for holes (p-type) and $0.067 m_0$ for electrons, when m_0 is electron mass. The damping constant is related to carrier mobility (μ) and m^* by the equation

$$\Gamma = \frac{e}{\mu m^*} \quad (3)$$

In our calculations, μ is taken to be $400 \text{ cm}^2/\text{V}\cdot\text{s}$ for holes [45] and $8000 \text{ cm}^2/\text{V}\cdot\text{s}$ for electrons [46]. As shown in Fig. 4(e), the difference between the refractive index of intrinsic GaAs and p+ GaAs ($6.48 \times 10 \text{ cm}^{-17}$) is approximately 0.15 over the wavelength range of interest. While intrinsic GaAs is essentially lossless in this regime, there is a increase in extinction coefficient (κ) upon carrier injection. Fig. 4(g) shows spatial variation of refractive index in the GaAs layer at 10 μm wavelength for 0 V and 1.4 V. For the perturbed structure, the refractive index (n) of the tunable GaAs layer varies with vertical co-ordinate (y). In our simulations, the tunable GaAs layer was divided into sublayers, each having a constant refractive index. The number of sublayers was increased until calculated absorptivity spectrum converged. Five sublayers were found to be sufficient to achieve convergence. The total variation in n is approximately 0.11. Within each layer, the variation in refractive index is approximately 0.02. All the subsequent calculations reported are done using five sublayers.

We simulate the absorptivity of the grating using the COMSOL wave optics simulation solver. The solver uses the finite-element, frequency-

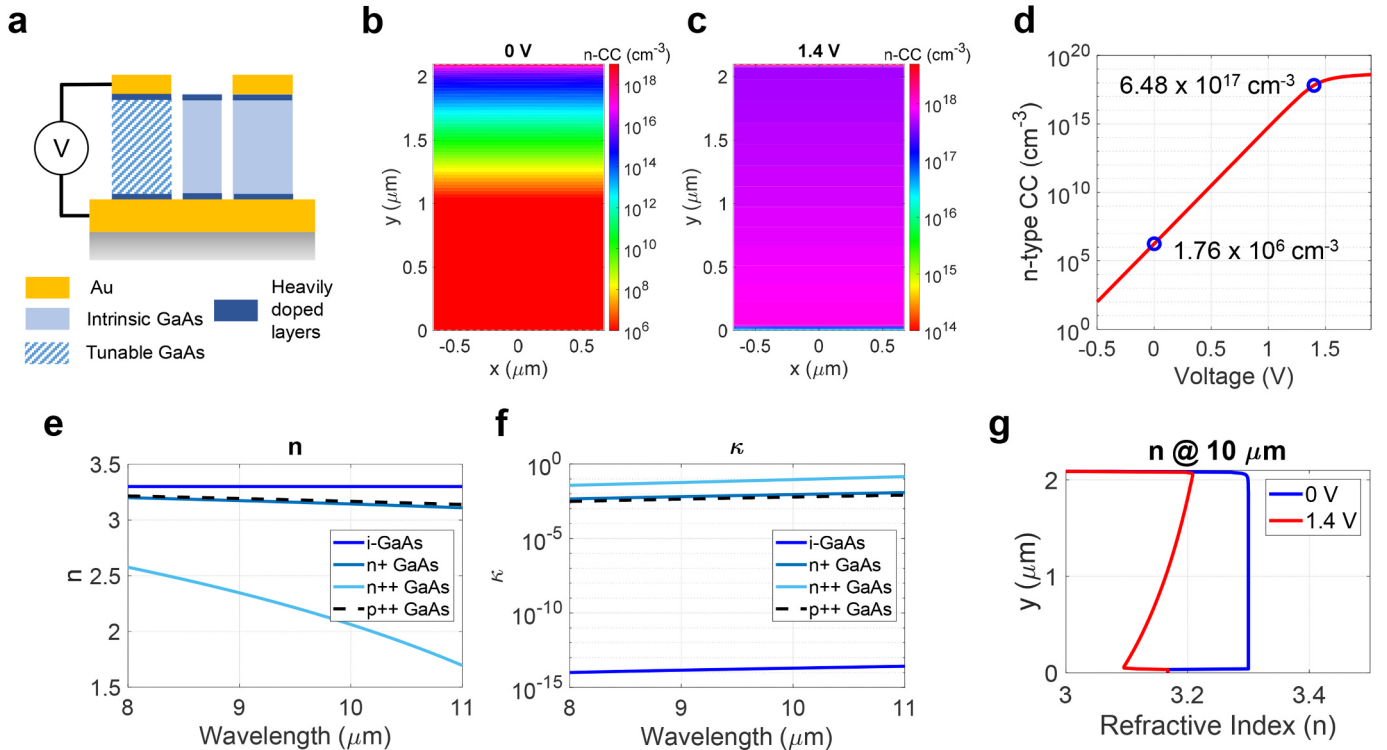


Fig. 4. (a) Proposed configuration to introduce index perturbation for dynamic symmetry breaking. Applying a voltage across the left stripe using the gold cap and the metallic substrate as contacts enables reversible n+ doping of the GaAs layer. The carrier concentration of electrons (n) in the GaAs layer at (b) 0 V and (c) 1.4 V. (d) The carrier concentration of electrons (n) at the center of the GaAs layer is plotted as a function of applied voltage. Refractive index n (e) and extinction coefficient κ (f) plotted as a function of wavelength for i-GaAs (0 V), n+ GaAs (1.4 V), n++ GaAs (top layer), and p++ GaAs (bottom layer). (g) Spatial variation in refractive index (n) of the dielectric layer at 10 μm as a function of y -coordinate for 0 V and 1.4 V.

domain method to solve Maxwell's equations. Bloch periodic boundary conditions were used for the left and right boundaries of the unit cell. The absorptivity (a) of the structure is given by $a = 1 - r$, where r is reflectivity. We note that a voltage bias to a p-i-n diode can change the chemical potential of photons emitted for the photons above the band gap of the semiconductor. This may lead to super-Planckian thermal emission [47]. However, in the present study, GaAs has a band gap of 1.424 eV (0.87 μm). The chemical potential of photons in the wavelength range of interest is unaffected. Therefore, Kirchhoff's law of thermal radiation holds. From Kirchhoff's law, emissivity (e) equals absorptivity.

The emissivity of the unperturbed grating at normal incidence is shown in Fig. 5(a). The spectrum shows a prominent peak around 10 μm . This peak corresponds to a bright mode. At the same time, a dark mode (BIC) exists at the wavelength highlighted by the dashed line. Due to symmetry, the normally incident wave cannot couple with the resonance, and no excitation is seen in the BIC field profile (shown in the inset). Fig. 5(b) shows the emissivity spectrum for the perturbed grating at 1.4 V. The spectrum displays an additional peak. Due to index perturbation, the symmetry is broken, and the dark mode becomes bright. As a result, the resonance can now be excited by a normally incident plane wave. The field profile of the excited resonance is shown in the inset. The asymmetric mode shape is apparent. Due to the reversible nature of voltage-tunable carrier injection, this method allows a pathway to ON-OFF switching of emissive resonances. An ON-OFF contrast ratio of ~ 40 is predicted.

The dependence of spectral emissivity on the angle of incidence (θ) is plotted in Fig. 6. The emissivity of the unperturbed grating is shown in Fig. 6(a) and exhibits two bright bands. These bands correspond to the resonances that can be excited by an external plane wave. The lower wavelength band shows a dark spot, or a hole, at $\theta = 0$, highlighting the location of the BIC. As this is a symmetry-protected BIC, it is dark only for $k_x = 0$. Off-normal plane waves have non-zero convolution with the mode profile and can excite the resonance, which explains the appearance of the hole in the contour plot. Fig. 6(b) plots the angular spectral emissivity for the perturbed grating at 1.4 V. The emissivity hole at the location of BIC is noticeably filled. As a result of the index perturbation, we also observe a shift in the bands and an increase in the gap between bands. Due to the shift in the band structure, off-normal thermal emission exhibits shift in resonance peaks.

The proposed grating can be fabricated by templated liquid-phase

crystal growth [48], or epitaxial transfer [49], followed by chemical vapor deposition of gold and etching. The electro-optic nature of the tuning mechanism also enables high-speed ON-OFF switching. The modulation speed of such a device can be estimated using the equivalent capacitor-resistor circuit. For the design presented in the paper, assuming a device footprint of 10,000 μm^2 , we estimate the device capacitance to be approximately 300 fF. Using a conservative value of contact resistance of 50 Ω and transmission line resistance of 50 Ω , we estimate that the device can operate up to 5 GHz. Electro-optic breaking of symmetry can be applied to any electro-optic material such as InAs, GaAs, ITO, and alloys of In, Ga, As, and Sb. Dimensions of the grating can be adjusted to excite resonances in the desired spectral range. By carefully designing the BICs, we expect that tunable emission can be attained at any wavelength.

4. Conclusions

In conclusion, we theoretically demonstrated the feasibility of using electro-optics to break symmetry and access a symmetry-protected BIC. Reversible index perturbation enabled by carrier injection allows switching resonance and tunable thermal emission. We predict a contrast ratio of 40 upon modulation. The design highlights a pathway for developing voltage-tunable narrowband thermal emitters and absorbers. Electro-optic driven symmetry breaking can have various implications for tunable thermal emission, especially when switching of narrowband resonances is desired. Such applications include image encryption [16] and communication [17]. Present work takes advantage of a mismatch (match) between Q_{rad} and Q_{abs} to turn the emission OFF (ON). Such a mismatch can also be induced at oblique angles of incidence, even in the absence of BICs. Hence, tunable light-matter interactions can be engineered at off-normal incident angles. Besides symmetry protected BICs, accidental BICs [28] that occur at oblique angles can also be studied for index perturbation and tuning of thermal emission. Therefore, we envision that the scheme of reversible symmetry breaking can be extended to angular resonances. The idea presented here can also be extended for two-dimensional gratings, giving rise to intriguing new possibilities of tunable thermal emission.

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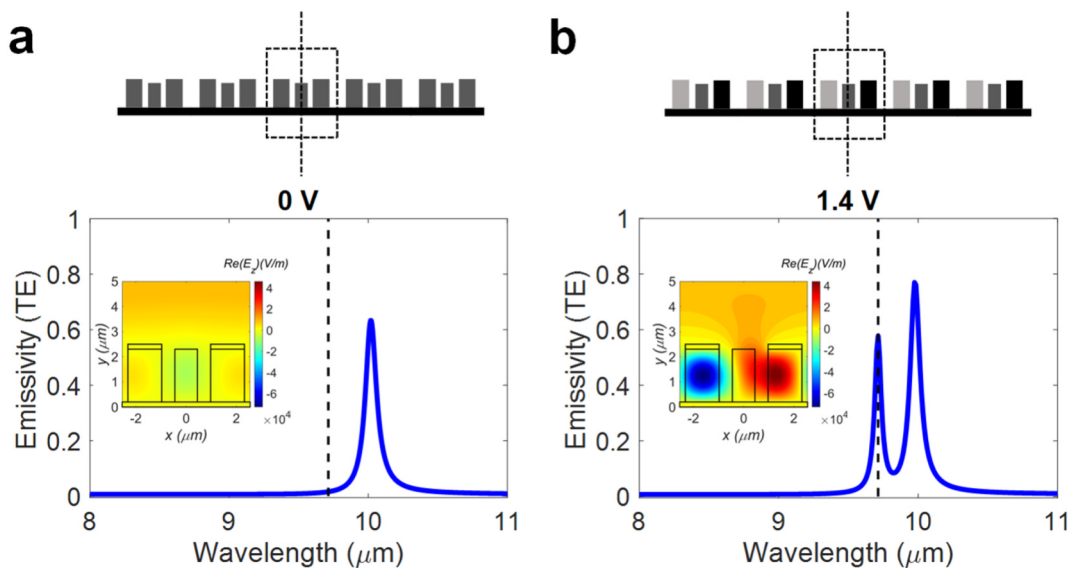


Fig. 5. (a) The emissivity of the unperturbed grating at normal incidence. The dashed line indicates the location of the dark mode with near-zero emissivity. The field profile of the dark mode is shown in the inset. (b) The emissivity of the perturbed grating with a broken symmetry at 1.4 V shows a new peak. The field profile of the corresponding resonance is plotted in the inset.

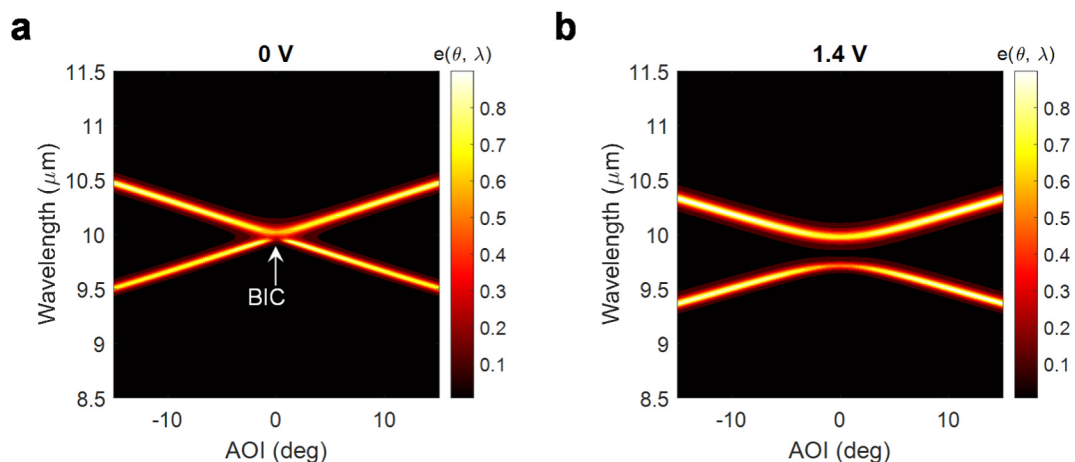


Fig. 6. (a) Emmissivity of the unperturbed grating plotted as a function of angle of incidence and wavelength. The flower bright band shows a 'hole' at 0 deg, indicating the BIC. (b). The emissivity of the structure with broken symmetry (at 1.4 V).

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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