


Narrow Bandwidth and Tunable Mid-Infrared Thermal Emitter Design Based on Double Asymmetric Dielectric Metasurfaces

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Abstract

Thermal emitters working in the mid-infrared (MIR) region are indispensable in many applications, such as sensing, thermophotovoltaics, and imaging. Resonance wavelength tunability, high efficiency, cost-effectiveness, and high quality (Q) factor are desirable properties of thermal emitters. Selective thermal emitters have been realized using metallic metasurfaces, which, due to ohmic losses, do not exhibit very sharp emission peaks. Recently, metasurfaces possessing very high Q factors made of dielectric materials with asymmetric features that exploit quasi-bound states in the continuum are introduced. The dielectric metasurface-based thermal emitters shown in the literature have a single type of asymmetry, such as a difference in the length of resonators or angular separation of resonators. However, resonance wavelength and thermal emissivity could be tuned by having multiple types of asymmetries. This study proposes a structure consisting of a zigzag array of silicon rectangular bars with different lengths as resonators. Gold is the choice of the substrate with a dielectric layer made of Al₂O₃ sandwiched between gold substrate and silicon bars. Based on the conducted simulations, an emissivity value exceeding 0.99 with a Q factor of 116 at the resonance wavelength of 5.818 µm was obtained when the silicon bars were separated by $\pi/25$ from the origin in opposite directions with a length asymmetry factor of 0.3. Additionally, independent tuning of emissivity intensity and resonance wavelength is displayed. Such findings can lead to bespoke thermal emitter designs.

Keywords: Thermal emitter, dielectric metasurface, high-Q resonators, tunable metasurface

I. INTRODUCTION

An object with a temperature above absolute zero emits electromagnetic energy to its surroundings, a phenomenon known as thermal radiation, which is intensely studied by scientists for a range of applications, including sensing, infrared camouflage, and thermal energy utilization [1]. Conventional thermal emitters are broadband, omnidirectional, and polarization-independent. These properties are undesirable for many use cases. For instance, certain chemicals such as polymers have sharp absorption bands, and it is highly convenient to have access to a thermal emitter that matches the absorption band of the analyte of interest rather than coupling broadband thermal emitters with filters, which waste most of the energy coming from the emitter [2]. Furthermore, in a thermophotovoltaic system, a wavelength-selective emitter that matches the bandgap of a photovoltaic cell is required [3]. Hence, tunable high Q factor thermal emitters are essential to various technologies. One-dimensional [4] or two-dimensional photonic crystals [5], plasmonic metasurfaces [6], and dielectric metasurfaces [7] with micro/nanometer resolution have been proposed in the literature to satisfy such requirements. Kirchhoff's and Planck's law state that emissivity equals to absorptivity for reciprocal systems; highly efficient thermal emitters also act as highly efficient absorbers in the wavelengths of interest. Thus, a designed structure emits at the same wavelength at which it absorbs once heated to a high enough temperature. The most common way to explain the resonance quality is to use the Q (quality) factor, which is the resonance wavelength divided by the width at half the intensity. A higher Q factor means sharper absorption/emissivity peaks. One of the most employed designs utilizes an insulator spacer layer sandwiched between two metal layers, which is popular due to ease of design and fabrication [8]. Unfortunately, Ohmic losses in the metal widen the absorption peak, resulting in lower Q factors. Indeed, metal-insulator-metal configurations reported in the literature have Q factors of less than 20 [2, 9]. Structures using dielectrics to support resonances are proposed to overcome the plasmonic ohmic losses and heating problems, and they have been shown to perform with higher Q factors [10].

Bound states in the continuum (BIC) are non-radiative states localized inside the continuum spectrum [11]. Initially appeared in quantum mechanics, BIC has found applications in diverse areas such as acoustics and hydrodynamics as well as photonics to make high Q factor resonators [7, 12]. One type of BIC is called symmetry-protected BICs, characterized by infinite Q factors [13] and displaying a different symmetry than incoming waves, making them not excitable [14]. These states can be excited if the symmetry is broken through geometrical means making them quasi-BICs with finite but high Q factors [15]. Metasurface geometries are carefully selected to tune asymmetry parameters, leading to well-tuned resonance wavelengths and intensities. Geometries with broken symmetries include, among others, differently oriented elliptical disks [16], a pair of rectangular rods with different lengths [17], and a cylinder-ellipse pair [18]. All designs proposed in the literature have a single type of asymmetry, except where the design has different widths of bars and gap sizes in a grating designed for refractive index sensing whose geometrically tuning capability has yet to be shown [19]. Geometry parameters are not the only flexibility in designing structures that support quasi-BICs. A recent study shows the refractive index contrast between the surrounding medium and the structure is influential [20]. Additionally, nanocube based resonators with polarization-independent optical response was shown through computational studies and can be used in sensing applications [21]. Very recently, a silicon cube-based design with carved features demonstrated asymmetry in optical response to light handedness, resulting in high circular dichroism [22]. It is evident that structures that support quasi-BICs with different materials and topologies are currently being investigated by researchers for various use cases.

In this work, we propose a novel type of dielectric narrowband MIR thermal emitter having two different geometric asymmetries. Quasi-BIC modes are realized by employing two rectangular rods made of silicon with different lengths and orientations. The substrate of choice is gold and Al₂O₃ for spacer layer material. Through delicate tuning, the proposed design supports a sharp and intense (>0.995) emission/absorption band with a Q factor of 116 at a resonance wavelength of 5.818 μm. Furthermore, the intensity and the resonance wavelength can be tuned by changing angular orientation and length asymmetry, respectively. The results show that by using a dielectric metasurface on a conductive substrate, narrowband and tunable thermal emitters can be made by employing the quasi-BIC phenomenon.

II. MATERIALS AND METHODS

2.1. Definition of Structure

The structure of a double asymmetric dielectric metasurface-based MIR thermal emitter is shown in Figure 1. It is made of two differently oriented 400 nm

thick rectangular rods separated by a 780 nm thick spacer layer that sits on a conductor substrate thick enough to block light transmission. The structure's unit cell is a square lattice with a period of 4000 nm. The centers of the two rods within the unit cell are separated by 1700 nm. Both rods have widths of 1200 nm but have differing lengths. The long rod is 3100 nm long, whereas the short one is 2170 nm. The length asymmetry parameter (α_l) for the proposed structure is defined according to [12]:

$$\alpha_l = \frac{\Delta L}{L} = \frac{3100 - 2170}{3100} = 0.3 \quad (1)$$

where L is the bar's original length, and ΔL is the length removed from the original length. Furthermore, to induce a secondary asymmetry in the suggested structure, the rectangular rods are rotated by angles (θ) of $\pi/25$ in opposite directions. The resonance wavelength and intensity are highly dependent on the asymmetry parameters, and non-zero values of asymmetry parameters would result in exciting quasi-BIC states that lead to narrowband emission. The studied wavelength region lies between 5.6 and 6.2 μm.

2.2. Materials

To investigate the emission performance of the suggested structure, we rely on the properties reported in the literature. For the substrate, gold is chosen, whose refractive index (n) and extinction coefficient (k) values are obtained from [23]. As the spacer layer, Al₂O₃ is chosen, with n values taken from [24]. For k values, a constant value of 0.001 is used for all wavelengths in the study, similar to [2].

Silicon is chosen as the dielectric metasurface material. Constant values of n=3.42 and k=0 were used for all the wavelengths in the study [25]. It is important to note that using a material with higher refractive indices, such as germanium [26] or Bi₂Te₃ [27], would result in higher Q factors, but we chose silicon as it is one of the most widely used materials.

2.3. Simulation Parameters

As Kirchhoff's law of thermal radiation states, an object's absorptivity (A) equals its emissivity (E). An incoming light can be transmitted through, reflected off, or absorbed by an object. In our investigation, as the substrate is thick gold, the transmission can be neglected, reducing the problem of finding the reflectivity (R) of the structure for the wavelengths of interest. So, the spectral emissivity of the thermal emitter is:

$$E(\lambda) = A(\lambda) = 1 - R(\lambda) \quad (2)$$

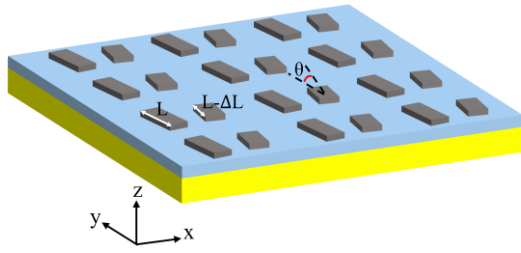


Figure 1. The schematic of the dielectric metasurface based thermal emitter. Each unit cell has two rectangular rods of different lengths, rotated opposite each other at an angle of θ to induce asymmetries.

We use the source TORCWA library to calculate emissivity values [28], a rigorous coupled-wave analysis (RCWA) tool that provides semi-analytical solutions by computing the scattering matrix for periodic stacked structures. In RCWA, relative permittivity is expanded in Fourier series, which must be truncated for calculations [29]. A truncation order of 7 is used in the simulations. The unit cell is assumed to be periodic in both the x and y directions. The incident light is normal to the surface and polarized in the x direction. The spatial resolution is chosen to be 1 nm, and emissivity values are calculated for every 2.5 nm between 5.6 and 6.2 μm .

The quality (Q) factor of a resonator is calculated as the ratio of wavelength of emissivity peak to full width at half maximum of the peak and can be formulated as:

$$Q = \frac{\lambda}{\Delta\lambda} \quad (3)$$

III. RESULTS AND DISCUSSION

3.1. Performance Evaluation of Proposed Structure

We start evaluating the proposed design where the bars, with a length asymmetry of 0.3, are rotated by $\pi/25$ in opposite directions. Figure 2 (a) shows the dielectric metasurface-based thermal emitter's calculated emission spectrum. A single emission/absorption peak at 5.818 μm exceeding an emissivity of 0.995 is obtained from the simulations. The inset zooms into the resonance wavelength area, and the full width at half maximum of the emission is calculated to be 50 nm, which corresponds to a Q factor of 116. Considering that metal-based thermal emitters reported in the literature achieve Q factors of less than 20, dielectric resonator-based structures have the potential to be used in various applications.

The high Q factor resonance that we observe in the suggested structure is supported by quasi-BIC. To prove the symmetry-protected properties of quasi-BIC resonances, the real part of the electric field distribution E_y in the xz plane at the resonance wavelength is shown in Figure 2 (b). As expected, no electric field exists inside the gold substrate ($z = -500$ nm to $z = 0$ nm). The anti-symmetric electric field profile, where one rod

experiences the minimum of the electric field while the other one holds the maximum electric field, conveys the existence of quasi-BIC resonance [30]. Additionally, it can be clearly seen that the field enhancement is mostly contained inside the silicon rectangular rods, and some leakage to the surrounding vacuum and spacer layer occurs.

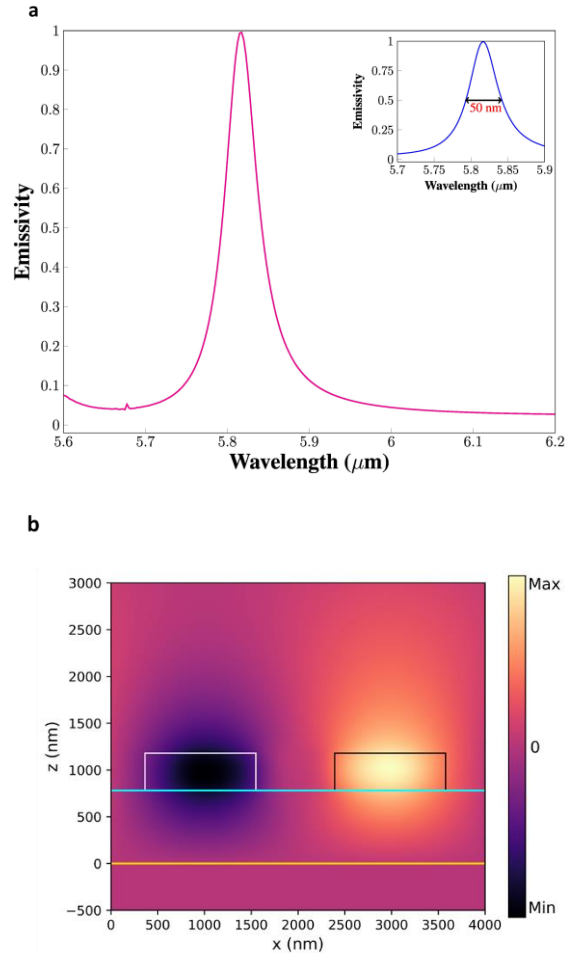


Figure 2. (a) Emissivity spectrum and (b) simulated cross-sectional profile of E_y from the double asymmetric dielectric metasurface. The yellow line indicates the top of the gold substrate, and the cyan line depicts the top of the spacer layer. The silicon resonators are within the black and white rectangles.

3.2. Parameter Sweep of Separation Angle

In the double asymmetric dielectric metasurface-based thermal emitter, rotating rectangular rods by $\theta = \pi/25$ produce almost unity emissivity when the length asymmetry is 0.3. However, the emissivity intensity can be tuned by changing the rotation angle without changing the resonance wavelength.

Figure 3 shows the rotation angle sweep results. In all these cases, the length asymmetry value (α_1) is 0.3. The sweep starts from $\theta = 0$, depicting the case of two perfectly parallel bars to $\theta = \pi/15$. We did not go beyond $\pi/15$ as those values correspond to the case of

two bars touching each other. As can be seen, when there is no asymmetry in rotation ($\theta = 0$ case), no resonance is supported, leading to an emissivity of 0, which means all the incoming light is reflected from the structure. In other words, no quasi-BIC resonance is observed. As θ increases, the emissivity values increase up to $\pi/25$, where it reaches almost unity. Further increase in θ results in lower emissivity values. It is important to stress that emissivity intensity can be tuned by only changing the relative orientation without moving the resonance wavelength, which can be handy in sensing applications.

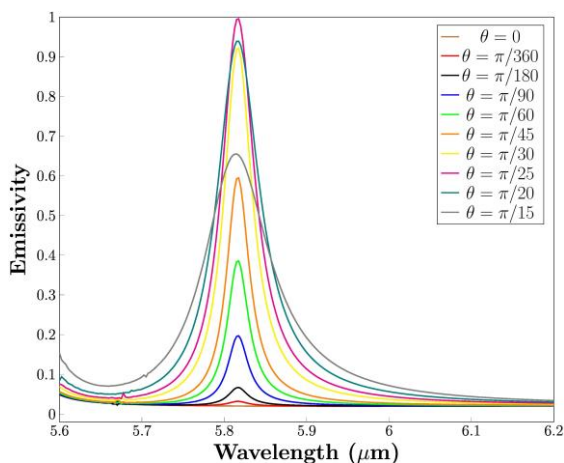


Figure 3. Emissivity spectra of dielectric metasurface thermal emitter with different angles of rotation.

3.3. Parameter Sweep of Length Asymmetry

Another asymmetry parameter is introduced by having rectangular rods with different lengths by changing length asymmetry, which is defined as the original length of the bar, which is the length of the more extended bar, and the length difference, which is the removed length in the shorter bar. Like the separation angle sweep case, we only tune one parameter. So, in all the numerical simulations done in this section, the bars are rotated by $\pi/25$ in opposite directions.

Figure 4 (a) shows emissivity of dielectric metasurfaces when the length asymmetry (α_l) is tuned from 0 to 0.4. The length of the original shorter band becomes equal to the longer rod (3100 nm) when α_l is 0. The length of the shorter rod decreases as α_l increases and becomes 1860 nm for $\alpha_l = 0.4$. As can be clearly seen, resonance wavelength redshifts, and resonance intensity drops when α_l is reduced from the original value of 0.3. Any further increase of α_l from the original value results in a blueshifted resonance wavelength accompanied by lower emissivity intensity.

Figure 4 (b) displays the resonance wavelength vs length asymmetry parameter. The resonance wavelength linearly decreases with increasing α_l values. So, it is possible to design a bespoke thermal emitter at the intended resonance wavelength. One of the most important realizations of this figure is that the

resonance condition occurs even when the bars are of the same length; that is α_l is 0, which is expected as the rods are still rotated away from each other and very similar structures using elliptical disks with same lengths instead of rectangular rods can be found in the literature [14].

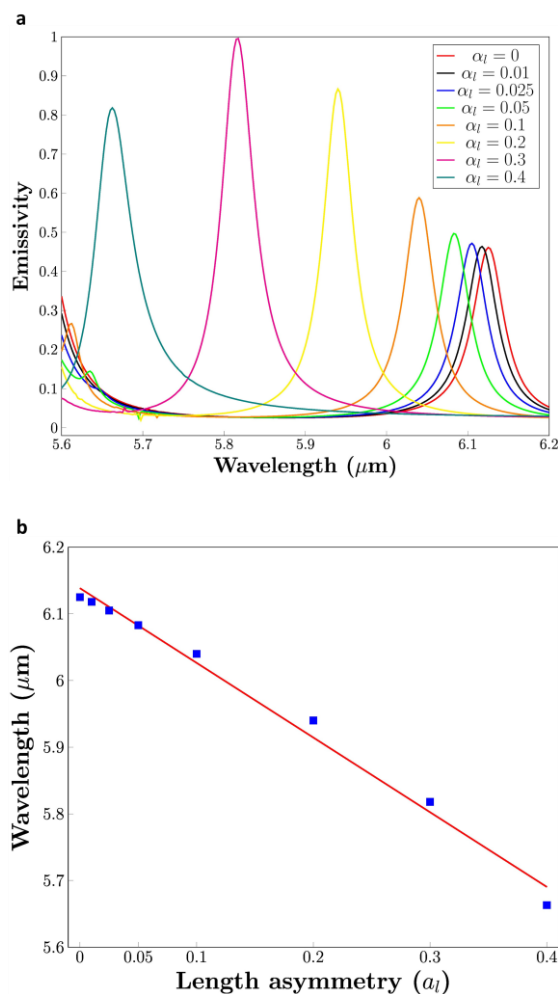


Figure 4. (a) Emission spectra of the thermal emitter with eight different length asymmetry parameters and (b) resonance wavelength with respect to asymmetry parameter.

IV. CONCLUSIONS

This study introduces a narrowband thermal emitter structure with tunable emissivity intensity and resonance wavelength. The structure consists of dielectric rectangular rods with different lengths and opposite orientations to induce quasi-BIC resonance. Silicon rods sit atop a spacer layer of Al_2O_3 and are placed on a gold substrate. Based on numerical studies, an emissivity value exceeding 0.99 is obtained at the resonance wavelength of $5.818 \mu\text{m}$ by diligently tuning asymmetry parameters.

The quasi-BIC inside the dielectric metasurface supports the resonance. The linewidth of emissivity is found to be 50 nm, corresponding to a Q factor of 116

which is roughly an order of magnitude higher than metal-based emitters. We also show that resonance wavelength can be tuned by changing the length asymmetry, whereas emissivity intensity can be tuned by modifying the rotation angle without changing the resonance wavelength. Although we study the effect of length asymmetry and rotation separately, this study can be extended to evaluate possible nonlinear dependencies between these two parameters. To our knowledge, this is the first thermal emitter design with double asymmetric features.

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