Thermal emission from finite photonic crystals

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ABSTRACT

We present a microscopic theory of thermal emission from truncated photonic crystals and show that spectral emissivity and related quantities can be evaluated via standard bandstructure computations without any approximation. We then analyze the origin of thermal radiation enhancement and suppression inside photonic crystals and demonstrate that the central quantity that determines the thermal radiation characteristics such as intensity and emissive power is the area of the iso-frequency surfaces and not the density of states as is generally assumed. We also identify the physical mechanisms through which interfaces modify the potentially super-Planckian radiation flow inside infinite photonic crystals, such that thermal emission from finite-sized samples is consistent with the fundamental limits set by Planck's law. As an application, we further demonstrate that a judicious choice of a photonic crystal's surface termination facilitates considerable control over both the spectral and angular thermal emission properties. Finally, we outline design principles that allow the maximization of the radiation flux, including effects associated with the isotropy of the effective Brillouin zone, photonic band gap size and flatness of the band structure in the spectral range of interest.

Keywords: photonic crystals, photonic band gaps, thermal radiation

1. INTRODUCTION

Photonic crystals (PhCs) offer the potential to controllably alter light-matter interaction and light propagation on a fundamental level.\textsuperscript{1–3} Early theoretical studies have unveiled profound modifications of the fluorescence properties of individual emitters embedded in PCs, but despite significant progress, experimental investigations of such systems remain rather challenging. Experimentally more accessible is thermally driven fluorescence, i.e. thermal emission from emitters embedded in PhCs.\textsuperscript{4–6} Besides the scientific relevance of the investigation of thermal emission from PhCs, numerous technological application, such as thermo-photovoltaic energy conversion devices and light sources, will benefit from a detailed understanding of the underlying physics.\textsuperscript{6–9}

Here, we address the effect interfaces on the thermal radiation flux emitted by PhCs. Our formalism is an extension of our earlier work\textsuperscript{10,11} and solely relies on a natural modal expansion of the electromagnetic field that can be related to standard photonic bandstructure computations without invoking any approximation. Such a general framework enables several significant advances. First, while our theory for infinite PhCs shows that the thermal radiation intensity may exceed the free-space blackbody (BB) limit,\textsuperscript{10,11} it is, on thermodynamic grounds\textsuperscript{7} (verified by direct simulation\textsuperscript{12,13}), clear that the introduction of an interface must limit the maximally allowed thermal emission from truncated PhCs to the BB limit set by Planck’s law. Understanding the balance between these two physical mechanisms (energy transport velocity effects of infinite PhCs and reflection at PhC interfaces) is, thus, essential for the analysis of thermal emission from finite PhC samples. Second, our formalism allows to evaluate the spectral and angular characteristics of thermal emission from PhCs "bottom-up" (i.e., without invoking Kirchhoff’s law or any variation thereof) and can be used to design future applications based on the ability to engineer the electromagnetic modes properties, such as group velocity and reflection at interfaces.

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2. THERMAL RADIATION IN INFINITE PHOTONIC CRYSTALS

The strong scattering of light inside PhCs leads to a redistribution of the photonic modes and thus to significant modifications of the thermal flux as compared to the case of homogeneous bodies. In particular, it has been shown that the area of the iso-frequency surface is the central quantity that determines the thermal radiation characteristics at frequency $\omega$, and that the thermal radiation flux may display striking focusing effects.\textsuperscript{10,11} We briefly review here the microscopic theoretical framework describing thermal radiation emission in infinite PhCs that are in thermal equilibrium.\textsuperscript{10,11}

The flow of electromagnetic energy in PhCs is described by the time-averaged Poynting’s vector which is defined as the energy per unit time per unit area that is carried by a the electromagnetic field. The time-averaged Poynting vector can be resolved into the individual Bloch modes according to

\[
\mathbf{S}(r) \equiv \text{Re} \left[ \mathbf{E}(r,t) \times \text{Re} \left[ \mathbf{H}(r,t) \right] \right] = \sum_{n,k} \mathbf{S}_{n,k}(r),
\]

where $\mathbf{E}$ and $\mathbf{H}$ are the electric and magnetic field, respectively, and $\text{Re}$ denotes the real part of a complex number. The group velocity is defined as the energy per unit time per unit area that is carried by a electromagnetic field. The time-averaged Poynting vector can be resolved into the individual Bloch modes according to

\[
\mathbf{S}_{n,k}(r) \equiv \text{Re} \left[ \mathbf{E}_{n,k}(r) e^{-i\omega_n k \cdot r} \right] \times \text{Re} \left[ \mathbf{H}_{n,k}(r) e^{-i\omega_n k \cdot r} \right]
\]

In the following, we adopt a simplified approach and spatially average the flow of the electromagnetic radiation over a PhC unit cell. To this end, we introduce the energy velocity for a given Bloch mode in the form

\[
\mathbf{v}_{n,k}^{(c)} = \frac{1}{V} \int d\mathbf{r} \mathbf{S}_{n,k}(r) = \mathbf{v}_{n,k}^{(g)} \mathbf{e}_{n,k},
\]

where $V$ is the volume of a unit cell and we have decomposed the group velocity into its magnitude $v_{n,k}^{(g)}$ and direction $\mathbf{e}_{n,k}$. It can be shown\textsuperscript{14} that in a PhC the energy velocity coincides with the group velocity $v_{n,k} \equiv \nabla_\mathbf{k}\omega_{n,k}$ such that the spatially averaged energy current of electromagnetic radiation for a given Bloch mode, $J_{n,k}(T)$, reads as

\[
J_{n,k}(T) = \frac{1}{V} \int d\mathbf{r} \mathbf{S}_{n,k}(r) = i_{n,k}(T) \mathbf{e}_{n,k}.
\]

Here, we have introduced

\[
i_{n,k}(T) = v_{n,k}^{(g)} u_{n,k}(T).
\]

We now proceed and introduce certain physical quantities that are usually used to describe thermal radiation:\textsuperscript{15}

(i) $i(\omega, \theta_s, \phi_s, T)$, the directional spectral intensity defined as the energy emitted per unit time, per unit frequency interval $d\omega$ around $\omega$, per unit elemental projected surface area $dA_p$ normal to the direction $\mathbf{s}$ (defined by $\theta_s, \phi_s$), and into a unit elemental solid angle $d\Omega_s$ around the direction $\mathbf{s}$.

(ii) $e(\omega, \theta_s, \phi_s, T)$, the directional spectral emissive power defined as the energy emitted per unit time, per unit frequency interval $d\omega$ around $\omega$, per unit elemental surface area $dA$, and into a unit elemental solid angle $d\Omega_s$ around the direction $\mathbf{s}$,

\[
e(\omega, \theta_s, \phi_s, T) = i(\omega, \theta_s, \phi_s, T) \cos \theta_s.
\]
(iii) $I(\omega, T)$, the average spectral intensity, defined as the average energy per unit time, per unit frequency interval $d\omega$ around $\omega$, per unit elemental projected surface area $dA_p$, emitted into the $4\pi$ solid angle,

$$I(\omega, T) = \frac{1}{4\pi} \int_0^{\pi/2} \int_0^{\pi/2} \sin \theta_s \sin \theta_e \, \omega_{n,k} \, \eta_{n,k}(\omega, \theta_s, \phi_s, T).$$

(7)

(iv) $E(\omega, s, T)$, the hemispherical spectral emissive power, defined as the energy per unit time, per unit frequency interval $d\omega$ around $\omega$, per unit elemental surface area $dA$ normal to the direction $s$, emitted into the positive $s$ semi-plane,

$$E(\omega, s, T) = \int_0^{\pi/2} \int_0^{\pi/2} \sin \theta_s \sin \theta_e \, \epsilon_{n,k}(\omega, \theta_s, \phi_s, T).$$

(8)

(v) $I(T)$, total intensity, defined as the energy per unit time, per unit elemental projected surface area $dA_p$, emitted into the positive $s$ semi-plane,

$$I(T) = 4\pi \int d\omega \, I(\omega, T) = \int_0^{\pi/2} \int_0^{\pi/2} \sin \theta_s \sin \theta_e \, i(\omega, \theta_s, \phi_s, T).$$

(9)

(vi) $E(s, T)$, hemispherical total emissive power, defined as the energy per unit time, per unit elemental surface area $dA$, emitted into the positive $s$ semi-plane,

$$E(s, T) = \int d\omega \, E(\omega, s, T).$$

(10)

Given that, for a specific Bloch mode, the group velocity and its $k_e$-vector index may have different orientations, the evaluation of the angle-dependent spectral intensity and emissive power raises the conceptual problem of how to map the reciprocal space representation of, say, the averaged energy current (5) onto the desired real-space quantities. To facilitate this, we introduce

(i) $i_{n,k}(T)$, the directional mode-intensity defined by the energy per unit time, per mode $\{n, k\}$, per unit elemental projected surface area $dA_p$ normal to the direction $e_{n,k}$ (defined by $\theta_{e_{n,k}}, \phi_{e_{n,k}}$).

(ii) $e_{n,k}(T)$, the directional mode-emissive power defined by the energy per unit time, per mode $\{n, k\}$, per int elemental surface area $dA$ normal to the direction $e_{n,k}$ (defined by $\theta_s, \phi_s$),

$$e_{n,k}(T) = i_{n,k}(T) \cos \theta_{e_{n,k}}.$$

(11)

Then, the total intensity and hemispherical total emissive power, can be represented as

$$I(T) = \sum_{n,k} i_{n,k},$$

(12)

$$E(s, T) = \sum_{\{n,k\}, e_{n,k} \cdot \hat{s} \geq 0} e_{n,k} = \sum_{n,k} i_{n,k} \cos \theta_{e_{n,k}}.$$  

(13)

Here, we have chosen the $z$-axis of our system to be oriented along $s$ and have introduced the restricted summation $\sum'$ over modes for which $e_{n,k} \cdot \hat{s} \geq 0$.

With the help of (5b) of $i_{n,k}(T)$, we obtain

$$I(T) = \sum_{n,k} \hbar \omega_{n,k} n_{n,k}(T) \nu_{n,k},$$

(14)

$$E(s, T) = \sum_{n,k} \hbar \omega_{n,k} n_{n,k}(T) \nu_{n,k} \cdot \hat{s}.$$  

(15)
We note the fact that, in general, the group velocity cannot be represented as a functional of the dispersion relation

\[ v_{n,k}^{(g)} \equiv \nabla_k \omega_{n,k} \neq \mathcal{F}(\omega_{n,k}), \]

This means that it is not possible to convert the expressions of the radiation flux in Eq. (14) Eq. (15) into a simple frequency integral involving only the photonic DOS. Rather, in order to arrive at spectral representations, we have to employ a procedure similar to the introduction of the local DOS\(^{16}\) in spontaneous emission calculations: We insert the identity \(1 = \int_0^\infty d\omega \delta(\omega - \omega_{n,k})\) into Eq. (14) Eq. (15) and convert the \(k\)-space integration via the well-known rules for the Dirac \(\delta\)-function into an integration over an iso-frequency surface \(\Sigma_\omega\) within the 1BZ. As a result, the magnitude of the group velocity cancels from Eq. (14) Eq. (15) and we obtain

\[
\begin{align*}
I(T) &= \Omega_d \int_\omega d\omega I(\omega, T), \\
E(s, T) &= \int_\omega d\omega E(s, \omega, T), \\
I(\omega, T) &= \frac{1}{\Omega_d} \frac{1}{(2\pi)^d} \hbar \omega n(\omega, T) A(\Sigma_\omega), \\
E(s, \omega, T) &= \frac{1}{(2\pi)^d} \hbar \omega n(\omega, T) A'_p(\Sigma_\omega).
\end{align*}
\]

Here, \(d\) represents the dimensionality of the system and have introduced the solid angle in a \(d\)-dimensional space, \(\Omega_d = 2, 2\pi, 4\pi\) for \(d = 1, 2, 3\), respectively. Furthermore, \(A(\Sigma_\omega)\) denotes the total surface area of \(\Sigma_\omega\) and \(A'_p(\Sigma_\omega)\) stands for the total area that is obtained when \(\Sigma_\omega\) is projected onto a plane normal to \(\hat{s}\). For actual computations, the corresponding expressions for \(A(\Sigma_\omega)\) and \(A'_p(\Sigma_\omega)\) may be decomposed into contributions from individual bands according to

\[
\begin{align*}
A(\Sigma_\omega) &= \sum_n A(\Sigma_n(\omega)), \\
A'_p(\Sigma_\omega) &= \sum_n A'_p(\Sigma_n(\omega)),
\end{align*}
\]

where we have introduced the abbreviations

\[
\begin{align*}
A(\Sigma_n(\omega)) &= \int_{\Sigma_n(\omega)} dS, \\
A'_p(\Sigma_n(\omega)) &= \int_{\Sigma'_n(\omega)} dS \cos \theta_s.
\end{align*}
\]

Here, \(\Sigma_n(\omega)\) represent the contributions to the iso-frequency surface \(\Sigma_\omega\) that are associated with band \(n\). Similarly, \(\Sigma'_n(\omega) \equiv \Sigma_n(s, \omega)\) is that portion of the \(k\)-space surface \(\omega_{n,k} = \omega\) that lies within the first Brillouin zone and for which the condition \(s \cdot v_{n,k} \geq 0\) is satisfied.

In the above expressions, \(I(\omega, T)\) and \(E(s, \omega, T)\) denote, respectively, the average spectral radiation intensity and the spectral emissive power within the PhC. Due to the cancellation of the group velocity in the expressions in Eqs. (16), it is now clear that the mechanism associated with Van Hove singularities (small group velocities) that provides the basis for the strong enhancement of the spectral energy density, is not present anymore. In other words, while a PhC may present a large energy density for a certain spectral region, the spectral flow of the radiation may be reduced because the effective group velocity is usually reduced in these spectral regions (for example, at a band edge of a low-dimensional PhC, the density of states is enhanced, while the group velocity is vanishing). However, from Eqs. (16) we notice that the spectral flow of radiation strongly depends on the geometrical details of the dispersion relation and, depending on the frequency, may be enhanced or inhibited.
We now turn to an investigation of the angular resolution of the intensity and the hemispherical emissive power via the evaluation of the associated directional quantities. Basically, we follow the same procedure as described by Chigrin in Ref. 17 in order to account for the fact that the intensity and the emissive power have a natural angular resolution. The directional mode-intensity and mode-emissive power defined in Eqs. (5b) and (11) characterize the flow of thermal radiation in the direction of the mode’s group velocity $v_{n,k}$. The key concept in this analysis is the notion of stationary points.\(^\text{17}\) For a given position-space direction $\hat{r} \to \{\theta_r, \phi_r\}$, we define the set of stationary points $\{k'_n\}_\nu$, as the set of modes (labeled by band index $n$ and $k$-vectors) that belong to the iso-frequency surface $\omega=\text{const}$ and whose mode-group velocity points into a prescribed direction $\hat{r}$.

\[
\omega_{k'_n} = \omega, \quad (19a)
\]

\[
v_{k'_n} \uparrow \hat{r}. \quad (19b)
\]

For a given real-space direction $\hat{r}$ and a given frequency $\omega$ it is possible to have zero, one or more stationary points. Clearly, the absence of a stationary point corresponds to a stop-band along the corresponding $k$-space direction.

We then rewrite the area of the iso-frequency surface, $A(\Sigma_\omega)$, as a sum over angular integrals around the stationary points (labeled by $\nu$) on the iso-frequency surface

\[
A(\Sigma_\omega) = \sum_n \int_{\Sigma_n(\omega)} d^2k_n = \sum_\nu \sum_n \int d\Omega'_k \frac{|k'_n|^2}{\cos \varphi}. \quad (20)
\]

After a series of coordinate changes,\(^\text{17}\) we obtain

\[
A(\Sigma_\omega) = \sum_{\nu,n} \int d\Omega_r \frac{1}{K_{k'_n}}, \quad (21)
\]

where we have introduced the Gaussian curvature of the stationary points

\[
\frac{1}{K_{k'_n}} = \frac{dA'(\Sigma_n(\omega), \theta_r, \phi_r)}{d\Omega_r}. \quad (22)
\]

A similar analysis for the projected surface area $A'_p(\Sigma_\omega)$ yields

\[
A'_p(\Sigma_\omega) = \sum_{\nu,n} \int d\Omega_r \frac{\cos \theta_r}{K_{k'_n}}. \quad (23)
\]

The directional spectral intensity and spectral power can now be expressed in a form that does not depend on the photonic DOS but rather on the geometric details of the photonic band structure

\[
i(\omega, \theta_r, \phi_r, T) = \frac{\hbar \omega n(\omega, T)}{\Omega_d (2\pi)^d} \sum_\nu \frac{1}{K_{k'_n}}, \quad (24a)
\]

\[
e(\omega, \theta_r, \phi_r, T) = \frac{\hbar \omega n(\omega, T)}{(2\pi)^d} \cos \theta_r \sum_\nu \frac{1}{K_{k'_n}}, \quad (24b)
\]

and it is straightforward to verify

\[
I(\omega, T) = \Omega_d \int d\Omega_r i(\omega, \theta_r, \phi_r, T), \quad (25a)
\]

\[
E(\omega, r, T) = \int d\Omega_r e(\omega, \theta_r, \phi_r, T). \quad (25b)
\]
3. THERMAL RADIATION IN FINITE PHOTONIC CRYSTALS

We now consider a half-space problem where a semi-infinite, lossless dielectric PhC is separated from free space by a planar interface. This system is in thermal equilibrium at temperature T. The periodicity of the infinite PhC gives rise to the existence of propagating Bloch modes with frequency $\omega_{n,k}$, where n and k, respectively, label the band index and (real-valued) wave vector associated with a given mode. The wave vector is confined to the first Brillouin zone (BZ). In thermal equilibrium, emitters that are embedded in the PhC populate the available propagating Bloch modes and it is readily seen\cite{10,11} that their occupation number obeys Bose-Einstein statistics $ar{n}(\omega,T) = \left( e^{\hbar \omega/k_B T} - 1 \right)^{-1}$. The excited Bloch modes can couple to free space and this will lead to the emission of radiation into the far field of the propagating Bragg orders. We compute the corresponding transmittance coefficients via a generalization of an on-shell (fixed frequency $\omega$) bandstructure method that allows for real- and complex-valued wave vectors, i.e., propagating and evanescent Bloch modes\cite{18}. Within our approach, the plane-wave expansion of a Bloch mode $\{n,k\}$ into the reciprocal lattice vectors of the infinite PhC’s Bravais lattice, is rearranged as an expansion into plane waves $G_\parallel$ that are obtained by stripping each
reciprocal lattice vector $G$ of its component normal to the surface. On the air side, a corresponding expansion of the electromagnetic field into the same set of plane waves $G_{\parallel}$ is employed. Upon splitting the Bloch mode’s wave vector $k$ into parallel and perpendicular contributions, $k_{\parallel,n}$ and $k_{\perp,n}$, the continuity of the tangential electric and magnetic fields across the interface can be enforced by comparing the terms that belong to different plane waves $G_{\parallel}$. For a surface that is oriented along a high-symmetry direction of the PhC, our generalized approach thus coincides with the method of Ref. 18. In particular, although evanescent Bloch modes do not carry energy (and can thus not be excited by the emitters), they do give important contributions to the near fields. 18 Therefore, a sufficient number of them are required to ensure accurate computations of the transmittance coefficients for the propagating Bloch modes into the (generalized) propagating Bragg orders. An analogous statement applies for the (generalized) evanescent Bragg orders on the air side.

In general, an excited Bloch mode $\{n, k\}$ will transmit energy into several Bragg orders so that the corresponding time-averaged Poynting vector on the air side is

$$S_{n,k}^{\text{air}} = \sum_{G_{\parallel}} S_{n,k,G_{\parallel}}^{\text{air}},$$

(26)

Here, each summand contains the square of the transmittance coefficient of the excited Bloch mode $n, k$ into the corresponding propagating Bragg order that is characterized by its surface-parallel wave vector $k'_{\parallel} = k_{\parallel,n} + G_{\parallel}$. Since the total wave number of such a propagating Bragg order is $\omega/c$, we can also determine the corresponding real-space direction of energy flow in terms of the angle $\phi$ relative to the surface normal as $|k'_{\parallel}| = (\omega/c)\sin\phi$.

Figure 3. (Color online) Directional spectral emissivity from a 2D hexagonal lattice of air pores in a dielectric matrix (see text for details). The plane of the interface is perpendicular to (a) the $\Gamma$-$M$ or (c) the $\Gamma$-$K$ direction. The corresponding photonic bandstructure is shown in (b).

In order to determine the energy density current on the air side generated by the excited Bloch mode $\{n, k\}$, the Poynting vector (26) is weighted by the (directional) density of states

$$\rho(\omega, k_{\parallel,n}) = \frac{1}{(2\pi)^2} \frac{1}{v_{\perp,n,k}},$$

(27)

along the iso-frequency surface, i.e., at frequency $\omega$ along the parallel wave vector $k_{\parallel,n}$. Here $v_{\perp,n,k}$ denotes the group velocity component that is perpendicular to the surface and can be obtained via standard bandstructure computations. 19 Consequently, the energy current density that the Bloch modes around $\{n, k\}$ emit into the propagating Bragg orders is

$$J_{n,k} = \sum_{G_{\parallel}} \frac{1}{(2\pi)^2} \frac{1}{v_{n,k,\parallel}} S_{n,k,G_{\parallel}}^{\text{air}} dk_{\parallel},$$

(28)
0
 0.2
 0.4
 0.6
 0.8
 1
 0  0.1  0.2  0.3  0.4  0.5  0.6  0.7
ωa/2πc
ε(ω)
α(ω)
Figure 4. (Color online) Hemispherical spectral emissivity (solid line) and absorptivity (symbols) of the 2D model PhC described in Fig. 3.

For a plane wave in air, we find that the infinitesimal angle \(d\phi\) around \(\phi\) is
\[
d\phi = \frac{k'_{\parallel}}{k'_{\perp,G}} d\phi_{G_{\parallel}}\] (where \(k'_{\perp,G} = (\omega^2/c^2 - |k'_{\parallel}|^2)^{1/2}\)) so that we may express (28) in terms of the real space direction described by the angle \(\phi\) as
\[
J_{n,k} = \sum_{\phi_{G_{\parallel}}} \frac{1}{(2\pi)^2} \frac{k'_{G_{\parallel},G_{\parallel}}}{v_{\perp,n,k}} \bar{n}_{n,k} \epsilon_{\text{air},\phi_{G_{\parallel}}} d\phi_{G_{\parallel}}.
\] (29)

Here, the infinitesimal angles \(d\phi_{G_{\parallel}}\) are around \(\phi_{G_{\parallel}}\), where \(\phi_{G_{\parallel}}\) denotes the direction that belongs to \(k'_{G_{\parallel}}\). Finally, we obtain the directional spectral intensity \(i_{\text{PhC}}(\omega,\phi,T)\) by collecting the contributions from all modes associated with a certain emission angle \(\phi\) and weighting them by the occupation \(\bar{n}(\omega,T)\) of the modes
\[
i_{\text{PhC}}(\omega,\phi,T) = \sum_{\{k,n\},G_{\parallel}} \bar{n}(\omega,T) \frac{k'_{G_{\parallel},G_{\parallel}}}{(2\pi)^2} v_{\perp,n,k} |S_{n,k}^{\text{air},\phi_{G_{\parallel}}}|.
\] (30)

More precisely, (30) represents the energy flux from the PhC into the infinitesimal angle around \(\phi\) on the air side within the frequency interval \([\omega - d\omega, \omega + d\omega]\) and at temperature \(T\). The summation in (30) is restricted such that \(k'_{G_{\parallel}} = k_{\parallel,n} + G_{\parallel}\) is fulfilled and \(|k'_{\parallel}| = (\omega/c) \sin \phi\) corresponds to the emission angle \(\phi\). If we normalize the directional spectral intensity (30) to that of a BB, we obtain the directional spectral emissivity (DSE)
\[
\varepsilon(\omega,\phi) = \frac{i_{\text{PhC}}(\omega,\phi,T)}{(h\omega^2/4\pi^2c) / (e^{h\omega/k_BT} - 1)}.
\] (31)

The DSE is a measure of the thermal radiation flux of a given structure relative to the one emitted by a BB. If we assume that the PhC’s bandstructure remains unaltered by temperature, the directional spectral emissivity is temperature independent.

4. RESULTS

In the following, a 2D model PhC will help to illustrate several features of thermal emission from PhCs that are generic to PhCs and not limited to this particular model. We consider a hexagonal lattice (lattice constant \(a\)) of pores (radius \(r/a = 0.427\)) in a silicon matrix \((\epsilon = 11.56)\) where emitters populate the H-polarized modes. We display the corresponding bandstructure in Fig. 3(b) along with the DSE for two distinct surface terminations, Fig.3(a) and (c).

Consistent with thermodynamics, the DSE is bounded from above by unity for all frequencies and angles. In the long-wavelength limit and for frequencies up to the lower edge of the stop band in \(\Gamma\)-\(M\) direction, the PhC behaves as an effective (homogeneous) medium with an refractive index \(n_{\text{eff}}\) so that the angular behavior
is dominated by refraction and total internal reflection. At higher frequencies, we observe a strong angular dependence: For frequencies just below the lower edge of the stop band in Γ-M direction, the Γ-K termination leads to very strong emission for very large angles up to 90 degrees. This behavior is the remnant of the super-Planckian emission inside the infinite PhC for frequencies near the first stop band.\textsuperscript{10,11} For frequencies just above the lower edge of the stop band in Γ-M direction, we find that the Γ-M termination leads to a preferred emission into large angles, the Γ-K termination induces a pronounced forward emission. As a matter of fact, these effects can be directly linked to the radiation focusing effects of the infinite PhC near the photonic band gap (PBG) of the model system.\textsuperscript{10,11} For frequencies beyond the PBG, the iso-frequency contours of the infinite PhC develop into multi-valued surfaces that lead to complex and highly-directional behavior: For certain frequencies narrow angular emission ranges can be suppressed while for certain frequencies emission can effectively be funneled into certain angular ranges.

Next, we demonstrate that our "bottom-up" approach for evaluating DSE is consistent with the "top-down" approach where the directional spectral absorptance is calculated in a independent way.\textsuperscript{13} Instead of exciting modes in the PhC and tracking their behavior at the PhC-air interface, we consider the reverse situation and analyze (with our generalization of the method of Ref.\textsuperscript{18}) the scattering of plane waves at the PhC structure. We have verified that the results of these calculations agree with those obtained from the well-known Fourier Modal Method.\textsuperscript{20} Since the PhC is semi-infinite, we have to treat all the radiation that is transmitted into the PhC as being absorbed by the PhC, so that the absorptance \( \alpha(\omega, \phi) = 1 - r(\omega, \phi) \) for a plane wave (with frequency \( \omega \) and angle \( \phi \) to the surface normal) is given by in terms of the total reflectance \( r(\omega, \phi) \). Next, we evaluate the hemispherical spectral emissivity \( \varepsilon(\omega) \) (absorptivity \( \alpha(\omega) \)) according to

\[
\left( \begin{array}{c} \varepsilon(\omega) \\ \alpha(\omega) \end{array} \right) = \int_{-\pi}^{\pi} \left( \begin{array}{c} \varepsilon(\omega, \phi) \\ \alpha(\omega, \phi) \end{array} \right) \cos \phi \, d\phi
\]  

(32)

In Fig. 4, we demonstrate that hemispherical spectral emissivity equals absorptivity. Actually, this equality also holds for the directional spectral emissivities and absorptivities for arbitrary angles (not shown). In other words, Kirchhoff’s law is a consequence of our microscopic theory and not part of its conceptual basis.

As a final illustration, we show in Fig. 5 how a judicious choice of a PhC’s surface termination facilitates far-reaching control of the thermal emission characteristics. We consider a semi-infinite hexagonal lattice of
silicon rods (dielectric constant $\epsilon = 1.156$ and radius $r/a = 0.176$) in air where emitters populate the E-polarized modes. Besides a PBG, this structure exhibits in its bandstructure a Dirac-point that leads to unusual transport properties in the presence of disorder.\textsuperscript{21} We observe that for frequencies near this Dirac point ($\lambda/\lambda \approx 0.545$) the thermal emission for a $\Gamma$-$M$ terminated PhC is effectively channeled into the angular range around $\pm 37.5$ degree whereas for a $\Gamma$-$K$ terminated PhC this channeling occurs into the forward direction over a large frequency range (emission limited to a $\pm 23$ degree window over a frequency range of about 15\% around the frequency of the Dirac point).

5. CONCLUSIONS

In summary, we have developed a microscopic theoretical framework for analyzing the thermal radiation emission from finite PhC samples in thermal equilibrium. Without any further assumptions, this framework obey the fundamental laws of thermodynamics. Therefore, this theory represents an ideal starting point for an analysis of the non-equilibrium properties of such systems. With this "bottom-up" framework, we have further demonstrated that the spectral as well as angular thermal emission characteristics from PhCs may be controlled over a wide range via a combination of focusing effects associated with the infinite PhC and the PhC’s surface termination. Our study suggests numerous applications for highly efficiency and highly directional light sources as well as for optimized thermo-photovoltaic setups where the thermal emission properties have to be matched to the properties of available low-cost photovoltaic cells.

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