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Finite dipole model for extreme near-field thermal radiation between a tip and planar SiC substrate

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ABSTRACT

Recent experimental studies have measured the infrared (IR) spectrum of tip-scattered near-field thermal radiation for a SiC substrate and observed up to a 50 cm^{-1} redshift of the surface phonon polariton (SPhP) resonance peak [1,2]. However, the observed spectral redshift cannot be explained by the conventional near-field thermal radiation model based on the point dipole approximation. In the present work, a heated tip is modeled as randomly fluctuating point charges (or fluctuating finite dipoles) aligned along the primary axis of a prolate spheroid, and quasistatic tip-substrate charge interactions are considered to formulate the effective polarizability and self-interaction Green's function. The finite dipole model (FDM), combined with fluctuational electrodynamics, allows the computation of tip-plane thermal radiation in the extreme near-field (i.e., $H/R \lesssim 1$, where H is the tip-substrate gap distance and R is the tip radius), which cannot be calculated with the point dipole approximation. The FDM provides the underlying physics on the spectral redshift of tip-scattered near-field thermal radiation as observed in experiments. In addition, the SPhP peak in the near-field thermal radiation spectrum may split into two peaks as the gap distance decreases into the extreme near-field regime. This observation suggests that scattering-type spectroscopic measurements may not convey the full spectral features of tip-plane extreme near-field thermal radiation.

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1. Introduction

Thermal radiation in the near-field is very different from the far-field phenomenon. Previous theoretical studies have predicted that in the near-field, or when the emitter-receiver separation is less than the thermal wavelength, thermal radiation can exceed Planck's blackbody limit by up to several orders of magnitude due to radiation tunneling of evanescent electromagnetic (EM) waves [3–6], and that its spectrum becomes quasi-monochromatic if surface modes are excited [5,7,8]. Recently, significant efforts have been made to experimentally validate the near-field enhancement of thermal radiation for plane-plane [9–15] and sphere-plane [16–19] configurations. However, in these configurations, achieving sub-10 nm vacuum gap distances is challenging due to technical difficulties in precision emitter-receiver gap control. The smallest vacuum gap distances achieved to date for the plane-plane and sphere-plane geometry are 60 nm and 20 nm, respectively [14,19].

In efforts to explore extreme near-field thermal radiation within sub-10 nm gap distances, scanning probe microscopy has been used due to its capability of controlling the tip position with sub-nanometer resolution. To measure near-field radiative heat transfer from a heated substrate to a tip, Kittel's group used a thermocouple-integrated needle probe to measure the tip temperature for different tip-substrate gap distances down to 1 nm in an ultra-high vacuum scanning tunneling microscope [20]. A similar experiment was conducted by measuring the near-field thermal conductance between a scanning thermal microscope probe and suspended microheater device [21]. However, their results are not consistent with each other, leaving open questions about the extreme near-field behaviors of thermal radiation. Tip-based near-field optical measurement is another scheme to investigate extreme near-field thermal radiation. De Wilde et al. [22] imaged the electromagnetic local density of states by collecting tip-scattered thermal emission from a metallic tip scanning over a heated substrate. Recently, tip-scattered near-field thermal radiation between a tip and SiC substrate was spectroscopically analyzed to demonstrate that thermal emission can excite surface phonon polaritons (SPhPs) on a SiC substrate to emit quasi-monochromatic thermal radiation [1,2]. However, they observed a spectral redshift of the SPhP resonance peak up to 50 cm^{-1}, which could not be explained with the conventional point dipole model [1,2]. This trait of scattering-type thermal infrared near-field spectroscopy (TINS) necessitates the development of a comprehensive model to understand the underlying physics of extreme near-field thermal radiation in the tip-plane geometry.

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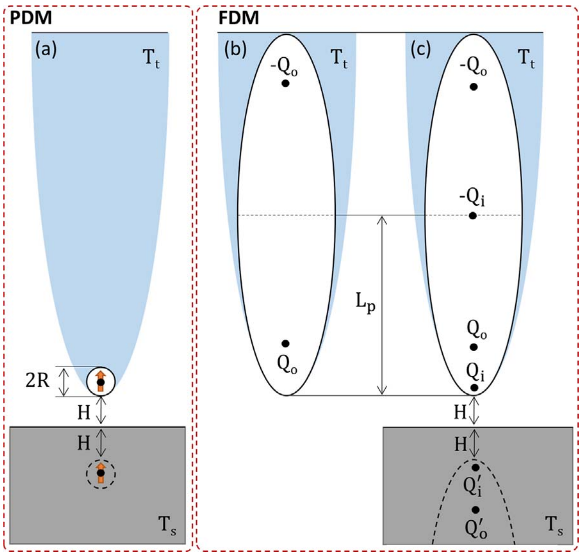

Fig. 1. Schematic of a tip with radius R and temperature T_t a distance H above a surface at temperature T_s as modeled by (a) the PDM, (b) the FDM with no surface, and (c) the FDM near the surface. The FDM uses a prolate spheroidal geometry with semi-major axis L_p. The non-perturbed charge distributions, Q_o and $-Q_o$, are formed by incident electric field without the surface while the induced charge distributions, Q_i and $-Q_i$, are induced by the near-field interaction between the tip and surface quantified by Q'_o and Q'_i.

The point dipole model (PDM) is a conventional model that reduces the complex tip geometry to a spherical point dipole located at the tip end [7,23–25]. Fig. 1(a) illustrates the schematic of the PDM, where R represents the tip (or dipole) radius and H is the tip-substrate separation equivalently defined throughout the paper. Quasistatic tip-substrate interactions are derived by mirroring the entire dipole in the surface and developing recursive interactions between the tip and image dipoles. The mathematical formulation of the PDM has been well developed for different tip-substrate configurations [7,24–26], and it has been used to understand tip-substrate near-field interactions in tip-based optical nanospectroscopy and near-field thermal radiation experiments [1,20,27,28]. However, the PDM is only valid for tip-substrate separations much larger than the tip radius to satisfy the uniform electric field condition of the model [24]. This limitation leads to a discrepancy between the PDM and the measured near-field IR spectrum for polar materials [1,28,29–31]. For example, Babuty et al. [1] had to use the tip geometry of R = 1.6 μm and H = 100 nm to replicate the observed spectral redshift of tip-scattered thermal radiation with the PDM, which is an unrealistic tip geometry outside the valid regime of the PDM. Aside from the simple PDM, various numerical methods have been developed to compute near-field thermal radiation between arbitrary geometries, such as the finite difference time domain method [32,33], molecular dynamics [34], and thermal discrete dipole approximation [35,36]. However, these numerical schemes are computationally expensive to be routinely used in conjunction with experiments.

In this article, we implement the finite dipole model (FDM) to calculate tip-plane near-field thermal radiation for tip-plane separations less than those permitted by the PDM while maintaining computational simplicity. In Section 2, we provide a detailed description of the PDM to evaluate its limitations, followed by the FDM and its adaptation with fluctuational electrodynamics to formulate the effective polarizability and self-interaction Green's function. Section 3 presents and discusses the results obtained by the FDM, comparing them with both the PDM and experimentally obtained spectra from the literature.

2. Modeling

Near-field radiative heat transfer between a tip and a planar surface can be modeled by treating the tip as a randomly fluctuating electric dipole, $\mathbf{p}_t$. Based on fluctuational electrodynamics, the net spectral radiative heat transfer from the dipole at T_t to a planar surface at T_s or vice versa can be written as [23,24,37,38]

$$P_{\text{net}}^{t\to s}(\omega) = \frac{2}{\pi}\left[\Theta(\omega, T_t) - \Theta(\omega, T_s)\right] \times \text{Tr}\left[\text{Im}(\overleftrightarrow{\alpha}_{\text{eff}})\text{Im}[\overleftrightarrow{\mathbf{G}}_R(\mathbf{r}_t, \mathbf{r}_t)]\right], \tag{1}$$

where $\Theta(\omega, T)$ is the mean energy of a Planck oscillator at the angular frequency ω in thermal equilibrium at temperature T and is given as $\Theta(\omega) = \hbar\omega/[\exp(\hbar\omega/k_B T) - 1]$, where $\hbar$ is the reduced Planck constant and k_B is the Boltzmann constant. The effective electric polarizability tensor is denoted by $\overleftrightarrow{\alpha}_{\text{eff}}$, and $\overleftrightarrow{\mathbf{G}}_R(\mathbf{r}_t, \mathbf{r}_t)$ is the dyadic reflection Green's function for the electric field at the dipole position, $\mathbf{r}_t$, referred to as the *self-interaction Green's function* throughout this paper. Eq. (1) clearly indicates that the effective polarizability of the dipole representing the tip and the self-interaction Green's function are the key variables for tip-plane near-field thermal radiation.

For a point dipole in free space subjugated to the unperturbed, uniform electric field, $\mathbf{E}_o$, the dipole moment is solely induced by $\mathbf{E}_o$ to formulate $\mathbf{p}_o = \overleftrightarrow{\alpha}_o^{PD}\mathbf{E}_o$, where $\overleftrightarrow{\alpha}_o^{PD}$ is the bare electric polarizability tensor of the point dipole. For the special case of a spherical point dipole as shown in Fig. 1(a), $\overleftrightarrow{\alpha}_o^{PD}$ is given by [7]

$$\overleftrightarrow{\alpha}_o^{PD} = 4\pi R^3\left(\frac{\varepsilon_t - 1}{\varepsilon_t + 2}\right)\overleftrightarrow{\mathbf{I}} \tag{2}$$

where ε_t is the tip's dielectric function and $\overleftrightarrow{\mathbf{I}}$ is the unit tensor. When the point dipole approaches a surface, the dipole moment is induced by the total electric field to yield $\mathbf{p}_t = \overleftrightarrow{\alpha}_o^{PD}\mathbf{E}_{\text{tot}}(\mathbf{r}_t)$, where $\mathbf{E}_{\text{tot}}$ includes the reflection of the electric field radiated from the dipole itself. The total electric field at the dipole position, $\mathbf{r}_t$, is thus written as [24]

$$\mathbf{E}_{\text{tot}}(\mathbf{r}_t) = \mathbf{E}_o + \overleftrightarrow{\mathbf{G}}_R(\mathbf{r}_t, \mathbf{r}_t)\mathbf{p}_t. \tag{3}$$

where $\overleftrightarrow{\mathbf{G}}_R(\mathbf{r}_t, \mathbf{r}_t)$ is the self-interaction Green's function and for a point dipole can be approximated as [24,39]

$$\overleftrightarrow{\mathbf{G}}_R^{PD}(\mathbf{r}_t, \mathbf{r}_t) = \frac{\beta}{32(H+R)^3\pi\varepsilon_o}\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix} \tag{4}$$

using the image dipole method. Here, ε_o is the vacuum permittivity, and β is the quasistatic Fresnel reflection coefficient for p-polarization written as $\beta = (\varepsilon_s - 1)/(\varepsilon_s + 1)$, where ε_s is the dielectric function of the substrate. The effective electric polarizability that accounts for the near-field interaction between a point dipole and a planar surface can be derived from Eq. (3) [1,24]:

$$\overleftrightarrow{\alpha}_{\text{eff}}^{PD} = \frac{\overleftrightarrow{\alpha}_o^{PD}}{\overleftrightarrow{\mathbf{I}} - \overleftrightarrow{\alpha}_o^{PD}\overleftrightarrow{\mathbf{G}}_R^{PD}(\mathbf{r}_t, \mathbf{r}_t)}. \tag{5}$$

The total dipole moment $\mathbf{p}_t$ can thus be expressed with $\overleftrightarrow{\alpha}_{\text{eff}}^{PD}$ to yield $\mathbf{p}_t = \overleftrightarrow{\alpha}_{\text{eff}}^{PD}\mathbf{E}_o$.

As illustrated in Figs. 1(b) and (c), the FDM simplifies a conductive tip to a vertically aligned prolate spheroid to better represent the field enhancement due to the antenna-like nature of the actual tip geometry within the quasistatic approximation ($2L_p < \lambda$) [29]. In fact, the FDM has shown good correlations with the experimental near-field optical spectra of polar materials [29,30,31]. Due to the antenna-like tip shape, the electric field

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