Thermal Transport at Nanoscale Point and Line Constrictions and Interfaces

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The objective of this project was to collaborate with the University of Central Paris Laboratory EM2C to foster technical expertise and expand current knowledge of numerical modeling and simulation of thermal transport across nanometer scale point and line constrictions and interfaces that are important for a number of existing and emerging technologies, including (i) nanoscale point contacts in scanning probe microscopy, thermally assisted magnetic recording, carbon nanotube thermal interface materials, and nanowire thermoelectric devices; (ii) nanoscale line interfaces in Si FINFET nanotransistors, nanowire and nanotube electronic devices, and metal/dielectric interconnect structures for next-generation ultra-large-scale-integrated (ULSI) circuits.

INTRODUCTION

Thermal transport at nanoscale constrictions and interfaces is a fundamental problem that has been encountered in various new applications but has not been adequately studied. Recently, we have conducted Molecular Dynamics (MD) simulation of thermal transport at a nanoscale circular point constriction in silicon [1], and measured the contact thermal resistance between a planar surface and a carbon nanofiber [2], an InAs nanofilm [3], or a CrSi2 nanowire [4]. We have collaborated with Dr. Ravi Prasher at Intel to calculate the thermal resistance at nanoscale constrictions and interfaces.

Analytical work to date clearly predicts a major increase in radiative transfer between bodies spaced at sub-wavelength distances, with the effect increasing dramatically as the separation distance is decreased. Hence, we will investigate the influences of near- and far- field radiation transfer on the temperature distribution and thermal resistance at the interface between a nanostructure and a substrate in contact or in close proximity to each other. To accomplish this goal, we collaborated with Profs. Jean Taine and Jean-Jacques Greffet at the University of Central Paris to explore the most recent methods in numerical heat transfer and near field radiation analysis. Near fields are especially relevant, as much of the cutting edge research on the physics of near fields has been done in Paris. Prof. Greffet is in fact currently chairing a school studying near-field thermal heat transfer. His recent references are devoted to this research area [5-12].

We collaborated with Prof. Greffet's group to extend our existing finite-difference time-domain (FDTD) model to study near-field radiative interactions between a heated stylus and a substrate, and will be combined with MD simulation of phonon transfer between the stylus and the substrate. This combined approach will provide predictions of combined-mode transfer between the stylus and substrate, allowing prediction and comparison of interface resistance. This work is funded by NSF through the University of Texas at Austin. Mr. Nathan Malcolm, a US citizen, was chosen for this program. He is a graduate research assistant on the existing grant, and had sufficient background in modeling at the time of the visit (proposed for Summer, 2008) to carry out effective interaction with his French counterparts and also learn from them. He was be prepared for the visit through orientation with the College of Engineering Study-Abroad Program, which has an effective interchange program with other French Universities.

RESEARCH ACTIVITIES AND ACCOMPLISHMENTS OF THE INTERNATIONAL COOPERATION

The solution of the near field radiation that augments energy transfer from a particle to the substrate will be modified to compute the radiative energy transfer from the sharp tip or a line source to the substrate. We will predict the radiative transfer from the probe or line to the substrate using near-field analysis, and will include the effect of radiation field reflection from the substrate and its interaction with the incident field. (Reflection was neglected in the results of [13]). The results of Heltzel et al. indicate an important effect of probe-substrate spacing when approximations are removed from the near-field Maxwell equations for Mie theory, resulting in the oscillations of incident radiation with radius shown in Fig. 1. We will determine whether the near-field solutions for radiation from the probe tip or line source to the substrate show similar effects when the external excitation source is removed. In addition, we will also simulate the far-field radiation exchange between the side surfaces of the tip and line source and the substrate surface, and compare near- field radiation exchange with far-field radiation transfer.

An additional computational tool that will assist the understanding of the near-field radiation between tip and substrate is the finite-difference time-domain (FDTD) method for solving Maxwell's equations. The partial differential form of the magnetic and electric field components are discretized and solved explicitly in a leapfrog manner. The FDTD technique has been successfully employed for grids containing up to billions of nodes, with an extensively developed computational theory. The direct solutions of Maxwell's equations also have been verified in both near-field and far-field, and have successfully described laser radiation enhancement surrounding an AFM tip [15]. The field enhancement due to laser/microsphere interaction has been characterized using a 3-D capable program. Figure 2 shows a snapshot of the electric field component in the x-direction taken midway through the cubic grid. A distinctly enhanced local field exists at the sphere/substrate contact point, agreeing with analytical theory and experiment. Figure 3 shows the effect an AFM-tip sized perfect electric conductor (bottom of grid) has on an incident laser waveform. The inclusion of appropriate magnetic and electric properties will accurately simulate the local effects generated by an etched silicon or silicon nitride microprobe coated with a conducting layer.

The FDTD method is a versatile direct simulation tool. Arbitrary radiation sources can be applied in user-defined scattering and absorption problems. The introduction of Berenger's perfectly-matched-layer absorbing boundary condition [16] allows long duration simulations without accumulated error.

Treatment of thermal radiation heat transfer between a nanoscale object and surface poses a more complex, but feasible, set of modeling challenges than the monochromatic excitations of Figs. 2 and 3. The objects themselves are radiation sources rather than scatterers, producing the full spectrum of intensities based on temperature and emissive properties. With the spectrum known, a finite number of wavelength intensities can be modeled, approximating the energy emitted from an arbitrary object. The electromagnetic intensity can be calculated within a solid volume by the Poynting vector, providing input for a joint heat transfer simulation. Prof. Greffet's group is one of the leading groups to simulate nanoscale thermal radiation transport and especially between a nano tip and a surface. [9] The collaboration with them will have mutual benefits for the education of the participating students and sharing the knowledge gained from this study.

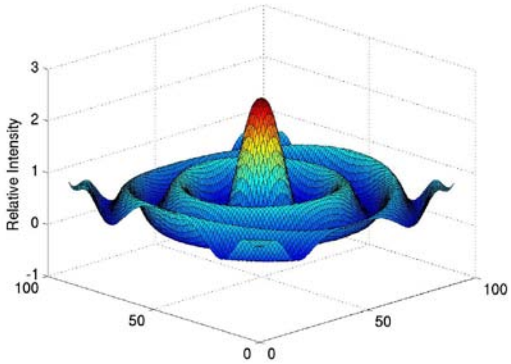

Fig. 1: Intensity of radiation on a flat substrate beneath a dielectric sphere of diameter 880 nm, refractive index 1.37, irradiated by a laser of wavelength 355 nm; sphere separated from the substrate by 675 nm. Results include near-field augmentation.

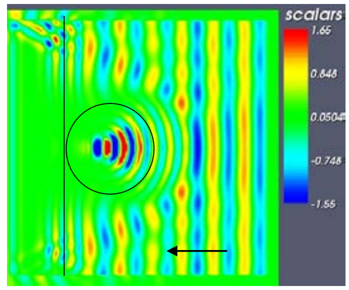

Fig. 2: FDTD simulation of laser/microsphere interaction

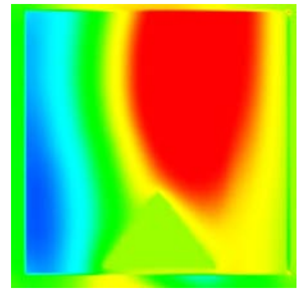

Fig. 3: FDTD simulation of laser/AFM tip interaction

BROADER IMPACTS OF THE INTERNATIONAL COOPERATION

The proposed collaborative interactions will provide an international perspective and feedback on the work being carried out under the existing NSF grant at The University of Texas from a highly respected international research group. The graduate student carrying out the work will assimilate new tools, and the interaction and information exchange among the UT PIs and the French researchers will be strengthened. In addition, the PIs' and the graduate student's familiarity with the foreign language, culture, and applicable technological trends was enhanced, particularly the graduate student's through foreign language study before and during the trip.

DISCUSSION AND SUMMARY

Most recently, we have collaborated with the University of Central Paris to explore the most recent methods in numerical heat transfer solving and near field analysis. Near fields are especially relevant, as much of the cutting edge research on the physics of near fields has been done in Paris. Greffet is in fact currently chairing a school studying near-field thermal heat transfer. We modeled thermal transport at nano- point and line constrictions and interfaces that are highly relevant to existing and new engineering applications over a large temperature range. A MD method was used to calculate the temperature distribution and thermal resistance at nano- constrictions and interfaces. In addition to heat conduction, our calculation investigated the influences of near- and far- field radiation transfer on the temperature distribution and thermal resistance. The effects of the constriction size and impurity doping concentration was investigated in the experiments and calculations. The research program consists of tasks undertaken jointly by Dr. Shi, Dr. Howell, and graduate student Nathan Malcolm.

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BRIEF BIOGRAPHIES OF RESEARCHERS

Nathan Malcolm received a B.S. degree in Mechanical Engineering with minors in Mathematics, Physics, and Spanish from the University of Arkansas in 2006. He is currently finishing an M.S. degree in Mechanical Engineering specializing in Radiation and Nanotechnology. He has been involved with numerous student groups and outreach programs, serving as Vice-President of the Graduate Engineering Council since 2007, and serving as Director for the Graduates and Industry Networking Conference 2008, to name a few.

Li Shi is a faculty member of the Thermal/Fluid Systems program of the Mechanical Engineering Department. He has served on the College of Engineering faculty since 2002. Dr. Shi is also a fellow of the Center for Nano and Molecular Science and Technology in the University of Texas at Austin Texas Materials Institute. He received a CAREER award from the National Science Foundation (NSF) for his work on thermal transport and thermoelectric measurements of nanotransistors, nanowires, and superlattices in 2003, and a Young Investigator Award from the Office of Naval Research for research of nanostructured thermoelectric materials in 2004. He received an Outstanding Reviewer Award from the ASME Journal of Heat Transfer, which honors those reviewers who have made exemplary contributions to the Journal.

John Howell is a faculty member of the Thermal/Fluid Systems program of the Mechanical Engineering Department. He has served on the College of Engineering faculty since 1978 and previously taught at the University of Houston. He served as departmental chair from 1986 to 1990 and as Associate Dean for Research in the College of Engineering for three years until August 31, 1999. He worked to improve safety awareness, renovation procedures, communication between the College and the central administration on issues ranging from renovations to intellectual property. He also chaired the committee to develop a Strategic Plan for the College. He coauthored *Thermal Radiation Heat Transfer*, Taylor and Francis, now in 4th ed (2002) (with Robert Siegel), and *Fundamentals of Engineering Thermodynamics*, McGraw Hill, 2nd ed. 1992 (with Richard Buckius), and has published over 200 articles, papers and reports. He maintains a web page of thermal radiation shape factors at http://www.me.utexas.edu/~howell/. He received the ASME/AIChE Max Jakob Award (1997), the ASME Heat Transfer Memorial Award (1991) and the AIAA Thermophysics Award (1990) for his work in radiative transfer, and the ASEE Ralph Coats Roe Award in 1987 as Outstanding Mechanical Engineering Educator. He is a Fellow of ASME and AIAA, and was elected a Foreign Member of the Russian Academy of Science (1999). In 2004 the College of Engineering recognized Dr. Howell's outstanding research contributions with the Billy and Claude R. Hocott Distinguished Centennial Engineering Research Award.