Supplementary Material
Near-field radiative thermal transfer between a nano-structured periodic material and a planar substrate

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In this supplementary material, we start in the first section by calculating the Green's functions for stratified media. In the next section, the expressions for the Green's functions are generalized for periodic structures. Using those Green's functions, the thermal transfer is calculated in such structures.

Green's functions for stratified media:

For the calculation of thermal transfer, we need to calculate the Green's functions which determine the produced electromagnetic fields in one object (say object 1) that result from current sources in the other object (say object 2). For stratified media composed of a stack of different layers (See Fig. S1a), the contribution of an infinitesimal current $\vec{J}\,(k_x, k_y)\,dz'$ to the total electric field produced by it at its own position, denoted by z' in object 2, is given by:

$$\overrightarrow{dE_{inc}}\,(z') = \frac{-\omega\mu_0}{2k_z}\,(\hat{p}_{2+}\hat{p}_{2+} + \hat{s}\hat{s})\cdot\vec{J}dz' \tag{S1}$$

where $\hat{p}_{2+}$ and $\hat{s}$ refers to the P and S polarization directions for a wave with transverse wave-vector components of k_x, k_y. Note that $+$ sign denotes the wave with the wave-vector direction from object 2 toward object 1. From the transfer matrix method, the electric field produced by that element in a location different from its own location, denoted by z in material 1, is given by:

$$\overrightarrow{dE_{inc}}\,(z) = \frac{-\omega\mu_0}{2k_z}\,(t^p_{21}\hat{p}_{1+}\hat{p}_{2+} + t^s_{21}\hat{s}\hat{s})\cdot\vec{J}dz' \tag{S2}$$

where $\hat{p}_{1+}$ refers to P polarization direction in object 1, and t^s_{21} and t^p_{21} refers to transmission coefficients from z' to z, for S and P polarizations, respectively.

Accordingly, the dyadic Green's function is given through the following expression:

$$\overleftrightarrow{G}\,(z, z') = \frac{-\omega\mu_0}{2k_z}\,(t^p_{21}\hat{p}_{1+}\hat{p}_{2+} + t^s_{21}\hat{s}\hat{s}) \tag{S3}$$

This exactly follows Sipe's derivation for the Green's function.

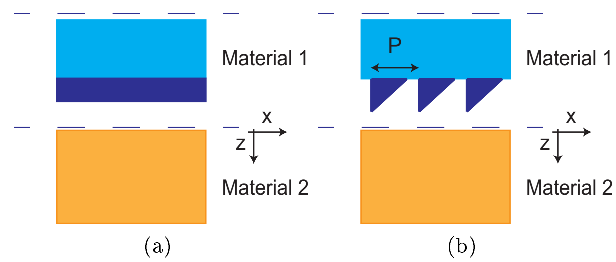

Figure S1: Schematic of (a) planar structured materials and (b) a planar and an arbitrary shaped periodic structure (This is the same figure as Fig. 1 in the main manuscript)

In the simple case of a slab adjacent to air, this formalism can be simplified further. In this case, we assume the boundary between them is located at $z = 0$ and the observation point be located inside air at $z = 0$. Moreover, we assume that a current source to be located inside the slab at a distance z' from the object's surface.

Denoting the transversal wave vector by $\beta\hat{\beta} = k_x\hat{x} + k_y\hat{y}$, the total wave vector in the air and slab can be expressed as:

$$\vec{k_1} = \beta\hat{\beta} + k_{zv}\hat{z} \tag{S4}$$
$$\vec{k_2} = \beta\hat{\beta} + k_z\hat{z} \tag{S5}$$

Also the S and P polarization directions can be expressed as:

$$\hat{p}_{1+} = \frac{c}{\omega}\left(\beta\hat{z} - k_{zv}\hat{\beta}\right) \tag{S6}$$
$$\hat{p}_{2+} = \frac{c}{\sqrt{\epsilon}\omega}\left(\beta\hat{z} - k_z\hat{\beta}\right) \tag{S7}$$
$$\hat{s} = \hat{\beta}\times\hat{z} \tag{S8}$$

Moreover in this case, t^p_{21} and t^s_{21} are simple Fresnel coefficients:

$$t^p_{21} = \frac{2\sqrt{\epsilon}k_z}{k_z + \epsilon k_{zv}}e^{-ik_zz'} \tag{S9}$$
$$t^s_{21} = \frac{2k_z}{k_z + k_{zv}}e^{-ik_zz'} \tag{S10}$$

So the dyadic Green's function can easily be derived as:

$$\overleftrightarrow{G} = -\frac{\mu_0 c^2 e^{-ik_z z'}}{\omega\left(k_z+\epsilon k_{zv}\right)}\left(\beta\hat{z}-k_{zv}\hat{\beta}\right)\left(\beta\hat{z}-k_z\hat{\beta}\right) - \frac{\mu_0 \omega e^{-ik_z z'}}{k_z+k_{zv}}\left(\hat{\beta}\times\hat{z}\right)\left(\hat{\beta}\times\hat{z}\right) \tag{S11}$$

with the following components:

$$\overleftrightarrow{G} = \begin{bmatrix} \frac{-k_x^2}{\omega\epsilon_0\beta^2}\frac{k_{zv}k_z e^{-ik_z z'}}{k_z+\epsilon k_{zv}} - \frac{\omega\mu_0}{\beta^2}\frac{k_y^2 e^{-ik_z z'}}{k_z+k_{zv}} & \frac{-k_x k_y}{\omega\epsilon_0\beta^2}\frac{k_{zv}k_z e^{-ik_z z'}}{k_z+\epsilon k_{zv}} + \frac{\omega\mu_0}{\beta^2}\frac{k_x k_y e^{-ik_z z'}}{k_z+k_{zv}} & \frac{1}{\omega\epsilon_0}\frac{k_{zv}k_x e^{-ik_z z'}}{k_z+\epsilon k_{zv}} \\ \frac{-k_y k_x}{\omega\epsilon_0\beta^2}\frac{k_{zv}k_z e^{-ik_z z'}}{k_z+\epsilon k_{zv}} + \frac{\omega\mu_0}{\beta^2}\frac{k_x k_y e^{-ik_z z'}}{k_z+k_{zv}} & \frac{-k_y^2}{\omega\epsilon_0\beta^2}\frac{k_{zv}k_z e^{-ik_z z'}}{k_z+\epsilon k_{zv}} - \frac{\omega\mu_0}{\beta^2}\frac{k_x^2 e^{-ik_z z'}}{k_z+k_{zv}} & \frac{1}{\omega\epsilon_0}\frac{k_y k_{zv} e^{-ik_z z'}}{k_z+\epsilon k_{zv}} \\ \frac{1}{\omega\epsilon_0}\frac{k_x k_z e^{-ik_z z'}}{k_z+\epsilon k_{zv}} & \frac{1}{\omega\epsilon_0}\frac{k_y k_z e^{-ik_z z'}}{k_z+\epsilon k_{zv}} & \frac{-\beta^2}{\omega\epsilon_0}\frac{e^{-ik_z z'}}{k_z+\epsilon k_{zv}} \end{bmatrix} \tag{S12}$$

These components become the more known results if k_y is assumed to be zero, as shown for instance in reference[S1]:

$$\overleftrightarrow{G} = \frac{1}{\omega\epsilon_0} \times \begin{bmatrix} \frac{-k_{zv}k_z e^{-ik_z z'}}{k_z+\epsilon k_{zv}} & 0 & \frac{k_{zv}k_x e^{-ik_z z'}}{k_z+\epsilon k_{zv}} \\ 0 & \frac{-\omega^2\mu_0\epsilon_0 e^{-ik_z z'}}{k_z+k_{zv}} & 0 \\ \frac{k_x k_z e^{-ik_z z'}}{k_z+\epsilon k_{zv}} & 0 & \frac{-k_x^2 e^{-ik_z z'}}{k_z+\epsilon k_{zv}} \end{bmatrix} \tag{S13}$$

It is clear that these results can be easily generalized to more complicated planar structures by deriving more general expressions for the Fresnel coefficients.

Generalization of the Green's functions to periodic structures:

In the general case of periodic structures (See Fig. S1b), we have:

$$\overleftrightarrow{G_E}\left(\omega,x,y,z,\beta\hat{\beta},z'\right) = -\frac{\omega\mu_0}{2k_z}\overrightarrow{Res_E}\left(\omega,x,y,z,\beta\hat{\beta},z',\hat{p}_{2+}\right)\hat{p}_{2+} - \frac{\omega\mu_0}{2k_z}\overrightarrow{Res_E}\left(\omega,x,y,z,\beta\hat{\beta},z',\hat{s}\right)\hat{s} \tag{S14}$$

where $\overrightarrow{Res_E}\left(\omega,x,y,z,\beta\hat{\beta},z',\hat{p}_{2+}\right)$ and $\overrightarrow{Res_E}\left(\omega,x,y,z,\beta\hat{\beta},z',\hat{s}\right)$ are electric field responses at position x, y, z to the P and S polarized incident plane wave with transversal wave-vector $\beta\hat{\beta}$ and unity electric field amplitude at position z' and angular frequency ω. This is the modified version of Sipe's formalism[S2].

Similarly, for the magnetic field, the following Green's function is defined:

$$\overleftrightarrow{G_H}\left(\omega,x,y,z,\beta\hat{\beta},z'\right) = -\frac{\omega\mu_0}{2k_z}\overrightarrow{Res_H}\left(\omega,x,y,z,\beta\hat{\beta},z',\hat{p}_{2+}\right)\hat{p}_{2+} - \frac{\omega\mu_0}{2k_z}\overrightarrow{Res_H}\left(\omega,x,y,z,\beta\hat{\beta},z',\hat{s}\right)\hat{s} \tag{S15}$$

where $\overrightarrow{Res_H}\left(\omega,x,y,z,\beta\hat{\beta},z',\hat{p}_{2+}\right)$ and $\overrightarrow{Res_H}\left(\omega,x,y,z,\beta\hat{\beta},z',\hat{s}\right)$ are magnetic field responses at position x, y, z to the P and S polarized incident plane wave, again with transversal wave vector $\beta\hat{\beta}$ and unity electric field amplitude at position z' and angular frequency of ω.

From these, in the general case of periodic structures, for the current density of $\vec{J}\left(\omega,k'_x,k'_y,z'\right) = \vec{J}\left(\omega,k_x,k_y,z_0\right)\delta\left(k'_x-k_x\right)\delta\left(k'_y-k_y\right)\delta\left(z'-z_0\right)$, the generated electric and magnetic field components at position x, y, and $z=0$ are given by:

$$\overrightarrow{E_a}\left(\omega,x,y,z=0,k_x,k_y,z_0\right) = \frac{-\omega\mu_0}{2k_z}e^{-ik_z(k_x,k_y)z_0} \times \sum_b \left(\left(\overrightarrow{Res_E}\left(\omega,x,y,z=0,\beta\hat{\beta},z'=0,\hat{p}_{2+}\right)\hat{p}_{2+} + \overrightarrow{Res_E}\left(\omega,x,y,z=0,\beta\hat{\beta},z'=0,\hat{s}\right)\hat{s}\right)_{ab}\right. \times \vec{J}_b\left(\omega,k_x,k_y,z_0\right) \tag{S16}$$

$$\overrightarrow{H_a}(\omega,x,y,z=0,k_x,k_y,z_0)=\frac{-\omega\mu_0}{2k_z}e^{-ik_z(k_x,k_y)z_0}$$
$$\times\sum_b\left(\overrightarrow{Res_H}\left(\omega,x,y,z=0,\beta\hat{\beta},z'=0,\hat{p}_{2+}\right)\hat{p}_{2+}\right.$$
$$\left.+\overrightarrow{Res_H}\left(\omega,x,y,z=0,\beta\hat{\beta},z'=0,\hat{s}\right)\hat{s}\right)_{ab}$$
$$\times\vec{J}_b(\omega,k_x,k_y,z_0) \tag{S17}$$

We assumed the z direction to be toward the substrate and normal to its plane. The convention used for the x direction is also shown in Fig. S1b. In the above equations, $z=0$ is chosen as the place of the substrate. In fact for a periodic material with infinite thickness, we are interested only in the calculation of electromagnetic fields in this location; since by knowing the transverse components of $\vec{E}$ and $\vec{H}$ field in this plane, we can calculate the Poynting vector which determines the heat transfer. This plane is shown with the bottom dashed line in Fig. S1b.

For simplification of the later equations, we define $\overrightarrow{G_E^a}(\omega,x,y,z,k_x,k_y)$ and $\overrightarrow{G_H^a}(\omega,x,y,z,k_x,k_y)$ as the following:

$$\overrightarrow{G_E^a}(\omega,x,y,z,k_x,k_y)\triangleq\frac{-\omega\mu_0}{2k_z}$$
$$\times\sum_b\left(\overrightarrow{Res_E}\left(\omega,x,y,z,\beta\hat{\beta},z'=0,\hat{p}_{2+}\right)\hat{p}_{2+}\right.$$
$$\left.+\overrightarrow{Res_E}\left(\omega,x,y,z,\beta\hat{\beta},z'=0,\hat{s}\right)\hat{s}\right)_{ba}\hat{e}_b \tag{S18}$$

$$\overrightarrow{G_H^a}(\omega,x,y,z,k_x,k_y)\triangleq\frac{-\omega\mu_0}{2k_z}$$
$$\times\sum_b\left(\overrightarrow{Res_H}\left(\omega,x,y,z,\beta\hat{\beta},z'=0,\hat{p}_{2+}\right)\hat{p}_{2+}\right.$$
$$\left.+\overrightarrow{Res_H}\left(\omega,x,y,z,\beta\hat{\beta},z'=0,\hat{s}\right)\hat{s}\right)_{ba}\hat{e}_b \tag{S19}$$

where $\hat{e}_b$ is the unity vector in direction b, which takes on the unity vectors in x, y, and z directions in the summation. These are the electric and magnetic fields at position x, y, and z, produced by the unity component a of the current density at $z'=0$. Note that $\overrightarrow{Res_E}$ and $\overrightarrow{Res_H}$ are the electromagnetic responses of the system that can be obtained through the RCWA method. Consequently, $\overrightarrow{G_E^a}(\omega,x,y,z,k_x,k_y)$ and $\overrightarrow{G_H^a}(\omega,x,y,z,k_x,k_y)$ can be calculated directly from the RCWA method, as well.

Therefore, for a general current density distribution $\vec{J}(\omega,x_0,y_0,z_0)$ in the substrate material, we can write $\vec{E}$ and $\vec{H}$ at position x, $y=0$, and $z=0$, in the following general form:

$$\vec{E}(x,y=0,z=0,t)=\frac{1}{(2\pi)^3}\int_{\omega=0}^{+\infty}d\omega e^{i\omega t}\int d\vec{r}_0$$
$$\times\sum_a\int_{k_y=-\infty}^{+\infty}\int_{k_x=-\infty}^{+\infty}dk_xdk_ye^{-ik_xx_0-ik_yy_0-ik_z(k_x,k_y)z_0}$$
$$\times\overrightarrow{G_E^a}(\omega,x,y=0,z=0,k_x,k_y)$$
$$\times\vec{J}_a(\omega,x_0,y_0,z_0)+\text{c.c.} \tag{S20}$$

$$\vec{H}(x,y=0,z=0,t)=\frac{1}{(2\pi)^3}\int_{\omega=0}^{+\infty}d\omega e^{i\omega t}\int d\vec{r}_0$$
$$\times\sum_b\int_{k_y=-\infty}^{+\infty}\int_{k_x=-\infty}^{+\infty}dk_xdk_ye^{-ik_xx_0-ik_yy_0-ik_z(k_x,k_y)z_0}$$
$$\times\overrightarrow{G_H^b}(\omega,x,y=0,z=0,k_x,k_y)$$
$$\times\vec{J}_b(\omega,x_0,y_0,z_0)+\text{c.c.} \tag{S21}$$

where a, b denotes the three possible components of the current density, and $\overrightarrow{G_E^a}(\omega,x,y=0,z=0,k_x,k_y)$ and $\overrightarrow{G_H^b}(\omega,x,y=0,z=0,k_x,k_y)$, are defined in the above. Also c.c. refers to complex conjugate.

According to the above equations, the following expression for the Poynting vector is found:

$$\vec{P}(x,y=0,z=0)=\frac{1}{(2\pi)^6}\sum_{a,b}\int_{\omega=0}^{+\infty}\int_{\omega'=0}^{+\infty}d\omega'd\omega$$
$$\times e^{i(\omega-\omega')t}\int\int d\vec{r_0}d\vec{r_0'}\left\langle\vec{J}_a(\omega,\vec{r_0})\vec{J}_b^*\left(\omega',\vec{r_0'}\right)\right\rangle$$
$$\times\int_{k_y'=-\infty}^{+\infty}\int_{k_x'=-\infty}^{+\infty}\int_{k_y=-\infty}^{+\infty}\int_{k_x=-\infty}^{+\infty}dk_xdk_ydk_x'dk_y'$$
$$\times\left(\overrightarrow{G_E^a}(\omega,x,y=0,z=0,k_x,k_y)\right.$$
$$\left.\times\overrightarrow{G_H^{b*}}\left(\omega',x,y=0,z=0,k_x',k_y'\right)\right)$$
$$\times e^{-ik_xx_0-ik_yy_0-ik_zz_0+ik_x'x_0'+ik_y'y_0'+ik_z'^*z_0'}+\text{c.c.} \tag{S22}$$

Random thermal motions of charges inside a material generate fluctuating current densities. These current densities, for a material that is in the thermodynamic equilibrium at temperature T, obey the following correlation relation known as fluctuation dissipation theorem[S3,S4]:

$$\left\langle\vec{J}_a(\omega,\vec{r_0})\vec{J}_b^*\left(\omega',\vec{r_0'}\right)\right\rangle=4\pi\epsilon_0\epsilon''(\omega)\hbar\omega^2$$
$$\times\left(e^{\hbar\omega/k_bT}-1\right)^{-1}\delta_{ab}\delta(\omega-\omega')\delta\left(\vec{r_0}-\vec{r_0'}\right) \tag{S23}$$

After making a simplification using the fluctuation dissipation theorem, we have:

$$\overrightarrow{P}(x,y=0,z=0)=\frac{1}{16\pi^5}\sum_a\int_{\omega=0}^{+\infty}d\omega\int d\vec{r}_0\epsilon_0$$
$$\times\,\epsilon''(\omega)\,\hbar\omega^2\left(e^{\hbar\omega/k_bT}-1\right)^{-1}$$
$$\times\int_{k'_y=-\infty}^{+\infty}\int_{k'_x=-\infty}^{+\infty}\int_{k_y=-\infty}^{+\infty}\int_{k_x=-\infty}^{+\infty}dk_xdk_ydk'_xdk'_y$$
$$\times\Big(\overrightarrow{G_E^a}(\omega,x,y=0,z=0,k_x,k_y)$$
$$\times\,\overrightarrow{G_H^{a*}}(\omega,x,y=0,z=0,k'_x,k'_y)\Big)$$
$$\times\, e^{i(k'_x-k_x)x_0+i(k'_y-k_y)y_0}e^{i(k'^*_z-k_z)z_0}+\text{c.c.}\tag{S24}$$

after interchanging the order of integrations, we arrive at:

$$\overrightarrow{P}(x,y=0,z=0)=\frac{1}{16\pi^5}\sum_a\int_{\omega=0}^{+\infty}d\omega\epsilon_0\epsilon''(\omega)$$
$$\times\int_{k'_y=-\infty}^{+\infty}\int_{k'_x=-\infty}^{+\infty}\int_{k_y=-\infty}^{+\infty}\int_{k_x=-\infty}^{+\infty}dk_xdk_ydk'_xdk'_y$$
$$\times\Big(\overrightarrow{G_E^a}(\omega,x,y=0,z=0,k_x,k_y)$$
$$\times\,\overrightarrow{G_H^{a*}}(\omega,x,y=0,z=0,k'_x,k'_y)\Big)$$
$$\times\,\hbar\omega^2\int_{z_0=0}^{\infty}\int_{y_0=-\infty}^{\infty}\int_{x_0=-\infty}^{\infty}dx_0dy_0dz_0e^{i(k'^*_z-k_z)z_0}$$
$$\times\, e^{i(k'_x-k_x)x_0+i(k'_y-k_y)y_0}\left(e^{\hbar\omega/k_bT}-1\right)^{-1}+\text{c.c.}\tag{S25}$$

which reduces to:

$$\overrightarrow{P}(x,y=0,z=0)=\frac{1}{4\pi^3}\sum_a\int_{\omega=0}^{+\infty}d\omega\epsilon_0\epsilon''(\omega)$$
$$\times\int_{k'_y=-\infty}^{+\infty}\int_{k'_x=-\infty}^{+\infty}\int_{k_y=-\infty}^{+\infty}\int_{k_x=-\infty}^{+\infty}dk_xdk_ydk'_xdk'_y$$
$$\times\Big(\overrightarrow{G_E^a}(\omega,x,y=0,z=0,k_x,k_y)$$
$$\times\,\overrightarrow{G_H^{a*}}(\omega,x,y=0,z=0,k_x,k_y)\Big)$$
$$\times\,\hbar\omega^2\left(e^{\hbar\omega/k_bT}-1\right)^{-1}\delta(k_x-k'_x)\,\delta\left(k_y-k'_y\right)$$
$$\times\int_{z_0=0}^{\infty}e^{i(k'^*_z-k_z)z_0}dz_0+\text{c.c.}\tag{S26}$$

Finally we obtain that:

$$\overrightarrow{P}(z=0,y=0,x)=\frac{1}{4\pi^3}\sum_a\int_{\omega=0}^{+\infty}d\omega\epsilon_0\epsilon''(\omega)\,\hbar\omega^2$$
$$\times\left(e^{\hbar\omega/k_bT}-1\right)^{-1}\int_{k_y=-\infty}^{+\infty}\int_{k_x=-\infty}^{+\infty}dk_xdk_y$$
$$\times\,\frac{1}{Im(k_z)}\Re\Big\{\Big(\overrightarrow{G_E^a}(\omega,x,y=0,z=0,k_x,k_y)$$
$$\times\,\overrightarrow{G_H^{a*}}(\omega,x,y=0,z=0,k_x,k_y)\Big)\Big\}\tag{S27}$$

If the periodic material has infinite extent, the z component of this quantity measures the total thermal transfer. However, if as denoted in Fig. S1b, the periodic material has a finite height, the Poynting vector at the top dashed line should also be calculated. We assume that the top dashed line be located at $z=-h$. Thermal transfer in this case is the difference of these two contributions. Moreover, thermal conductance can be obtained from thermal transfer through differentiating with respect to temperature:

$$S_{total}(x)=\frac{1}{4\pi^3}\sum_a\int_{\omega=0}^{+\infty}d\omega\epsilon_0\epsilon''(\omega)\left(e^{\hbar\omega/k_bT}-1\right)^{-2}$$
$$\times\int_{k_y=-\infty}^{+\infty}\int_{k_x=-\infty}^{+\infty}dk_xdk_y\frac{e^{\hbar\omega/k_bT}}{Im(k_z)}\frac{\hbar^2\omega^3}{k_bT^2}$$
$$\times\,\Re\Big\{\Big(\overrightarrow{G_E^a}(\omega,x,y=0,z=0,k_x,k_y)$$
$$\times\,\overrightarrow{G_H^{a*}}(\omega,x,y=0,z=0,k_x,k_y)$$
$$-\,\overrightarrow{G_E^a}(\omega,x,y=0,z=-h,k_x,k_y)$$
$$\times\,\overrightarrow{G_H^{a*}}(\omega,x,y=0,z=-h,k_x,k_y)\Big)_z\Big\}\tag{S28}$$

In fact, what is measured as the total heat conductance is the average of the above function across a period, which we show here with the same symbol:

$$S_{total}=\frac{1}{P}\int_{x=0}^{P}S_{total}(x)\,dx\tag{S29}$$

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