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Ultrabroadband super-Planckian radiative heat transfer with artificial continuum cavity states in patterned hyperbolic metamaterials

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Localized cavity resonances due to nanostructures at material surfaces can greatly enhance radiative heat transfer (RHT) between two closely placed bodies owing to stretching of cavity states in momentum space beyond the light line. Based on such understanding, we numerically demonstrate the possibility of ultrabroadband super-Planckian RHT between two plates patterned with trapezoidal-shaped hyperbolic metamaterial (HMM) arrays. The phenomenon is rooted not only in HMM’s high effective index for creating subwavelength resonators but also its extremely anisotropic isofrequency contour. The two properties enable one to create photonic bands with a high spectral density to populate a desired thermal radiation window. At submicron gap sizes between such two plates, the artificial continuum states extend outside the light cone, tremendously increasing overall RHT. Our study reveals that structured HMM offers unprecedented potential in achieving a controllable super-Planckian radiative heat transfer for thermal management at nanoscale.

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Near-field-mediated radiative heat transfer (RHT) exceeding the far-field blackbody limit [1] has attracted increased attention in recent years [2], not only because it unfolds an unexplored fundamental scientific field, but also because it holds technological importance towards nanogap thermophotovoltaics, scanning near-field thermal microscopy, thermal logics, etc. Commonly, materials supporting surface-guided waves at infrared frequency were investigated for achieving such phenomenon, since surface modes especially at frequency close to their resonances offer extra channels of energy transfer due to evanescent-wave coupling at small gaps. Surface-wave-bearing materials at infrared include polar dielectrics supporting surface phonon polaritons [3, 4], doped silicon supporting surface plasmon polaritons [5], and more recently grooved metal surfaces supporting the so-called spoof surface plasmon polaritons [6–9]. The presence of surface modes leads to spectrally enhanced quasimonochromatic heat flux around their resonance frequencies. Contrary to the extensive attentions paid to surface modes, localized resonant modes were rarely mentioned for achieving near-field-enhanced RHT. Localized or cavity resonances at infrared or even optical frequencies can be readily created using today’s nanofabrication technologies. Spatial localization of such modes usually corresponds to enormous extension of the modes in momentum (wave vector k) dimension. Such flat bands can potentially lie outside the light cone (bounded by k = ω/c) in frequency-momentum representation. Similar to surface-mode-based RHT scenario, presence of photonic states outside the light cone implies near-field energy transfer between two bodies, which can potentially amount to super-Planckian RHT. A direct advantage of cavity-resonance-based RHT is that one can arrange nanocavities with different resonant frequencies within unit cells of two plates to achieve enhanced RHT at multiple frequencies. With an exotic resonator design, as the current work will reveal, an ultrabroadband super-Planckian RHT can even be achieved.

Referring to Fig. 1, we consider RHT between two plates each consisting of a gold substrate and an array of trapezoidal-shaped hyperbolic metamaterial (HMM). The HMM is formed by a multilayer metal-dielectric stack. The two plates are separated by a vacuum gap g. The thicknesses of dielectric and metal are 95 and 20 nm, respectively. Each HMM cavity contains 20 dielectric-metal pairs. The cross section of a single cavity resembles a trapezoid with short base of wL = 0.4 μm, long base of wH = 1.9 μm, and height of h = 2.3 μm. The period of the HMM arrays is fixed at a = 2.0 μm. The relative permittivities of dielectric (Si) and metal (Au) are ϵSi = 11.7 and ϵAu(ω) = 1 − ωp4/(ω2(ω + iγ)2), in which ωp = 9 eV, and γ = 35 meV, respectively. Such structure can be fabricated with focused ion beam milling of deposited metal-dielectric multilayers [10], or with shadow deposition of dielectric and metal layers [11, 12].

The HMM, when truncated, helps to create subwavelength electromagnetic cavities, while the trapezoidal geometry is responsible for producing such resonances over a broad wavelength range. To simplify our argument in this paragraph, we neglect the gold substrates [13] and consider only k, wave-vector direction. A single HMM plate, when unpatterned, has an indefinite diagonal effective permittivity tensor, with negative x and y components and positive z component. Such an anisotropic slab, for the given geometry, guides a set of x-propagating p-polarized modes [14]. For frequency up to 300 × 1012 rad/s and even higher, the modes have almost similar linear dispersion curves, based on which one calculates the effective index (n_eff) of the HMM as ~3.77. When laterally truncated, p-polarized wave bounces between two truncation facets; each HMM patch therefore is a 2D high-index resonator. High-index material is essential for creating small-dimension resonators, especially at the upper wavelength limit for broadband RHT, that fit into a grating period a. Note also that, for achieving super-Planckian RHT at a wavelength λr, a needs to satisfy a < λr/2 in order for

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the resonance to cross the light line in the first Brillouin zone of the plate’s mode spectrum. The lower wavelength limit \( \lambda_{\text{min}} \) of desired broadband RHT would set \( a < \lambda_{\text{min}} / 2 \). The most intriguing property of such a HMM resonator, as will be further clarified in Fig. 3, is the weak dependence of its resonant frequencies on mode orders (with nodal breaking along \( z \)), or equivalently the resonator’s thickness. This sets the fundamental difference between using HMM and using an isotropic dielectric material. A trapezoidal profile-patterned HMM can therefore be treated as a series of vertically-stacked thin HMM resonators of varying widths, and in turn varying resonant frequencies, for achieving broadband operation.

We mention that a single array of such HMM resonators was previously found to exhibit broadband absorption of far-field radiation [15]. Near-field properties with implications to RHT were insofar left unexplored. There were also studies of RHT based on unpatterned HMM plates [16–21]; the results, as we will show later, can be radically different from RHT between patterned HMMs, principally due to lack of localized resonances. Here, using a rigorous full-wave scattering-matrix method [6,9], we calculate the RHT flux between two patterned HMM plates and numerically confirm ultrabroadband super-Planckian RHT at small gap sizes. In addition, we utilize a finite-element based eigenmode solver [22,23] to reveal the modal properties of the double-plate structure and identify that cavity modes play critical roles in enhancing RHT.

The radiative heat flux between two 1D periodic arrays can be expressed by

\[
q(T_1, T_2) = \frac{1}{2\pi} \int_0^\infty \left[ \Theta(\omega, T_1) - \Theta(\omega, T_2) \right] \Phi(\omega) d\omega,
\]

where \( \Theta(\omega, T) = \hbar \omega / \exp(\hbar \omega / k_B T) - 1 \) is the mean energy of Planck oscillators at temperature \( T \) and angular frequency \( \omega \). \( \Phi \) is integrated transmission factor

\[
\Phi(\omega) = \frac{1}{4\pi^2} \sum_{m,s,p} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} T_j(\omega, k_x, k_y) d k_x d k_y,
\]

\( T_j(\omega, k_x, k_y) \) is the transmission factor that describes the probability of a thermally excited photon transferring from one plate to the other, given polarization \( s \) or \( p \), and surface-parallel wave vector \( k_x \equiv (k_x, k_y) \) at \( \omega \).

Figure 2 plots the transmission-factor distributions \( (T \text{ maps}) \) over frequency and \( k_x \), while \( k_y \) is kept zero, for three types of plate configurations: unpatterned HMM plates [panels 2(a) and 2(b)], rectangular-profiled HMM plates [2(d) and 2(e)], and trapezoidal-profiled HMM plates [2(g) and 2(h)]. All configurations are mirror-symmetric. Note the \( T \) maps are shown only for \( k_x \) direction, along which the mode spectra of truncated HMM structures exhibit marked difference against the untruncated scenario. The calculation is repeated for two gap sizes: 1000 and 50 nm. For comparison purpose, in some \( T \) maps we selectively superimpose dispersion curves obtained from eigenmode calculations. In Fig. 2(a), when HMM is untruncated (\( g = 1000 \text{ nm} \)), the \( T \) map shows a thin line of states just below the light line. The states originate from a gap plasmon mode (GPM) confined mostly in the vacuum gap between the two HMM plates, as confirmed by the mode distribution [mode I in panel (c), or c-I] from eigenmode analysis. Further below the GPM states, there are a set of modes (c-II, c-III, c-IV) guided mostly in the HMMs; the number of modes is decided by the number of metal-dielectric layer pairs constructing the HMMs [14]. Only the bonding-type HMM-guided modes are shown. Owing to their strong confinements and the relatively large gap size, the fields in two HMM plates are hardly coupled, therefore having almost no contribution to the RHT process. Even when separation between the two plates is reduced to \( g = 50 \text{ nm} \), the contribution of the HMM-guided modes to RHT is trivial, as shown by the \( T \) map in Fig. 2(b), as well as its inset with a down-limited color scale. When HMM is truncated, mode structure in the two-plate system changes drastically. The GPM remains (f-I), but now with its field confined between the two gold substrates; an antibonding GPM (f-II) also emerges due to relatively large separation between two gold plates. Then, importantly, each HMM patch becomes a cavity; localized resonances happen (modes f-III, f-IV). The cavity mode fields are tightly confined laterally, which leads to almost flat dispersion curves of the modes, as shown in Fig. 2(d). The contribution of these cavity modes to RHT is evident in Fig. 2(d) with \( g = 1000 \text{ nm} \), and even more so in Fig. 2(e) with \( g = 50 \text{ nm} \).

Unlike resonators made of isotropic dielectric materials, the resonant frequencies of the HMM modes with different order numbers due to nodal breaking along \( z \) are quite close to each other. This can be understood by examining the iso-frequency contours of the HMM in bulk, shown in \( k_x \) and \( k_z \) axes (\( k_y = 0 \)) in Fig. 3. Three hyperbolic contours correspond to relatively close frequencies at 235, 245, and 255 \times 10^{12} \text{ rad/s} \). Given a 2D rectangular HMM cavity (of width \( w \) ) in Fig. 2(f), resonant frequencies of modes are decided by the modes’ corresponding \( k_x \) and \( k_z \) values. The fundamental mode has approximately \( k_x = \pi / w \) and \( k_z = 1.5 \pi / h \) [24]. For next higher-order mode with a nodal breaking along \( z \), \( k_z \) remains the same, and it has \( k_x = 2.5 \pi / h \), and so on. The first three cavity modes are indicated by three yellow dots in Fig. 3, vertically aligned. They are positioned quite near to \( 245 \times 10^{12} \text{ rad/s} \), which is in reasonably good agreement with Figs. 2(d) and 2(e). The fact that the modes with nodal breaking along \( z \) stay close in frequency is fundamentally decided by the extremely anisotropic hyperbolic isofrequency curves of the HMM. This is confirmed by a re-plot of Fig. 3 in its inset using equal axis scales. The hyperbolic curves are almost vertically lines. The isofrequency plot in Fig. 3 also suggests that it is the width of a 2D HMM cavity which determines the resonant frequencies of its modes. The cavity height (even very thin) does
not influence much the resonant frequencies. Knowing this, one can potentially create a cavity that supports resonances at multiple frequencies. Trapezoidal-profiled HMM structure as illustrated in Fig. 1 is a straightforward solution. Indeed, the computed $T$ map for $g = 1000$ nm exhibits ultrabroadband transmission factors [Fig. 2(g)]. The states contributing to RHT are so densely packed such that they form almost a continuum. The lower cut-off frequency of the continuum is determined by the bottom width of the trapezoids. High transmission factors extend beyond the light line, and at certain frequencies reach the first Brillouin zone edge. When the gap becomes smaller, at $g = 50$ nm, the continuum states extend to larger $k_x$ values; more evanescent states contribute to RHT. This lends the possibility of achieving an ultrabroadband super-Planckian RHT between two plates using trapezoidal-profiled HMMs. From eigen-mode calculations, we obtain modes responsible for the RHT process. Besides the GPM pair (modes i-I, i-II), we show modes i-III and i-IV, which offer a glimpse of cavity modes in the continuum. As characterized by their hot spots, the cavity modes now have very tight confinement, or correspondingly large $k_z$. The positions of hot spots reveal the mechanisms of their resonances. Mode i-III has hot spots at the middle section of the trapezoidal HMM cavity; it well corresponds to a resonant frequency just below $200 \times 10^{12}$ rad/s. Slight complication arises at higher frequencies. Mode i-IV, for example, has its hot spots located at both narrow- and wide-width sections of the HMM cavity; a wide HMM section can support a high-frequency resonance through nodal breaking along $x$ direction.

A full characterization of RHT between two plates requires a calculation of transmission factors for all $k_x$ over concerned frequency range. In Supplemental Material [25], we selectively plot $T_{\pm p}(k_x, k_y)$ maps at $\omega = 173 \times 10^{12}$ rad/s for various gap sizes. There we also explain the modal origin of the RHT states with the help of eigenmode analysis especially when $k_z = 0$ and $k_z \neq 0$. Generally speaking, as $k_z$ deviates
Integrated transmission-factor spectra, $\Phi(\omega)$, for the three types of HMM plate configurations as mentioned in Fig. 3 at gap sizes of 1000 and 50 nm. The trapezoidal-profiled HMM plates clearly exhibit the highest $\Phi$ over almost the whole frequency range when $g = 1000$ nm; at $g = 50$ nm, it has the highest $\Phi$ among the three structures at high frequencies (above $\sim 110 \times 10^{12}$ rad/s). At low frequencies, the homogeneous HMM plates have better RHT performance at small gap sizes.

That is because the effect of eddy current generation through magnetic-field coupling ($s$ polarization) between metal plates becomes prominent [9,26]; and the surface area at the nearest proximity between two plates decides the degree of such coupling (i.e., Derjaguin proximity approximation starts to apply). The broadband high $\Phi$ for the trapezoidal is dominantly due to the cavity mode continuum as shown in Figs. 3(g) and 3(h). The rectangular-profiled HMM plates show high $\Phi$ bands at certain frequencies (mainly at $\sim 235 \times 10^{12}$ rad/s) linked to cavity resonances in the HMM patches, as indicated in Fig. 3(d) and 3(e). It is worth noticing that the peak $\Phi$ value of the rectangular-profiled HMM structure is smaller than that of the trapezoidal-profiled HMM structure at the same frequency. This is due to the fact that the trapezoidal one can have extra resonances due to nodal breaking in $x$ direction, while similar high-order resonances do not exist for the rectangular counterpart in the considered frequency range. The homogeneous HMM structure shows featureless $\Phi$ spectra, because they do not sustain any cavity resonances but linearly dispersive guided modes [Figs. 3(a) and 3(b)]. As the gap size decreases down to 50 nm, the $\Phi$ spectrum of the trapezoidal-profiled HMM structure surpasses that of blackbody structure over the whole frequency range; ultrabroadband super-Planckian RHT occurs.

We further calculate spectral heat flux $q(\omega)$ between two plates with temperatures at 301 and 300 K for the mentioned HMM structures [Fig. 4(b)]. At $g = 50$ nm, the trapezoidal structure performs significantly better than blackbody plates, with 155% increase in $q$ at the highest-$q$ frequency of the blackbody-plate scenario (i.e., $150 \times 10^{12}$ rad/s). Note that the structure presented in this work is for demonstrating the flexibility of HMM-based plates for tailoring enhanced near-field RHT [$\Phi$ spectra in Fig. 4(a)] without considering specific plate temperatures in the first place. The actual heat transfer in measurable values [as $q$ spectra in Fig. 4(b)] depends further on exact temperature settings. In reality, towards a particular application, one should design the profile patterning (period, resonator width, trapezoid shape, etc.) such that one maximizes near-field RHT in measurable quantities either at a desired frequency range or over the whole spectrum.

The profile patterning of HMM layers is currently one dimensional, which results in inferior RHT when $k_i$ has inclination towards the $y$ direction. We envisage that a 2D periodic structuring of the HMM layer (pyramid array) [10] can give rise to isotropic enhancement in RHT in all $k_i$ directions owing to true localization of the cavities modes. In addition, in this work we have not optimized the metal and dielectric layer thicknesses (as well as the dielectric material type) in the HMM. It is likely one can have even higher effective index of the HMM by choosing appropriate geometrical and material parameters, so that one can further adjust the frequency range of the cavity mode continuum as well as the Brillouin zone size.
In conclusion, we numerically demonstrated one can achieve an ultrabroadband super-Planckian RHT with two closely spaced trapezoidal-profiled HMM plates. The design rests on two key properties of HMMs: high effective index for creating subwavelength resonators and extremely anisotropic isofrequency curves responsible for cavity-width-dependent resonance frequencies. The superiority of the trapezoidal-profiled patterning in achieving ultrabroadband enhanced RHT is explained through its capability of forming a cavity mode continuum. The transmission-factor maps derived from the scattering-matrix method were confirmed by dispersion curves calculated using an eigenmode mode solver. The contributing modes were further elucidated with the obtained mode field distributions. Our study reveals that highly localized cavity resonances, besides surface waves, do enhance RHT at small separation of two bodies. In this respect, structured hyperbolic media offers unprecedented control in creating cavity modes for achieving a controllable super-Planckian RHT.

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[13] The gold substrates are mainly to prevent transmission leakage; their presence also induces a surface mode between HMM and gold. However, the main contribution to near-field RHT is the cavity modes, whose existence persists even without the gold substrates.
[24] Extra 0.5π phase change is due to nearly perfect magnetic conductor condition at boundary in contact with gold.