Design of thermal metamaterials beyond the effective medium theory: Direct numerical simulation via the Thermal Discrete Dipole Approximation (T-DDA)

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1. INTRODUCTION
1.1. Objective, broader impacts and intellectual merit
The objective of this research is to establish a computational toolbox for designing metamaterials, with user-defined thermal radiative properties, beyond the effective medium theory. This will be accomplished by direct calculation of near-field thermal emission via a novel approach called the Thermal Discrete Dipole Approximation. The establishment of thermal metamaterials with unique designer properties will expedite the development of technologies such as infrared cloaking and nanoscale-gap thermophotovoltaic power generation.

Metamaterials are composite materials that display exotic electric and magnetic properties resulting from sub-wavelength functional inclusions (“meta-atoms”) [1]. The ability to engineer metamaterials with specific electric permittivity and magnetic permeability enables tailoring media with unique thermal radiative properties [2]. PI’s group demonstrated via the effective medium theory (EMT) that quasi-monochromatic near-field thermal emission in the near infrared is achievable at a temperature as low as 400 K via Mie resonance-based metamaterials made of dielectric inclusions, while, according to Wien’s law, a temperature greater than 1000 K is required for dominant emission in the near infrared via naturally occurring materials [3,4]. The application of such metamaterials to nanoscale-gap thermophotovoltaic (nano-TPV) power generators will allow low temperature waste heat recovery in a variety of electronic devices, such as cell phones and photovoltaic cells [5-11]. Among the devices that can be powered by nano-TPV systems or whose functionality can be improved are several used by the Army in its mission to provide prompt, sustained land dominance in military operations: computers, communication devices (e.g., radios) and night vision cameras. Worth noting is that the design of thermal metamaterials with user-defined properties will have other applications, such as optical cloaking. In particular, the ability to control the thermal spectrum will pave the way for developing materials invisible to infrared cameras. Such passive infrared camouflage is also relevant to military operations.

Metamaterials’ electromagnetic properties are usually predicted via the EMT, where a heterogeneous medium is conceptualized as homogeneous with effective electric permittivity and magnetic permeability [1]. However, when considering the near-field electromagnetic spectrum emitted at a distance smaller than the size of the meta-atoms or their separation distance, approximating a heterogeneous layer as homogeneous may lead to significant errors. The validity of the EMT was verified recently in the near field of hyperbolic metamaterials made of thin films [12-14]. This analysis was made possible since direct calculation of near-field thermal emission by layered media is well understood [15]. Liu and Shen [16] performed direct simulation of near-field thermal emission by hyperbolic metamaterials via the Wiener chaos expansion method. However, it is not clear how this numerical approach can be employed for computing the near field of a thermal source made of complex three-dimensional (3D) inclusions. Therefore, it is safe to conclude that current methods do not allow direct calculation of near-field thermal emission by metamaterials made of 3D inclusions such as split-ring resonators and dielectric particles. Additionally, the EMT does not account for all the microscopic interactions between the meta-atoms, the host medium and electromagnetic waves.
When directly calculating near-field thermal emission by metamaterials, all the complex interactions between the different material constituents are accounted for. Direct numerical simulation thus allows a better understanding of the underlying physics, which will lead to better design of thermal metamaterials.

The proposed research is radically different from the state-of-the-art, as it will provide for the first time a computational toolbox for designing thermal metamaterials made of 3D arbitrarily-shaped inclusions beyond the EMT. The objective of this research will be fulfilled by accomplishing three specific tasks: (1) Implementation of a novel computational method developed in PI’s lab, called the Thermal Discrete Dipole Approximation (T-DDA) [17], for modeling near-field radiative heat transfer in 3D complex geometries, (2) Application of the T-DDA to direct calculation of near-field thermal emission by metamaterials and assessment of the validity of the EMT, and (3) Design of metamaterials maximizing nano-TPV power generator performances. This project will have major impacts in metamaterial design, thermal radiation at the nanoscale and waste heat recovery, and will pave the way to the development of novel metamaterial-based technologies such as nano-TPV power generation and infrared cloaking to name only a couple.

1.2. Previous research by the PI

The PI has been contributing to the emerging area of near-field thermal radiation over the past few years, and, as a result, he co-wrote a chapter for the fifth edition of *Thermal Radiation Heat Transfer* [18]. He demonstrated that near-field thermal spectra can be tuned via coupling of surface phonon-polaritons in nanostructures [19-23] and Mie resonance-based metamaterials [3,4,24]. The PI also successfully implemented a coupled near-field thermal radiation, charge and heat transport model for predicting nano-TPV performances [10], and he obtained the NSF CAREER Award in 2013 for experimentally demonstrating enhanced power generation in nano-TPV systems due to radiative heat transfer exceeding the blackbody limit [25]. Other research by the PI focuses on radiative polaritons in thin films [26,27], optical tomography [28,29] and characterization of nanoparticles [30-35]. For this last project, the PI built an experimental device, performed measurements in the microwave band in collaboration with the Fresnel Institute (Marseille, France) [35], and is involved in the inversion procedure [32-34]. The PI has a pending patent regarding a cascaded PV / nano-TPV system for optimizing solar energy conversion [36].

2. BACKGROUND AND LITERATURE SURVEY

2.1. Fundamentals of near-field thermal radiation

Radiation heat transfer between bodies separated by distances greater than the dominant thermal wavelength as predicted by Wien’s law \((\lambda_{\text{max}} T = 2898 \, \mu\text{m} \cdot \text{K}) [18]\) is limited by Planck’s blackbody distribution [18,37,38]. In this far-field regime, radiative heat exchange predictions in 3D complex geometries are tractable using well-established numerical techniques such as the discrete ordinates method and Monte Carlo approaches [18,38]. In the near-field regime of thermal radiation, which refers to the case where bodies are separated by sub-wavelength gaps, heat transfer can exceed by several orders of magnitude the blackbody limit [18,39-54]. The enhancement beyond Planck’s distribution is due to the extraneous contribution to energy transport by waves evanescently confined within a distance of about a wavelength normal to the surface of a thermal source. These modes include evanescent waves generated by total internal reflection of propagating waves at the material-gap interface as well as resonant surface waves such as surface phonon-polaritons and surface plasmon-polaritons. These surface polaritons, with
evanescent fields exponentially decaying on both sides of the material-gap interface, can lead to quasi-monochromatic heat exchange [7,19,42,55-57].

Near-field heat transfer problems are modeled via Maxwell’s equations combined with fluctuational electrodynamics [18,39,47,58]. In this formalism, thermal emission is conceptualized as the result of random fluctuations of charged particles inside a body caused by thermal agitation [39]. On a macroscopic level, this chaotic motion of charged particles is introduced via a stochastic current density $J'$ which is added into Maxwell’s equations to model thermal emission. The random nature of the thermal current thus makes the Maxwell equations stochastic. Assuming $e^{-i\omega t}$ for the time-harmonic fields, the stochastic Maxwell equations in the frequency domain can be written as:

\[
\begin{align*}
\nabla \times \mathbf{E}(\mathbf{r}, \omega) &= i\omega \mu_0 \mathbf{H}(\mathbf{r}, \omega) \\
\nabla \times \mathbf{H}(\mathbf{r}, \omega) &= -i\omega \varepsilon_0 \varepsilon \mathbf{E}(\mathbf{r}, \omega) + J'(\mathbf{r}, \omega) \\
\nabla \cdot \mathbf{D}(\mathbf{r}, \omega) &= \nabla \cdot \mathbf{B}(\mathbf{r}, \omega) = 0
\end{align*}
\]

where $\mathbf{E}$, $\mathbf{H}$, $\mathbf{D}$ and $\mathbf{B}$ are respectively the electric field, the magnetic field, the electric flux density and the magnetic induction at location $\mathbf{r}$ and at angular frequency $\omega$, $\varepsilon_0$ and $\mu_0$ are the vacuum permittivity and permeability, and $\varepsilon$ is the dielectric function. The above set of equations is subjected to the following assumptions: the bodies are isotropic, non-magnetic and their electromagnetic responses are described by frequency-dependent dielectric functions local in space. The first moment of the random current is zero (i.e., $\langle J' \rangle = 0$), which implies that the mean radiated fields are also zero [39]. In heat transfer analysis, however, the quantities of interest are the flux and the energy density which are proportional to the ensemble average of the spatial correlation function of currents [58]. This correlation function is provided by the fluctuation-dissipation theorem linking the thermal current to the local temperature of the emitter [39]:

\[
\langle J'(r',\omega) \cdot (J'(r,\omega))^\dagger \rangle = \frac{4\omega \varepsilon_0 \varepsilon''}{\pi} \Theta(\omega, T) \delta(r' - r) \mathbf{I}
\]

where $\dagger$ is the Hermitian operator (conjugate transpose), $\varepsilon''$ is the imaginary part of the dielectric function of the thermal source, $\mathbf{I}$ is the unit dyadic and $\Theta$ is the mean energy of a Planck oscillator in thermal equilibrium [47]. The application of the fluctuation-dissipation theorem requires that the media are in local thermodynamic equilibrium.

So far, near-field radiative heat transfer predictions have been mainly restricted to simple canonical geometries. This is due to the fact that the vast majority of near-field thermal radiation problems have been solved by deriving analytical expressions for the dyadic Green’s function (DGF) relating a source point $\mathbf{r}'$ to a field observed at $\mathbf{r}$; this approach is referred to as the DGF method. The DGF method provides exact solutions to near-field thermal radiation problems, but becomes intractable when dealing with 3D arbitrarily-shaped objects. Over the past years, the DGF approach has been applied to various cases: two bulks [40-42,58-62], two films [20-23,63], two structured surfaces [64], two nanoporous materials [65], one-dimensional (1D) layered media [15,66,67], cylindrical cavity [68], two dipoles [69-71], two large spheres [72], dipole-surface [73], dipole-structured surface [74], sphere-surface [75], two long cylinders [76], two nanorods [77,78] and two gratings [79].

The limitations associated with the numerical solution of the stochastic Maxwell equations applied to near-field thermal radiation prevent accurate predictions of near-field emission by
metamaterials. As such, there is an urgent need for predicting near-field heat exchange in 3D complex geometries. Beyond the application to thermal metamaterial design, modeling near-field thermal radiation in complex 3D geometries will benefit a wide variety of technologies such as imaging [80], nanomanufacturing [81,82], thermal management of electronic devices [83] and thermal rectification [84,85] to name only a few. It is worth noting that numerical procedures, namely the finite-difference time-domain (FDTD) method [16,86,87], the finite-difference frequency-domain (FDFD) method [88] and the boundary element method (BEM) [89] have been applied recently to near-field thermal radiation calculations. Both FDTD and FDFD suffer from large computational time, while the BEM is difficult to apply when dealing with heterogeneous materials.

2.2. State-of-the-art for predicting near-field thermal emission by metamaterials

Near-field thermal emission by a metamaterial is schematically depicted in Fig. 2.1, where the symbol \( <u> \) represents the energy density characterizing the near-field thermal spectrum. The energy density is calculated at a distance \( \Delta \) away from the interface 1-2. When \( \Delta \) is of the same order of magnitude as, or less than, the dominant wavelength emitted (~10 \( \mu \)m at room temperature), the thermal spectrum is composed of propagating and evanescent waves. Figure 2.1(a) illustrates the EMT, where a metamaterial is conceptualized as a homogeneous layer with effective electric permittivity \( \varepsilon_{\text{eff}} \) and magnetic permeability \( \mu_{\text{eff}} \). These effective properties are computed using a simplified model (e.g., Clausius-Mossotti [1]) and are then employed to predict \( <u> \) via the DGF method for an emitting bulk with electric and magnetic response. The EMT has been applied by a few groups for predicting near-field thermal emission from metamaterials [3,4,24,67,90-92]. These studies demonstrated that effectively magnetic materials open a new channel through which energy can flow in the form of TE-polarized surface polaritons. Of particular interest for nano-TPV power generation are the results of Fig. 2.2 [4], where it is shown that a metamaterial made of silicon (Si) inclusions can lead to resonance of the near-field thermal spectrum in the near infrared (0.53 eV) at a temperature as low as 400 K. According to Wien’s law, a temperature of about 1200 K is needed for dominant (but not quasi-monochromatic) thermal emission at 0.53 eV. Physically, the quasi-monochromatic behavior observed in Fig. 2.2 is due to the high permittivity of Si in the near infrared [93]. However, one must keep in mind that the accuracy of the results in Fig. 2.2 is not guaranteed since these simulations were generated using the EMT while \( \Delta \) was fixed at 50 nm.

In Fig. 2.1(b), \( <u> \) is calculated by considering the metamaterial as heterogeneous, which can be accomplished by directly calculating thermal emission by the host medium and the inclusions. When \( \Delta \) is smaller than the inclusions and/or their separation distance, it is expected that the particles near the
interface 1-2 in Fig. 2.1(b) have a greater influence on $\langle u \rangle$ than the particles located far from that interface (“non-local effects” [13]), such that a homogenization approach as done in the EMT is clearly inappropriate. It is therefore necessary to directly calculate thermal emission by metamaterials operating in the near field.

A very few studies, restricted to simple geometries, have been devoted to direct calculation of near-field thermal emission by metamaterials. Smith and Schurig [94] introduced the idea of indefinite media with hyperbolic dispersion, or hyperbolic metamaterials, and identified 1D layered media (i.e., thin films are the meta-atoms) as an avenue for generating such metamaterials. The application of hyperbolic metamaterials, made of thin films, to near-field thermal emission has recently attracted some interest [12-14,95-97]. Bihs et al. [95] showed that hyperbolic metamaterials can be considered the near-field analog of a blackbody, since the near-field enhancement from such structures is broadband. Tschikin et al. [12] questioned the validity of the EMT for hyperbolic metamaterials made of thin films and, as expected, observed that the EMT did not provide accurate results in the near field when surface polaritons are present. Similar results were shown by Guo et al. [14] in their study on hyperbolic metamaterials.

Direct calculation of near-field thermal emission by structures made of thin films is well established [15]. Current methods, however, do not allow performing such predictions for metamaterials made of 3D inclusions such as split-ring resonators and spherical particles. Very recently, Liu and Shen [16] proposed to directly calculate near-field thermal emission by metamaterials via the Wiener chaos expansion method implemented by the FDTD technique. They considered the case of a 10 $\mu$m-thick silicon carbide (SiC) layer and a metamaterial, made of metal wire arrays, separated by a vacuum gap. In the simulations, SiC was considered as emitting while the metamaterial layer as purely absorbing (0 K). It was pointed out that the main challenge in the Wiener chaos expansion method is to find the proper current modes of the thermal source. The current modes in the homogeneous SiC emitter have sinusoidal forms; for more complicated geometries (e.g., medium made of 3D inclusions), the current modes can be generated using spherical harmonics. While the authors argue that the flux emitted by the metamaterial and absorbed by the SiC layer can easily be determined using reciprocity, it is not clear how the Wiener chaos expansion method can accommodate near-field heat transfer calculation between two metamaterials where thermal emission truly needs to be calculated directly from a medium made of 3D inclusions. Nevertheless, simulation results for wires (modeled as perfect electric conductors) with 50 nm radii and a periodicity of 300 nm revealed that direct calculation of near-field thermal emission and the EMT diverged for a vacuum gap smaller than 300 nm. For a 10-nm-thick vacuum gap, the EMT over-predicted the spectrally integrated radiative heat flux by more than one order of magnitude, thus showing the great importance of direct calculation of near-field thermal emission by metamaterials.

In this project, a novel computational method called the Thermal Discrete Dipole Approximation (T-DDA) is proposed for solving near-field thermal radiation problems in 3D complex geometries and for direct calculation of near-field thermal emission by metamaterials. As explained in the next section, the T-DDA is based on discretizing bodies into electric point dipoles such that this method can accommodate any type of complex objects. The T-DDA also has the following advantages: (i) conceptually simple, (ii) non-stochastic, (iii) computationally cheap when compared to FDTD and FDFD approaches, (iv) allows direct thermal radiation emission calculation from particulate media, (v) does not require any complicated expansion into spherical harmonics, and (vi) allows near-field heat transfer predictions of problems involving
objects with sizes of various orders of magnitude (e.g., nanosize particles bounded by semi-infinite surfaces).

3. PROPOSED RESEARCH

The proposed research is divided into three main tasks. For each task, deliverables are provided. Before going through the details of the research plan, the T-DDA recently developed in PI’s lab, which is the backbone of this project, is described in section 3.1 [17].

3.1. Description of the T-DDA and proof-of-concept

The T-DDA is formulated based on the schematic shown in Fig. 3.1. A total of \( m = 1, 2, \ldots, M \) objects at temperatures \( T_m \) are submerged in air or vacuum (medium 0) and are exchanging thermal radiation. The \( M_e \) emitters are made up of source points \( r' \) while the \( M_a \) absorbers are composed of points \( r \) where the fields are calculated. As discussed in section 2.1, the bodies are assumed to be in local thermodynamic equilibrium, isotropic, non-magnetic (the constituents are non-magnetic, but the collective responses of the bodies may be effectively magnetic) and their electromagnetic responses are described by frequency-dependent dielectric functions \( \varepsilon_m = \varepsilon'_m + i\varepsilon''_m \) local in space. No assumptions are made on the shape of the objects and their separation distances.

The Discrete Dipole Approximation (DDA) is extensively used for predicting electromagnetic wave scattering by particles [82,98-104]. In this framework, objects are approximated by a finite number of discrete electric point dipoles. The T-DDA proposed here follows the same general procedure as the DDA, except that the incident field is induced by thermal fluctuations. The starting point of the T-DDA is to decompose the (total) electric field \( E \) as the sum of an incident field, \( E_{inc} \), and a scattered field, \( E_{sca} \), that satisfy the following vector wave equations:

\[
\nabla \times \nabla \times E_{inc}(r, \omega) - k_0^2 E_{inc}(r, \omega) = i\omega \mu_0 J'(r, \omega) \tag{3.1a}
\]

\[
\nabla \times \nabla \times E_{sca}(r, \omega) - k_0^2 E_{sca}(r, \omega) = (k^2 - k_0^2) E(r, \omega) \tag{3.1b}
\]

The incident field is interpreted as the field produced by the stochastic current \( J' \) in the absence of scatterers (i.e., field propagating in free space). The scattered field accounts for the multiple interactions between the objects and can be interpreted as the field generated by an equivalent source function \( (k^2 - k_0^2) E \) propagating in free space. Solutions for the incident and the scattered electric fields are obtained using the free space DGF [105] denoted as \( \overline{G} \):

\[
E_{inc}(r, \omega) = i\omega \mu_0 \int_{V_e} \overline{G}(r, r', \omega) \cdot J'(r', \omega) dV' \tag{3.2a}
\]

\[
E_{sca}(r, \omega) = \int_{V} (k^2 - k_0^2) \overline{G}(r, r', \omega) \cdot E(r', \omega) dV' \tag{3.2b}
\]

where \( V_e \) is the volume of the emitters, while \( V (= V_e + V_a) \) is the total volume where \( V_a \) is the volume of the absorbers. It can be seen in Eq. (3.2a) that the integration is performed over \( V_e \).
only where the thermal source is non-zero, while the integration in Eq. (3.2b) is performed over the total volume $V$ to account for the interactions between all objects.

A volume integral equation for the (total) electric field is obtained by substituting the scattered field (Eq. (3.2b)) into $E = E_{\text{inc}} + E_{\text{sca}}$:

$$\frac{\varepsilon(r) + 2}{3} E(r,\omega) - \frac{k_0^2 P.V.}{3} \int_V [\varepsilon(r') - 1] G(r,r',\omega) \cdot E(r',\omega) dV' = E_{\text{inc}}(r,\omega)$$  \hspace{1cm} (3.3)

where the principal value method ($P.V.$ in Eq. (3.3) stands for principal value) has been employed in order to handle the singularity of the DGF at $r = r'$. In the principal value method, an infinitesimal volume containing the singularity point is excluded from the integral [101,106].

A system of linear equations is derived from Eq. (3.3) by approximating the emitting and the absorbing bodies by $N$ cubical sub-volumes on a cubical lattice. The first $N_e$ sub-volumes are located in the emitters, while the $N_a$ $(= N - N_e)$ remaining sub-volumes are allocated to the absorbers. The discretization should be fine enough such that the dimension of each sub-volume is small compared to the radiation wavelength ($\sim 1/10$ to $1/20$ of the wavelength within the material). If this condition is satisfied, it can be assumed that the electromagnetic properties, the electric field, and the DGF are uniform inside each sub-volume. After some manipulations, the discretized version of the volume integral equation is given by [17]:

$$\left[ \frac{\varepsilon_i + 2}{3} - \frac{2(\varepsilon_i - 1)}{3} \right] \Delta V_i \sum_{j \neq i} \varepsilon_j^{-1} A \varepsilon_j G_{ij} \cdot E_j = E_{\text{inc},i}, \ i = 1, 2, \ldots, N \hspace{1cm} (3.4)$$

where the subscripts $i$ and $j$ refers to sub-volumes, while $a_i$ is the effective radius of sub-volume $i$, with volume $\Delta V_i$, defined as $(3\Delta V_i/4\pi)^{1/3}$. Equation (3.4) is a system of $N$ vector equations where the electric field $E_i$ in each sub-volume is the unknown.

From now on, each sub-volume is assumed to be an electric point dipole, such that Eq. (3.4) can be expressed in terms of unknown equivalent dipole moments $p_i$ instead of unknown electric fields $E_i$ using the relation [101]:

$$E_i = \frac{3 \alpha_i^{CM}}{\varepsilon_i + 2} p_i \hspace{1cm} (3.5)$$

where $\alpha_i^{CM}$ is the Clausius-Mossotti polarizability. The incident field can also be expressed in terms of a thermally fluctuating dipole moment instead of a random current via the following relation [105]: $J_i = (-i\omega / \Delta V_i) p_i$. The system of equation given by Eq. (3.4) can thus be re-written in terms of unknown dipole moments $p_i$:

$$\frac{1}{\alpha_i} p_i - k_0^2 \sum_{j \neq i} G_{ij} p_j = E_{\text{inc},i}, \ i = 1, 2, \ldots, N \hspace{1cm} (3.6)$$

where $\alpha_i$ is the radiative polarizability of dipole $i$ defined in Refs. [101,104]. The incident field written in terms of thermally fluctuating dipole moment is given by:

$$E_{\text{inc},i} = \begin{cases} 0 & i = 1,2,\ldots,N_e \\ \mu_0 \omega^2 \sum_{k=1}^{N_e} G_{ik} p_k & i = N_e + 1, N_e + 2,\ldots,N \end{cases} \hspace{1cm} (3.7)$$
Equation (3.7) stipulates that the thermally generated field is nil in the emitters \((j = 1, 2, \ldots, N_e)\), while the incident field within the absorbers \((i = N_e + 1, N_e + 2, \ldots, N)\) is due to the \(k = 1, 2, \ldots, N_e\) emitting dipoles. As for the random current, the mean of the thermally fluctuating dipole moment is equal to zero. The random dipole moments are related to the local temperature of the medium via a modified version of the fluctuation-dissipation theorem (see Eq. (2.2)) \[107\]:

\[
\langle \mathbf{p}_i \cdot (\mathbf{p}_i^\dagger) \rangle = \frac{4\varepsilon_0}{\pi \omega} \text{Im}(\alpha_i^{CM}) \Theta(\omega, T) \mathbf{I}
\tag{3.8}
\]

The system of \(3N\) scalar equations with \(3N\) unknowns given by Eq. (3.6) (each dipole \(i\) has three orthogonal components) can also be written in a compact form using the following matrix notation: \(\mathbf{A} \cdot \mathbf{P} = \mathbf{E}_{inc}\), where \(\mathbf{P}\) is the \(3N\) stochastic column vector containing the unknown dipole moments \(\mathbf{p}_i\), \(\mathbf{E}_{inc}\) is the \(3N\) stochastic column vector containing the known incident fields \(\mathbf{E}_{inc,i}\), while \(\mathbf{A}\) is the \(3N\) by \(3N\) deterministic interaction matrix consisting of \(N^2\) 3 by 3 sub-matrices. Each sub-matrix \(\mathbf{A}_{ij}\) represents the interactions between dipoles \(i\) and \(j\). The specific composition of the vectors and the interaction matrix is provided by Edalatpour and Francoeur \[17\].

The T-DDA allows calculations of many quantities of interest (e.g., energy density, power absorbed, scattering and absorption cross-sections). Here, for purpose of verification against analytical results, the power absorbed is considered. The mean energy dissipated in the absorbers \((i = N_e + 1, N_e + 2, \ldots, N)\) at a given frequency \(\omega\) is calculated as \[100, 101\]:

\[
\langle Q_{abs, \omega} \rangle = \frac{\omega^2}{2} \sum_{i=N_e+1}^{N} \left( \text{Im}(\alpha_i^{-1})^* - \frac{2}{3} k_0^2 \right) \text{tr} \left( \langle \mathbf{p}_i \cdot \mathbf{p}_i^\dagger \rangle \right)
\tag{3.9}
\]

where \(*\) denotes complex conjugate. According to Eq. (3.9), the unknown dipole moments \(\mathbf{p}_i\) do not need to be calculated directly. Instead, the trace of the dipole auto-correlation function, \(\text{tr}(\langle \mathbf{p}_i \cdot \mathbf{p}_i^\dagger \rangle)\), is needed in order to compute the power absorbed. The procedure for calculating the auto-correlations \(\langle \mathbf{p}_i \cdot \mathbf{p}_i^\dagger \rangle\) is briefly described below.

From the linear system of equations \(\mathbf{A} \cdot \mathbf{P} = \mathbf{E}_{inc}\), the dipole moment vector can be calculated as \(\mathbf{P} = \mathbf{A}^{-1} \cdot \mathbf{E}_{inc}\). The mean value of the dipole moment vector is \(\langle \mathbf{P} \rangle = \mathbf{A}^{-1} \cdot \langle \mathbf{E}_{inc} \rangle = 0\), since the first moment of the thermally fluctuating dipoles contained in the incident field vector is zero. The correlation matrix of the zero-mean dipole moment vector, defined as \(\mathbf{R}_{PP} = \langle \mathbf{P} \cdot \mathbf{P}^\dagger \rangle\), is given by the following expression after substitution of \(\mathbf{P} = \mathbf{A}^{-1} \cdot \mathbf{E}_{inc}\) and after using the identity \((\mathbf{A}^{-1} \cdot \mathbf{E}_{inc})^\dagger = \mathbf{E}_{inc}^\dagger \cdot (\mathbf{A}^{-1})^\dagger\):

\[
\mathbf{R}_{PP} = \mathbf{A}^{-1} \mathbf{R}_{EE} (\mathbf{A}^{-1})^\dagger
\tag{3.10}
\]

where \(\mathbf{R}_{EE} = \langle \mathbf{E}_{inc} \cdot \mathbf{E}_{inc}^\dagger \rangle\) is the correlation matrix of the incident field. In Eq. (3.10), both correlation matrices \(\mathbf{R}_{PP}\) and \(\mathbf{R}_{EE}\) are \(3N\) by \(3N\) matrices consisting of \(N^2\) sub-matrices, \(\mathbf{R}_{PP,i} = \langle \mathbf{p}_i \cdot \mathbf{p}_j^\dagger \rangle\) and \(\mathbf{R}_{EE,i} = \langle \mathbf{E}_{inc,i} \cdot \mathbf{E}_{inc,j}^\dagger \rangle\), correlating the dipole moments and the incident fields in dipoles \(i\) and \(j\), respectively.
Referring to Eq. (3.9), only the traces of the auto-correlation matrices \( \overline{R}_{pp} \) are needed for computing the power absorbed. To perform these calculations, it is necessary to first compute the incident field correlation matrix \( \overline{R}_{EE} \) (see Eq. (3.10)). A given sub-matrix between dipoles \( i \) and \( j \) is calculated as follows after application of the fluctuation-dissipation theorem (see Eqs. (3.7) and (3.8)):

\[
\overline{R}_{Ei Ej} = \frac{4\varepsilon_0 \mu_0^2 \omega^3 \Theta(\omega, T)}{\pi} \sum_{k=1}^{N} \text{Im}(\alpha_k^{CM}) G_{ik} \cdot G_{jk}^\dagger, \quad i, j \geq N_e + 1
\]  

(3.11)

Equation (3.11) is employed to populate the incident field correlation matrix \( \overline{R}_{EE} \), which is in turn substituted into Eq. (3.10) in order to compute \( \overline{R}_{PP} \). The diagonal elements of \( \overline{R}_{PP} \), corresponding to the auto-correlation of the dipole moments, are finally used for calculating the power absorbed by the \( M_a \) objects made of \( N_a \) dipoles via Eq. (3.9). From this result, the power absorbed by the \( M_e \) objects due to thermal emission from the \( M_a \) bodies can easily be obtained using the reciprocity of the DGF [108]. As such, the net radiative heat transfer between the emitters and the absorbers can be calculated.

As a proof-of-concept, the T-DDA is verified hereafter by computing the spectral radiative conductance between two spheres and by comparing the results against those obtained from the analytical solution (i.e., DGF method) of Narayanaswamy and Chen [72]. The thermal conductance between two objects is defined as follows. Assuming that the first object is at temperature \( T \) while the second object is at temperature \( T + \delta T \), the spectral conductance \( G_\omega \) is calculated as:

\[
G_\omega = \lim_{\delta T \to 0} \frac{<Q_{net,\omega}>}{\delta T}
\]  

(3.12)

where \( <Q_{net,\omega}> \) is the net spectral heat transfer rate between the two objects.

The benchmark problem, shown in Fig. 3.2(a), involves computation of the spectral conductance between two silica spheres. The diameters \( D \) of the spheres and their separation distance \( d \) are fixed at 0.5 \( \mu m \), while the temperature is kept at 400 K. Note that the number in parentheses in Fig. 3.2 indicate the amount of dipoles used for discretizing each object.

![Figure 3.2](image-url)

Figure 3.2. Spectral conductance between two objects made of silica: (a) two spheres, and (b) two cubes. The T-DDA is compared against analytical results in panel (a). In both set of results, the temperature \( T \) is fixed at 400 K.
A good agreement between the T-DDA and the analytical solution is observed for all numbers of dipoles considered in the simulations. Additionally, the resonant frequencies are predicted accurately via the T-DDA. For 552 dipoles in each sphere, the relative difference between the total conductance (i.e., spectrally integrated conductance) calculated from the T-DDA and the analytical solution within the spectral band of from 0.04 eV to 0.16 eV is 5.7%.

Similar results are shown in Fig. 3.2(b) for two cubes having side lengths $D$ and separation distance $d$ of 0.5 µm (the temperature $T$ is again fixed at 400 K). Note that an analytical solution does not exist for this problem, thus showing the flexibility of the T-DDA. A fast convergence of the T-DDA is observed in Fig. 3.2(b). This is in good agreement with Yurkin et al. [109], where it was observed that the error associated with cubically shaped objects is smaller than for curved geometries.

The accuracy of the T-DDA is subjected to the same validity criteria as the DDA. Draine [99] identified three validity criteria associated with the DDA: (i) the number of dipoles should be large enough in order to describe the geometries of the objects accurately, (ii) the discretization should be small enough when compared to the wavelength in the material and to the attenuation length of the wave within the material, and (iii) the electric point dipoles must be small enough such that magnetic dipole effects are negligible. Using the criteria suggested by Draine and the associated equations provided in Ref. [99], it was found that the shape error dictates the minimum number of dipoles to be employed in the simulations of Fig. 3.2. For the case of Fig. 3.2(a), it was found that 688,160 dipoles were necessary to achieve a fractional accuracy of 0.01. On the other hand, Fig. 3.2(a) clearly shows that 552 dipoles were sufficient for accurate predictions of the spectral radiative conductance between two spheres. The accuracy and the convergence of the T-DDA can significantly be improved by using the methods discussed in Task 2.

This section demonstrated that the T-DDA, which is the backbone of this research, is an appropriate tool for predicting near-field thermal radiation in 3D complex geometries. The details of the research plan are provided next.

3.2. Research plan

Task 1: Implementation of the T-DDA

The deliverable of Task 1 is a freely available open-source code for modeling near-field thermal radiation in 3D complex geometries via the T-DDA. A user guide will be published in the Journal of Quantitative Spectroscopy and Radiative Transfer and the code will be updated frequently (at least once a year). Task 1 regroups three steps: addition of surface interactions, optimization of the code, and generalization of the T-DDA via calculation of various outputs. Task 1 will be accomplished in years 1 and 2.

Surface interactions. It is assumed in the procedure described in section 3.1 that the objects are embedded in a homogeneous infinite medium (see Fig. 3.1). In many applications, such as for direct calculation of near-field thermal emission by metamaterials, it is necessary to account for the interactions between the objects and semi-infinite surfaces. Figure 3.3 shows two dipoles $i$ and $j$ above a large surface considered as semi-infinite. The presence of the surface modifies the formulation of section 3.1 in two ways. First, the incident field $E_{\text{inc}}$...
consists of the superposition of waves generated at \( \mathbf{r}' \) in the emitter that reach the point \( \mathbf{r} \) in the absorber, as before, and waves emitted at \( \mathbf{r}' \) that reflect off the surface before reaching \( \mathbf{r} \). Secondly, the interaction mechanism between dipoles \( i \) and \( j \) is modified by adding an extraneous contribution due to radiation from dipole \( j \) that reflects off the surface before reaching dipole \( i \), as shown in Fig. 3.3. In the presence of a surface, the linear system of equations to be solved becomes: \((\mathbf{A} + \overline{\mathbf{R}}) \cdot \mathbf{P} = \mathbf{E}_{\text{inc}}\), where \( \overline{\mathbf{R}} \) is the \( 3N \times 3N \) deterministic reflection-interaction matrix. Once \( \mathbf{E}_{\text{inc}} \) is modified and \( \overline{\mathbf{R}} \) is populated, the solution procedure of section 3.1 can be applied.

Electromagnetic light scattering prediction by objects close to a surface via the DDA was first proposed by Taubenblatt [110,111] and implemented in a few other studies [82,101,102,104]. The integration of surface interactions within the DDA and the T-DDA is essentially based on the work of Sommerfeld that analyzed electric dipole radiation above a semi-infinite plane [112]. Electric dipole oscillations can be separated into two components: horizontal electric dipole (HED) oscillations and vertical electric dipole (VED) oscillations. For a HED, the dipole moment is in the \( \rho-\phi \) plane, while the dipole moment is oriented along the \( z \)-axis for a VED (see Fig. 3.3). The primary electric field at \( \mathbf{r} \) generated by a dipole is:

\[
\mathbf{E}(\mathbf{r}, \omega) = \frac{k_0^2}{\varepsilon_0} \left[ \frac{\mathbf{i} + \nabla}{k_0^2} \right] \cdot \frac{e^{i k_0 4 \pi r}}{4 \pi r} \mathbf{p}
\]  (3.13)

where \( \mathbf{p} \) is dipole moment vector (oriented following the HED and VED conventions), while \( r \) is the magnitude of \( \mathbf{r} \). Equation (3.13) represents propagation of spherical waves. The electric field reflected off the surface is calculated from the primary field using the Sommerfeld identity [106]:

\[
\frac{e^{i k_0 4 \pi r}}{4 \pi} = i \int_{k_{\rho 0}}^{k_0} \frac{k_{\rho} J_0(k_{\rho} \rho) e^{i k_{\rho} \rho}}{k_{\rho}^2 - k_0^2} dk_{\rho}
\]  (3.14)

where \( k_{\rho} \) and \( k_{\rho 0} \) are respectively the wavevectors parallel and perpendicular to the surface, while \( J_0 \) is the Bessel function of the zeroth order. The purpose of the Sommerfeld identity is to decompose spherical waves into a summation of cylindrical waves propagating parallel to the surface and plane waves propagating along the \( z \)-direction. As such, the cylindrical waves do not interact with the surface; only the plane waves interact with the surface, and this interaction is calculated via the standard Fresnel reflection coefficients [105].

By performing this analysis for the HED and the VED, the electric fields reflected off the surface in both TM and TE polarizations due to dipole radiation are calculated. These reflected electric fields are then added to the incident field vector \( \mathbf{E}_{\text{inc}} \). The reflected electric fields are also employed for populating the reflection-interaction matrix. This is done by considering the reflected field at \( \mathbf{r}_i \) due to dipole radiation at \( \mathbf{r}_j \) [101]:

\[
\mathbf{E}_{\text{ref},i} = \overline{\mathbf{R}}_{ij} \cdot \mathbf{p}_j
\]  (3.15)

Using the reflected electric fields in combination with Eq. (3.15), the expression for the local reflection-interaction matrix \( \overline{\mathbf{R}}_{ij} \) for all dipole pairs is derived. Then, the global reflection-interaction matrix \( \overline{\mathbf{R}} \) can be populated. The mathematical details are omitted here due to lengthy equations. At the end of this step, near-field thermal radiation problems in 3D complex geometries involving objects much greater and much smaller than the wavelength will be...
tractable for the very first time. It is worth noting that the extension to multiple surfaces is straightforward via calculation of plane wave reflection and transmission from multiple plane layers [113].

**Optimization of the code.** For an ensemble of objects, tens of thousands of dipoles might be needed for accurate simulations. It will therefore be necessary to optimize the code in order to reduce the number of operations, to parallelize the code, and to improve the convergence rate for objects with large electric permittivity. The current version of T-DDA is not optimized. For instance, the simulations of Fig. 3.2(a) for 552 dipoles required 100 hours on a personal laptop computer. A technique such as the fast Fourier transform can be applied to the T-DDA in order to reduce the numbers of operations and storage requirements [101]. The optimization of the code will be performed after inclusion of the surface interactions. The T-DDA is subjected to the same errors as the DDA. As such, the literature regarding the convergence of the DDA is also applicable to the T-DDA. The DDA suffers from convergence problems when the refractive index of the objects is much greater than unity [99,114]. Indeed, as the refractive index of a material increases, the wavelength within that material decreases, such that the number of dipoles for convergence increases. Two methods have been proposed in the DDA literature in order to circumvent this bottleneck. The first approach, suggested by Piller and Martin [115], is called the Filtered Couple Dipole (FCD) method. In the T-DDA formulation described in section 3.1, each sub-volume is approximated as an electric point dipole where the electric field and the DGF are assumed to be uniform. Generally speaking, the purpose of the FCD method is to account for spatial variations of the field and the DGF within a sub-volume using the concepts of sampling theory. Piller and Martin showed that the application of the FCD increased the accuracy of the DDA by a factor of 100 [115]. Later, Yurkin et al. [114] included the FCD in the publicly available ADDA code [116] and reported similar improvements. The second approach is based on an extrapolation technique. Yurkin et al. [117] showed that the error of the DDA is bounded by a quadratic function. In this second method, an extrapolation technique is applied to find the constants of the quadratic error function. This error function is then employed in combination with the DDA results in order to estimate the exact solution. Yurkin et al. reported that the error associated with DDA decreased by two orders of magnitude when employing the extrapolation technique [118].

**Generalization of the T-DDA.** The code will be made as general as possible by implementing the calculation of various outputs such as the power absorbed, the net radiative flux and the energy density to name only a few. It is important to understand that calculation of these various outputs is straightforward, as it does not change the solution procedure outlined in section 3.1. Indeed, all energy related quantities are proportional to the trace of the dipole auto-correlation function tr(<p_i ⋅ p_i^†>) (see Eq. (3.9)). More details are provided in Task 2 regarding the computation of the energy density for direct calculation of near-field thermal emission by metamaterials.

**Task 2: Application of the T-DDA to direct calculation of near-field thermal emission by metamaterials and assessment of the validity of the EMT.**

The **deliverables** of Task 2 are: the application of the T-DDA to direct calculation of near-field thermal emission by metamaterials, and the determination of the conditions for which the EMT cannot be applied to thermal metamaterial design. Task 2 will be accomplished in years 2 and 3.

**Direct calculation of near-field thermal emission by metamaterials.** Figure 3.4 depicts a hypothetical case where the energy density <u_ω> is calculated at location r above a metamaterial made of spherical inclusions. The point r can be in the near field or in the far field of the
metamaterial, and any complex-shaped inclusions can be considered (spheres are depicted for simplicity). A general expression for the energy density characterizing the near-field thermal spectrum at \( r \) due to emission by the metamaterial is given by [47]:

\[
\langle u_{\omega}(r) \rangle = \varepsilon_0 \langle |E(r, \omega)|^2 \rangle + \mu_0 \langle |H(r, \omega)|^2 \rangle
\] (3.16)

where the square of the magnitude of the electric and the magnetic fields are proportional to the trace of the stochastic current auto-correlation function. Therefore, after discretizing Eq. (3.16), the energy density becomes proportional to the trace of the dipole auto-correlation function \( \text{tr}(\langle \mathbf{p}_i \cdot \mathbf{p}_i^\dagger \rangle) \) as for the power absorbed. The only difference between the power absorbed and energy density calculations is in the initialization of the problem. When calculating the power absorbed, \( M_e \) objects are defined as emitters while \( M_a \) objects are classified as absorbers. For energy density calculations, all inclusions in the metamaterial contribute to thermal emission and absorption. As such, each inclusion must be treated as an emitter and an absorber. The incident field vector \( \mathbf{E}_{\text{inc}} \) can thus be calculated as follows for a metamaterial made up of \( m = 1, 2, \ldots, M \) inclusions:

1. Consider a given inclusion \( m = m_i \) as the emitter, while all other inclusions are treated as absorbers.
2. Calculate the incident field produced in all inclusions, except in \( m = m_i \), due to emission by inclusion \( m = m_i \).
3. Repeat steps 1 and 2 for all \( m = 1, 2, \ldots, M \) in order to compute the overall incident field in all inclusions.

Additionally, direct calculation of near-field thermal emission by metamaterials will require an iterative process. Indeed, metamaterials can be made of thousands of inclusions, while only those close to the material-air interface are likely to play a key role in near-field thermal emission. An example of an iterative process is schematically shown in Fig. 3.4 (a 2D structure is depicted for simplicity, but realistic 3D structures will be considered). First, the energy density is calculated by considering the inclusions contained in box 1. Calculations are repeated for a larger number of inclusions (box 2), and are compared against the results obtained using box 1. The process is repeated until the relative difference of energy density between two successive calculations is less than a prescribed convergence criterion (e.g., 1%).

The method proposed in Task 2 is applicable to any type of metamaterial. However, during the three-year period of the research activities, the focus will be on Mie resonance-based metamaterials [119]. These structures use dielectric sub-wavelength inclusions (~ 50 nm – 1 \( \mu \)m), such as spheres and cylinders, embedded in a dielectric host medium to create materials with isotropic designer permittivity and permeability. The electric and magnetic responses of the inclusions can be conceptualized as meta-atoms dictating the electromagnetic properties of the metamaterial. A large collection of these resonators can induce surface polaritons that are crucial for controlling near-field heat transfer. The choice of focusing on Mie resonance-based metamaterials is motivated by the fact that isotropic electromagnetic responses can easily be
achieved [119-121]. Secondly, resonant surface polaritons can conveniently be generated in the near infrared using dielectric inclusions with high permittivity in that spectral band (e.g., Si, see Fig. 2.2). This characteristic is crucial for the development of nano-TPV power generators [8,10,11]. Additionally, fabrication of metallic-based metamaterials made of intricate structures such as split-ring resonators or fishnet patterns requires sophisticated lithography techniques, which make it difficult to manufacture 3D macroscale samples to be used in engineering devices. Finally, while hyperbolic metamaterials made of thin films, as discussed in section 2.2, are easier to fabricate than 3D structures, the broadband enhancement of the near-field thermal spectrum is not suitable for many applications. For instance, 3D meta-atomic structures are preferable in order to achieve quasi-monochromatic near-field thermal emission, which is needed for viable and highly efficient nano-TPV power generation [8,10,11]. PI’s group is currently fabricating Mie resonance-based metamaterials via an ultrasound manipulation technique that can arrange nanostructures in 3D patterns in a macroscale volume (~ mm to cm) [4,122].

For macroscale metamaterials, it is not necessary to model all interfaces; only the material-air interface above which the energy density is calculated is necessary in the simulations. For smaller sample size (~ µm and below), other interfaces might need to be accounted for, and this can be easily handled via the technique described in Task 1. The number of interfaces to be used in the simulations can be determined by analyzing the radiation penetration depth [20,21,23]. For the aforementioned Mie resonance-based metamaterials, the host medium has very low absorption, and thus very low emission. As such, thermal emission by the host material is likely to be negligible when compared to thermal emission by the inclusions. This assumption will be verified by comparing near-field thermal emission by a bulk made of the host medium against thermal emission by the inclusions. In the exceptional case that emission by the host material is non-negligible, the energy density at \( r \) will be computed by superposing the energy density due to the inclusions with the energy density due to a bulk made of the host material weighted by the porosity of the host matrix (since thermal emission is a volumetric process) [58].

**Assessment of the validity of the EMT.** The assessment of the validity of the EMT will be done by comparing results from the T-DDA against those from the EMT. Again, the focus during the three-year period of this research will be on Mie resonance-based metamaterials for nano-TPV power generation. In EMT predictions, the metamaterial is assumed to be a homogeneous layer with effective electromagnetic properties. Various approaches exist for predicting the effective electric permittivity and magnetic permeability of metamaterials. PI’s group employed the scattering-corrected Clausius-Mossotti relations for predicting near-field thermal emission by Mie resonance-based metamaterials [3,4,24,120,121]. Smith et al. [123] proposed a more general approach for effective property prediction called the S-parameter method. This approach is based on computing the complex transmittance and reflectance of a metamaterial slab illuminated by a propagating wave in order to retrieve the effective permittivity \( \varepsilon_{\text{eff}} \) and permeability \( \mu_{\text{eff}} \). Details about the S-parameter method can be found in the monograph of Cai and Shalaev [1].

Metamaterial effective permittivity and permeability predicted from the scattering-corrected Clausius-Mossotti relations and the S-parameter approach will serve as input for computing the energy density from an effectively homogeneous slab. The code for performing these calculations, based on the DGF method, is available in PI’s lab and described in Ref. [3]. The transition to the EMT will be studied as a function of various parameters, such as \( r \) (see Fig. 3.4), the temperature, the size of the meta-atoms and the volume filling fraction of inclusions to name only a few. At the end of this task, the conditions for the applicability of the EMT to thermal metamaterial design will be clearly defined. This analysis will be useful not only for the
proposed research activities, but also for researchers designing structures selectively emitting and absorbing thermal radiation both in the near- and far-field regimes.

**Task 3: Design of metamaterials maximizing nano-TPV power generator performances**

The **deliverable** of Task 3 is a metamaterial design for harvesting low temperature waste heat through nano-TPV power generation. Task 3 will be accomplished in year 3.

Figure 3.5 depicts a schematic for a nano-TPV apparatus. A radiator at temperature $T_{rad}$ is separated from a cell, consisting of a p-n junction, by a sub-wavelength distance $d$ ($\sim$ 10 nm to 200 nm). Radiation with energy greater than or equal to the absorption bandgap of the cell produces electron-hole pairs, which in turn may generate electricity. Francoeur et al. [10] showed via a coupled near-field thermal radiation, charge and heat transport model that marked enhancement of radiation heat transfer in the near field does not automatically yield more electricity. This is because the near-field radiative heat transfer enhancement is broadband, contributing not only to increased photocurrent generation but also to heating the cell due to absorption by the lattice and the free carriers, electron-hole pair recombination and thermalization [10,124]. Figure 3.6 shows the influence of the cell temperature on the near-field power enhancement of a nano-TPV device made of a tungsten radiator ($T_{rad} = 2000$ K) and indium gallium antimonide cells. For a 10-nm-thick vacuum gap, the near-field power enhancement is about 36 when $T_{cell}$ is fixed at 300 K, but decreases rapidly as the cell temperature increases. Numerical simulations suggest that it is quite challenging to maintain $T_{cell}$ around room temperature when using naturally occurring materials, such as tungsten, for the radiator. For instance, when considering a 20-nm-thick vacuum gap, simulations results revealed that the TPV cell reached a temperature of 470 K even when a forced convection thermal management system is employed, thus reducing the conversion efficiency to about 7%. The results presented by the PI in Ref. [10] demonstrate that naively spacing the radiator and the cell by a few tens of nanometers is not a viable solution.

The key to developing viable, highly efficient nano-TPV devices is to tune near-field radiation heat transfer from the radiator to the cell so that most of the radiative energy is used for generating electricity. Polar crystals such as SiC support surface phonon-polaritons in the infrared leading to quasi-monochromatic near-field thermal emission. However, low energy (i.e., long wavelength) surface phonon-polaritons modes in polar crystals ($\sim$ 0.12 eV) are difficult to convert into electricity due to current TPV cell technological limitations [125]. Instead, quasi-monochromatic near-field thermal sources with resonance in the near infrared ($\sim$ 0.5 eV to 0.8 eV), which are difficult to find in nature [8,126], are needed for viable, highly efficient nano-TPV power generation. Mie resonance-based metamaterials made of Si inclusions have been shown to exhibit tunable surface polariton resonance in the near infrared at a temperature as low as 400 K (see Fig. 2.2).
surface polariton modes in Mie resonance-based metamaterials can be controlled by varying adjustable parameters, which include the shape, material, orientation, size, size distribution, arrangement, and the concentration of inclusions, as well as the material used for the host medium. According to Wien’s law, a temperature above 1000 K is required for dominant (but not quasi-monochromatic) thermal emission in the near infrared. Operating nano-TPV power generators at low temperature (i.e., ~400 K instead of 1000 K – 2000 K usually discussed in the literature) brings the possibility of harvesting low temperature waste heat in a multitude of electronic devices (e.g., cell phones, computers, solar photovoltaic cells), and even harvesting heat from the human body. Additionally, thermal management of TPV cells is much easier to handle if nano-TPV devices are operated at low temperature.

Ilic et al. [11] suggested optimal electromagnetic properties for TPV radiators using simple analytical relations. These relations were however determined by neglecting the thermal effects in the TPV cell, and thus cannot be applied to real nano-TPV systems. Due to the complexity of the coupled near-field thermal radiation, charge and heat transport model [10], it is impossible to derive simple analytical equations for determining optimal radiators (for instance, all properties of the cell are temperature-dependent). Determination of optimal radiators will be achieved via a genetic algorithm [127]. The idea is to employ a Mie resonance-based metamaterial as the radiator, and to determine the adjustable parameters maximizing nano-TPV power generation. Note that a genetic algorithm for thermal radiative property control has been used by Drevillon and Ben-Abdallah [128]. In this work, a genetic algorithm is applied for determining 1D multilayer structures leading to desired far-field thermal spectra.

The main steps of the design process are described as follows. A nano-TPV system as shown in Fig. 3.5 is considered. The cell architecture (e.g., material, doping levels), the gap thickness $d$, the temperature of the radiator $T_{rad}$ and the thermal management device are fixed. As discussed earlier, the temperature $T_{rad}$ will be maintained around 400 K in order to achieve low temperature power generation. A natural convection thermal management system will be employed. A target near-field power enhancement will be specified. It is expected that enhancements beyond a factor of 36, as shown in Fig. 3.6, are achievable via metamaterials. The input parameters in the genetic algorithm are the metamaterial adjustable parameters. In order to minimize the number of unknowns and to constrain the genetic algorithm, a formal sensitivity analysis will be performed by computing sensitivity coefficients as done in Ref. [31]. The sensitivity coefficients provide the variation of an output to perturbation of the adjustable parameters. This sensitivity analysis will serve in preselecting a few materials for the inclusions and the host medium that exhibit resonance in the near infrared. It is important to note that the T-DDA will need to be included in the coupled nano-TPV model. Indeed, near-field heat transfer between two objects is a function of both the emitter (radiator) and the absorber (TPV cell) [8,20,21]. The method for including the surface interactions described in Task 1 can easily accommodate such calculations. The determination of an optimal metamaterial-based radiator via a genetic algorithm can be summarized in a few steps [127,128]:

1. A population of various radiators with different parameters is generated. For each configuration, the near-field power enhancement is calculated.
2. The discrepancy between the target power enhancement and the actual power enhancement of the structures generated in step 1 is calculated via a fitness function.
3. Using the fitness function, some members in the population are selected in order to produce children. Configurations not chosen are discarded.
4. To avoid convergence of the algorithm in a local minimum, mutations are performed in the population.
5. Steps 1 to 4 are repeated until the target power enhancement is achieved.

Note that the publicly available genetic algorithm code PIKAIA [129] will be employed for this task.

Task 3 will lead to the design of radiators (metamaterials) maximizing direct thermal-to-electrical energy conversion at low temperature. The optimal metamaterials will eventually be fabricated and tested experimentally. The experimental aspect of the project is externally funded by the NSF [25]. It is worth mentioning that the NSF CAREER Award is not concerned with the optimization of nano-TPV power generation, but with the experimental demonstration that enhanced power generation can be achieved due to radiative heat transfer exceeding the blackbody limit.

4. PROJECT TIMELINE AND RESOURCES
Completion of the proposed work will require three years (suggested dates: 01/10/2014 to 01/09/2017). Task 1 will be pursued in years 1 and 2, Task 2 during years 2 and 3, and Task 3 in year 3. The total cost for the project is $150,000 ($50,000 per year). This is based on a total of 1.5 person-month for the PI, support for three years for a PhD student and cost for participating in national conferences. No equipment nor material is requested.

Sheila Edalatpour, a PhD candidate in PI’s lab, will be supported by the award. Ms. Edalatpour is an expert in near-field thermal radiation simulations, and she developed along with the PI the T-DDA approach described in this document [17]. PI’s lab is equipped with desktop computers and the necessary compilers (e.g., Matlab, Fortran, C, etc.) for carrying on the proposed research. Large simulations involving multiple objects, such as direct calculation of near-field thermal emission by metamaterials, will be performed on multiple processors at the Center for High Performance Computing (CHPC) of the University of Utah [130]. These computational resources are freely available for faculty members, given that brief reports summarizing the research activities, milestones and the accomplishments are provided to the administration of the CHPC.

5. SUMMARY AND DISSEMINATION PLAN
This research will provide a computational toolbox for designing metamaterials, with user-defined thermal radiative properties, beyond the EMT. The T-DDA, which is the backbone of the proposed research, will provide for the first time a methodology for predicting near-field radiative heat transfer in 3D complex geometries between objects much smaller and much greater than the wavelength. The near-field thermal radiation code developed during the first two years of the research activities will be made freely available to the public. This code is expected to impact various fields such as thermal metamaterials, thermal management of micro/nanoscale devices and thermal rectification through a vacuum gap to name only a few. The application of the T-DDA to direct calculation of near-field thermal emission by metamaterials will allow quantitative assessment of the validity of the EMT. Such an analysis will be useful for researchers designing metamaterials. Finally, the combination of the T-DDA, the coupled nano-TPV performance code and a genetic algorithm will allow for the first time determination of metamaterials maximizing nano-TPV performances. This project will have major impacts in metamaterial design, radiation heat transfer at the nanoscale, selective thermal emission and low temperature waste heat recovery.

The findings of this research will be disseminated in high impact journals (e.g., Physical Review Letters, Physical Review B, Applied Physics Letters, Journal of Quantitative Spectroscopy and
Radiative Transfer) and at national conferences. Additionally, the outcome of this research will be integrated into an undergraduate / graduate Nanoscale Heat Transfer class developed by the PI in 2011, where half of the course content focuses on near-field thermal radiation, thermal metamaterials and direct thermal-to-electrical energy conversion.

6. OTHER REQUIRED INFORMATION

6.1. Description of the organization

The purpose of the University of Utah Research Foundation (UURF) is to promote, conduct, encourage and facilitate research, development and dissemination of knowledge, and the application of knowledge in all fields of learning including, but not limited to, science, technology, medicine, pharmacy, engineering, natural resources, energy, business, and education. Any contract, grant, gift, funds, property or assets acquired by the Foundation shall be used exclusively for the scientific, educational and charitable purpose of assisting the University of Utah in achieving its educational objectives as the Board of Directors shall direct.

6.2. Other agencies receiving proposal

This proposal in its current format has not been submitted to other funding agencies. Some aspects of this proposal regarding direct calculation of near-field thermal emission by metamaterials have been included in proposals sent to NSF and DOE in February 2013 (both proposals are pending).

The PI would like to point out that the NSF CAREER Award he received in 2013 [25] is concerned with the experimental demonstration of enhanced power generation in nano-TPV systems due to radiative heat transfer exceeding the blackbody limit. The project focuses on experiments, and does not involve any optimization nor radiator design. The only numerical component is the comparison between the experimental results against prediction from the coupled near-field thermal radiation, charge and heat transport model already implemented in PI’s lab [10].

6.3. Environmental impact

Not Applicable.

6.4. Class I and Class II ozone depleting substances

Not applicable.

6.5. Effort and type of support requested

The total cost for the project is $150,000 ($50,000 per year). This is based on a total of 1.5 person-month for the PI, support for three years for a PhD student and cost for participating in national conferences. No other type of support is requested.