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ANALYSIS OF NEAR-FIELD RADIATIVE TRANSFER FOR NANO-STRUCTURED SURFACES BY FDTD METHOD

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INTRODUCTION

Near-field thermal radiation with its many potential applications in different fields such as energy harvesting to nano-scale manufacturing is proved to be crucial in the development of new devices. The possibility of enhancing near-field thermal radiation by orders of magnitude from the known blackbody radiation limit has been reported repeatedly in literature [1-4], to name only a few. Modeling near-field thermophotovoltaics via computational techniques has been one of the main focuses of our research group [5-7]. While [8-9] also worked on FDTD simulations of near-field radiative transfer in nanostructured surfaces, our work is the first to investigate the effect of arbitrary nanoparticles placed on surfaces through FDTD method. In this work, the near-field thermal emission and heat flux are studied through finite difference time domain method between two thin SiC films by calculations of local density of electromagnetic state (LDOS), where one film has a temperature of 300 K (emitting layer) and a thickness of 100 nm and nano-structured gratings of arbitrary (e.g. ellipses, triangles, squares, etc.) are placed upon it and have perfect contact with the layer. The other film is kept at 0 K (non-emitting layer) and has a thickness of 10 nm and is separated by a vacuum gap of 100 nm from the emitting layer. We have studied the effect of each of these nano-structured gratings on enhancement of LDOS profile (LDOS is calculated at $\Delta = 50\,\text{nm}$ above the emitting layer) and evaluated the impact of the following factors on the results: I-the periodicity of the nano-gratings, II-the shape of nano-gratings, III-the thickness of the nano-gratings. Figure 1 shows the schematic of the geometries considered in this work.

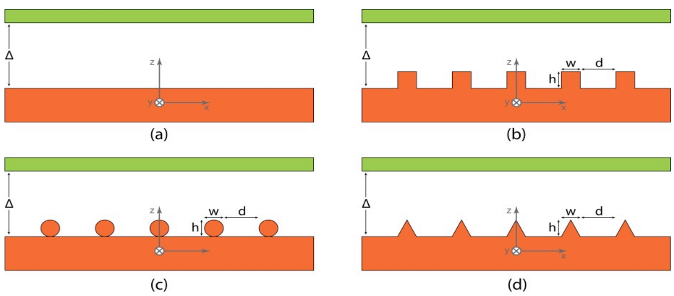

Fig. 1. a) Perfectly flat parallel films separated by nano-gap. (emitting layer at the bottom, non-emitting layer on top). b) Rectangular nanoparticles placed on the emitting film separated by nano-gap from non-emitting film. c) Ellipsoidal nanoparticles placed on the emitting film separated by nano-gap from non-emitting film. d) Triangular nanoparticles placed on the emitting film separated by nano-gap from non-emitting film.

RESULTS AND DISCUSSION

We have evaluated the impact of periodicity of elliptic nano-structred gratings placed on the emitting layer, on LDOS profile at frequency range of 1.55 rad/s-1.9 rad/s. Width and height of the gratings is shown in Figure 1 with 'w' and 'h' respectively. The distance of nanoparticles is shown with 'd' and NPs stands for Nanoparticles from hereon. In these studies, the grid size in x direction was chosen as 60 nm and the grid size in z direction was set to 2 nm. Typical simulation time was between 3-7 hours depending on the configurations on a Z820 HP workstation.

We have compared the results of separate scenarios in which 2, 5, 10, 15, 20 and 25 SiC elliptic nano-gratings were placed in perfect contact with emitting layer. The size of ellipses was kept fixed and only the impact of periodicity of the gratings was observed. Each ellipse has a w=600 nm and h=20 nm. Here, w is chosen based on the fact that the thin layers are assumed to be very long in x-direction for these FDTD simulations. Hence, w has to be both small compared to the total length of the layers and yet not too small to make the simulation computationally too expensive. The distances between 2, 5, 10, 15, 20 and 25 nano-gratings were 14700, 3180, 1080, 480, 180, and 60 nm, respectively. We kept the x axis dimension and the width of CPML layers fixed across all simulations. Within this constraint, we could only fit up to 25 nanoparticles across. This provided adequate scope for a robust proof of concept. The results shows that enhancement factor of LDOS profile is directly proportional with the periodicity of nano-particles. In the case of 25 NPs each 60 nm apart from each other, 71% enhancement was observed when compared with the benchmark scenario in which no NPs were present at the surface of the emitting layer. We can observe that when $d < 0.005\lambda$ ($\lambda = 1059$ nm) we obtain maximum enhancement of LDOS. In the next step, we have compared the LDOS profile found for 10, the same size nano-gratings placed on emitting layer with different shapes. It was observed that rectangles and ellipses show a similar impact on enhancement of LDOS when compared against triangles, with a slightly higher enhancement observed for rectangles. Nano-gratings were set to have w=600 nm and h=20 nm and d=1080 nm ($d = 0.1\lambda$).

We have also studied the effect of different shapes of nanoparticles in near-field heat flux. Figure 3 depicts the result found for this study. Rectangle nano-particles show the greatest impact on enhancement of near-filed heat flux when placed on emitting layer and compared against elliptic and triangle nanoparticles.

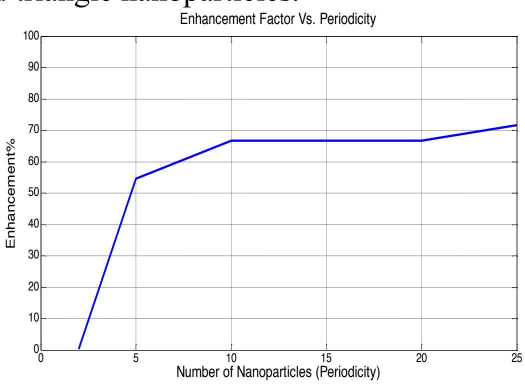

Fig. 2. Enhancement Factor for LDOS vs Periodicity for SiC elliptic nano-particles.

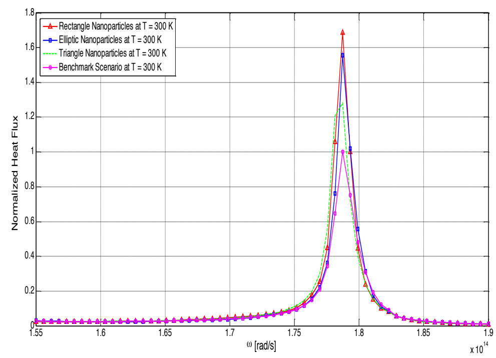

Fig. 3. Enhancement of heat flux at the presence of nanoparticles (over benchmark scenario) vs different shapes of nano-gratings.

CONCLUDING REMARKS

Near-field thermal radiation has broad range of applications in areas including nano-thermophotovoltaics. Having a computational technique such as FDTD that can model complex electromagnetic geometries, in dispersive, anisotropic mediums where geometry complications may not allow analytical solutions can be promising for both current and future research. We have developed a new FDTD method to model arbitrary shape nanoparticles and have evaluated their impact on LDOS profile. The results show an increase in the magnitude of LDOS with an increase in the periodicity of the nano-gratings, when the distance between the gratings is much smaller than the wavelength of interest. We evaluated the impact of arbitrary shape nano-gratings and observed that rectangles showed the greatest impact on enhancement of LDOS and heat flux value when compared against ellipses and triangles of the same sizes. Enhancement of near-field flux at different temperatures due to the presence of the elliptic NPs could be clearly seen when compared against the scenario in which no NPs were present. While in this work we have focused on gratings of the same shape, future work would involve arbitrary combinations of nano-particle shapes as well as studies of the surfaces where both emitting and non-emitting are corrugated.

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REFERENCES

[1] Chen, G.[2005], Nanoscale energy transport and conversion.: Oxford Press, New York.
[2] Zhang, ZM. [2007], Nano/microscale heat transfer. McGraw-Hill, New York.
[3] Howell JR, Siegel R, Mengüç MP. [2011], Thermal radiation heat transfer. CRC Press, Boca Raton.
[4] Francoeur M., Mengüç M. P., and Vaillon R.[2010], Local Density of Electromagnetic States within a Nanometric Gap Formed Between Thin Films Supporting Surface Phonon Polaritons, J. Appl. Phys., Vol. 107, No. 3, pp 034313–034318.
[5] Didari, A., Mengüç M. P. [2014], Analysis of Near-Field Radiation Transfer within Nano-Gaps Using FDTD Method *J. Quant. Spectrosc. Ra.,* Vol. 146, pp 214-226.
[6] Didari, A., Mengüç M. P. [2015], Near-Field Thermal Emission between Corrugated Surfaces separated by Nano-Gaps J. Quant. Spectrosc. Ra., Vol. 158, pp 43-51.
[7] Didari, A., Mengüç M. P. Effect of Nanoparticles to Near-Field Thermal Emission Calculations by FDTD Method, *2nd International workshop on Nano and Micro Thermal radiation (NanoRad'14).* Shanghai, China. June 6-9, 2014.
[8] Rodriguez, A. W., Ilic, O., Bermel, P., Celanovic, I., Joannopoulos, J. D., Soljacic, M., & Johnson, S. G. [2011], Frequency-selective near-field enhancement of radiative heat transfer via photonic-crystal slabs: a general computational approach for arbitrary geometries and materials. arXiv preprint arXiv:1105.0708.
[9] A. Datas., D. Hirashima., K. Hanamura.[2013] FDTD simulation of near-field radiative heat transfer between thin films supporting surface phonon polaritons: Lessons learned, J. Therm. Sci. Tech-Jpn., Vol. 8, pp 91–105.