Coherent thermal conductance of 1-D photonic crystals

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1. Introduction

Recently there has been a growing interest in exploring nanoscale heat transfer theoretically and experimentally which is triggered by the fact that radiative heat flux at the nanoscale can be much larger than that between two black bodies [1] and quasi-monochromatic [2,3] which makes it very promising for near-field thermophotovoltaics [4–8]. The tremendous increase in the amount of transferred energy for distances much smaller than the thermal wavelength (λth = hc/kBT) which can be several orders of magnitude larger than the value predicted by Stefan–Boltzmann’s law can for dielectrics be attributed to the contribution of a large number of coupled surface phonon polariton modes [9,10].

The contribution of surface modes (SMs) is indeed very important for nanoscale heat fluxes and many researchers have tried to enhance the amount of transferred heat by using this effect. Volokitin and Persson [11] have pointed out that thin metallic coatings on a substrate can increase the nanoscale heat flux, Bihs et al. [12,13] and Francoeur et al. [14] have shown that one can use the coupling of SMs in thin metallic or dielectric films to enhance the nanoscale heat flux, Ben-Abdallah and coworkers [15–19] and Francoeur et al. [20] have also considered this effect between two finite slabs or media with several layers, Fu and Zhang [21] have studied how doping affects the surface mode contribution, van Zwol et al. [22] have shown that large nanoscale heat fluxes in phase change materials are due to SMs, and Svetovoy et al. [23] and Ilic et al. [24] have pointed out that thin sheets of graphene allow do control or modulate the surface mode contribution. Very recent works have also considered heat fluxes for artificial structures and/or meta-materials supporting SMs in the infrared regime [19,25–28], or the surface mode coupling in many particle systems [29].

It should also be mentioned that very recent experiments could unambiguously show that the radiative heat flux increases for distances smaller than the thermal wavelength [30–32], and can exceed the Stefan–Boltzmann law [33,34]. The effect of modulation of heat fluxes by means of phase change materials could also be demonstrated very recently [35]. The overall agreement between the theoretical predictions based on the fluctuational electrodynamics [1] and the experimental results is very good [34–36].

In this work, we will revisit the theory of thermal conductance by photons within a 1-D photonic crystal (PC) as depicted in Fig. 1. We will provide an exact expression for the thermal conductance inside a 1-D PC for arbitrary dispersive and dissipative material slabs. In particular, this allows us to determine the transmission coefficients (TC) for the Bloch states inside the PC. In previous works Lau and co-workers [37] have assumed that the TC equals its maximum value of one for an infinite PC when losses can be neglected. With our method we can show that this expectation does not remain true for a finite PC placed between two half spaces (HSs), as sketched in Fig. 1. If the HSs are filled by vacuum the TC for frustrated total internal reflection modes, i.e., modes with wave vectors larger than the vacuum wave vector, goes to zero and not to its maximum value. On the other hand, if the HSs are filled with the slab material the TC for the frustrated modes converges in the limit of vanishing losses to values which are generally smaller than one independent of the number of slabs. In fact, we find that the TC is very sensitive to the losses inside the PC slabs. In addition, we show that the surface mode contribution can be crucial for the thermal conductance inside a PC.
2. Heat flux expression

In order to derive the expression for the radiative heat flux inside a PC, we assume that we have first two identical 1-D bilayer finite PCs placed between two HSs of the same material as depicted in Fig. 1. The bilayer structure has a period of \( a = l_1 + l_2 \) where \( l_1 \) is the thickness of the material layer with complex permittivity \( \epsilon_1 = \epsilon_1' + i \epsilon_1'' \) and \( l_2 \) is the thickness of the vacuum layer with \( \epsilon_2 = 1 \). The heat flux

\[
\phi_{lt} = h_{lt}(T_1, d) A T_{lt}
\]

between two such semi-infinite structures having a temperature difference \( \Delta T_{lt} = T_1 - T_2 \) across the vacuum gap of distance \( d \) can be derived from the expression given by Polder and van Hove [1].

The heat transfer coefficient (HTC) within an infinite PC can then be obtained by setting \( d = l_2 \)

\[
h_{lt} = \sum_{i=s,p} \int_0^{\infty} \frac{d\omega}{2\pi} f(T_i) \int \frac{d^2k}{(2\pi)^2} T_i(\omega, \kappa; d = l_2).
\]

Here, the time derivative of the Bose–Einstein function is given by

\[
f(T) = \frac{(h\omega)^2}{(k_BT)^2} e^{h\omega/k_BT} / (e^{h\omega/k_BT} - 1)^2
\]

and evaluated at the temperature \( T_1 \) of the last slab of the PC at the left-hand side. The TCs \( T_i(\omega, \kappa; d) \) for s- and p-polarized waves \( (i = s, p) \) are given in terms of the reflection coefficients \( R_s \) and \( R_p \) in Ref. [1]

\[
T_i(\omega, \kappa; d) = \begin{cases} 
\frac{(1-|R_i|^2)(1-|R_i''|^2)}{|D_i|^2}, & \kappa < \omega/c, \\
\frac{4 \text{Im}(R_i') \text{Im}(R_i'') e^{-2ikd0^f}}{|D_i|^2}, & \kappa > \omega/c,
\end{cases}
\]

where \( D_i^2 = 1 - R_i^1 R_i^2 e^{2\pi i k^0 d} \) is a Fabry–Pérot-like denominator with \( k_0^2 = \omega^2/c^2 - \kappa^2 \) and \( \kappa^2 = k_s^2 + k_p^2 \). Here \( R_i^1 = R_i^p \) and can be calculated with the standard S-matrix method for layered media [14, 15,38].

3. Impact of dissipation

Now, we are in a position to compare results from the exact expression in Eq. (2) with the results in Ref. [37]. First we note, that in the approach in Ref. [37] the authors assume that the TCs equal their maximum value of one for all propagating Bloch modes inside the PC. That means, the integral in Eq. (2) over all parallel wave vectors \( \kappa \) is replaced by

\[
A(\omega) = \sum_{i=s,p} \int \frac{d^2k}{(2\pi)^2} T_i \to 2 \int \frac{d^2k}{(2\pi)^2} \equiv A'(\omega).
\]

Here the prime notes that the integral is for each frequency \( \omega \) carried out over the whole parallel wave vector range which allows for propagating solutions inside the PC, i.e., over the photonic Bloch bands. The photonic Bloch bands can be determined for infinite PCs from the dispersion relation for the Bloch modes (see Ref. [38])

\[
\cos(k_s A) = -\frac{1}{2} \left( \frac{k_{s1}}{P_{s1}k_{s2}} + \frac{P_{s2}}{k_{s1}k_{s2}} \right) \sin(k_{s1}l_1) \sin(k_{s2}l_2) \\
+ \cos(k_{s1}l_1) \cos(k_{s2}l_2).
\]

Here, \( k_{s1} = \epsilon_1 \omega^2/c^2 - \kappa^2 \) and \( k_{s2} = k_0^2 \). and \( P_s = 1 \) and \( P_p = \epsilon_1 \) depending on the polarization state. Hence, the results from Ref. [37] for the coherent thermal conductance give the upper limit for the contribution of the propagating Bloch modes. As we will see in the following, the exact result can be very different from such a calculation due to finiteness of the investigated structure, losses, resonant SMs as well as evanescent Bloch modes.

In Fig. 2(a) the TC \( T_{s1} \) is plotted choosing \( \epsilon_1 = 12 + 0.001 \) for a PC with 100 slabs placed between two HSs with the same permittivity. It can be seen that although the imaginary part...
of the permittivity is very small, corresponding to a system with vanishing losses, the TC is less than one for most parts of the Bloch bands. We find similar results for the p-polarized modes. In Fig. 2(b) we present the numerical results for $A(\omega)$ when integrating the TC over $k$ using Eq. (4). The plotted values are normalized to the maximum value possible for propagating modes $A_{\text{max}} = \frac{1}{2\pi}(\omega/c)^2$ inside the vacuum gap. The solid black line represents the result from Ref. [37] and the colored dashed curves represent the exact results using the same $\epsilon_1$ as in Ref. [37] but for different $\epsilon_\|$. The best agreement with the black curve is found for $\epsilon_\| = 0.1$. When decreasing the losses by making $\epsilon_\|$ smaller than $0.1$ then $A(\omega)$ decreases as well for nearly all frequencies so the deviation from the black curve gets larger. This means that for vanishing losses the TC for a finite PC does not converge to its maximum value for all Bloch modes. On the other hand, when making $\epsilon_\|$ larger than $0.1$ the skin depth $\delta_s = \frac{1}{\sqrt{\epsilon_1\omega/c^2}}$ inside the material slabs decreases and attains for $\epsilon_\| = 10$ (dashed magenta curve) values on the order of the period $a$ of the PC so that the field is screened at this scale. Hence, the heat flux is not coherent anymore and the Bloch band structure in $\mathcal{T}_{\text{frus}}$ disappears. In fact, then the heat flux is due to Fabry–Pérot modes of the cavity formed by separation gap explaining the smooth and weak oscillating behaviour of $A(\omega)$ for $\epsilon_\| = 10$ [Fig. 2(b)].

Finally, in Fig. 2(c) we compare the HTCs $h^\text{frus}_{\|}$ for the PC between the two half spaces increases and converges for large penetration depths to a limiting value $> h^\text{frus}_{\|}$. Now, for the PC between the half space materials ($N = 10, 50, 100$) the curves show a maximum of $h^\text{frus}_{\|} \approx h^\text{frus}_{\|}$ at a given penetration depth. The exact position of this maximum depends on the number of slabs. For very large penetration depths the HTC of the PCs with $N = 10, 50, 100$ drops slightly and converges to a fixed value smaller than $h^\text{frus}_{\|}$. It can be seen, that for an increasing number of slabs the position of the maximum is shifted to larger $\delta_s$. This position can be identified as $\delta_s \approx aN$. Therefrom, we can conclude that the observed drop of the HTC for large penetration depth is due to the finite size of the PC. The observed drop of the HTC for large penetration depths is even more dramatic in the case of $N = 11$, i.e., the PC slabs are embedded in vacuum, where we find that the HTC $h^\text{frus}_{\|}$ goes to zero for large $\delta_s$. Hence, the ‘universal’ value found in Ref. [37] can be considered as the correct value for lossless PCs in the case of an infinite number of slabs only. Apart from this restriction, it is clear that the value found in Ref. [37] still represents the upper limit for the HTC of a lossless PC.

4. Role of surface modes

Here below we examine the behaviour of structures supporting SPPs. Surface phonon polaritons (SPPs). To do that we consider an Al$_2$O$_3$/vacuum PC with 100 slabs at $T_1 = 300$ K. For this material combination SPPs not only exist for the p-polarized modes but also play the important role for heat transfer at subwavelength distances. In Fig. 4(a) we have plotted the TC for p-polarized modes in $\omega-k$ plane. It is obvious that not only the Bloch modes and Bloch SPPs contribute to the heat conductance but also coupled SPP modes which can be identified in the frequency bands $\Delta_1$ and $\Delta_2$ where $\epsilon_1 (-1)$. To compare our exact calculations with results from [37] for the Al$_2$O$_3$/vacuum PC we have plotted in Fig. 4(b) the HTC $h^\text{frus}_{\|}$ versus the vacuum gap $l_1$ for different $l_2$. The results are normalized to the HTC $h^\text{frus}_{\|}$ from Ref. [37] for which $A(\omega) = A'(\omega)$ [see Eq. (4)]. It can be seen that the exact HTC can be nearly four orders of magnitude larger than the HTC calculated with the approximative method at $l_2 = 10$ nm. This can be attributed to the SPP mode contribution which is proportional to $1/l_2^2$ for small gap sizes [39].


5. Conclusions

In summary, we have revisited the radiative heat flux within a bilayer photonic crystal presenting an approach which allows for an exact calculation. In comparison with a previous approach we have shown (i) that the transmission for a finite PC vitally depends on losses inside the photonic crystal and (ii) that the impact of the surface modes can become crucial. In the latter case, we show in particular that heat flux calculated with our exact approach can exceed the heat flux calculated with previous approaches by three to four orders of magnitude.

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