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Modified thermal radiation in three-dimensional photonic crystals

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Thermal radiation from an empty blackbody cavity follows the conventional Wien's displacement law. At a temperature $T=2500$ K, the maximum monochromatic radiation intensity lies at a wavelength of 1.16 μm, and radiation into the visible band occupies only 3% of the total radiation energy. In this paper, we show that when the cavity is filled with a three-dimensional photonic crystal, a strong thermal radiation band can appear in the visible regime, significantly improving the luminescence efficiency. This is attributed to the redistribution of photon density of states (DOS) in different frequency ranges in the photonic crystal leading to orders-of-magnitude enhancement of DOS in the visible wavelength over that in the infrared wavelengths.

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In the past decade it has been well known that a three-dimensional (3D) photonic crystal can modify atomic spontaneous emission in a way drastically different from in vacuum.[1–6] This is achieved via the redistribution of the photon density of states (DOS) in different frequency ranges in the photonic crystal. When the atom transition frequency is located within a photonic band gap (PBG), spontaneous emission is completely forbidden, because there is no photon state that can be coupled with the atomic transition. Outside the PBG, the spontaneous emission rate is directly correlated with the photon DOS, and may vary drastically from one frequency to another, and from one site to another within the photonic crystal.[2,3] In this paper, we point out that such a redistribution of photon DOS can also significantly modify thermal radiation in a blackbody cavity filled with a 3D photonic crystal, and improve the luminescence efficiency of a thermal object in the visible band at modest temperature. In Ref. 6, the suppression of thermal emission using a 3D photonic crystal was discussed. However, there the photonic crystal thin film is placed on the surface of a hot object and serves only as a filter to thermal emission.

We consider an empty blackbody cavity. At a temperature T, the cavity is filled with thermal radiation (photons) that is in thermodynamical equilibrium with the blackbody cavity wall (absorbing all photons impinged on it and reradiating them out to the cavity space). According to Planck's law, the thermal radiation energy within a unit volume inside this blackbody cavity between a frequency range $\omega-(\omega+d\omega)$ is given by $E(\omega)d\omega=n(\omega,T)(\hbar\omega)\rho(\omega)d\omega$, where $n(\omega,T)$ is the average number of thermal photons at temperature T, described by the Bose-Einstein statistics, $n(\omega,T)=1/(e^{\hbar\omega/kT}-1)$, $\hbar\omega$ is the single-photon energy, and $\rho(\omega)$ is the photon DOS. For an empty cavity, $\rho(\omega)=\omega^2/(\pi^2c^3)$, so $E(\omega)d\omega=(\hbar\omega^3 d\omega)/[\pi^2c^3(e^{\hbar\omega/kT}-1)]$. Here c is the light speed in vacuum, k is the Boltzmann constant, and $\hbar=h/(2\pi)$, where h is the Planck constant. Equivalently the thermal radiation energy within a wavelength range $\lambda-(\lambda+d\lambda)$ is

$$E(\lambda)d\lambda=u(\lambda,T)\rho(\lambda)d\lambda=\frac{8\pi hc\,d\lambda}{\lambda^5[e^{hc/\lambda kT}-1]}, \qquad (1)$$

where $u(\lambda,T)=hc/[\lambda(e^{hc/\lambda kT}-1)]$ is the average energy of a thermal photon and $\rho(\lambda)=8\pi/\lambda^4$ is the photon DOS in the empty cavity. The thermal radiation intensity from the blackbody cavity is proportional to this radiation energy density inside the cavity. From Eq. (1) one can derive the conventional Wien's displacement law, according to which the maximum radiation intensity at a temperature T is located at the wavelength λ_m given by $\lambda_m T=2.90\times10^{-3}$ m K. Therefore, for $T=2500$ K, the radiation is strongest at $\lambda_m=1.16$ μm, while for $T=2000$ K, $\lambda_m=1.45$ μm. To have the radiation peak located in the visible band, say $\lambda_m=0.6$ μm, a temperature as high as $T=4900$ K is required. When the radiation peak lies in the infrared band, the total thermal radiation emitted into the visible band occupies only a small fraction of the whole radiation energy. For example, a simple calculation from Eq. (1) shows that the energy emitted into the visible band between 0.4–0.7 μm occupies only 3% and 1% percent of the total emission energy for a 2500- and 2000-K blackbody cavity, respectively; therefore, the luminescence efficiency is quite low. Most of the thermal energy is emitted into infrared bands, and thus, turned into heat.

In Eq. (1), the first factor $u(\lambda,T)$ is determined only by the cavity temperature, while the second factor $\rho(\lambda)$, the photon DOS, is determined by the cavity configuration and the material from which the thermal photons emerge. At a fixed temperature, $u(\lambda,T)$ is fixed, so the only available way to change the thermal radiation behavior is to modify the photon DOS by changing of the material filled inside the cavity. If we fill the empty cavity with a homogeneous medium of refractive index n, then the radiation energy density becomes $E(\lambda)d\lambda=(8\pi n^3hc\,d\lambda)/[\lambda^5(e^{hc/\lambda kT}-1)]$. The conventional Wien's displacement law is still upheld. To have a nontrivial redistribution of photon DOS among different frequency bands, an inhomogeneous medium is required to fill in the empty cavity. Since a 3D photonic crystal can promise easy control and design of the photon DOS, we will restrict our discussion to this type of periodic inhomogeneous medium. Now within the cavity, it is the Bloch photons (photons characterized by Bloch's modes) that are in thermodynamical equilibrium with the walls of the blackbody cavity.

We start from the conventional Wien's displacement law for an empty blackbody cavity. At temperature $T=2500$ K, the radiation energy density peak E_m lies at $\lambda_m=1.16$ μm. The radiation energy density at other wavelengths is

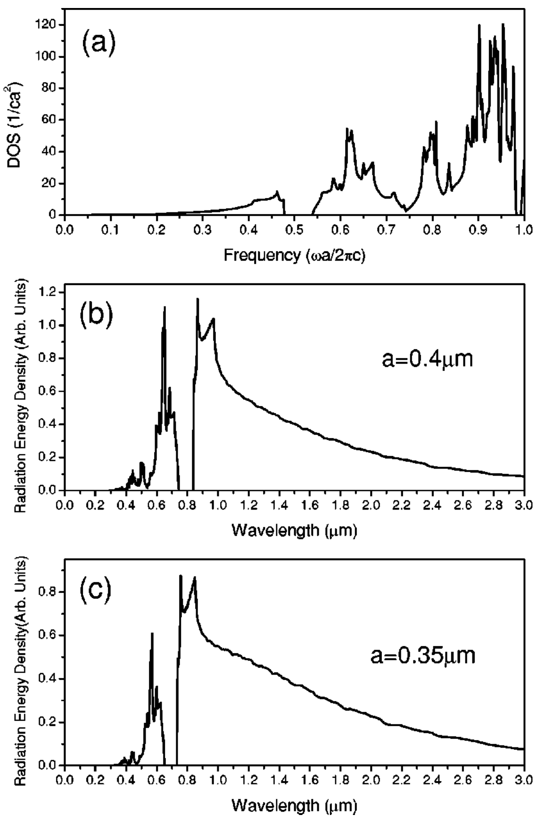

FIG. 1. (a) Photon DOS for a diamond lattice of dielectric spheres in air with $f=0.3$ and $n=3.6$. (b) and (c) show the calculated monochromatic thermal radiation energy density in a $T=2500$ K blackbody cavity filled with a diamond structure of $a=0.4$ and 0.3 μm, respectively.

given by $E(\lambda)/E(\lambda_m)=[u(\lambda,T)/u(\lambda_m,T)][\rho(\lambda)/\rho(\lambda_m)]\approx(\lambda_m/\lambda)\exp[(hc/kT)(1/\lambda_m-1/\lambda)](\lambda_m/\lambda)^4$. The radiation energy density at 0.6, 0.5, and 0.4 μm in the visible band are given by $E(0.6\ \mu\mathrm{m})/E(1.16\ \mu\mathrm{m})=(1/54)\times 14=0.26$, $E(0.5\ \mu\mathrm{m})/E(1.16\ \mu\mathrm{m})=(1/304)\times 29=0.095$, and $E(0.4\ \mu\mathrm{m})/E(1.16\ \mu\mathrm{m})=(1/4350)\times 71=0.016$. It is seen that in order for $E(\lambda)>E(\lambda_m)$, the photon DOS in the inhomogeneous medium must redistribute such that $\rho(\lambda)/\rho(\lambda_m)>u(\lambda_m,T)/u(\lambda,T)$, namely, at $T=2500$ K we must have $\rho(0.6\ \mu\mathrm{m})/\rho(1.16\ \mu\mathrm{m})>54$, or $\rho(0.5\ \mu\mathrm{m})/\rho(1.16\ \mu\mathrm{m})>304$, or $\rho(0.4\ \mu\mathrm{m})/\rho(1.16\ \mu\mathrm{m})>4350$. The DOS for a 3D photonic crystal depends in a complex way on a variety of geometrical and physical properties of the crystal itself, such as the lattice type and the refractive index contrast. However, a general rule of thumb can be followed: The presence of a complete PBG usually means a strong redistribution of photon DOS. Therefore, we first look at systems with a complete PBG. Two structures are known to possess a complete PBG: Diamond structures[7] and inverse-opal structures.[8] Let us first look at a photonic crystal composed of a diamond lattice of dielectric spheres in the air background. The sphere has a refractive index of $n=3.6$ and a filling fraction of $f=0.3$. The corresponding DOS is plotted in Fig. 1(a). The result has been obtained by the solution of the photonic band structure within an irreducible Brillouin zone of the lattice by means of a plane-wave expansion method.[3,7] The abscissa is in units of normalized frequency $\omega=x(2\pi c/a)$ (equivalently $\lambda=a/x$), where a is the cubic lattice constant. Normalized frequency is used because it can be scaled to different lattice sizes of photonic crystals, leading to great convenience in our discussions. The DOS is written as $\rho(\omega)=\rho(x)(1/ca^2)$. Under the dimensionless quantities x and $\rho(x)$, the radiation energy density between λ and $(\lambda+d\lambda)$ can be derived as

$$E(\lambda)d\lambda=\frac{hcx}{a[e^{hcx/akT}-1]}\,\frac{2\pi x^2\rho(x)d\lambda}{a^4}=\frac{2\pi hcx^3\rho(x)d\lambda}{a^5[e^{hcx/akT}-1]}. \tag{2}$$

Equation (2) allows one to calculate the radiation energy density at a given wavelength and temperature using the numerical solution of the dimensionless DOS. Due to the complex distribution of $\rho(x)$, the maximum energy density occurs at a wavelength depending in a subtle way on both the temperature and the photonic crystal structure.

From Fig. 1(a) one can find a complete PBG within $0.478-0.538(2\pi c/a)$, and this complete PBG indeed does induce a remarkable redistribution of DOS around the band gap: A strong DOS peak located at about $0.62(2\pi c/a)$ stands out far above the value expected for an effective homogeneous medium of this lattice. Below the band gap, the DOS [at frequencies under $0.35(2\pi c/a)$] stays at a low level. This means if we set $\lambda_m=1.16\ \mu$m (at $T=2500$ K) at this low-DOS range, a strong radiation peak will appear around $\lambda=0.6\ \mu$m, and the corresponding lattice constant of the crystal should be $a\approx 0.62\times 0.6\ \mu\mathrm{m}=0.37\ \mu$m. Our calculation has verified such an analysis. Figures 1(b) and 1(c) display the calculated thermal radiation energy density for a photonic crystal with $a=0.4$ and 0.3 μm, respectively, at 2500 K. A strong radiation band in the visible region is found for both systems. The energy density peak for the 0.4-μm crystal is located at 0.65 μm and is over two times the density at 1.16 μm. The peak for the 0.3-μm crystal is now shifted to 0.57 μm, and is still 20% larger than at 1.16 μm. Besides large enhancement at discrete spectrum lines, the energy emitted into the whole visible band occupies 8% and 4.5% of the total radiation energy, respectively, also a remarkable enhancement over the 3% value for an empty cavity. Although the two DOS peaks in this band [located at $0.462(2\text{-}c/a)$ and $0.476(2\pi c/a)$] are four to five times smaller than the principal peak at $0.62(2\pi c/a)$, the radiation energy is dominant in this band due to a relatively large average single-photon energy. The exponential decay of the average thermal photon energy with respect to the frequency in short-wavelength bands also leads to an almost negligible thermal radiation at the violet band and beyond, although a vary sharp peak in the DOS curve is present in this frequency range [see the spike around $0.95(2\pi c/a)$ in Fig. 1(a)].

Now let us turn to the inverse-opal structures. This is a photonic crystal composed of a face-centered-cubic (fcc) lattice of close-packed air spheres in a dielectric background. With a large enough refractive index contrast, a complete PBG is opened at high photonic bands. The calculated DOS is plotted in Fig. 2(a) for 74% filling fraction of air spheres

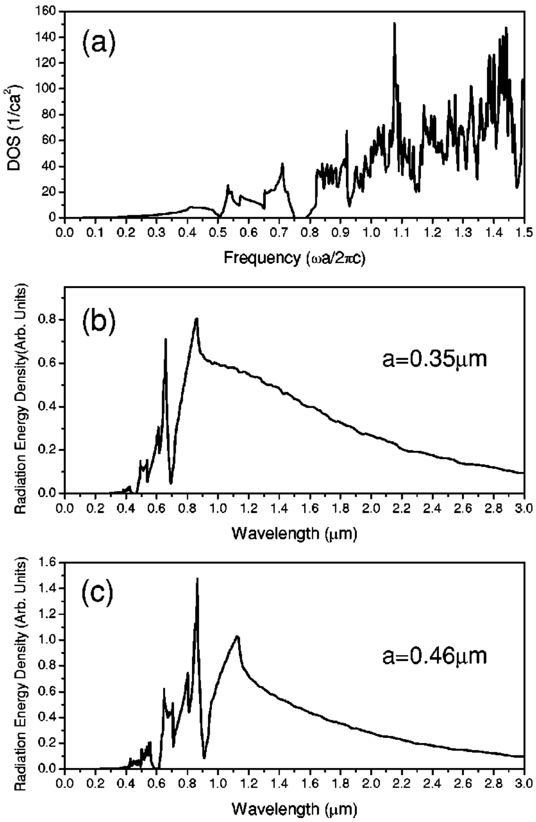

FIG. 2. (a) Photon DOS for an inverse-opal structure with $f=0.74$ and of $n=3.6$. (b) and (c) show the calculated monochromatic thermal radiation energy density in a 2500-K blackbody cavity filled with an inverse structure of $a=0.35$ and 0.46 μm, respectively.

and a refractive index contrast of 3.6. A complete PBG lies within $0.748-0.788(2\pi c/a)$. At about $0.506(2\pi c/a)$ the DOS is close to zero, corresponding to a pseudogap lying at low photonic bands. Around these two gaps two sharp peaks stand at $0.532(2\pi c/a)$ and $0.71(2\pi c/a)$, and the corresponding DOS is $25(1/ca^2)$ and $42(1/ca^2)$, respectively. In comparison, the DOS at $0.266(2\pi c/a)$ and $0.355(2\pi c/a)$ is $1.8(1/ca^2)$ and $3.9(1/ca^2)$, respectively. As $\rho(0.532)/\rho(0.266)>\rho(0.71)/\rho(0.355)$, it is preferable to use the 0.532 peak to enhance thermal radiation into the visible band. Let this peak correspond to a radiation wavelength of 0.65 μm, the lattice constant of the inverse opal should be around $a=0.532\times0.65=0.346$ μm. Figure 2(b) displays the monochromatic radiation energy density within a 2500-K cavity filled with an inverse opal of $a=0.35$ μm. A strong radiation band is found corresponding to the high-DOS band between the pseudogap and the complete band gap. The radiation band is centered at 0.6 μm and a sharp peak is located at 0.66 μm. Similar to the diamond structure, a dominant fraction of energy is radiated into a band between λ_m and the visible band, due to the balance between the DOS and the average energy of a single thermal photon in this band. An overwhelmingly small single-photon average energy results in negligible contribution of the high-DOS band above the complete PBG to the thermal radiation.

The DOS peak at $0.71(2\pi c/a)$ is induced by the appearance of the complete PBG. To make use of this peak, we choose $a=0.71\times0.65$ μm$=0.46$ μm. The calculated monochromatic radiation energy density for a 2500-K cavity filled with such an inverse opal is shown in Fig. 2(c). A modest radiation band is found between 0.6 and 0.7 μm. In contrast, the radiation band corresponding to the 0.532 peak induced by the pseudogap now becomes dominant, and its density is over two times that of the 0.71 peak. Besides, the radiation band around λ_m is also stronger than the visible band. As a result, the 0.71 peak is not an optimum candidate to modify the thermal radiation. For the same reason, the higher and sharper DOS peak located at $1.08(2\pi c/a)$ also is not a good choice.

We have found in the inverse opal that a pseudogap may contribute more to enhance thermal radiation into the visible band than a complete PBG. We also find that to optimally enhance the thermal radiation, what we need is only a significantly enhanced DOS spike and far smaller DOS in the whole band below this spike extending into the frequency around λ_m. Therefore, it seems that a photonic crystal without a complete PBG or even without an apparent pseudogap can also be utilized to redistribute the DOS so as to enhance thermal radiation into the visible wavelengths at modest temperature. This release of limitation surely will greatly expand our freedom to design an optimum photonic crystal structure for thermal radiation modification. Since there are so many photonic crystal structures available for choice, we need in the first step to investigate the photonic band structures for a specific crystal structure observed. Some characteristics prove to be useful guides. For instance, a flat photonic band may correspond to a high DOS. In addition, if this flat band happens to occur at low frequency, then it is likely that we have found an optimal crystal structure for our purpose. Figure 3(a) shows such an example, where the photonic band structures for a fcc lattice of dielectric spheres ($f=0.3$,$n=3.6$) in air are plotted. The 3, 4, and 5 photonic bands are quite flat and very close to each other around $0.57(2\pi c/a)$ in a large k space extending from the center of the Brillouin zone (Γ point) to its boundary (L and X points). This suggests the presence of a very sharp spike of DOS around $0.57(2\pi c/a)$. The calculation of the full DOS has verified this expectation, where the result is displayed in Fig. 3(b). Indeed, a DOS spike occurs right at $0.57(2\pi c/a)$. With a value of $135(1/ca^2)$, this spike is over one hundred times stronger than the DOS at the frequency $0.285(2\pi c/a)$ [with a value of $1.21(1/ca^2)$] in the long-wavelength regime, and still over six times larger than another low-frequency DOS peak at $0.494(2\pi c/a)$. From all these features we can expect in this photonic crystal a promising function to modify thermal radiation.

In Figs. 4(a) and 4(b) we plot the calculated results of monochromatic radiation energy density within a 2500-K blackbody cavity filled with the above photonic crystal with a lattice constant of 0.35 and 0.3 μm, respectively. The sharp thermal radiation peak is located at 0.614 and 0.526 μm for the two crystals, which are about eight and four times the radiation density at $\lambda_m=1.16$ μm, respec-

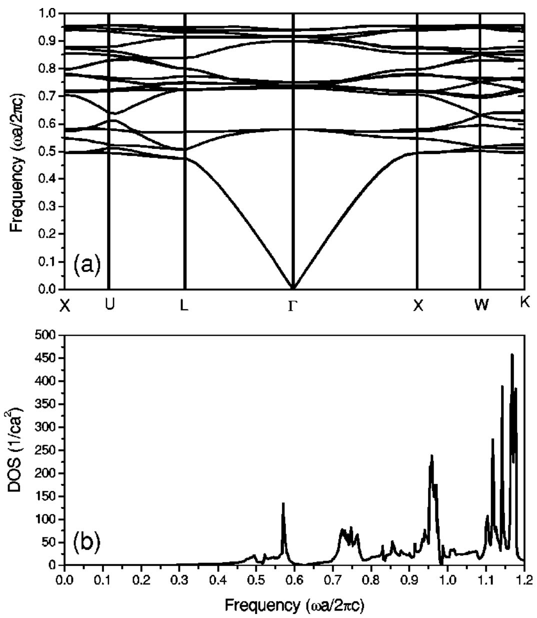

FIG. 3. (a) Photonic band structures for a fcc lattice of dielectric spheres in air with $f=0.3$ and $n=3.6$. (b) Corresponding photon DOS.

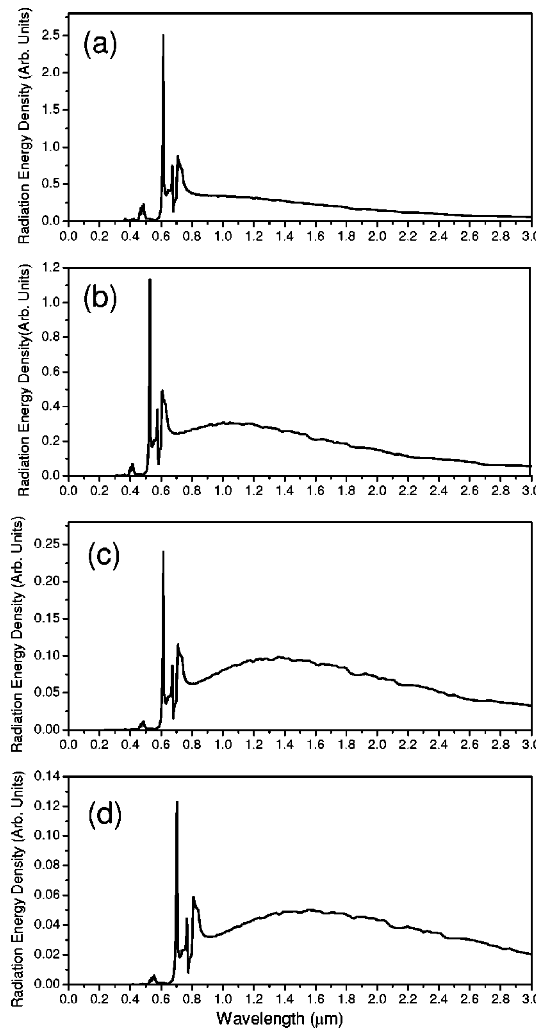

FIG. 4. Calculated monochromatic thermal radiation energy density in a blackbody cavity filled with the photonic crystal material shown in Fig. 3. (a) $T=2500$ K, $a=0.35$ μm; (b) $T=2500$ K, $a=0.3$ μm; (c) $T=2000$ K, $a=0.35$ μm; (d) $T=1750$ K, $a=0.4$ μm.

tively. In addition, the total radiation into the visible band adds up to 10.9% and 10.6% of the total radiation, respectively, a significant enhancement over the empty cavity case (3%). Now one can see that this fcc lattice is superior to the above diamond and inverse-opal crystals in thermal radiation modification, despite the absence of any appreciable band gaps (complete or incomplete). With two-orders-of-magnitude enhancement of the DOS, the modification of thermal radiation can still be significant at lower temperatures. Figure 4(c) shows the monochromatic thermal radiation energy density within a 2000-K cavity filled with the above photonic crystal of $a=0.35$ μm, while the result for $T=1750$ K and $a=0.4$ μm is displayed in Fig. 4(d). A sharp and narrow radiation spectrum line is found in both cavities at wavelengths of 0.614 and 0.702 μm, respectively. The peak radiation density for both is about 2.5 times the radiation density at λ_m. Even at 1500 K, a thermal radiation spectrum line can still be found in the visible band with an energy density comparable to that at λ_m (1.93 μm).

In summary, we have shown that a 3D photonic crystal can induce strong redistribution of the photon DOS among different frequency bands. This redistribution can be used to modify thermal radiation from a blackbody cavity when the photonic crystal is filled in an otherwise empty cavity. In a designed photonic crystal, orders-of-magnitude enhancement of the DOS can occur adjacent to a low-DOS band in the long-wavelength regime. This leads to significantly enhanced thermal radiation spectrum lines in the visible band for a modest cavity temperature, whose wavelength can be freely adjusted by changing the lattice constant of the crystal. It is expected that this modification of thermal radiation can also be achieved by other more general inhomogeneous media.

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