Supporting Information for Vertical single-wall carbon nanotube forests as plasmonic heat pipes

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Expression for the heat flux between SWNT forest and dielectric substrate

The heat flux between vertical forest of SWNTs and dielectric substrate is given by

$$\dot{q}(\omega) = \frac{N\omega^3 \operatorname{Re}\sigma_{zz}(\omega) \operatorname{Im}\varepsilon_{\rm sub}(\omega)}{2\pi^2 c^4} \left(\Theta(\omega, T_{\rm sub}) - \Theta(\omega, T_{\rm nt})\right) \times \int\limits_{S_{\rm nt}} d\mathbf{R}_{\rm nt} \int\limits_{V_{\rm sub}} d\mathbf{R}_{\rm sub} \sum_{\alpha=x,y,z} |G_{\alpha z}(\mathbf{R}_{\rm sub}, \mathbf{R}_{\rm nt}, \omega)|^2, \tag{1}$$

where electric field Green dyadic, $\underline{\underline{G}}(\mathbf{r}, \mathbf{r}', \omega)$, for an isolated SWNT placed above the substrate is defined as

$$\left[\left(\nabla_{\mathbf{r}} \times \underline{\underline{I}}\right) \cdot \left(\nabla_{\mathbf{r}} \times \underline{\underline{I}}\right) - k^2(\mathbf{r}) \underline{\underline{I}} \right] \cdot \underline{\underline{G}}(\mathbf{r}, \mathbf{r}', \omega) = 4\pi \underline{\underline{I}} \delta(\mathbf{r} - \mathbf{r}'), \tag{2}$$

where

$$k(\mathbf{r}) = \begin{cases} (\omega/c)\sqrt{\varepsilon_{\rm sub}}, & z < 0 \\ (\omega/c), & z > 0 \end{cases} \tag{3}$$

is the wavenumber, $\underline{\underline{I}}$ is the unit dyadic, $\delta(\mathbf{r} - \mathbf{r}')$ is the Dirac delta-function. The Green dyadic $\underline{\underline{G}}$ must also satisfy boundary conditions imposed on the SWNT surface (see Eqs. (7,8) in Ref.[1]). We look for the solution of Eq. (2) in the form

$$\underline{\underline{G}}(\mathbf{r}, \mathbf{r}', \omega) = \underline{\underline{G}}^{(hs)}(\mathbf{r}, \mathbf{r}', \omega) + \underline{\underline{G}}^{(sc)}(\mathbf{r}, \mathbf{r}', \omega), \tag{4}$$

where $\underline{\underline{G}}^{(hs)}$ is the half-space Green dyadic, satisfying inhomogeneous Eq. (2). The scattered Green dyadic $\underline{\underline{G}}^{(sc)}$, satisfying homogeneous Eq. (2) and the effective boundary conditions on the SWNT surface, is given by[1]

$$G^{(sc)}_{\alpha z}(\mathbf{r}, \mathbf{r}', \omega) = \frac{i\omega}{c^2} \int\limits_{S_{\rm nt}} d\mathbf{R}_{\rm nt} \, G^{(hs)}_{\alpha z}(\mathbf{r}, \mathbf{R}_{\rm nt}, \omega) \, \mathcal{J}\left(\mathbf{R}_{\rm nt}, \mathbf{r}', \omega\right), \tag{5}$$

where $\alpha = x,y,z$, $\mathcal{J}\,(\mathbf{R}_{\rm nt},\mathbf{r}',\omega) = \sigma_{zz}(\omega)\,G_{zz}(\mathbf{R}_{\rm nt},\mathbf{r}',\omega)$ is current density induced on the SWNT surface by a delta-source situated in point $\mathbf{r}'$ and polarized along z-axis of the Cartesian coordinate system. Hereinafter, we use the coordinate system with the origin on the substrate surface and z-axis oriented along the SWNT axis. Radius-vectors $\mathbf{R}_{\rm nt}$ and $\mathbf{R}_{\rm a}$ of the points on the SWNT surface and SWNT axis are defined as

$$\mathbf{R}_{\rm nt}(z,\varphi) = R(\cos\varphi\,\mathbf{e}_x + \sin\varphi\,\mathbf{e}_y) + \mathbf{R}_{\rm a}(z), \tag{6}$$

$$\mathbf{R}_{\rm a}(z) = (z - L/2 - d)\,\mathbf{e}_z, \tag{7}$$

where $z \in [-L/2, L/2]$, $\varphi \in [0, 2\pi)$, and $\mathbf{e}_\alpha$ are the unit basis vectors.

Substituting Eqs. (4),(5) in Eq. (1) and using the identity

$$\sum_{\alpha=x,y,z}\int\limits_{V_{\rm sub}} d\mathbf{r}\,\frac{\omega^2}{c^2}\,G^{(hs)}_{i\alpha}(\mathbf{r}_1,\mathbf{r},\omega)G^{*(hs)}_{j\alpha}(\mathbf{r}_2,\mathbf{r},\omega){\rm Im}\,\varepsilon_{\rm sub}(\omega) = 4\pi\,{\rm Im}G^{(hs)}_{ij}(\mathbf{r}_1,\mathbf{r}_2,\omega), \tag{8}$$

we obtain

$$\dot{q}(\omega) = \frac{N\omega^3\,{\rm Re}\,\sigma_{zz}(\omega)}{2\pi^2 c^4}(\Theta(\omega,T_{\rm sub}) - \Theta(\omega,T_{\rm nt}))(q_1(\omega)+q_2(\omega)+q_3(\omega)), \tag{9}$$

where

$$q_1(\omega) = \frac{4\pi c^2}{\omega^2}\int\limits_{S_{\rm nt}} d\mathbf{R}_{\rm nt}\,{\rm Im}G^{(hs)}_{zz}(\mathbf{R}_{\rm nt},\mathbf{R}_{\rm nt},\omega), \tag{10}$$

$$q_2(\omega) = -\frac{8\pi}{\omega}\int\limits_{S_{\rm nt}} d\mathbf{R}_{\rm nt}\int\limits_{S_{\rm nt}} d\mathbf{R}'_{\rm nt}\,{\rm Im}\mathcal{J}\left(\mathbf{R}'_{\rm nt},\mathbf{R}_{\rm nt},\omega\right){\rm Im}G^{(hs)}_{zz}(\mathbf{R}_{\rm nt},\mathbf{R}'_{\rm nt},\omega), \tag{11}$$

$$q_3(\omega) = \frac{4\pi}{c^2}\int\limits_{S_{\rm nt}} d\mathbf{R}_{\rm nt}\int\limits_{S_{\rm nt}} d\mathbf{R}'_{\rm nt}\int\limits_{S_{\rm nt}} d\mathbf{R}''_{\rm nt}\mathcal{J}(\mathbf{R}'_{\rm nt},\mathbf{R}_{\rm nt},\omega)\,\mathcal{J}^*(\mathbf{R}''_{\rm nt},\mathbf{R}_{\rm nt},\omega)\,{\rm Im}G^{(hs)}_{zz}(\mathbf{R}'_{\rm nt},\mathbf{R}''_{\rm nt},\omega). \tag{12}$$

Equations (10)-(12) can be simplified even further:

$$q_1(\omega) \approx \frac{8\pi^2 R c^2}{\omega^2} \int\limits_{-L/2}^{L/2} dz \,\mathrm{Im} G_{zz}^{(hs)}(\mathbf{R}_\mathrm{a}, \mathbf{R}'_\mathrm{a}, \omega), \tag{13}$$

$$q_2(\omega) \approx -\frac{16\pi^2 R^2}{\omega} \int\limits_{-L/2}^{L/2} dz \int\limits_{-L/2}^{L/2} dz' \,\mathrm{Im} G_{zz}^{(hs)}(\mathbf{R}_\mathrm{a}, \mathbf{R}'_\mathrm{a}, \omega) \,\mathrm{Im}\mathcal{J}_a\left(\mathbf{R}'_\mathrm{a}, \mathbf{R}_\mathrm{a}, \omega\right), \tag{14}$$

$$q_3(\omega) \approx \frac{8\pi^2 R^3}{c^2} \int\limits_{-L/2}^{L/2} dz' \int\limits_{-L/2}^{L/2} dz'' \,\mathrm{Im} G_{zz}^{(hs)}(\mathbf{R}'_\mathrm{a}, \mathbf{R}''_\mathrm{a}, \omega) \int\limits_{-L/2}^{L/2} dz \,\mathcal{J}_a\left(\mathbf{R}'_\mathrm{a}, \mathbf{R}_\mathrm{a}, \omega\right) \mathcal{J}_a^*\left(\mathbf{R}''_\mathrm{a}, \mathbf{R}_\mathrm{a}, \omega\right), \tag{15}$$

where we take into account that $\int_{S_\mathrm{nt}} d\mathbf{R}_\mathrm{nt} = R\int_0^{2\pi} d\varphi \int_{-L/2}^{L/2} dz$, and $\mathrm{Im} G_{zz}^{(hs)}(\mathbf{R}_\mathrm{nt}, \mathbf{R}'_\mathrm{nt}, \omega) \approx \mathrm{Im} G_{zz}^{(hs)}(\mathbf{R}_\mathrm{a}, \mathbf{R}'_\mathrm{a}, \omega)$.

As a next step we introduce the half-space Green dyadic, using the method of images (see Sec. 10.10 in Ref.[2]), as

$$G_{zz}^{(hs)}(\mathbf{r}, \mathbf{r}', \omega) = G_{zz}^{(fs)}(\mathbf{r}, \mathbf{r}', \omega) + \frac{\varepsilon_\mathrm{sub}(\omega) - 1}{\varepsilon_\mathrm{sub}(\omega) + 1} G_{zz}^{(fs)}\left(\mathbf{r}, \mathbf{r}'^{(im)}, \omega\right), \tag{16}$$

where points $\mathbf{r}$,$\mathbf{r}'$ lie above the substrate, $\mathbf{r}'^{(im)} = (x', y', -z')$ designates the image charge position, and

$$G_{zz}^{(fs)}(\mathbf{r}, \mathbf{r}', \omega) = \left(1 + \frac{1}{k_0^2}\frac{\partial^2}{\partial z^2}\right) \frac{e^{ik_0|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|} \tag{17}$$

is the free-space Green dyadic, $k_0 = \omega/c$. Equation (16) is valid only when the gap width and the SWNT length are much smaller than radiation wavelength.

Finally, we need to calculate current density, $\mathcal{J}_a$, given by

$$\mathcal{J}_a(\mathbf{R}_{\rm a},\mathbf{R}'_{\rm a},\omega) = \sigma_{zz}(\omega)\int\limits_0^{2\pi} d\varphi' G_{zz}(\mathbf{R}_{\rm nt},\mathbf{R}'_{\rm nt},\omega)$$
$$= \sigma_{zz}(\omega)\left(k_0^2+\frac{\partial^2}{\partial z^2}\right)\left(\Phi(z,z',\omega)+\frac{i\omega R}{c^2}\int\limits_{-L/2}^{L/2}\Phi(z,z'',\omega)\mathcal{J}_a(\mathbf{R}''_{\rm a},\mathbf{R}'_{\rm a},\omega)dz''\right), \quad (18)$$

where

$$\Phi(z,z',\omega) = \frac{1}{k_0^2}\int\limits_0^{2\pi}\frac{e^{ik_0 r(z,z',\phi')}}{r(z,z',\phi')}d\varphi' + \frac{2\pi}{k_0^2}\frac{\varepsilon_{\rm sub}(\omega)-1}{\varepsilon_{\rm sub}(\omega)+1}\frac{e^{ik_0 r_{im}(z,z')}}{r_{im}(z,z')}, \quad (19)$$

$r(z,z',\varphi') = \sqrt{(z-z')^2+4R^2\sin^2(\varphi'/2)}$, $r_{im}(z,z') = L+2d-z-z'$. Integro-differential equation (18) is transformed to the Hallen integral equation fo current density

$$\int\limits_{-L/2}^{L/2}\mathcal{K}(z,z'')\,\mathcal{J}_a(\mathbf{R}_{\rm a}(z''),\mathbf{R}_{\rm a}(z'),\omega)dz'' + C_1e^{-ik_1z}+C_2e^{ik_1z} = 2ik_0\Phi(z,z',\omega) \quad (20)$$

with the kernel

$$\mathcal{K}(z,z'') = \frac{e^{ik_1|z-z''|}}{\sigma_{zz}(\omega)} + \frac{2\omega^2R}{c^3}\Phi(z,z'',\omega). \quad (21)$$

Integral equation (20) is supplemented by the edge condition $\mathcal{J}_a(\mathbf{R}_{\rm a}(\pm L/2),\mathbf{R}_{\rm a}(z'),\omega)=0$.

The integral equation is solved by reducing it to the system of linear equations. For this purpose we divide the SWNT axis on N_p small pieces and assume that current $\mathcal{J}_a(\mathbf{R}_a(z''),\mathbf{R}_a(z'),\omega)$ is constant along each of these pieces. Formal solution of this system is given by

$$\mathbf{J}(\mathbf{R}_a(z')) = \mathcal{M}^{-1}\mathbf{\Phi}(z'), \quad (22)$$

where

$$J_l(\mathbf{R}_\mathrm{a}(z')) = \begin{cases} \mathcal{J}_a(\mathbf{R}_\mathrm{a}(z_l),\mathbf{R}_\mathrm{a}(z'),\omega), & l \neq 1, N_{eq}+1, \\ C_1, & l = 1, \\ C_2, & l = N_{eq}+1, \end{cases} \tag{23}$$

$$\mathcal{M}_{nl} = \begin{cases} \int\limits_{-z_l-h/2}^{z_l+h/2} \mathcal{K}(z_n,z'')dz'', & l \neq 1, N_{eq}+1, \\ e^{-ik_1 z_n}, & l = 1, \\ e^{ik_1 z_n}, & l = N_{eq}+1, \end{cases} \tag{24}$$

$\Phi_l(z') = 2ik_0\Phi(z_l,z')$, $h = L/N_p$, $z_l = -L/2 + (l-1)h$. It should be noted that $\Phi(z,z')$ has log-singularity when $z = z'$. However, this singularity is integrable and there are no singular terms in matrix $\mathcal{M}$. Moreover, singularity in $\mathbf{\Phi}(z')$ is also eliminated by substituting formal solution (22) into Eqs. (14),(15) and integrating over z'.

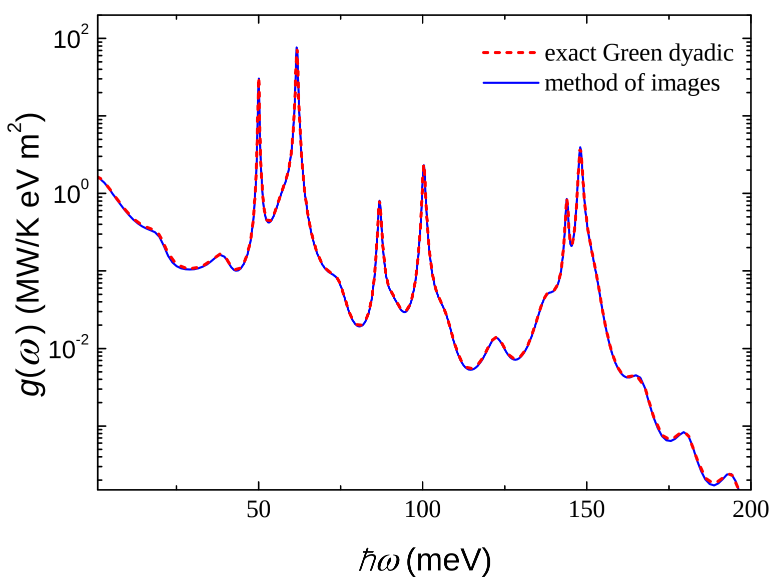

Figure 1: Spectral Kapitza conductance, $g(\omega)$, between quartz substrate and vertical forest of identical metallic (15,0) SWNTs of length $L = 500$ nm as a function of frequency. $d = 10$ nm, $T_{\mathrm{sub}} = 300$ K, $N = 10^{16}$ m^{-2}. Calculations are made using exact expression[1,2] for the half-space Green dyadic (dash red line) and method of images approximation (solid blue line).

In order to justify our choice of Green dyadic (16), we calculate spectral thermal conductance across a gap between forest of identical (15,0) SWNTs and quartz substrate, using both the exact expression[1,2] for the half-space Green dyadic (red dashed line in Fig. 1) and Eq. (16), obtained by method of images (solid blue line in Fig. 1). As one can see from Fig. 1, the method of images provides good approximation for the half-space Green tensor in the low-frequency region, when both the SWNT length and the gap width are much smaller than the radiation wavelength.

Dependence of the thermal Kapitza conductance on the radius of metallic SWNTs in the forest

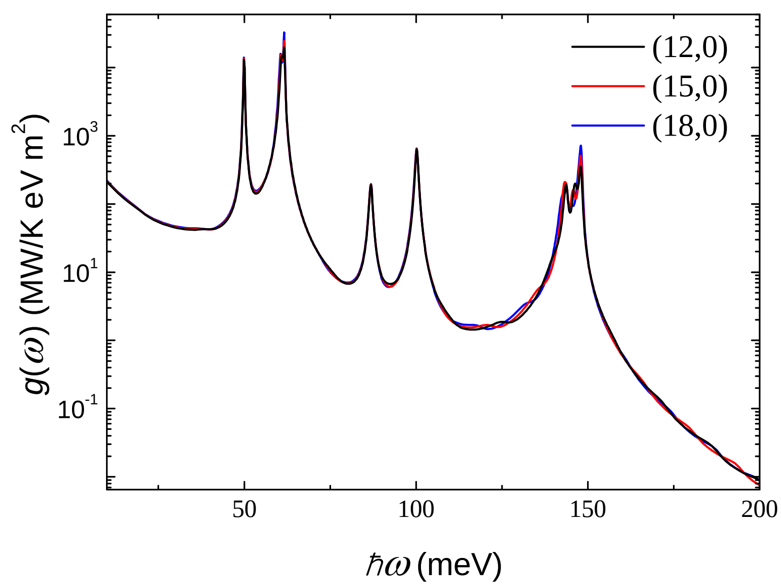

Figure 2: Spectral Kapitza conductance, $g(\omega)$, between quartz substrate and vertical forest of identical metallic SWNTs as a function of frequency. Chiralities of SWNTs in the forest are indicated in the figure. $d = 0.34$ nm, $T_S = 300$ K, $N = 10^{16}$ m^{-2}, $L = 500$ nm.

Thermal Kapitza conductance between a forest of metallic SWNTs and substrate depends insignificantly on the radius R of SWNTs in the forest (see Fig. 2). Particularly, interface thermal conductance is equal to 47.4 MW K^{-1} m^{-2} for a forest of $(12,0)$ SWNTs, 51.6 MW K^{-1} m^{-2} for a forest of $(15,0)$ SWNTs, and 57.4 MW K^{-1} m^{-2} for a forest of

(18,0) SWNTs. We explain this behaviour by the fact that the SWNT surface area increases proportionally to the SWNT radius, while the electric surface conductivity of metallic SWNTs decreases inversely proportional to the SWNT radius.[3] Thus increase in the SWNT absorption area is compensated by the decrease of the absorption strength per unit area, defined by the electric conductivity.

Interface thermal conductance of the forest of undoped semiconducting SWNTs

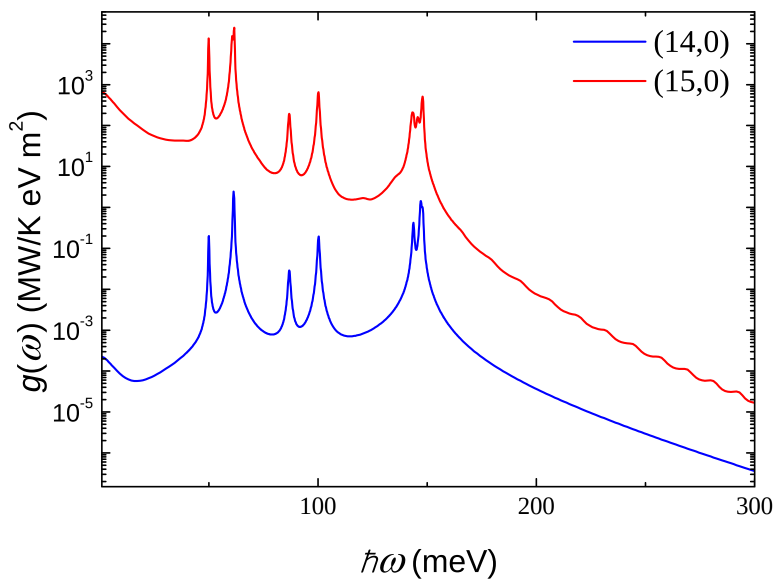

Figure 3: Spectral thermal conductance, $g(\omega)$, between quartz substrate and vertical forest of identical SWNTs as a function of frequency. Chiralities of SWNTs in the forest are indicated in the figure. $d = 0.34$ nm, $T_S = 300$ K, $N = 10^{16}$ m^{-2}, $L = 500$ nm.

Conductivity of an undoped semiconducting SWNT can not be described by the Drude model. Using the full quantum-mechanical expression for the conductivity[1] of semiconducting SWNTs, we calculate the interface thermal conductance between vertical forest of (14,0) SWNTs and quartz substrate (see Fig. 3). As one can see, the spectral thermal conductance contains pronounced polariton resonances, only. Plasmon resonances are absent in the spectrum, because of the strong attenuation of the surface plasmons in semiconducting SWNTs. Moreover, the thermal conductance across the gap between (14,0) SWNT forest and quartz is equal to 5.5 KW K^{-1} m^{-2}. This is more than three orders of magnitude lower than the interface thermal conductance values, obtained for metallic SWNT forest.

References

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