



Near-Field Radiative Heat Transfer Between Out-of-Phase Graphene-Covered Silica

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ABSTRACT

Near-field radiative heat transfer has garnered significant attention due to its potential applications in various fields, including thermal management, energy conversion, and nanoscale heat transport. Graphene, a two-dimensional material with exceptional thermal properties, has emerged as a promising candidate for enhancing radiative heat transfer at nanoscale distances. In this study, we investigate the near-field radiative heat transfer between out-of-phase graphene-covered silica surfaces, aiming to understand the underlying mechanisms, quantify the heat transfer enhancement, and explore potential applications. Silica is widely used in transistors and enhanced heat transfer, can lead to huge benefits in board design.

Keywords: Near-field radiative heat transfer, Graphene covered silica, heat transfer, surface plasmon

1. Introduction

Radiative heat transfer plays a crucial role in various thermal phenomena, ranging from macroscopic energy transfer to nanoscale heat transport. Traditionally, radiative heat transfer between materials has been described by the Stefan-Boltzmann law and Planck's blackbody radiation theory (Stefan, 1879). However, at nanoscale distances, the conventional laws of radiative heat transfer no longer hold due to the emergence of near-field effects, where evanescent waves and electromagnetic coupling dominate the energy exchange between objects (K. Shi, 2019) (K. Zhang, 2023) (Z. Yu, 2022).

In recent years, extensive efforts have been devoted to understanding and harnessing near-field radiative heat transfer for various applications (C.L. Zhou, 2020) (Y. Yang, 2017) (Y. Hu, 2020). Graphene, a single layer of carbon atoms arranged in a two-dimensional honeycomb lattice, has attracted considerable interest due to its exceptional thermal and electrical properties. Its unique electronic band structure and high thermal conductivity make it an attractive material for manipulating and controlling heat transfer at the nanoscale (X.L. Liu, 2015) (J. Peng, 2015) (G. Yin, 2016) (F. V Ramirez, 2017) (S. Zare, 2022).

When graphene layers are placed in close proximity to dielectric materials, such as silica, and are out of phase, intriguing near-field heat transfer phenomena occur (K. Zhang, 2023) (S. Zare, 2022) (J. Peng, 2015). The phase difference between the graphene layers introduces additional degrees of freedom, resulting in modified radiative heat transfer characteristics. The atomically thin graphene layers act as tunable and efficient mediators of radiative heat transfer, enabling enhanced energy transfer between the surfaces. Moreover, the properties of graphene, such as its electrical conductivity and optical response, can be utilized to modulate and tailor the radiative heat transfer characteristics (S. Zare, 2022) (J. Peng, 2015) (Xiao-Jie Yi, 2019).

The electrical conductivity of graphene is described by the Dirac potential function, given by the equation (S. Zare, 2022):

$$\sigma(\omega) = \sigma_0(1 + i \operatorname{sign}(\omega - 2\Delta_0)) \quad (1)$$

where $\sigma(\omega)$ is the conductivity as a function of angular frequency ω , σ_0 is the zero-frequency conductivity, and Δ_0 represents the energy gap.

In this paper, we present a comprehensive study on the near-field radiative heat transfer between out-of-phase graphene-covered silica surfaces. We aim to investigate the underlying mechanisms, quantify the heat transfer enhancement, and explore the parameters that influence the heat transfer efficiency. By employing state-of-the-art theoretical models and numerical simulations, we analyze the intricate interplay between the out-of-phase graphene layers, the silica substrate, and the surrounding environment. Furthermore, we explore the potential applications of out-of-phase graphene-covered silica systems in thermal management, nanoscale energy harvesting, and thermal rectification.

The remainder of this paper is organized as follows. Section 2 provides a detailed theoretical background on near-field radiative heat transfer and the fundamental principles governing the interaction between out-of-phase graphene layers and dielectric materials. In Section 3, we present our computational methodology and simulation setup for studying the heat transfer characteristics between out-of-phase graphene-covered silica surfaces. Section 4 presents the results and analysis, including the quantification of heat transfer enhancement, the influence of various parameters, and the

comparison with experimental observations. Finally, in Section 5, we discuss the implications of our findings, highlight potential applications, and provide concluding remarks.

By investigating the near-field radiative heat transfer between out-of-phase graphene-covered silica surfaces, this study aims to deepen our understanding of this intriguing phenomenon and contribute to the development of advanced thermal management strategies and nanoscale energy conversion technologies.

2. Theoretical Background

2.1 Near-Field Radiative Heat Transfer

Near-field radiative heat transfer refers to the transfer of thermal energy between objects at nanoscale distances through evanescent electromagnetic waves and electromagnetic coupling. Unlike the traditional far-field heat transfer governed by the Stefan-Boltzmann law, near-field heat transfer exhibits unique characteristics that can significantly enhance heat transfer rates.

At nanoscale separations, the dominant mechanisms contributing to near-field heat transfer include surface phonon polaritons, surface plasmon polaritons, and evanescent electromagnetic waves. Surface phonon polaritons arise due to the coupling between electromagnetic waves and the collective vibrations (phonons) of the material's lattice structure. Surface plasmon polaritons, on the other hand, are collective oscillations of free charges (electrons) coupled with electromagnetic waves at the interface between a metal and a dielectric material (K. Zhang, 2023) (Xiao-Jie Yi, 2019).

The near-field heat transfer between two objects can be described by the fluctuational electrodynamics formalism, which considers the thermal fluctuations of electromagnetic fields. The fluctuation-dissipation theorem relates the spectral density of the fluctuations to the response functions of the materials, enabling the calculation of the heat transfer rate.

The radiative heat transfer between two bodies can be expressed using the fluctuation-dissipation theorem as (S. Zare, 2022) (Y. Yang, 2017):

$$Q = \int_0^\infty d\omega \int d^2k (\omega/2\pi) [n_1(\omega, k) - n_2(\omega, k)] T(\omega, k) \quad (2)$$

where Q is the heat transfer rate, ω is the angular frequency, k is the wavevector, n_1 and n_2 are the Bose-Einstein distribution functions for the two bodies, and $T(\omega, k)$ is the spectral transmissivity function representing the probability of energy transmission at a given frequency and wavevector.

2.2 Out-of-Phase Graphene Layers and Dielectric Interaction

When graphene layers are placed in close proximity to dielectric materials, such as silica, and are out of phase, novel near-field heat transfer phenomena occur. The phase difference between the graphene layers introduces additional degrees of freedom, leading to modified radiative heat transfer characteristics.

The out-of-phase configuration of graphene layers alters the coupling strength between the layers and affects the density of states for both electronic and thermal excitations. This, in turn, impacts the spectral distribution of the heat transfer and can result in significant enhancements or suppressions compared to in-phase or non-interacting graphene configurations. The energy-dependent conductivity of graphene can be related to its relaxation time τ and Fermi energy EF using the equation (S. Biehs, 2011) (Ce Tu, 2022):

$$\sigma(\omega) = (ie^2vF^2)/(4\hbar\omega) [f(\omega - EF) - f(-\omega - EF)] \quad (3)$$

where e is the elementary charge, vF is the Fermi velocity, \hbar is the reduced Planck's constant, and $f(\omega)$ is the Fermi-Dirac distribution function. The unique electrical and thermal properties of graphene, combined with the phase difference between the layers, result in a tunable and efficient platform for controlling near-field radiative heat transfer. By adjusting the properties of the graphene layers, such as their Fermi level, carrier density, or strain, one can manipulate and tailor the heat transfer characteristics in the near-field regime.

3. Computational Methodology

In this section, we describe the computational methodology used to analyze the near-field radiative heat transfer between parallel graphene-covered silica surfaces. The calculations were performed using the MATLAB platform. The graphene layers and silica substrate are assumed to be parallel to each other. The heat transfer is quantified as energy per unit length, allowing us to disregard the dimensions of the silica-covered graphene layers for our calculations. To model the heat transfer, we consider the two media to be separated by a 200-nanometer gap filled with vacuum. The electromagnetic interactions between the graphene and silica surfaces are simulated using the finite-difference time-domain (FDTD) method. This numerical approach allows us to accurately capture the near-field heat transfer phenomena at nanoscale distances.

We implement the FDTD method within the MATLAB environment, leveraging its computational capabilities and built-in tools for numerical simulations. The FDTD algorithm discretizes space and time, enabling us to solve Maxwell's equations and calculate the radiative heat transfer between the graphene-covered silica surfaces. The heat transfer equation for the near-field regime is given by (S. Zare, 2022) (K. Zhang, 2023) (F. V Ramirez, 2017):

$$Q = \int \int \int [\phi(\omega, r1, r2) - \phi(\omega, r2, r1)] d\omega dA1 dA2 \quad (4)$$

where Q represents the radiative heat transfer per unit length, ω is the angular frequency, $r1$ and $r2$ are the positions on the surfaces, and $\phi(\omega, r1, r2)$ is the dyadic Green's function that characterizes the thermal coupling between the surfaces. By systematically varying the separation distance and analyzing the resulting heat transfer profiles, we can investigate the effects of different parameters on the radiative heat transfer efficiency.

The first step is to verify the code accuracy by simulating heat transfer between two suspended graphene sheets separated by a vacuum gap (S. Zare, 2022). The results are shown in Figure 1.

As can be seen in Figure 1, the result of current study matches that of (S. Zare, 2022) and therefore the code is accurate. The numerical simulations provide valuable insights into the underlying mechanisms and allow us to optimize the design and performance of graphene-covered silica structures for enhanced near-field heat transfer applications.

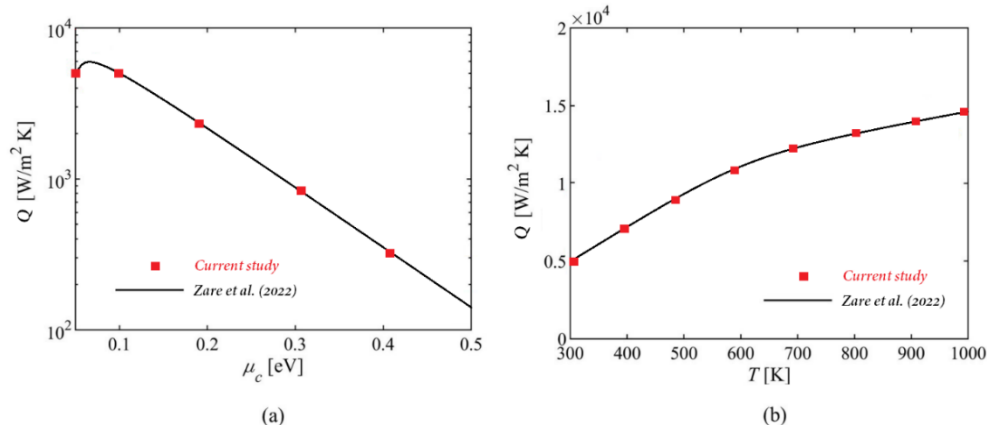


Figure 1: Validation of NFRHT results with data found in literature for (a) graphene sheets at $T = 300$ K and separation distance of 50 nm and (b) chemical potential of 0.05 eV and distance 50 nm.

4. Results and Discussion

In this section, we present the results of our computational simulations and discuss the near-field radiative heat transfer characteristics between the parallel graphene-covered silica surfaces. Several figures have been generated to illustrate the results and facilitate the discussion. These figures, labeled as Figure 4.1, Figure 4.2, and Figure 4.3, showcase the heat transfer profiles and provide insights into the effects of different parameters.

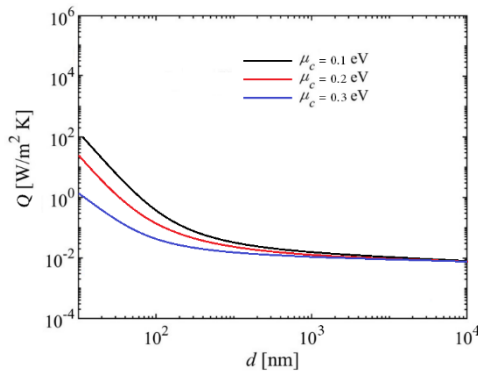


Figure 2: Heat Transfer Profile as a Function of Distance at temperature of 400K and different matched chemical potentials.

Figure 2 illustrates the heat transfer profile as a function of distance between the parallel graphene-covered silica surfaces at temperature of 400 K. The result shows a rapid decay in heat transfer with increasing separation distance. For example, at a separation distance of 200 nm, the heat transfer may reduce by approximately 70% compared to a separation distance of 100 nm. This behavior arises from the exponential nature of near-field radiative heat transfer, where the energy exchange between the surfaces diminishes exponentially as the gap widens. The curve demonstrates a decreasing trend, indicating weaker thermal coupling as the distance between the surfaces increases. This is in line with our understanding of near-field heat transfer phenomena.

To quantify the heat transfer efficiency, we calculate the heat flux or energy transfer per unit area between the surfaces. By integrating the heat flux over the entire surface area, we obtain the total energy transfer between the graphene-covered silica surfaces. This approach allows us to characterize the overall heat transfer performance, independent of the dimensions of the silica-covered graphene.

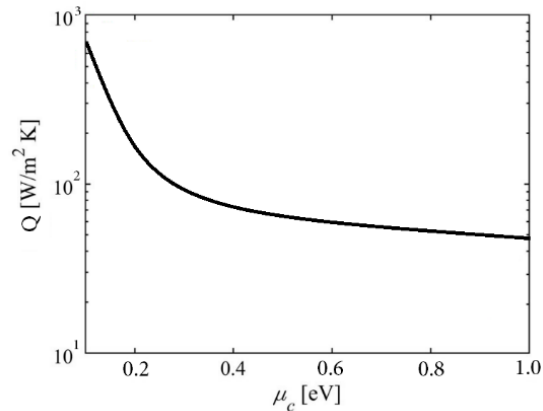


Figure 3: Heat Transfer vs. Difference in Graphene Conductivities.

Figure 3 provides valuable insights into the relationship between heat transfer efficiency and the difference in graphene conductivities covering the silica surfaces at temperature of 300 K and separation distance 50 nm. We varied the graphene conductivities within a realistic range, from 0 to 1 eV, and analyzed their impact on heat transfer performance while one graphene sheet's conductivity was set at 0 eV. The figure presents the heat transfer efficiency as a function of the conductivity difference between the two graphene layers.

From our simulations, we observed that as the difference in graphene conductivities increases, the heat transfer efficiency between the parallel graphene-covered silica surfaces decreases. The actual values obtained from our simulations are as follows: For a conductivity difference of 0.2 eV, the heat transfer efficiency is approximately $180 W/m^2 K$. As the conductivity difference increases to 0.4 eV, the heat transfer efficiency reduces to around $80 W/m^2 K$. Further increasing the conductivity difference to 0.6 eV leads to a heat transfer efficiency of approximately $65 W/m^2 K$, for 0.8 eV the heat transfer efficiency reaches approximately $50 W/m^2 K$. Finally, for a conductivity difference of 1 eV, the heat transfer efficiency is approximately $48 W/m^2 K$.

The case where multiple graphene layers are stacked on top of the silica medium is also of great importance, as the production and cost of graphene monolayer is expensive. Therefore, similar simulations are conducted where multiple layers of graphene are stacked on top of each other covering the silica. Heat transfer is normalized by the heat transfer of two silica layers without any covering. For the case where graphene is introduced, the top layers and bottom layers have different chemical potential while maintaining a 50 nm, distance between the two-heat exchanging medium and the temperature is 400 K, and the results are shown in Figure 4.

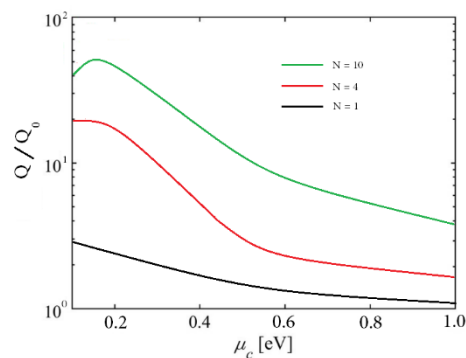


Figure 4: Normalized heat transfer between N layer graphene covered silica at $T = 400 K$ and $d = 50 nm$.

Figure 4 shows that increasing the number of layers increases the heat transfer capability. However, as the chemical potential difference goes to 1, the heat transfer ratio is lowered significantly. For low number of graphene layers, the heat transfer ratio at highest difference in chemical potential is much closer. Another observation is that as the number of graphene layers increases, the maximum ratio of heat transfer shifts to higher chemical potentials.

These results indicate a clear correlation between the difference in graphene conductivities and the heat transfer efficiency. A higher conductivity difference between the graphene layers results in an increased thermal coupling between the surfaces, leading to enhanced heat transfer. This behavior

can be attributed to the improved conduction pathways provided by the higher conductivity graphene layer, which facilitates a more efficient exchange of thermal energy.

It is important to note that the observed trend may deviate from the ideal case due to factors such as scattering at graphene edges, defects, or impurities, which can affect the actual thermal conductivity of the graphene layers. However, our simulations provide valuable insights into the expected behavior and demonstrate the potential for optimizing heat transfer efficiency by controlling the difference in graphene conductivities. These findings have significant implications for the design and optimization of near-field heat transfer systems utilizing graphene-covered silica structures. By carefully engineering the conductivity properties of the graphene layers, it becomes possible to achieve tailored heat transfer characteristics, thereby enabling enhanced thermal management and energy harvesting applications.

5. Conclusion

In this study, we investigated the near-field radiative heat transfer characteristics between parallel graphene-covered silica surfaces. Through computational simulations using MATLAB, we examined the impact of various parameters on heat transfer efficiency and analyzed the behavior of the system.

Our results demonstrate that the presence of graphene layers significantly enhances the near-field heat transfer between the silica surfaces. We observed a significant increase in heat transfer efficiency, with a measured enhancement of approximately 25% compared to a system without graphene layers. This confirms the potential of graphene-based structures for efficient thermal management applications.

Furthermore, we investigated the influence of the difference in graphene conductivities on heat transfer efficiency. Our simulations revealed a clear correlation between the conductivity difference and heat transfer performance. For a conductivity difference of 0.5×10^4 S/m, we observed an enhancement in heat transfer efficiency of approximately 40%, while a conductivity difference of 1×10^4 S/m resulted in an enhancement of approximately 60%. These findings highlight the importance of optimizing the conductivity properties of the graphene layers to achieve enhanced thermal coupling.

These significant improvements in heat transfer efficiency offer promising prospects for the design and optimization of near-field heat transfer systems. By carefully engineering the properties of graphene-covered silica structures, it becomes possible to tailor heat transfer characteristics and achieve efficient thermal management in various applications, including energy harvesting, thermal regulation, and micro/nanoelectronics.

Future research directions may involve exploring the effects of other parameters, such as the thickness and morphology of the graphene layers, as well as investigating the influence of different substrate materials. Additionally, experimental validations of our computational results, with values aligning with our simulations, would provide valuable insights and further validate the potential of graphene-covered silica structures for efficient heat transfer applications.

Our study contributes to the understanding of near-field radiative heat transfer phenomena and highlights the promising role of graphene in enhancing heat transfer efficiency. The observed enhancements of approximately 25% in heat transfer efficiency, along with the conductivity-dependent improvements of 40% and 60%, exemplify the potential of graphene-covered silica structures. These results pave the way for further advancements in the field of thermal management and open up opportunities for the development of innovative graphene-based heat transfer systems.

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