Enhanced radiative heat transfer between nanostructured gold plates

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Abstract. We compute the radiative heat transfer between nanostructured gold plates in the framework of the scattering theory. We predict an enhancement of the heat transfer as we increase the depth of the corrugations while keeping the distance of closest approach fixed. We interpret this effect in terms of the evolution of plasmonic and guided modes as a function of the grating’s geometry.

The far-field radiative heat transfer between good conductive metals is very low at room temperature, since they are very good reflectors at the infrared frequencies of blackbody radiation. The radiative heat transfer is enhanced in the near field, due to the contribution of evanescent surface modes \cite{1, 2, 3}. Polar materials like SiO\textsubscript{2} or SiC are in addition favored by the contribution of surface phonon polaritons whose resonance frequencies lie in the infrared \cite{4}. There is an analogous effect for metals arising from the surface plasmons resonances but those lie in the ultraviolet and do not contribute significantly to the heat transfer \cite{5}.

It has been shown recently that the radiative heat transfer can be controlled by nanostructuring the interfaces periodically. When the period $d$ is much smaller than the wavelength $\lambda$ and the separation distance $L$, the system can be treated using an effective refractive index for the equivalent homogeneous medium. It has been shown that the induced anisotropy introduces additional modes \cite{6} and also allows modulating the flux \cite{7}. For periods on the order of the wavelength, a full solution of Maxwell equations is needed. The heat transfer between two periodic slabs has been studied within a two dimensional approximation and for $p$-polarization using a finite difference time domain (FDTD) technique \cite{8}. A flux enhancement attributed to the excitation of the structure’s modes was found. While FDTD allows modeling complex shapes easily, dealing with bulk 3D media and accounting for polarization effects has not been achieved so far.

In this article, we compute the radiative heat transfer between 1D gold lamellar gratings in the framework of the scattering theory. We do include all propagation directions (the so-called conical diffraction) and all polarization states, which is of critical importance in order to deal quantitatively with cross-polarization effects \cite{9}. The scattering theory is the most successful technique for treating the Casimir effect between bodies at thermodynamic equilibrium \cite{10, 11}. The method determines the electromagnetic field in the space between the two bodies in interaction in order to compute the Maxwell stress tensor in terms of the reflection amplitudes on the two bodies. When the two bodies are not at the same temperature, there is a net flux.
of energy transferred from the warm body to the cold one. Recently, this heat transfer problem between two bodies kept at different temperatures has also been formulated in terms of the scattering properties of the bodies [12, 13, 14, 15].

In the following, we use the scattering amplitudes which have already been calculated for studying the Casimir interaction between 1D lamellar gratings [16] and deduce the heat flux when the two bodies are at different temperatures. We show that the heat flux is largely enhanced when the corrugation depth is increased while keeping the distance of closest approach fixed. We attribute the heat flux increase to the excitation of guided modes and surface plasmons whose frequencies change with the corrugation depth.

![Diagram](image-url)

**Figure 1.** The conventions used in the present paper. The grating period is $d$, the corrugation depth is $a$, the distance of closest approach of the two gratings is $L$. The lines of the grating are along the $y$ direction, while the Fabry-Perot cavity between the two gratings is along the $z$ direction.

We consider the cavity formed by two gratings separated by a distance of closest approach $L$ measured so as to vanish at contact (Fig. 1). The gratings are aligned and not displaced laterally. We model the gold permittivity with a Drude model $\epsilon(\omega) = 1 - \frac{\omega_p^2}{\omega^2 + i\gamma\omega}$ with $\omega_p = 9$ eV and $\gamma = 35$ meV. We write the heat flux $q$ between two bodies at temperatures $T_1$ and $T_2$ as [3]

$$q = \int \int \int (e_{T_1}(\omega) - e_{T_2}(\omega)) T_L(k, \omega) \frac{d\omega dk}{(2\pi)^3},$$

(1)

where $e_T(\omega) = \hbar \omega (e^{\hbar \omega/k_BT} - 1)^{-1}$ is the mean energy per mode of frequency $\omega$ at temperature $T$ while $T_L(k, \omega)$ is the sum (trace) of the transmission factors for all the modes of frequency $\omega$ and lateral wavevector $k$ between the two gratings separated by a distance $L$ [17, 18].
expression of this transmission factor is given by scattering amplitudes

\[ T_L(k, \omega) = \text{tr} \left( DW_1 D^i W_2 \right), \]  
(2a)

\[ D = (1 - S_1 S_2)^{-1}, \]  
(2b)

\[ W_1 = \Sigma_{\perp}^{\text{pw}} - S_1 \Sigma_{\perp}^{\text{pw}} S_1^\dagger + S_1 \Sigma_{\parallel}^{\text{ew}} - \Sigma_{\parallel}^{\text{ew}} S_1, \]  
(2c)

\[ W_2 = \Sigma_1^{\text{pw}} - S_2^\dagger \Sigma_1^{\text{pw}} S_2 + S_2 \Sigma_1^{\text{ew}} - \Sigma_1^{\text{ew}} S_2, \]  
(2d)

\[ S_1 = R_1(k, \omega), \]  
(2e)

\[ S_2 = e^{ik_s L} R_2(k, \omega) e^{ik_s L}. \]  
(2f)

Mode counting is defined over frequency \(\omega\) and lateral wavevector \(k\) restricted to the first Brillouin zone, due to the Bloch theorem. \(k_z = \sqrt{\omega^2/c^2 - \mathbf{k}^2}\) is the longitudinal wavevector for the Fabry-Perot cavity, with the principal square root used in its definition \(-\frac{\pi}{2} < \arg k_z \leq \frac{\pi}{2}\).

The operators \(\Sigma_n^{\text{pw/ew}} = k_n^\alpha \Pi^{\text{pw/ew}}\) involve the projectors \(\Pi^{\text{pw/ew}}\) on the propagative or the evanescent sector, respectively. The operator \(D\) is the so-called Fabry-Perot denominator which takes into account the multiple reflection of thermal photons inside the cavity formed by the two gratings. The operators \(W_i\) account for the absorption of thermal photons (in particular, in the propagative sector the operator \(W_i\) is proportional to the emissivity \(1 - |r_i|^2\) of body \(i\) for a particular mode; this consideration can be extended in the evanescent sector \([17]\)). \(S_1\) and \(S_2\) are scattering operators defined from the reflection operators \(R_1(k, \omega)\) and \(R_2(k, \omega)\). \(S_i\) are represented in the basis of the wavevectors \(\{k^{(n)}\}\) coupled by the grating. We define \(k^{(n)} = k + n\frac{2\pi}{\lambda} \hat{e}_x\) where \(d\) is the grating period, \(\hat{e}_x\) the direction perpendicular to the lines of the grating (see figure 1) and \(n\) runs from \(-N\) to \(+N\), where \(N\) is the highest diffraction order retained. The operators \(S_i\) are square matrices of dimension \(2(2N + 1)\) \([16]\) as well as all bold operators appearing in eqs. 2 (note that \(e^{ik_s L}\) where \(k_s = \sqrt{\omega^2/c^2 - (k^{(n)})^2}\) is not proportional to the identity \(1\)). All scattering operators appearing in eqs. 2 are represented in the \((s/p)\) (also denoted TE/TM) polarization basis, well adapted to propagative fields.

In the following, we apply formula (1) to compute the heat transfer coefficient \(h\) defined as

\[ h = \frac{T_1 - T_2}{T_1 + T_2} \]  
for two temperatures \(T_1\) and \(T_2\) close enough to each other, say for example \(T_1 = 310\) K and \(T_2 = 290\) K. We note that \(T_1 - T_2\) acts as a cutoff function for frequencies greater than the thermal frequency \(\omega_T\) which can be defined as \(\omega_T = 2\pi c/\lambda T \approx 2.5 \times 10^{14}\) rad s\(^{-1}\) \((\lambda T \approx 7.6\) \(\mu\)m\)). The transmission factor \(T_L(k, \omega)\) thus exhibits the mode structure for the problem under study (Fig. 1) while (1) integrates the contributions of all these modes to the heat transfer, taking into account the values of their frequencies with respect to \(\omega_T\) (more discussions below).

For a depth of the corrugation \(a = 0\), we recover the heat transfer coefficient \(h_0(L) = 0.16\) Wm\(^{-2}\)K\(^{-1}\) between two gold plates separated by a distance \(L = 1\) \(\mu\)m. For a non null depth \(a\), we introduce the factor of enhancement of heat transfer with respect to non corrugated plates

\[ \Omega = \frac{h(L)}{h_0(L)}. \]  
(3)

We present in Fig. 2 the enhancement factor \(\Omega\) as a function of the corrugation depth \(a\), with the distance of closest approach \(L = 1\) \(\mu\)m and the filling factor \(p = 0.5\) kept fixed (the filling factor is the width of the corrugations per unit of the period). The blue solid curve corresponds to a period \(d = 1\) \(\mu\)m for the gratings while the red solid curve corresponds to a period \(d = 2.5\) \(\mu\)m. The dashed curve corresponds to a period \(d = 10\) \(\mu\)m. As the corrugations become deeper, we see a striking increase in the heat transfer coefficient. We note that the enhancement factor is largely independent of the grating period up to a corrugation depth \(a \approx 1\) \(\mu\)m. For a period \(d = 1\) \(\mu\)m for which the effect is more important, we get an enhancement up to a factor 10 for
a = 6 \, \mu m. For a period \( d = 2.5 \, \mu m \), the enhancement reaches nearly a factor 4 for \( a = 6 \, \mu m \). For the largest period \( d = 10 \, \mu m \), the enhancement still reaches nearly a factor 2 at \( a = 6 \, \mu m \).

For comparison, we have shown as the dotted line in Fig. 2 the prediction of the proximity approximation (PA) which amounts to adding plane-plane heat transfer contributions, as if they were independent,

\[ \Omega^{PA} = p + (1 - p) \frac{h_0(L + 2a)}{h_0(L)}. \]

As expected, the PA predicts a decrease of \( \Omega \) when \( a \) is increased, in complete contradiction with the exact results shown by the solid and dashed curves.

In the remainder of this article, we analyze the electromagnetic mode structure in order to explain the increase of the heat transfer [17, 18]. To this aim, we use the scattering formula (1) and show that, as we increase the corrugation depth, some modes of the system are indeed brought to the infrared frequencies and thus are able to contribute to the heat transfer. The mode structure is described by the transmission factor \( T_L(k, \omega) \) which can reach its maximum value 1 at the resonances of the corrugated cavity. Our system is periodic so that the mode structure, distributed over the whole range of wavevectors in the absence of corrugations, now shows many branches folded in the first Brillouin zone. More precisely, there are \( 2(2N + 1) \) branches where the factor 2 is due to the two polarizations and the factor \( 2N + 1 \) is the number of orders (or branches) used when taking into account mode coupling by diffraction on the gratings.

We represent in Fig. 3 the sum of transmission factors \( T_L(k, \omega) \) over all polarizations and all branches. It is shown as a function of the frequency \( \omega \) and the depth of the corrugations \( a \) for a fixed value of the transverse wavevector \( k = (\frac{\pi}{d}, 0) \), here chosen to be in the middle of the positive-\( k_x \) first Brillouin zone. The plot corresponds to the period \( d = 2.5 \, \mu m \), which was shown as the solid curve in Fig. 2. The vertical red line represents the light line \( \omega = ck_x \approx 1.88 \times 10^{14} \, \text{rad s}^{-1} \).

It clearly appears in Fig. 3 that the transmission factor takes significant values only on resonances which correspond to the mode structure of the corrugated cavity. The transmission
Figure 3. The transmission factor for two gold gratings with period $d = 2.5 \, \mu m$ as a function of the frequency $\omega$ and the corrugations depth $a$. The lower curve is for plane-plane $a = 0$ while the upper one is for corrugations depth $a = 3 \, \mu m$. The vertical red line is the light line. The horizontal arrow at $a = 1.5 \, \mu m$ shows a cut of this plot represented on Fig. 4. (colors online)

factor $T_L(k, \omega)$ goes to a maximum value of 1 for each non degenerate mode $(k, \omega)$; it can be 2 if two modes cross and we see one of these occurrences in the figure. The general trend is clear on the diagram: as the depth $a$ of the corrugations is increased, new modes appear, with frequencies decreasing as $a$ increases. When these modes enter into the thermal window $\omega \lesssim \omega_T$ they contribute more and more to the heat transfer. This explains the enhancement of the heat flux, due to the presence of additional modes in the thermal window for a deeply corrugated structure.

We now examine in more detail the nature of the modes. While varying the corrugation depth $a$ from 0 to $3 \, \mu m$ we can follow the evolution of each mode. Note that, for $k_y = 0$, the polarizations $\sigma = s$ and $\sigma = p$ are not mixed (however, the computation of $h$ takes into account all modes for which polarization mixing is important).

We show in Fig. 4 the modes calculated for a particular corrugation depth $a = 1.5 \, \mu m$ indicated by the red horizontal arrow on Fig. 3. The position of the peaks have been confirmed through a direct mode calculation [19] of the eigenfrequencies of the structure modes obtained for $p$ (black arrows) and $s$ (red arrows) polarizations. In addition to the excellent agreement between the peaks of the transmission factor and the directly calculated modes (arrows on Fig. 4), direct mode calculations show the fields and, therefore, allow us identifying the first few modes. For the second $p$ polarization and the first $s$ polarization modes appearing at $\omega \approx 2.4 \times 10^{14} \, \text{rad} \, \text{s}^{-1}$ and $\omega \approx 6.5 \times 10^{14} \, \text{rad} \, \text{s}^{-1}$ in particular, the frequencies are largely independent upon the value of $k_x$, which is usually the signature of guided modes. By looking at the fields corresponding to those two modes, we indeed confirmed that the electric field is to some extent confined in the
Figure 4. The transmission factor for two gold gratings with period \( d = 2.5 \) \( \mu \)m and corrugation depth \( a = 1.5 \) \( \mu \)m as a function of frequency \( \omega \). The arrows indicate the position of the modes in a direct mode calculation (red for \( s \) polarization and black for \( p \) polarization). The dashed curve is the function \( \frac{e^{T_1} - e^{T_2}}{e^{T_1} + T_2} \). (colors online)

waveguides formed by the corrugations.

To further illustrate this fact, we show in Fig. 5 the dispersion diagram resulting by representing the transmission factor \( T_L(k, \omega) \) in the plane \((k_x, \omega)\) still fixing \( k_y = 0 \). The diagram is for a period \( d = 1 \) \( \mu \)m and a corrugation depth \( a = 3 \) \( \mu \)m. There is a strong coupling between the plasmonic mode and the guided modes which are represented in red and are essentially \( k_x \)-independent as expected. The electromagnetic field associated to these modes is essentially confined to the waveguides formed by the corrugations and nearly vanishes in the vacuum between the gratings. We have indicated by horizontal arrows the position of the guided modes predicted by the relation appearing in ref. [20]. The leading term in the energetic position of the guided modes verify \( \cos(\omega a/c) = 0 \). It follows that to a good approximation, the position of the first few guided modes is independent of the period \( d \) and behaves as \( 1/a \) with the corrugation depth. This mechanism of strong coupling between “geometrical” resonances (guided modes) and plasmon has been studied before and dubbed “Spoof Surface Plasmons” (SSP) by some authors [21, 22].

We can further correlate the position of the guided modes with respect to the thermal window with the enhancement factor \( \Omega \) shown in Fig. 3. We show in Fig. 6 the position of the first two guided modes for two gold gratings with period \( d = 1 \) \( \mu \)m as a function of the corrugation depth \( a \). As expected, the frequency of those guided modes decreases with increasing corrugation depth.

Remembering that the thermal frequency \( \omega_T \approx 3 \times 10^{14} \) rad s\(^{-1}\) we see that the first guided mode enters the thermal window for \( a \approx 1 \) \( \mu \)m. As for the second guided mode, it enters the thermal window for \( a \approx 4 \) \( \mu \)m. We can then discuss the enhancement factor in Fig. 3: for \( a < 1 \) \( \mu \)m, there is no guided mode in the thermal window which can contribute to the heat transfer. In this regime, only the plasmon mode can contribute and this mode is very close to the light line at those low frequencies. This is the reason why the enhancement factor is essentially independent of the grating period \( d \) for \( a < 1 \) \( \mu \)m.

For \( a > 1 \) \( \mu \)m, the first guided mode enters the thermal window and leads to an enhancement
Figure 5. The transmission factor for two gold gratings with period $d = 1 \mu m$ and corrugation depth $a = 3 \mu m$ as a function of transverse wavevector $k_x$ and frequency $\omega$. The red curves are the guided modes, nearly $k_x$-independent. The horizontal arrows indicate the position of those guided modes as predicted by [20]. The dashed line is the light line.

Figure 6. Calculated position of the first two guided modes for two gold gratings with period $d = 1 \mu m$ as a function of the corrugation depth $a$. The lower dotted curve gives the position of the first guided mode while the upper dotted curve the position of the second one. We have indicated the thermal frequency $\omega_T$ by the horizontal solid line.
in the heat flux. This enhancement strongly depends on the coupling between the plasmon mode and the guided mode which in turn depends on the size of the first Brillouin zone. This non-trivial coupling between plasmon and guided modes even leads to a slight decrease in the heat flux for the larger period \( d = 10 \mu \text{m} \).

Finally, for the period \( d = 1 \mu \text{m} \) where the effect is the more visible, we can see a further increase in the heat flux around \( a = 4 \mu \text{m} \) corresponding to the second guided mode entering the thermal window.

We have theoretically demonstrated the enhancement of the heat transfer between two nanocorrugated gold plates in comparison with flat plates with the same distance of closest approach. This enhancement is due to the emergence of Spoof Surface Plasmon resonances which can be brought in the thermal frequency window and hence contribute to the heat transfer by varying the geometrical parameters of the gratings. We have described all the relevant information about the mode structure in terms of the transmission factor \( T_L(k,\omega) \) which appears in the scattering formula for the heat flux. We have discussed the enhancement of the heat transfer in a regime where the three characteristic lengths of the problem (the distance \( L \) between the gratings, the period \( d \) of the gratings and the height \( a \) of the corrugations) are of the same order. We stress that neither the proximity nor the effective medium approximations can work in this regime. We have in fact shown that the proximity approximation predicts a decrease of the heat transfer, in complete contradiction with the striking enhancement of the heat flux observed in the exact results.

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