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Hyperbolic Metamaterials as an Analog of a Blackbody in the Near Field

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We study the near-field heat exchange between hyperbolic materials and demonstrate that these media are able to support broadband frustrated modes which transport heat by photon tunneling with a high efficiency close to the theoretical limit. We predict that hyperbolic materials can be designed to be perfect thermal emitters at nanoscale and derive an upper limit for the heat flux due to hyperbolic modes.

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A blackbody is usually defined by its property of having a maximum absorptivity and therefore also a maximum emissivity by virtue of Kirchhoff's law [1]. The energy transmission between two blackbodies having different temperatures obeys the well-known Stefan-Boltzmann law. This law sets an upper limit for the power which can be transmitted by real materials, but it is itself a limit for the far-field only, since it takes only propagating modes into account. In terms of the energy transmission between two bodies, the blackbody case corresponds to maximum transmission for all allowed frequencies ω and all wave vectors smaller than ω/c , where c is the vacuum light velocity. This means that all the propagating modes are perfectly transmitted across the separation gap.

In the near-field regime, i.e., for distances smaller than the thermal wavelength $\lambda_{\text{th}} = \hbar c/k_B T$ ($2\pi\hbar$ is Planck's constant, k_B is Boltzmann's constant, and T is the temperature) the radiative heat flux is not due to the propagating modes, but it is dominated by evanescent waves [2–4] and especially surface polaritons as confirmed by recent experiments [5–11]. The common paradigm is that the largest heat flux can be achieved when the materials support surface polaritons which will give a resonant energy transfer which is, however, restricted to a small frequency band around the surface mode resonance frequency [3,4,12,13]. Many researchers have tried to find materials enhancing the nanoscale heat flux due to the contribution of the coupled surface modes by using layered materials [14,15], doped silicon [16,17], metamaterials [18–20], phase-change materials [21], and recently graphene [22].

In the present Letter, the aim is twofold. (i) We show, that materials supporting a broad band of evanescent frustrated modes can outperform the heat flux due to surface modes. This provides new possibilities for designing materials giving large nanoscale heat fluxes which could be used for thermal management at the nanoscale, for instance. (ii) We predict that hyperbolic materials can be designed to be perfect thermal emitters for near-field

radiation and can, in fact, be used to realize the near-field analog of a usual blackbody. Such an emitter can be defined as a medium which absorbs all incoming evanescent modes. That means that the energy transmission coefficient (TC) between two such media must be equal to one for all frequencies and all wave vectors larger than ω/c when the separation distance goes to zero. In particular, we derive an upper limit of the heat flux achievable with hyperbolic materials.

With today's nanofabrication techniques, it is possible to manufacture artificial materials such as photonic band gap materials and metamaterials which exhibit very unusual material properties like negative refraction [23]. Because of such properties they are considered as good candidates for perfect lensing [24,25], for repulsive Casimir forces [26–29] and enhanced or tunable radiative heat flux at the nanoscale [18–20,30–32] to mention a few.

There exists a class of uniaxial metamaterials for which the permittivity and permeability tensor elements are not all of the same sign [33]. In particular, for such materials the dispersion relation for the solutions of Helmholtz's equation inside the material is not an ellipsoid as for normal uniaxial materials [34] but a hyperboloid [35–37]. For this reason such materials are also called hyperbolic materials. These materials have already been considered for super-resolution imaging [38] and enhanced thermal conductivity inside the material itself [39], for instance. Here we focus on the heat flux between two bodies consisting of hyperbolic materials showing that these materials can have large TCs for a broad frequency range resulting in large heat fluxes and that they can be used to realize a blackbody at the nanoscale.

The nanoscale heat flux Φ between two semi-infinite materials separated by a vacuum gap of thickness d having the temperatures $T + \Delta T$ and T can be written in terms of the quantum of thermal conductance $\pi^2 k_B^2 T/3h$ [40] and the sum over all transversal modes as [41]

$$\Phi = \frac{\pi^2 k_B^2 T}{3h} \left[\sum_{j=s,p} \int \frac{d^2 \kappa}{(2\pi)^2} \bar{\mathcal{T}}_j \right] \Delta T, \quad (1)$$

where $\boldsymbol{\kappa} = (k_x, k_y)^t$ is the lateral wave vector. The mean TC introduced here is defined as

$$\bar{\mathcal{T}}_j = \frac{\int du u^2 e^u (e^u - 1)^{-2} \mathcal{T}_j(u, \kappa)}{\int du u^2 e^u (e^u - 1)^{-2}}, \quad (2)$$

where $u = \hbar\omega/k_B T$ is a rescaled frequency or energy and $\mathcal{T}_j(\omega, \kappa)$ is the energy TC for s - and p -polarized modes in (ω, κ) space. For isotropic and anisotropic semi-infinite materials the explicit expression of this energy TC is known and can be found in Refs. [2,42,43].

From Eq. (1) it is obvious that the heat flux Φ can be increased on the one hand by increasing the mean TC for a transversal mode with a given κ or by increasing the number of modes contributing significantly to the heat flux on the other. As discussed in Refs. [4,41], the number of propagating modes contributing to the heat flux is limited due to the fact that the dispersion relation of these modes $\kappa^2 + k_{z0}^2 = \omega^2/c^2$ restricts for a fixed frequency the modes to a circle $\kappa \leq \omega/c$. For dielectric materials the frustrated internal reflection modes [44] which can also contribute to the heat flux for distances $d < \lambda_{th}$ the dispersion relation reads $\kappa^2 + k_{z1}^2 = \epsilon\omega^2/c^2$ so that in this case the contributing modes are for a fixed frequency restricted to a circle $\kappa < \sqrt{\epsilon}\omega/c$.

It is known that in presence of resonant surface modes such as surface phonon polaritons (SPhP) [45,46] in the infrared the heat flux at nanoscale can be increased by several orders of magnitude with respect to the blackbody value [12,13] (see Fig. 1). In terms of the mean TC $\bar{\mathcal{T}}_j$ it can be shown [41] that the transmission of these modes is very small (less than one percent, see Fig. 3 of Ref. [41]),

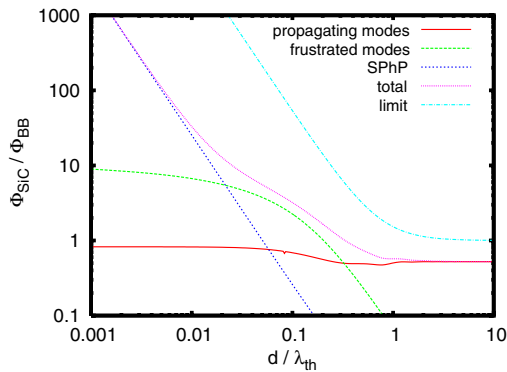


FIG. 1 (color online). Heat flux Φ from Eq. (1) between two semi-infinite SiC bodies over distance in units of thermal wavelength λ_{th} . Φ is normalized to the blackbody value Φ_{BB} for temperature $T = 300$ K and $\Delta T = 1$ K. The plot also shows the contribution of the propagating and frustrated modes and the SPhP and the limit consisting of the expression in Eq. (9) plus the usual blackbody value.

but the contributing modes for very small distances extend up to $\kappa < \log[2/\text{Im}(\epsilon)]/(2d)$. First, this means that the number of contributing modes goes like $1/d^2$ for very small distances so at very small distances the SPhP contribution to the heat flux becomes larger than the contribution of the frustrated total internal reflection modes. Therefore, the SPhP provide the dominant heat flux channel at the nanoscale despite the fact that their TC is rather small [41]. Second, the upper limit of the wave vectors κ for the contributing modes also depends on the intrinsic losses [41,47] of the material. Note, that there is a fundamental restriction to $\kappa < \pi/a$ where a is for polar materials given by the lattice constant so that there is also a definitive limit for the nanoscale heat flux [48,49].

Now we are in a position to discuss the heat flux for hyperbolic materials. Such materials are a special class of anisotropic uniaxial materials. The dispersion relation for extraordinary waves in uniaxial materials with an optical axis normal to the surface reads [34]

$$\frac{\kappa^2}{\epsilon_{\perp}} + \frac{k_{z1}^2}{\epsilon_{\parallel}} = \frac{\omega^2}{c^2}, \quad (3)$$

where ϵ_{\perp} and ϵ_{\parallel} are the permittivities for the electric field components perpendicular and parallel to the surface, respectively, having an opposite sign [33]. Hence, the dispersion relation describes not an ellipse in the (κ, k_z) plane but a hyperbolic function as illustrated in Fig. 2(b). This means that in principle without losses the κ which can fulfill the dispersion relation (3) extend up to the above mentioned fundamental restriction of π/a . In the following, we will call such modes hyperbolic modes (HM). If we consider the nanoscale heat flux for such materials then the number of contributing modes is for $d \gg a$ only restricted by the intrinsic cutoff in the energy TC which is $\mathcal{T}_j(\omega, \kappa) \propto \exp(-2\kappa d)$ for $\kappa \gg \omega/c$ [see Eq. (6)]. It follows that the heat flux due to the HM scales for small distances like $1/d^2$ as the contribution of the SPhP. When $\epsilon_{\parallel} > 0$ and $\epsilon_{\perp} < 0$ ($\epsilon_{\parallel} < 0$ and $\epsilon_{\perp} > 0$) the HM are

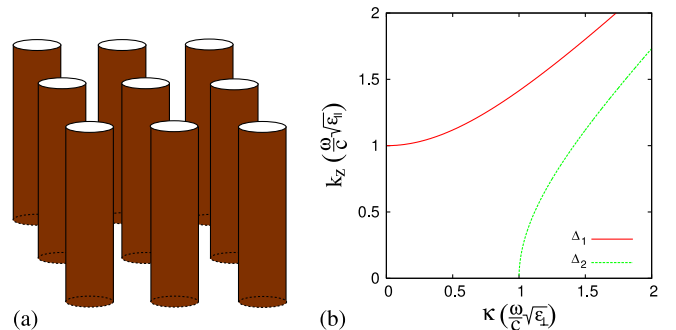


FIG. 2 (color online). (a) Sketch of a hyperbolic material consisting of a periodical array of nanowires. (b) Hyperbolic dispersion relation for a fixed frequency within the bands Δ_1 and Δ_2 in Fig. 3(a). For Δ_1 (Δ_2) we have $\epsilon_{\parallel} > 0, \epsilon_{\perp} < 0$ ($\epsilon_{\parallel} < 0, \epsilon_{\perp} > 0$).

evanescent in the vacuum gap and propagating inside the hyperbolic material for $\kappa > \omega/c$ ($\kappa > \epsilon_{\perp} \omega/c$). Since both kinds of HM are evanescent inside the vacuum region, i.e., for small distances $d \ll \lambda_{\text{th}}$ they are a special kind of frustrated internal reflection modes. As for usual frustrated modes we can expect a large mean TC for the HM up to $\kappa \approx 1/(2d)$ if they exist in a broad frequency band. Since the mean TC for the SPhP was found to be very small, because these modes are restricted to a small frequency band around the surface mode frequency, we can expect to have a heat flux due to the HM larger than that of the coupled SPhP.

In order to see whether our expectation is true, we consider a simple example of a uniaxial material which is given by periodically positioned nanowires [50] of SiC as sketched in Fig. 2(a). In the long wavelength limit [42] we can describe the effective material properties by the Maxwell-Garnett expressions [51]

$$\epsilon_{\parallel} = \frac{\epsilon(\omega)(1+f) + (1-f)}{\epsilon(\omega)(1-f) + (1+f)}, \quad (4)$$

$$\epsilon_{\perp} = (1-f) + \epsilon(\omega)f. \quad (5)$$

Here f is the volume filling fraction of the SiC wires and $\epsilon(\omega)$ is the permittivity of SiC [46]. As pointed out in Refs. [37,42], the effective medium theory is limited to distances $d > a/\pi$, where a is in contrast to the above given fundamental restriction the lattice constant of the nanowires. For smaller distances a nonlocal model for the permittivity would be necessary.

Since the optical axis of the considered material is perpendicular to the surface the s - and p -polarized modes decouple and we have only extraordinary waves for p polarization [34]. Then the energy TC \mathcal{T}_j for two identical half-spaces which enters into Eq. (2) reads [42]

$$\mathcal{T}_j(\omega, \kappa; d) = \begin{cases} (1 - |r_j|^2)/|D_j|^2, & \kappa < \omega/c \\ 4[\text{Im}(r_j)]^2 e^{-2|k_{z0}|d}/|D_j|^2, & \kappa > \omega/c, \end{cases} \quad (6)$$

for $j = \{s, p\}$, where $D_j = 1 - r_j^2 e^{2ik_{z0}d}$ is the Fabry-Pérot-like denominator, $k_{z0} = \sqrt{\omega^2/c^2 - \kappa^2}$, and

$$r_s(\omega, \kappa) = \frac{k_{z0} - k_s}{k_{z0} + k_s} \quad \text{and} \quad r_p(\omega, \kappa) = \frac{\epsilon_{\parallel} k_{z0} - k_p}{\epsilon_{\parallel} k_{z0} + k_p}, \quad (7)$$

introducing $k_s = \sqrt{\epsilon_{\parallel} \omega^2/c^2 - \kappa^2}$ and $k_p = \sqrt{\epsilon_{\perp} \omega^2/c^2 - \frac{\epsilon_{\parallel}}{\epsilon_{\perp}} \kappa^2}$. From the expression for the reflection coefficients it becomes obvious that only the extraordinary waves represented by r_p are sensitive to ϵ_{\perp} and ϵ_{\parallel} . Hence, only the p -polarized part can support HM. For magnetic materials also the s -polarized part can support HM.

In Fig. 3(a), we plot $\text{Re}(\epsilon_{\parallel})$ and $\text{Re}(\epsilon_{\perp})$ in a frequency range around the transversal and longitudinal phonon frequency of SiC ($\omega_T = 1.495 \times 10^{14}$ rad/s and $\omega_L =$

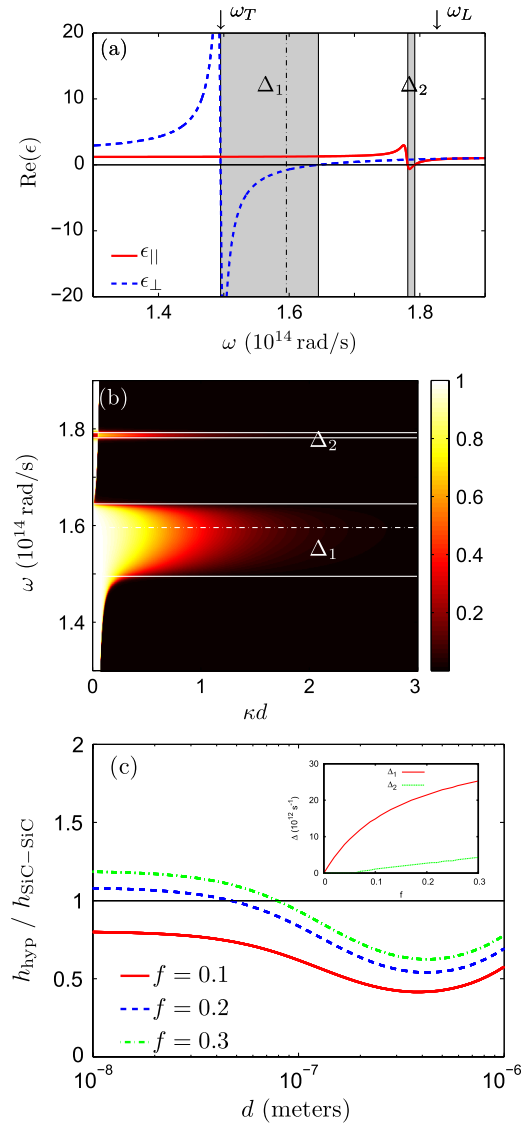


FIG. 3 (color online). (a) Real part of ϵ_{\parallel} and ϵ_{\perp} defined in Eqs. (4) and (5) with $f = 0.1$. The two gray areas mark the frequency regions Δ_1 and Δ_2 where both permittivities have different signs, i.e., where the modes fulfill a hyperbolic dispersion relation. Vertical dashed line: frequency where $\text{Re}(\epsilon_{\perp})\text{Re}(\epsilon_{\parallel}) = -1$. (b) Transmission coefficient $\mathcal{T}_p(\omega, \kappa)$ choosing $d = 100$ nm for the same frequency region and the same volume filling fraction showing high transmission for regions Δ_1 and Δ_2 . Horizontal dashed line: frequency where $\text{Re}(\epsilon_{\perp})\text{Re}(\epsilon_{\parallel}) = -1$. For this frequency κ has its maximum value (see Ref. [52]). (c) Heat transfer coefficient for two hyperbolic materials with $f = 0.1, 0.2, 0.3$ normalized to the value for two flat SiC half spaces ($T = 300$ K). Inset: Δ_1 and Δ_2 over f .

1.827×10^{14} rad/s) using $f = 0.1$. The regions Δ_1 and Δ_2 where the permittivities have different signs are highlighted. Within these frequency bands we have HM. In Fig. 3(b), it can be seen that the TC $\mathcal{T}_p(\omega, \kappa)$ is close to one for these modes up to $\kappa d \approx 1/2$. Furthermore, we observe in Fig. 3(b) that for the chosen parameters we

have no coupled SPhP in our hyperbolic material so that the heat flux is only due to the usual frustrated modes and the HM. It can be shown that for filling factors $f < 1/3$ there are no surface modes in our structure regardless of the material used for the nanowires [52].

By increasing the filling factor in our structure the two regions Δ_1 and Δ_2 supporting HM get broader [see inset of Fig. 3(c)] resulting in larger heat fluxes in the small distance regime around $d = 100$ nm. It can be seen in Fig. 3(c) that in this distance regime the heat flux due to HM can be larger than that by SPhP for two SiC media. This makes clear that the goal for designing a hyperbolic material with elevated heat fluxes is to make the bands for HM as broad as possible. This can be done by changing the constituents of the hyperbolic material and by considering different geometries like, for example, different nanowire structures or nanolayered materials.

Now we derive a theoretical limit for the heat flux due to HM. That means we will start with the general expression for the heat flux in Eq. (1) using the reflection coefficients in Eqs. (7) without assuming a special realization of the hyperbolic material as the example of the nanowired material. The only assumptions for the underlying structure made are that we have a uniaxial local medium with its optical axis parallel to the surface normal. Before we start, we remind the reader that the usual blackbody limit can be obtained from Eq. (1) by considering the limits $\text{Re}(\epsilon_{\perp}), \text{Re}(\epsilon_{\parallel}) \rightarrow 1$ and $\text{Im}(\epsilon_{\perp}), \text{Im}(\epsilon_{\parallel}) \rightarrow 0$ for all frequencies. Then the $r_p \rightarrow 0$ and therefore $\mathcal{T}_p \rightarrow 1$ for $\kappa < \omega/c$ and $\mathcal{T}_p \rightarrow 0$ for $\kappa > \omega/c$.

With a similar reasoning we will now derive the theoretical limit for near-field radiation by the HM. For convenience, we consider only the case $\text{Re}(\epsilon_{\parallel}) > 0$ and $\text{Re}(\epsilon_{\perp}) < 0$. Let us first again assume that $\text{Im}(\epsilon_{\perp}), \text{Im}(\epsilon_{\parallel}) \rightarrow 0$ for all frequencies then we can recast the reflection coefficient for p -polarized waves as

$$r_p = \frac{ai - 1}{ai + 1}, \quad (8)$$

where we have introduced the symbol $a = \sqrt{\epsilon_{\parallel}|\epsilon_{\perp}|}\gamma/\gamma_{\perp}$ with $\gamma^2 = \kappa^2 - \omega^2/c^2$ and $\gamma_{\perp}^2 = |\epsilon_{\perp}|\omega^2/c^2 + \kappa^2$. Since we consider only the frustrated total internal reflection modes ($\kappa > \omega/c$) a is a real number. Hence, as can be expected for total internal reflection modes we have $|r_p|^2 = 1$. Plugging this reflection coefficient into the TC for the evanescent modes in Eq. (6) we find that $\mathcal{T}_p = 1$ for $|k_{z0}|d \ll 1$. On the other hand, for $|k_{z0}|d \gg 1$ we find that \mathcal{T}_p has a maximum for $r_p = \pm i$. It follows from Eq. (8) that the condition for having perfect transmission is $a^2 = 1$ which translates in the quasistatic regime ($\kappa \gg \omega/c$) into $\epsilon_{\parallel}|\epsilon_{\perp}| = 1$.

Finally, we can derive the maximum heat flux due to the frustrated HM by plugging $r_p = \pm i$ into the expression for the TC in Eq. (6) and evaluating Eq. (1) for the heat flux.

Then, we find a maximum heat transfer coefficient ($\Phi = h\Delta T$) of

$$h_{\max,p} = \frac{1}{\pi d^2} \left(\frac{\pi^2 k_B^2 T}{3h} \right) \frac{\ln(2)}{2}. \quad (9)$$

Note, that this limit is a limit for the HM only and can in principle be exceeded by mechanisms which have large wave vector contributions to the TCs, i.e., for $\kappa > 1/(2d)$ as for example the surface mode contribution and adsorbates [4]. We note that the result in Eq. (9) is by a factor $\ln(2)/2$ smaller than the upper limit found in Ref. [53], which was derived for the surface mode contribution.

To illustrate the potential of hyperbolic materials for near-field heat fluxes, let us now compare the upper limit in Eq. (9) with known results. For $T = 300$ K, the heat transfer coefficient for a blackbody is about $6.1 \text{ W m}^{-2} \text{ K}^{-1}$. According to Eq. (9), its near-field counterpart is $h_{\max,p} \approx 3.1 \times 10^5 \text{ W m}^{-2} \text{ K}^{-1}$. Hence, $h_{\max,p}$ is by a factor of about 285 (36) larger than the heat flux between two gold (SiC) plates. Finally, we compare the limit for the heat transfer coefficient due to photon tunneling of HM from Eq. (9) with a numerically found upper limit for Drude materials for the heat transfer coefficient due to the coupling of surface plasmon polaritons (we have calculated the heat transfer coefficient using the parameter set A of Ref. [54], see also Ref. [52]). We find that this value is about 0.6 times $h_{\max,p}$ at $d = 100$ nm. When doing a similar procedure for our nanowire material we already find an optimum value of about 0.5 times $h_{\max,p}$ [52]. Further optimization of the design and the material components will certainly push the heat flux closer to $h_{\max,p}$.

In conclusion, we have studied the near-field heat transfer between hyperbolic materials and we have shown with a simple example that the broadband spectrum of frustrated modes supported by these media allows us to get heat fluxes which are larger than the heat flux due to narrow-band coupled surface polariton modes (see Ref. [52] for more details). We have demonstrated that hyperbolic materials can be used to achieve perfect transmission for wave vectors smaller than $1/(2d)$ and we have derived a theoretical limit of the heat flux due to HM. This opens up new possibilities to achieve large heat fluxes at the nanoscale by the design of hyperbolic materials. In particular, we find that hyperbolic structures are especially useful to turn poor near-field emitters into very good near field emitters [52].

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