SYMPOSIUM DD

Heat and Mass Transport at Nanoscale–From Fundamentals to Devices

March 29 - 31, 2005

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* Invited paper

SESSION DD1: Mass Flow at Nanoscale
Chair: Pawel Keblinski
Tuesday Morning, March 29, 2005
Room 3003 (Moscone West)

9:00 AM *DD1.1
Pearling Instability of Nano-flows Confined to a Chemical Channel. Joel Koplik[1], Tak Shing Lo[1], Markus Rauscher[2,3], Siegfried Dietrich[2,3] and Jayanth R. Banavar[4]; [1]Levich Institute, City College of New York, New York, New York; [2]Max-Planck-Institut fur Metallforschung, Stuttgart, Germany; [3]ITAP, Universitat Stuttgart, Stuttgart, Germany; [4]Physics Department, Pennsylvania State University, University Park, Pennsylvania.

We investigate the flow of a nano-scale incompressible liquid ridge along a "chemical channel" on a substrate: a long, straight completely wetting stripe sandwiched between two non-wetting solids. Molecular dynamics simulations, finite-element continuum calculations, and a simple long-wavelength approximation were used, and give qualitatively consistent results. While shallow liquid ridges are stable both statically and when flowing, a (linear) pearling instability develops when the thickness of the ridge exceeds half of the width of the channel. In the flowing case periodic bulges propagate along the channel and subsequently merge due to non-linear effects. However, the ridge does not break up even when the flow is unstable.

9:30 AM *DD1.2
Molecular Modeling of Macromolecules in Nanoscopic Systems: From Flow in Nanochannels to Dynamics in Nanoglasses. Juan J. de Pablo, Chemical Engineering, University of Wisconsin, Madison, Wisconsin.

An increasing amount of evidence suggests that the behavior of macromolecules under nanoscale confinement is considerably different from that in the bulk. This presentation will discuss how deviations from bulk behavior arise in the context of two examples that encompass a wide range of concentrations, from dilute solutions to concentrated polymer melts. The first example considers deviations from bulk behavior in the flow of DNA solutions in micro and nanofluidic channels, where confinement influences the conformation and dynamic properties of individual molecules. The second example considers ultrathin polymer films, where severe (nanoscale) confinement can alter the thermophysical and mechanical properties of polymeric materials considerably.

10:30 AM *DD1.3
Water Transport through Nanopores. Shekhar Garde[1], Gerhard Hummer[2] and Amrit Kalra[1]; [1]Chemical and Biological Engineering, Rensselaer Polytechnic Institute, Troy, New York; [2]NIDDK Laboratory for Chemical Physics, National Institutes of Health, Bethesda, Maryland.

Single walled carbon nanotubes are ideal model systems to study wetting/dewetting, selective partitioning, and transport of solution species such as water and other small solutes. We will report molecular dynamics simulation studies of molecular transport of solute species through open-ended carbon nanotube interior. Water penetrates the nanotube interior, forming well-ordered hydrogen-bonded water wires. Our simulations of water transport through nanotubes driven by osmotic driving forces highlight unique aspects of molecular scale flows. Specifically, we find that water transport through nanopores is stochastic in nature, encounters negligible friction, and is dominated by entry and exit barriers. We develop a molecular model for single-file transport of water and other solution species that quantitatively accounts for the flow observed in simulations. Our simulations also address the issues of water in nanoscopic confinements and shed light on behavior of water in one, two, and three-dimensional geometries. Thermodynamic and kinetics or solute partitioning and transport in nanotubes is analogous to that in biological nanopores and suggests exciting applications of nanotubes in nanoscale devices or separation systems.

11:00 AM *DD1.4
Water Flows in Carbon Nanotubes. Petros Koumoutsakos, Swiss Federal Inst of Technoloyg, Zurich, Switzerland.

We discuss the transport of water and ions through carbon nanotubes using non-equilibrium molecular dynamics and multiscale simulations. The hydrophobicity and water transport in the nanotubes is determined in terms of impurities on the nanotube walls and in the solute. We focus on water transport in single wall carbon nanotubes where we analyse the effect of electrostatic forces. Our results indicate that carbon nanotubes inhibit proton transport through the presence of L-defects on the water structure and that water flow can be regulated via appropriate nanotube wall modifications.

11:30 AM DD1.5
Interfacial Heat Transfer in Presence of Laminar Shear Flow. Rajesh Khare[2], Arun Yethiraj[3] and Pawel Keblinski[1]; [1]Department of Materials Science & Engineering, Rensselaer Polytechnic Institute, Troy, New York; [2]Department of Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, Wisconsin; [3]Department of Chemistry, University of Wisconsin-Madison, Madison, Wisconsin.

We use molecular dynamics simulations to study thermal resistance at a solid-liquid interface in the presence of a simple laminar shear flow. Thermal transport properties of two model liquids - a monoatomic liquid and a polymeric liquid composed of 20 repeat units - are studied when confined to thin films. The confining walls are modeled as atomistic FCC lattice surfaces and simulations are carried out at different strengths of the solid-liquid interaction. In each case, the interfacial thermal resistance in presence of shear flow was compared with a corresponding system but without the shear flow. We find that with no-slip velocity boundary condition, the mass flow does not affect the thermal interfacial resistance, whereas a slip in the velocity profile causes an increase of the interfacial resistance by about a factor of two. Interestingly, a polymeric system with strongly attractive solid-liquid interactions exhibits an effective negative interfacial thermal resistance due to the enhanced thermal conductivity of the liquid layer adjacent to the solid wall.

11:45 AM DD1.6
Surface Mediated Liquid Transport on Nanotubes. Kyungsuk Yum and Min-Feng Yu; Department of Mechanical and Industrial Engineering, University of Illinois at Urbana-Champaign, Urbana, Illinois.

The surface mediated liquid transport on nanotubes is studied. Liquid droplets with volumes of the order of femtoliters are formed on the outside surfaces of nanotubes using the nanopipette integrated with the nanomanipulation stage. If the spreading parameter S is larger than a threshold value S_c, the liquid spontaneously flows out from the droplet through a thin film formed on the nanotube surface. The liquid transport on the nanotubes is investigated by measuring the volume flow rate, which is obtained from a direct observation of the size of the droplet. The dynamics process is interpreted by balancing the viscous force and the pressure gradient generated by the surface tension driven Laplace pressure and the disjoining pressure due to the long-range liquid/solid interactions. The results are relevant to the nanoscale liquid transport systems for nanofabrication.

SESSION DD2: Nanotubes and Nanowires I
Chair: Dimos Poulikakos
Tuesday Afternoon, March 29, 2005
Room 3003 (Moscone West)

2:00 PM *DD2.1
Thermal Issues in Femtosecond Laser Assisted Growth of Nanowires. Sam Mao, Lawrence Berkeley National Lab, Berkeley, California.

This talk will provide an overview of recent progress of crystalline nanowire synthesis using femtosecond laser assisted vaporization/deposition approach. Thermal issues involved in catalytic one-dimensional nanocrystal growth and in nonequilibrium femtosecond laser vaporization process will be discussed. Also presented will be structural and optical characterization of nanowires grown by different synthesis approaches. As we recently demonstrated, femtosecond laser assisted vaporization/deposition offers a plausible method for achieving uniform nanowires with good optical properties.

2:30 PM DD2.2
An AFM Based Joule Heating Thermometry Technique for Thermal Characterization of Nanostructures. Abhishek Jain, Lisa Pietruszka and Theodorian Borca Tasciuc; Rensselaer Polytechnic Institute, New York, Troy, New York.

Thermal characterization of nanostructures is critical for understanding thermal transport at nanoscale and for design and operation of nanoelectronics and novel thermo-electric energy conversion devices. There is a need to develop fast and reliable techniques to measure the thermal response of individual nanostructures during operation when electric current passes through the nano-devices. Here we describe an AFM based technique for thermal characterization of electrically conductive individual nanowires. Nanowire samples are distributed on patterned electrodes on an electrically insulated substrate such that one end of the nanowires is connected to microscale electrodes while the other end is free standing. A conductive AFM tip is brought in contact with a single nanowire. The tip serves as an electrode to pass current through the individual nanowire. The passage of DC electric current

causes a DC temperature change in the nanowires due to Joule heating which results in the change in the resistance. By measuring average resistance the average temperature can be found out. Using heat transfer modeling techniques average temperature can be related to thermal properties of the nanostructures. The modeling takes into account the complexities of the three-dimensional tip structure and also the convection, conduction and radiation effects of individual nanowires and thermal and electrical contact resistance between the AFM tip and the nanowire. Strategies are explored to determine the unknown parameters such as heat transfer coefficient, thermal conductivity and thermal contact resistance. For example the experiment is repeated for different nanowire lengths by moving the tip to different positions along the nanowire. A proof-of-principle experiment is demonstrated.

2:45 PM DD2.3
Phonon Transport and Scattering in Semiconductor Nanowires. Patrick Kenneth Schelling[1], Brian Becker[1] and Simon Phillpot[2]; [1]AMPAC and Department of Physics, University of Central Florida, Orlando, Florida; [2]Materials Science and Engineering, University of Florida, Gainesville, Florida.

Thermal management is becoming an issue of increasing importance as feature sizes in devices shrink to the nanometer scale. However, our understanding of the mechanisms of phonon transport and scattering at the nanoscale is quite lacking. It seems clear that a combination of experimental and theoretical methods will be needed to elucidate the fundamental aspects of nanoscale thermal transport.
Molecular-dynamics (MD) simulation can make important contributions to thermal transport at the nanoscale. We have recently developed the method of wave packet dynamics to study detailed phonon scattering mechanisms, and applied this method to the study of interfacial scattering. The basic idea is to create a localized wave packet from the phonon modes of the bulk perfect crystal, and then allow this wave packet to propagate and scatter in a standard MD simulation. The detailed results obtained in this way can be regarded as complementary to more usual MD methods. In this talk, I will present recent results for phonon transport in silicon nanowires obtained using wave packet dynamics. In particular, we have studied phonon scattering at a simple interface as a function of the diameter of the wire. Our results for this simple model system show a surprising amount of structure and richness. In particular, we have found that phonon confinement effects result in qualitatively different transmission mechanisms when compared to a bulk system. Analysis of the transmitted and reflected phonon modes reveals intricate details as to the coupling across the interface. Finally, we will present preliminary results for a new technique in which a localized wave packet sampled from a broad range of frequencies and modes is used to obtain experimentally measurable transport properties in a single MD simulation.

3:30 PM DD2.4
Nanoscale Engineering: Atomistic Simulations for de Novo Design of Nanostructured Materials Optimized for Thermoelectric Applications. Markus J. Buehler[1], Paul von Allmen[2], Seungwon Lee[2], Haibin Su[1], Tahir Cagin[3] and William Goddard III[1]; [1]Division of Chemistry, California Institute of Technology, Pasadena, California; [2]Jet Propulsion Lab, Pasadena, California; [3]Department of Chemical Engineering, Texas A&M University, College Station, Texas.

It has always been the dream of scientists to predict the properties of new materials from a very fundamental, ab initio perspective. At the beginning of the new millennium, the advent of new very accurate quantum mechanical methods, the significant growth of computing power and breakthroughs in computer science have for the first time enabled scientists to foresee achieving this goal within the current decade. Since all properties of all materials are in principle describable by quantum mechanics (QM), one could conceivably replace current empirical methods used to model material properties by a first principles or de novo computational design of materials and devices. This approach will revolutionize material science with a rapid computational design followed by synthesis and experimental characterization only for materials and designs predicted to be optimum. In this paper we focus on ab initio-based nanostructure engineering to improve the figure of merit of thermoelectric materials. The past years have witnessed the tremendous success of continuum-based methods for the systematic materials and structural design, such as topology and shape optimization. These methods are, however, scarcely applied to small-scale materials applications, since continuum theories break down at this scale and the atomistic viewpoint needs to be taken account. Here we report the development of methods that demonstrate new approaches to design new materials with a series of ab initio based computations for small-scale materials. Using tight-binding and atomistic molecular dynamics methods, we carry out a series of studies to determine the optimal design of nanomaterials optimized in terms of thermoelectric properties. We use genetic algorithm optimization to find optimal designs based on calculating the objective function, the ZT figure of merit, from first principles. We optimize the geometry of Si and Ge nanowires that are used as building blocks of nanostructures. Among others, as design variables we choose parameters such as the aspect ratio of the wires, the length of Si and Ge nanowires and the material composition. We also explore the optimal design of multilayer systems, since recent progress in experimental techniques to grow such multilayer thin films may allow for the rapid experimental verification of the proposed structures. Finally, we demonstrate how Si-Ge-nanostructures can be optimized for highly anisotropic thermoelectric properties. Several structures are reported that may guide experimental work in developing new materials for thermoelectric applications. The computations are carried out within our newly developed multi-scale multi-paradigm environment CMDF that allows scale-agnostic calculation of material properties from first principles.

3:45 PM DD2.5
3D Modeling of Nanoscale Seebeck Measurements by Scanning Thermoelectric Microscopy. Zhixi Bian[1], Ali Shakouri[1], Ho-Ki Lyeo[2], Li Shi[3] and C.K. Shih[2]; [1]Electrical Engineering, University of California Santa Cruz, Santa Cruz, California; [2]Department of Physics, The University of Texas at Austin, Austin, Texas; [3]Department of Mechanical Engineering, The University of Texas at Austin, Austin, Texas.

The performance of a thermoelectric device is mostly determined by the dimensionless figure of merit ZT. Recently the search of high ZT materials has focused on the nanoscale structures due to the enhanced phonon scattering and improved thermoelectric power factor. Since the physical parameters are modified locally due to the nanoscale feature of the materials, the conventional characterization methods for bulk materials may not give accurate results. Scanning thermoelectric microscopy (SThEM) provides a way to measure the Seebeck coefficient directly with nanometer spatial resolution. However, the magnitude of the thermoelectric voltage at the transition region of a pn-junction was much lower than the one expected from one dimensional model. This is attributed to the finite sizes of the tip-sample nanocontact and the temperature gradient around the tip. Because the heat diffuses in a 3-dimentional manner from the sample to the tip, the temperature gradient and Seebeck voltage are distributed in the sample. In this paper, we present a 3-dimentional modeling of the Seebeck profiling of a GaAs p-n junction by scanning thermoelectric microscopy. In the bulk materials, the heat conduction is described by continuum equation. However, the phonon scattering mechanism must be taken into account for nanostructures because the phonon mean free path is at about the same scale as the structure dimensions. Thus, we treat the solution of the temperature profile in two regions separately in this model: around the tip-sample nanocontact and in a distance of a phonon mean free path to the contact, we assume the temperature does not change since there is very few phonon scattering in such a short length; out of this region, the temperature change is derived by continuum equation of heat conduction. The electron and hole densities can be solved numerically from the Poisson equation. We divided the planar pn-junction to 48x48x24 cubic cells of resistor and voltage source network. A system of linear equations are then written and solved, giving the thermoelectric voltage at the STM tip. We studied the size effects of the tip-sample contact and phonon mean free path. It is concluded that the spatial resolution of this nanoscale measurement technique much depends on the phonon mean free path, and the size of the tip-sample contact. The 3D effects can not be simplified as an averaging of the 1D modeling of thermoelectric power in the adjacent region of the tip-sample contact. However, the local thermoelectric power can only be defined and calculated within a uniform volume larger than the relaxation lengths of energy/charge carriers and the inter-dopant spacing due to its statistical nature. Thus, this nanoscale Seebeck measurement technique can almost achieve a spatial resolution of the physical limit (the contact size can be made as small as 1 nm and below).

4:00 PM DD2.6
Atomistic Simulation of Nanostructure Effects on Thermoelectric Properties in Si/Ge Nanowires. Haibin Su[1], Paul von Allmen[2], Seungwon Lee[2], Tahir Cagin[3] and William A. Goddard III[1]; [1]Caltech, Pasadena, California; [2]Jet Propulsion Lab, Pasadena, California; [3]Department of Chemical Engineering,, Texas A&M University, College Station, Texas.

Understanding the thermal conductivity and heat transfer processes in nanostructures is critical for the development of thermoelectric devices. Experimental results on the thermal conductivity of superlattices have been reported in recent years for Si/Ge materials. These studies demonstrate that the thermal conductivity of a superlattice can be much lower than that estimated from the bulk values of its constituent materials, and even smaller than the thermal conductivity of the equivalent composition alloys. The thermal

conductivity reduction, coupled with the possible increase of the Seebeck coefficient and electrical conductivity due to quantum confinement effects in these superlattices, makes the Si/Ge superlattice system a good candidate for highly efficient thermoelectric energy conversion. Here we will combine tight-binding and atomistic molecular dynamics approaches to study the effects of nano-patterning on thermoelectric properties. The lattice contribution to the thermal conductivity, which is dominant in semiconductors, will be obtained from a Green Kubo relationship. We will calculate the electrical conductivity, the electronic contribution to the thermal conductivity, and the Seebeck coefficient using linear response theory with the empirical tight binding approach, which is suitable for the study of self-assembled nanostructures containing millions of atoms. Finally, we will discuss the systematic engineering of nanostructure to improve the figure of merit.

4:15 PM DD2.7
Elastic Deformation Effect on Transport Properties of Nanowires of Pure and Sn, Te-Doped Bismuth.
Albina Alexandrovna Nikolaeva[1,3], Tito E. Huber[2], Leonid Alexandrovich Konopko[1,3] and Gheorghe Ivanovich Para[1]; [1]Institute of Applied Physics, Chisinau, Moldova; [2]Department of Chemistry, Howard University, Washington, Washington; [3]International Laboratory of High Magnetic Fields and Low Temperatures, Wroclaw, Poland.

We report on investigation of the elastic deformation influence on the electric, thermoelectric and magnetothermoelectric properties of Bi nanowires doped with acceptor and donor impurities (Sn, Te) at electron topological transition (ETT) induced by elastic deformation up to 2-3% residual elongation. Glass covered single crystal Bi wires of strictly cylindrical form with d=50÷1000nm were obtained by the liquid phase casting by the Ulitovsky-Tailor method. Orientation of the samples of all the diameters was the same: the wire axis made up an angle of ~20° with the bisector axis C_2 in the bisector-trigonal plane. The diameter was controlled with the help of SEM and AFM microscopes. The Fermi level position and its change at doping with Sn and Te was estimated by the Shubnikov-de Haas (ShdH) oscillations. The ShdH oscillations were also used to control the transformation of the Fermi surface (FS) topology and to observe electron topological Lifshits transitions under elastic stretch of nanowires. It was found that the deformation curves of the resistance and thermopower show peculiarities at the ETT, which significantly depend on the density of states of disappearing or appearing new FS. Calculation and estimations of the Fermi level (FL)-ϵ_F, concentration of the carriers under stretch allowed us to conclude that if ϵ_F is in the region L of the conduction band and T-holes then the elastic stretch of nanowires leads to intensification of the electron contribution to the thermopower, and in the case when ϵ_F is localized in the region of L-holes the stretch intensifies the hole contribution and the thermopower increases. There were estimated the magnetic field intensities the positive contribution to the thermopower. Our study of the influence deformation, magnetic field and temperature on the thermopower suggest a model where the electron and holes mobilities are restricted by collision with the wire walls. **Acknowledgements** This work is supported by Civilian Research and Development Foundation (CRDF), CGP # MO-E1-2603-SI-04.

SESSION DD3:Nanofluids
Chair: Ho-Soon Yang
Wednesday Morning, March 30, 2005
Room 3003 (Moscone West)

8:30 AM *DD3.1
Nanofluids: New Frontiers in Thermal Science. Steve Choi, Energy Technology, Argonne National Lab, Argonne, Illinois.

Many industries face a need for next-generation coolants. Cooling of high-tech devices and systems represents a fundamental challenge to thermal scientists and engineers. As a new direction in liquid cooling technology, our ANL research group has created nanofluids, which consist of nanoparticles suspended in a conventional fluid. The novel feature of nanofluids is in the use of nanometer-size particles to achieve and control particle stability and thermal properties at the molecular and nanometer scales. This constitutes a new paradigm for making highly stable and conductive coolants. Nanofluids have been an active area of research over the last few years, and the discovery of the better-than-predicted thermal properties of nanofluids has aroused considerable interest across the world. This presentation will first review studies by our nanofluids group and others. The talk will cover methods for making and characterizing nanofluids and measurements of their thermal properties, which were completely unexpected. With regard to the latter, nanofluids were found to conduct heat an order-of-magnitude faster than scientists had predicted possible and to exhibit strongly temperature-dependent conductivity. These remarkable experimental discoveries have created a theoretical challenge to explain and model the observations. Newly proposed mechanisms and models for thermal conduction in nanofluids will be discussed. The emphasis will be on a new model that uses Brownian motion to account for the fundamental molecular and nanoscale nature of nanoparticles suspended in fluids, and is distinct from all previous models developed for micro- and meso-sized particles. Also, earlier research focused on the thermal properties of nanofluids at rest, but more recent research has started to focus on the thermal properties of nanofluids in single- and two-phase flow. I will briefly address the latest advances in convection and two-phase flow of nanofluids. Finally, I will present some future directions for basic and applied nanofluid research. Nanofluids offer theoretical and practical challenges and new frontiers.

9:00 AM *DD3.2
Stability and Thermo-physical Properties of Nanofluids and Its Application. Jae-Keun Lee, Yu-jin Hwang, Hyeong-soo Park and Jin-wook Jung; Mechanical Engineering, Pusan Nation University, Busan, South Korea.

Nanofluid is a kind of new engineering material consisting of nanometer-sized particles dispersed in base fluid. Nanofluids could have various applications such as magnetic fluids, heat exchanger working fluids, lubricants, drug delivery and so on. In present study, various nanoparticles, such as MWCNT (Multi-walled Carbon Nanotube), fullerene, copper oxide, silicon dioxide and silver, are used to produce nanofluids. As base fluids, DI-water, ethylene glycol, mineral oil, silicon oil and PAO (Poly α-olefin oil) are used. To investigate the thermo-physical properties of nanofluids, thermal conductivity and kinematic viscosity are measured. Stability estimation of nanofluid is conducted with a zeta potential analyzer and UV-vis spectrophotometer. In this study, the high pressure homogenizer is the most effective method to produce nanofluid with the prepared nanoparticle and base fluid. Excellently stable nanofluids are produced with the magnetron sputtering system. Thermal conductivity of nanofluid increases with increasing particle volume fraction except water-based fullerene nanofluid since the thermal conductivity of fullerene, 0.4 W/mK, is lower than that of water. In case of mineral oil-based nanofluid, fullerene nanofluid has higher thermal conductivity than MWCNT nanofluid. It is believed that fullerene nanofluid is much better stable than MWCNT nanofluid. Stability of nanofluid is influenced by the characteristics between base fluid and the suspended nanoparticles. For the higher functions and reproducible properties, stability of nanofluids have great importance. Also the industrial applications for nanofluids, such as micro heat exchangers, heat pipe systems, lubricants, and automobile coolants are introduced in details.

9:30 AM DD3.3
pH-Dependent Thermal Conductivity of Nanofluids. Jie Wu and Jeffrey A. Eastman; Materials Science Division, Argonne National Laboratory, Argonne, Illinois.

Nanofluids (suspensions of nano-sized particles in liquids) are of interest as potentially important heat transfer media for energy-efficient applications due to their enhanced thermal conductivity. In this study, several nanofluid systems (Al_2O_3/water, Al_2O_3/ethylene glycol, TiO_2/water, TiO_2/ethylene glycol) have been produced and the thermal conductivity of these nanofluids has been determined using 3ω method. It has been found that a significant enhancement of the thermal conductivity can be achieved by adjusting the pH value of nanofluids. For example, 95% higher thermal conductivity than that of pure water has been observed at pH = 11.4 in the Al_2O_3/water system containing 0.5 vol% of Al_2O_3 nanoparticles, while there is only 3% improvement for the Al_2O_3/water containing the same volume fraction of particles at pH = 8.4. In contrast, in the absence of nanoparticles, increasing the pH of water from 8.4 to 11.4 results in only ~ 40% increase in thermal conductivity. Possible mechanisms responsible for the thermal conductivity enhancement including the roles of the particle surface charge on both the particle dispersion behavior and the resulting heat transfer mechanism in the nanofluids will be discussed.

9:45 AM DD3.4

Open Discussion

10:30 AM *DD3.5
Giant Thermal Conductance between Polar Nanoparticles. Sebastian Volz, Ecole Centrale Paris/CNRS, Chatenay Malabry, France.

Nanofluids have raised much attention since it was proven that nanoparticles improve their heat conduction capability by a few to a dozen of percents. Several attempts were made to understand this behavior. Most of them relied on mass transfer and geometric

arguments. They either fail or involve questionable assumptions. We propose a new physical mechanism based on near field heat transfer. When the volume fraction exceeds a few percents, the mean distance between particles is of the order of the particle diameter. For nanoparticles, this distance is much lower than the dominant wavelength of far-field radiation (i.e. when photons are emitted or absorbed) and near-field radiation (i.e. Coulomb interaction) may become important. Heat transfer between two planes separated by sub-wavelength distances through electromagnetic interaction has been first investigated by many groups. It was shown that this mechanism has a very large resonance at the optical phonon frequency for polar materials. In this contribution, we explore the heat transfer between two nanoparticles separated by a distance of the order of a few nanometers. We introduce a thermal conductance that can be related to the fluctuations of the heat flux by using the fluctuation-dissipation theorem. We then implement a molecular dynamics simulation to compute the thermal conductance as a function of the separation distance. An alternative approach is based on a direct derivation of the heat flux between the two nanoparticles modelled by fluctuating dipoles. We find that both models agree for distances larger than a few diameters. In the case of silica nanoparticles, a very large enhancement of the conductance is observed when the distance decreases. The near field heat transfer then becomes two to three orders of magnitude more efficient than bulk heat conduction and than the heat transfer when the NPs are in contact. Polar materials such as oxides and SiC are the best amplifiers for the near field heat exchange. Those are also the materials used in nanofluids. Near-field heat transfer might be the leading mechanism explaining the enhancement of the effective thermal conductivity in nanofluids.

11:00 AM DD3.6
A Microconvection Model for Thermal Conductivity of Nanofluids. Hrishikesh Eknath Patel[1], T. Sundararajan[1], T. Pradeep[2] and Sarit Kumar Das[1]; [1]Mechanical Engineering, Indian Institute of Technology Madras, Chennai, Tamilnadu, India; [2]Chemistry, Indian Institute of Technology Madras, Chennai, Tamilnadu, India.

Nanofluids are found to have enhanced heat transfer capabilities. This implies the enhanced cooling in many applications like cooling of electronic equipment, lasers, fuel-cells, etc. The enhanced thermal conductivity of these fluids with small particle concentration was found beyond the explanation of existing theories for slurries, so it has been tried to model the enhancement using liquid layering, particle clustering, fractal theory etc.; however all are found to be unsatisfying. Also none of them show any dependence of the enhancement on temperature. In recent times, the models proposed by Jang et al [1] and Hemanth Kumar et al [2] show a dependence on particle size as well as temperature. Jang et al [1] have considered three modes of heat transfer in nanofluid viz. through liquid, through particles and by micro convection around particles. Hemanth Kumar et al [2] have considered two parallel paths of heat flow, one through the liquid particles and other through the nanoparticles. The effective thermal conductivity of particles is modeled using Brownian motion. Both these models use one or more adjustable parameters. No model till now fits to the experimental data varying over wide range of parameters. In view of the above, in the current work, efforts have been made to present a comprehensive model which will predict the thermal conductivity of nanofluids over a wide range of parameters. The heat flow through liquid and solid is modelled in the same way as that by Hemanth Kumar et al [2]. The model shows direct dependence of enhancement on particle volume fraction and inverse dependence on particle size. The Brownian motion effect is added to this to account for the temperature effect, instead of accounting it into effective thermal conductivity of particle itself, as done by Hemanth Kumar et al [2]. The motion of particles is modelled as creeping flow over spheres rather than effective conductivity of moving particle. The model brings out the physics behind the enhancement to a great deal in the form of microconvection. Above all, the model does not use any adjustable constant. It has been validated against almost all the experimental data available. It satisfactorily predicts the thermal conductivity for various nanofluids with base liquids like water (0.6 W/mK) to synthetic oil (0.14 W/mK), the particle materials like multiwalled carbon nanotubes (2000 W/mK) to copper oxide (18 W/mK), particle concentration from 0.3 % to 5 % as well as particle sizes from 10 nm to 100 nm. It is interesting to observe that enhancement from 4 % to 150 % are predictable appropriately by a single model. It also predicts the increase in the enhancement with temperature. References: 1. Jang S.P. and Choi S.U.S., 2004, Applied Physics Letters, 84(21), pp.4316-4318. 2. Hemanth K.D., Patel H.E., Rajeev K.V.R., Sundararajan T., Pradeep .T and Das S.K., 2004, Physical Review Letters, 93(14), pp. 144301.

11:15 AM DD3.7
Dual Lattice-Boltzmann Simulation of Heat Conduction in Nanofluids. Xuejiao Hu and Kenneth E. Goodson; Mechanical Engineering, Stanford University, Stanford, California.

A fluid containing a small volume fraction of suspended nanoparticles is called a "nanofluid". It has been shown that nanofluids may have larger conductivities than the pure liquid matrix, and there is some evidence that classical effective medium theory does not fully account for the difference [1-4]. Related to this problem is that the heat conduction mechanism of nanofluids is not well understood, especially the physics of conduction in the vicinity of the particle-liquid interface. Very recently, Jang and Choi [5] observed that the following nanoscale effects may be important: Brownian motion/advection of heat by suspended particles, fluid advection induced by particle Brownian motion, ballistic heat conduction within and near particles, and acoustic mismatch resistance at particle-liquid interfaces. Detailed assessments of these phenomena are very difficult due to the large scale range of motions from molecules and phonons to nanoparticles. Keblinski et al [6] reported a molecular dynamics simulation, and Bhattacharya et al [7] recently conducted a Brownian dynamics simulation, but these studies did not include the impact of associated fluid motion, which is critical for predicting the thermal conductivities of nanofluids according to [5]. The proposed work makes an effort to estimate the impact of Brownian transport, sub-continuum conduction, and acoustic mismatch resistance, on the conductivity of nanofluids. The particle Brownian motion and fluid convection are modeled using a hydrodynamic-based lattice-Boltzmann equation [8], which accounts both for fluid and particle advection. The solutions provide a framework for heat conduction simulations using the phonon lattice-Boltzmann transport equation. [9-11]. Boundary conditions between liquid and solid consider acoustic impedance. The impacts of Brownian motion, ballistic heat conduction on the thermal conductivity of a nanofluid are compared for varying particle and fluid combinations. The thermal conductivities of a nanofluid versus particle volume fractions and temperatures is modeled and compared with experimental results. [1] S. Lee, S. U. S. Choi, S. Li, J. A. Eastman, J. Heat Transfer 121, 280, (1999) [2] X. Wang, X. Xu, S. U. S. Choi, J. Thermophys. Heat Transfer 13, 474, (1999) [3] Y. Xuan, Q. Li, Int. J. Heat Fluid Flow 21, 58, (2000) [4] J. A. Eastman, S. U. S. Choi, S. Li, W. Yu, L. J. Thompson, Appl. Phys. Lett. 78, 718, (2001) [5] S. P. Janga, S. U. S. Choi, Appl. Phys. Letter, 84, 4316, (2004) [6] P. Keblinski, S. R. Phillpot, S. U. S. Choi, J. A. Eastman, Int. J. Heat Fluid Flow 45, 855, (2002) [7] P. Bhattacharya, S. K. Saha, A. Yadav, P. E. Phelana, R. S. Prasher, J. Appl. Phys., 95, 6492, (2004) [8] for a review, see S. Chen, G. D. Doolen, Annu. Rev. Fluid Mech., 30, 329, (1998) [9] W. Zhang, T. S. Fisher, Proc. IMECE'02 [10] R. A. Escobar, S. S. Ghai, C. H. Amon and M. S. Jhon, Proc. IMECE'03 [11] W. S. Jiaung and J. R. Ho, J. Appl. Phys., 95, 958, (2004)

11:30 AM DD3.8
Tunneling Photons and Heat Transfer in Nanofluids with Near-Spherical Nanoparticles. Shiu-Wing Tam and Stephen U. S. Choi; Energy Technology Division, Argonne National Laboratory, Argonne, Illinois.

For nanoparticles with aspect ratio near to 1 a low volume concentration of them (e.g., < a few volume percent) when dispersed randomly in a fluid medium will not allow a percolative transition, in contrast to what is possible for carbon-nanotube (CNT)-based materials [1]. Therefore in order to account for the experimentally observed enhancement in heat transfer in these classes of nano-fluids new physics need to be invoked. We suggest that a major contributing mechanism is radiative heat transfer (but in a form that is different from conventional radiative heat transfer as governed by the Stefan-Boltzmann law). The source of radiative heat transfer is the charge fluctuation within the source body (which is macroscopically electrically neutral) induced by thermal fluctuation. The charge fluctuation generates electromagnetic (EM) radiation. This conventional mode of radiative heat transfer is effected through the propagating photon modes in which the wave vectors of the photon states are real. These propagating photon modes can carry heat current over indefinite spatial distances in the vacuum. However, fluctuating charge and/or current sources may also generate EM fields that contain photon modes in which the wave vectors have components that are complex (i.e., with a finite imaginary part) in the propagation direction [2]. These modes are called evanescent (or tunneling) modes. They can transport significant thermal energy only over very small distances ($\sim$ 1000 nm) in the ambient temperature regime even in vacuum and are limited by the uncertainty principle. We demonstrate that these evanescent photon modes may become a significant contributor to radiative heat transfer in nanofluid whose nano-particles' aspect ratio is near 1. We have examined quantitatively from a theoretical perspective the effects of nano-particle concentration and temperature and the results were found to be consistent in magnitude and trends with experimental observation in near-spherical particle-based nanofluids [3]. The issue of the near-field EM contribution and the impact of the matrix fluids would discussed. In this framework the temperature dependence arises in a natural manner from the Bose-Einstein distribution. The

implications for this tunneling photon based heat transfer mechanism in nanofluids and other nanomaterials would be addressed. [1] Shiu-Wing Tam et. al., MRS Spring Meeting, 2003, Symposium S, Nanoscale Thermal Transport: From Fundamental And Devices, S1.6, p.385; [2] S. M. Rytov, Rep. AFCRC-TR-59-162 (Air Force Cambridge Research Center, Bedford, Mass., 1959); [3] J. A. Eastman, et. al., Appl. Phys. Lett. 78, 718 (2001). Work is supported by Office of FreedomCar and Vehicle Technologies, U. S. Department of Energy.

SESSION DD4: Nanowires and Nanotubes II
Chair: Patrick Schelling
Wednesday Afternoon, March 30, 2005
Room 3003 (Moscone West)

2:00 PM *DD4.1
Thermal and Thermoelectric Properties of Carbon Nanotubes and Nanotube-based Composite Materials.
Alan T. Johnson, Physics and Astronomy, Univ of Pennsylvania, Philadelphia, Pennsylvania.

I review results of experiments from the Penn group on thermal transport through nanotube material and nanotube-based composites, as well as measurements of the thermoelectric properties of single nanotubes. Thermal conductance data from bulk nanotube samples of show evidence that phonon confinement to the small nanotube circumference causes carbon nanotubes to act as one-dimensional phonon systems at low temperature. The observed 1D - 3D crossover temperature differs from that seen in specific heat measurements. The thermal conductivity of nanotube/epoxy composites is strongly enhanced over that of the neat epoxy, even at nanotube loading as small as 0.2 wt %. We attribute this observation to effective coupling of heat from the epoxy matrix to a percolative network of large aspect-ratio nanotubes. The measured thermoelectric power (TEP) voltage is used to probe the electronic properties of an individual p-type semiconducting nanotube. In the Coulomb Blockade regime, the TEP oscillates as predicted by theory. The baseline (average) TEP is first positive but becomes negative as the nanotube nears depletion. We attribute this to the creation of n-type barrier regions within the nanotube. We demonstrate that the TEP may be used as a probe of localized states along the nanotube even if these states carry negligible transport current.

2:30 PM *DD4.2
Interfacial Heat Flow in Nanoscale Composite and Suspensions. Sergei Shenogin, Arun Bodapati, Natalia Shenogina and Pawel Keblinski; Materials Science & Engineering, Rensselaer Polytechnic Institute, Troy, New York.

The thermal energy flow in composites and suspension involving nanoparticles and nanofibers is critically affected by interfacial thermal resistance between nanoparticles/nanofibers and surrounding matrix/fluid. We use classical molecular dynamics simulations to investigate the nature of heat flow between carbon nanotubes or fullerenes and soft organic matrix. In both cases weak coupling between vibration spectra of hard inclusion and soft organic matrix results in high thermal resistance on the interface (Kapitza boundary resistance), which for these systems is equivalent to resistance of the matrix layer with thickness of 5 to 20 nm . This dramatically reduces effective conductivity of carbon nanotube-polymer composites . Finite-Element Method (FEM) calculations were used to demonstrate that the interfacial resistance effectively eliminates a possibility of a rapid heat flow along the percolating network of highly conductive carbon nanotubes. Good thermal contact between nanotubes and the matrix is therefore the key factor to taking full advantage of very high aspect ratios of the nanotubes and their excellent thermal conductivity. To improve this contact we considered chemical functionalization of the nanoparticles with short organic chains2. The functionalization widens the overlap between the vibrational spectra of carbon nanostructures and the matrix and thus reduces interfacial resistance, however at the same time decreases the intrinsic high thermal conductivity along nanotubes. The effective medium theory based analysis indicates that for carbon nanotubes with low and moderate aspect ratios high concentration of side groups will lead to best thermal transport properties. For large aspect ratio tubes preserving the high conductivity of pristine tubes remains the optimal choice.

3:30 PM *DD4.3
Molecular Dynamics Simulation of Thermal Boundary Resistance between a Carbon Nanotube and Surrounding Materials. Shigeo Maruyama, Dept. of Mech. Eng., The University of Tokyo, Tokyo, Japan.

Several kind of thermal boundary resistance related to single-walled carbon nanotubes (SWNTs) are considered using molecular dynamics (MD) simulations. The Brenner potential (Brenner, 1990) with the simplified form (Yamaguchi and Maruyama, 1998) is employed as the potential function between carbon and carbon within a nanotube. The heat transfer from an SWNT to various surrounding materials is simulated by MD simulations. Heat transfers between nanotubes in a bundle of nanotubes and between a nanotube and water are considered. The heat transfer rate can be well expressed by the thermal conductance (or thermal boundary resistance) at the boundaries. The value of thermal conductance of various systems such as nanotube-junction, SWNT bundle and water-nanotubes are compared. For the thermal boundary resistance between SWNTs in a bundle, we consider a 5 nm SWNT bundle, which consists of 7 armchair type (5, 5) SWNTs with the diameter of 0.693 nm. In addition to the Brenner potential between carbon atoms within an SWNT, van der Waals force between carbon atoms in different SWNTs was expressed as 12-6 Lennard-Jones potential. After keeping the whole system at 300 K for 100 ps, the temperature of only the central SWNT was suddenly increased to 400 K using the velocity scaling method for a time period of 10 ps. The decay of the temperature difference of central and surrounding tubes is well approximated with a single exponential function. This encourages us to consider an SWNT as a solid material and express the heat transfer from the central tube to surrounding tubes by thermal conductance. Adopting the lumped capacity method, since the characteristic length of an SWNT is extremely small, the thermal conductance was estimated. Then, the thermal boundary resistance between an SWNT and water was considered. Water molecules were expressed by SPC/E potential (Berendsen et al., 1987) The potential function between water molecules and carbon atoms are represented by Lennard-Jones function and the quadropole interaction term (Walther et al., 2001). One (10, 10) SWNT with length 20.118 nm and 192 water molecules inside it were prepared in the 20.118x10x10 nm fully-periodic simulation cell. At the initial stage of simulation, water molecules and the SWNT were equilibrated at temperature of 300 K. Then, only the temperature of the SWNT was suddenly heated up to 400K. And all temperature control was stopped. The temperature difference between SWNT and water exhibited the exponential decay in a similar manner to the previous case of SWNT bundle simulation. The thermal conductance is estimated using the lump method similarly to the previous case. Finally, the thermal boundary resistance between a nanotube and Lennard-Jones fluids in different thermodynamics conditions was examined. The general mechanism of thermal boundary resistance is thought.

4:00 PM DD4.4
Phonon Dynamics in Carbon Nanotubes. Arun Bodapati[1], Pawel Keblinski[1] and Patrick Schelling[2]; [1]Materials Science, Rensselaer Polytechnic Institute, Troy, New York; [2]Physics, University of Central Florida, Orlando, Florida.

To date theoretical studies of thermal transport in carbon nanotubes focused on determination of overall conductivity of pristine and defected tubes as well as the influence of interactions with surroundings on thermal transport. In this work, to gain a more detailed understanding of thermal energy flow in carbon nanotubes we investigate the dynamics of well-defined phonon wave-packets by molecular dynamics simulation. In pristine tubes, we monitored the decay mechanism of longitudinal acoustic modes due to thermal scattering by other phonons and determined the temperature dependence of the scattering mechanism. The nature of scattering of phonons from structural defects will be also discussed.

4:15 PM DD4.5
Thermal Boundary Resistance between Carbon Nanotubes. Hongliang Zhong and Jennifer R. Lukes; Mechanical Engineering and Applied Mechanics, University of Pennsylvania, Philadelphia, Pennsylvania.

Due to their interesting thermal properties, carbon nanotubes are promising for thermal management in a wide variety of applications. Recent studies on interfacial heat transfer in nanofluids and nanocomposites indicate that the thermal boundary resistance is the key factor limiting heat flow in these materials. Therefore it is important to understand the thermal transport between tubes at a fundamental level. In real systems, the tube networks have configurations that depend on processing conditions. The effect of configuration parameters such as tube length, overlap, orientation and spacing on tube-tube thermal transport is not fully understood. Classical molecular dynamics simulations are performed in the present work to determine the effect of these parameters on thermal boundary resistance between two carbon nanotubes.

4:30 PM DD4.6
Thermal Transport in Aligned Carbon Nanotube Films Deposited on Si Substrates. Theodorian Borca-Tasciuc[1], Saeid Vafaei[1], Robert Vajtai[2] and Pulickel Ajayan[2]; [1]Mechanical, Aerospace, and Nuclear Engineering, Rensselaer Polytechnic Institute,

Troy, New York; [2]Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, New York.

This work reports the anisotropic thermal diffusivity of aligned multiwalled carbon nanotube films grown by Chemical Vapor Deposition on silicon substrates deposited with a thin layer of silicon dioxide. A photothermoelectric technique is employed to perform the measurements. In this method a modulated laser beam from an IR diode laser with 1.5 micrometer wavelength is used to create a micro-scale thermal wave in the film by focusing the light through the transparent silicon substrate. The generated thermal wave is detected by a fast responding thermocouple formed between the film surface and the tip of a sharp probe. By scanning the laser beam around the thermocouple, the amplitude and phase distributions of the thermal wave are obtained with micrometer resolution. The thermal diffusivity along directions parallel and perpendicular to the nanotube growth direction are obtained by fitting the detected thermal signals with an anisotropic heat conduction model. The work also investigates the importance of the carbon nanotube/substrate interface in these films by comparing measurements performed on carbon nanotube samples with different lengths.

SESSION DD5: Poster Session: Heat and Mass Transport at Nanoscale
Chair: Pawel Keblinski
Wednesday Evening, March 30, 2005
8:00 PM
Salons 8-15 (Marriott)

DD5.1
The Use of Ultra-Thin Layers Structure to Obtain a Self Cleaning Nuclear Reactor Fuel. Liviu Popa-Simil, AFCI-D5, Los Alamos National Laboratory, Los Alamos, New Mexico.

The actual development of the nuclear power production is slowed down by the disadvantages of the actual fuel materials. The low thermal conductivity makes that the operation temperature to be low and the conversion efficiency to be low so the thermal pollution at the power plants location to be high. After use the fuels becomes highly radioactive and reprocessing and storage are difficult processes. The radioactive waste is one of the most dangerous type of waste for environmental dispositioning. The scale of the fission energy release phenomena is less than 30 um in diameter. The range of the diffusion length of the fission products in the fuel is less than a 1/2 micron. These observations drives to the idea that if a several tenth of a micron layers of nuclear fuel into a draining fluid are used the fission products will stop both in the drainage fluid and fuel and by using an appropriate chemical structure and clusterization the fission products stopped in fuel will be drifted to the fuel-drain liquid interface. If to the drain liquid accumulating the fission products a smooth nano-flow is imposed, in a such a manner that in about 1 week the fluid to cross the reactor length, to a separator unit, the fission products can be removed. This mechanism, similar to the living beings, brings many advantages for the nuclear reactors like: lower over-criticality, single fuel load, low remnant radioactivity, increased operating temperature due to higher thermal conductivity, continuos isotopes (fission and/or n-capture products) delivery. The paper discusses various simulations of nuclear fuels and the consequences for the nuclear electric power production overall costs.

DD5.2
Abstract Withdrawn

DD5.3
Perturbed Molecular Dynamics Study of Thermal Conductivity for Development of Thermal Barrier Coatings. Masato Yoshiya[1], Akihiko Harada[2], Munetaka Takeuchi[2] and Hideaki Matsubara[1]; [1]Japan Fine Ceramics Center, Nagoya, Japan; [2]Fujitsu Limited, Chiba, Japan.

Thermal conductivities of zirconia-based materials, candidates for thermal barrier coatings (TBCs), were calculated using perturbed molecular dynamics which was modified for ionic materials based on so-called Evans-Gillan method. Partial thermal conductivity which is newly defined in this study showed that heat conduction in zirconia-based materials are governed by oxygen-dominating phonons, in accordance with earlier speculations. However, mean field analysis about the scattering species in Y_2O_3-doped ZrO_2 indicated that reduction of thermal conductivity as a result of aliovalent oxide addition cannot be ascribed only to scattering by oxide ion vacancy, and impurity metal cations are found to scatter phonons as much as oxide ion vacancies, decreasing thermal conductivity. This indicates that cation substitution is an effective way to decrease thermal conductivity without introducing porosity in the TBC. Based on these results, dependence of thermal conductivity on substitutional species was examined. It is found that heavy cations, such as Lu^{3+} or Yb^{3+}, are not effective to decrease thermal conductivity, though an earlier theory by Lawson predicted that thermal conductivity is inversely proportional to square root of density. In contrast, it is found that addition of light species such as Al^{3+} decreases thermal conductivity significantly since vibration of Al^{3+} deviates greatly from that of Zr^{4+} due to its light mass. In addition, addition of large cations such as La^{3+} also decreases thermal conductivity as much as Al^{3+}. Although vibration of La^{3+} does not differ from Zr^{4+} very much, lattice expansion due to large ionic radius causes decrease of thermal conductivity. Concentration dependences of these substitutional species are different from each other, which enables to optimize composition in balance with other important properties of TBC.
Acknowledgment: This work was performed as a part of the Nanostructure Coating Project carried out by the New Energy and Industrial Technology Development Organization.

DD5.4
Monte Carlo Calculation of the Effective Diffusivity and Conductivity in Nanocrystalline Materials. Graeme Murch and Irina Belova; School of Engineering, The University of Newcastle, Callaghan, New South Wales, Australia.

The problem of determining the effective continuum diffusivity and conductivity in nanocrystalline materials is addressed by mapping the problem onto a pseudo-lattice and making use of random walk theory. Nano sized cubes and spheres in various arrangements and diffusivities are analysed. Monte Carlo methods are used to calculate the effective diffusivity and conductivity in the assembly and compared with analytical expressions including the Hart-Mortlock formalism that is frequently used for microcrystalline systems and the Maxwell-Garnett formalism. It is shown that the Hart-Mortlock formalism invariably gives a poor description of the effective diffusivity for these materials. On the other hand, Maxwell-Garnett expressions, when correctly formulated, usually provide very good description except in the vicinity of a percolation threshold.

DD5.5
MeV Si Ion Bombardment Induced Thermal Conductivity Reduction of Bi_xTe_3/Sb_2Te_3 Thin Films. Zhigang Xiao, Claudiu Muntele, Robert Lee Zimmerman and Daryush Ila; Center for Irradiation of Materials, Alabama A&M University, Normal, Alabama.

Nanoscale Bi_xTe_3/Sb_2Te_3 multilayer thin films were deposited from solid antimony (III) telluride and bismuth (III) telluride sequentially using the ion-beam assisted deposition (IBAD) system at AAMU. The deposited multilayer films had a periodic structure consisting of alternating Bi_xTe_3 and Sb_2Te_3 layers, 10 nm thickness each. Rutherford backscattering spectrometry (RBS) analysis indicated that the deposited antimony telluride film had the desired stoichiometry of Sb_2Te_3 and the bismuth telluride film was $Bi_{1.1}Te_3$. 5 MeV Si ion bombardment was used to produce nanoscale structures in multi-layered Bi_xTe_3/Sb_2Te_3 in order to reduce thermal conductivity of the multilayer system by increasing phonon scattering sites. The 3ω method was used to measure the thermal conductivity of the multilayer thin films [D. G. Cahill, Rev. Sci. Instrum. 61, 802 (1990)]. We measured the thermal conductivity of the multilayers at room temperature before and after ion bombardment, finding 5.1 mW/cm K and 3.8 mW/cm K, respectively. The MeV Si ion bombardment was found to decrease the thermal conductivity of the multilayer thin films. *Research sponsored by the Center for Irradiation of Materials, Alabama A&M University and by the AAMURI Center for Advanced Propulsion Materials under the contract number NAG8-1933 from NASA. **Corresponding author: D. ILA; Tel.: 256-372-5866; Fax: 256-372-5868; Email: ila@cim.aamu.edu

DD5.6
Calculation of the Evolution of the Formation of Hollow Nanospheres by Chemical Interdiffusion. Irina Belova and Graeme Murch; School of Engineering, The University of Newcastle, Callaghan, New South Wales, Australia.

Recently, Yin and coworkers found that when nanocrystals of cobalt are exposed to sulphur, hollow nanospheres of cobalt sulphide are produced. It is believed that the large diffusive flux of cobalt atoms leads to a counterflux of vacancies that coalesce to form a cavity. This is an extreme type of Kirkendall porosity that is common in interdiffusion problems in microcrystalline systems. We set up the phenomenological diffusion equation for this finite size problem and solved it iteratively for various physically reasonable boundary conditions. This enabled the determination of the evolution of the atomic and vacancy composition profiles as interdiffusion proceeds and the nanocavity grows. We analysed the effect of different efficiencies and locations of vacancy sources and sinks within the nanocrystal. The results were also compared with Monte Carlo simulations based on random walk methods.

DD5.7

Thermal Transport in Carbon Nanotube Composites. Arun Bodapati, Sergei Shenogin and Pawel Keblinski; Materials Science, Rensselaer Polytechnic Institute, Troy, New York.

Carbon nanotubes due to their very high aspect ratio and very high thermal conductivity are considered as a potential filler material in composites to enhance thermal transport properties. However, high tube-matrix interfacial resistance and tube-tube contact resistance limit the effectiveness of carbon nanotubes. In this work, using classical molecular dynamics simulations we investigate the role of chemical bonding between nanotubes and the matrix on the heat flow in nanocomposite. Indeed, the introduction of chemical bonds significantly reduces tube-matrix thermal boundary resistance but at the same time reduces the intrinsic (axial) tube conductivity. Interestingly, tube axial conductivity decreases with increasing chemical functionalization but with 1% or more C atoms being functionalized becomes independent of the density of functionalized sites. This suggest important role of long wavelength phonon in thermal transport process. A quantitative analysis of the effect of interfacial bonding on composite conductivity is made using effective medium theory. This analysis predicts an increase by a factor of two in the conductivity of the composite due to functionalized nanotubes with an aspect ratio of within 100-1000 range.

DD5.8

Thermal Characterization of Electrolytic Fluid Flow with Electrically Charged Nanoparticles in Micro and Nano-Channels. Abhishek Jain, Rensselaer Polytechnic Institute, New York, Troy, New York.

The evolution of the microfabrication technologies has resulted in various Micro and Nano Electro Mechanical Systems (MEMS and NEMS). A potential application of these devices is micro and nano channels for efficient cooling of chips, which serve as an effective tool for removal of heat fluxes by significant amount due to increase in effective heat transfer coefficient [1]. When dealing with the micro or nanofluidics, particularly electrolytic flow in micro and nanochannels, the interfacial effect (phenomenon happening at the surface of the channel) comes into picture [2], which is negligible in bulk fluid flow. The presence of nanoparticles in the micro and nanochannels together with the electrokinetic effect results in an increase in effective heat transfer coefficient and hence Nusselt Number. In the present work we have studied the effect of nanoparticles in the micro and nanochannels through which the electrolytic flow is maintained. Analytical modeling is done to express the behavior of nanoparticles in the fluid flow. The channels considered are 10 μm and 100 nm in depth having length 100 μm and 1000 nm so that the flow can be approximated as the one between infinite parallel plates. The Navier-Stokes equations are modified to take into account the size effect of nanoparticles and the electrostatic force, generated due to interaction between the ionic charges in the electrolyte and the counter-ions present on the surface. The expressions for velocity profile in the developed regions are developed with and without the presence of nanoparticles and electrokinetic effect. Nanoparticles have been found to decrease the velocity. The expression for Nusselt number is developed and it is found that Nusselt number increases by 8% from the conventional value of 8.235 (without the electrokinetic effect and neglecting the presence of nanoparticles). Thus the presence of nanoparticles in the channels tends to increase the turbulence thereby enhancing the heat transfer. The dependence of characteristic thickness of the electric double layer, the C_fRe product and Nusselt number on the ionic strength of the electrolyte and the number concentration of nanoparticles is presented and interpreted in the physical domain.

DD5.9

A New Efficiency Kinetic Monte Carlo Method for Annealing Simulation. Min Yu[1], Ru Huang[1], Xing Zhang[1], Yangyuan Wang[1], Jinyu Zhang[2] and Hideki Oka[3]; [1]Institute of Microelectronics, Peking University, Beijing, China; [2]Fujitsu R&D Center Co. Ltd., Beijing, China; [3]Fujitsu Laboratories Ltd., Atsugi, Japan.

Kinetic Monte Carlo (KMC) method is proved to have great potential in simulating annealing process for shallow junction technology of integrated circuits. Improvement to the sampling algorithm of this method is necessary to reduce computing burden, which is still too heavy for engineer users. A new efficiency KMC method proper for annealing simulation is presented here. The new method with specially designed sampling algorithm avoids the time-consuming process of summing up rate of all possible movement and randomly selecting movement by considering rate ratio, which is applied in normal algorithm. Simulation experiment shows that computing speed based on the new algorithm is about 5 times that based on normal algorithm. The new algorithm, named event-list algorithm, is derived from the statistic results of random walk of a particle. This is possible because total energy of system is not necessary here in evaluating the rate of particles random walk, as is the approximation applied in annealing simulation. The rate of particle movement is determined by migration energy barrier, the prefactor and temperature. Impact from surrounding atoms on the rate of movement is not considered. By assuming that random walk of particle obeys Poisson statistic law, the probability density function and probability function of waiting time, during which particles wait for hop, is educed. By this result, the time when random hop happens can be predicted. All possible movements are predicted and arranged in order of time in a list called event list, after which the new algorithm is named. Here events refer to movement of particles, emission of clusters and other possible dynamic activities. All events are arranged in order of time, thus almost no computing time cost is need to select event. The only problem is the maintenance of the event list. Whenever a particle is changed due to the interaction with others, its position in event list must be updated. Considering that interactions are much less than movements, this additional cost is not so large. An index enhanced searching method is developed to make the maintenance of event list efficient. Simulation experiments are carried out to verify the algorithm. New algorithm increases the computing speed by a factor of about five. Computing time saved is in proportional to the total steps needed in simulation. Computing efficiency is even higher in case of even bigger number of particles. Analysis on computing process is presented in this paper to show how the algorithm works. Same simulation results are achieved from new method and normal results, which indicate the validity of the method.

DD5.10

Thermal Equation of State of Fe and V: Linear Response Quasiharmonic Lattice Dynamics. Xianwei Sha and Ronald E. Cohen; Carnegie Institution of Washington, Washington, District of Columbia.

First-principles calculations based on linear response linear muffin tin orbital (LMTO) method have been performed to examine the lattice-dynamical, transport and thermodynamic properties of Fe and V under high pressures and high temperatures. The calculated phonon dispersion, phonon density of states and transport properties such as thermal conductivities and electrical resistivities all agree well with experiment. Helmholtz free energy functional for bcc V, bcc and hcp Fe have been developed, and various thermodynamic properties, such as thermal equation of states, bulk modulus, thermal expansion coefficients as functions of temperatures and pressures have been derived. A detailed comparison with available experimental and theoretical investigations has been made.

DD5.11

Theoretical Calculation and Thermoreflectance Measurement of the Temperature Distributions in Broad Contact Diode Lasers. Tomasz J. Ochalski[1], Anna Kozlowska[2], Michal Szymanski[1], Tomasz Piwonski[1], Dorota Wawer[1] and Maciej Bugajski[1]; [1]Institute of Electron Technology, Warszawa, Poland; [2]Institute of Electronic Materials Technology, Warszawa, Poland.

Performance of diode lasers is strictly related to the temperature profiles in the laser structures and thus depends on the laser design, materials used for its construction and operational conditions. In this work we calculate temperature distribution in high power broad contact lasers across the laser resonator in the plane parallel to its mirrors. The solution to be heat problem is based on analytical solution of stationary, 2-D heat conduction equation $\nabla(\lambda(x)\nabla T(x,y))=-g(y)$, where T denotes relative temperature, λ - thermal conductivity, g- is a heat source function, x and y are the transverse and lateral co-ordinates, respectively. The heat conduction equation is subjected to the following boundary conditions: constant temperature at the bottom of the structure, convection cooling at the top, and no heat escape from the sidewalls.We will present 2-D maps of relative temperature T distribution for p-side down mounted GaAsP/AlGaAs (808nm) quantum well lasers with different resonators construction and different coating of the laser mirrors. The calculations are compared with experimental results obtained by thermoreflectance mapping. For verification the calculated data we have developed a new technique to monitor the laser facets temperature in real time and to correlate these measurements with device performance and reliability. The method is based on thermoreflectance, which is a modulation technique relaying on periodic facet temperature modulation induced by pulsed current supply of the laser. The periodic temperature change of the laser induces variation of the refractive index and consequently modulates probe beam reflectivity. The technique has a spatial resolution below 500nm and temperature differences of a degree can be measured. It should be noted that the temperature at the facet has a critical role in device reliability and performance. Catastrophic optical damage (COD) failure of a laser device occurs at the facet and is caused by absorption of light at the facet which leads to a local band-gap reduction with consequent increased absorption and temperature rise. The runaway effect leads to device failure. Thus the local facet temperature is indicative of these processes. The developed theoretical

method can be easily adapted for calculating temperature distribution across a 1-D laser array. Results of such calculations performed for arrays with different filling factor τ will be presented. They turned out to be very helpful when optimizing the geometry of 1-D laser arrays.

DD5.12
Effect of Dispersion of Fe and TiO2 Nanoparticles in Fluid on Thermal Conductivity. Ho-Soon Yang[1], Tae-Keun Hong[1] and C. J. Choi[2]; [1]Physics, Pusan Nat'l, Busan, South Korea; [2]Korea Institute of Machinery and Materials, Changwon, South Korea.

Fluids have typically very low thermal conductivity compared with crystalline solids. It has been recognized that suspensions of solids in fluids can show significant enhancement in thermal conductivity. The enhanced thermal conductivity of fluids contributes to improve the efficiency of heat transfer fluids. Furthermore, it can be possible to reduce the size of heat exchange system which has been limited due to the poor thermal transport property of fluids. The large enhancement in nanofluids could not be predicted by conventional theories on the effective thermal conductivity of two-component materials. Many factors such as particle size, effect of surfactant, dispersion of particles, and thermal property of dispersed particles have been expected to influence thermal property of nanofluids. This work focuses on the effect of well-dispersion of nanoparticles in fluids on thermal transport properties of the nanofluids. We present study of thermal conductivity of nanofluids containing Fe and TiO2 nanoparticles with average diameters of 10 and 20 nm, respectively. Since nanofluids are prepared with nanopowder and basefluid, nanoparticles exist as clusters in nanofluid. To improve dispersion of nanoparticles in fluids, highly-powered sonication with ultrasonic pulses is used in the preparation of nanofluids. Thermal conductivity of nanofluid is obtained with the transient hot wire method as changing sonication time. The average size of clusters of nanoparticles is also measured with a laser light scattering method. It is shown that thermal conductivity of nanofluids is related with an average size of clusters. The effect of intrinsic thermal property of dispersed nanoparticles is also studied as compared with other nanofluids containing metallic or ceramic nanoparticles.

DD5.13
Chemical Potential and Current Density Maps on Non-Equilibrium Surfaces. Ramana M. V. Murty, JDS Uniphase, San Jose, California.

Mass flow on a crystalline surface with facets has been modeled in the literature by several continuum, mesoscopic and Monte Carlo methods. However, the assumptions in a continuum or mesoscopic method, especially the description of the cusp have not been independently verified. In this work, thermodynamic parameters that appear in continuum theory such as chemical potential μ and current density are obtained directly from kinetic Monte Carlo simulations. The method that has been developed is applicable to any rough surface and includes the neighborhood of steps. Chemical potential and current density maps have been obtained for typical geometries such as an evolving sinusoidal surface and a train of steps. The simulations show that the chemical potential varies on a plateau corresponsing to the cusp orientation (it is assumed to be constant in certain models). The irreversible thermodynamics relation $\mathbf{j} \propto -\nabla\mu$ is satisfied everywhere including the plateau. The various continuum and mesoscopic methods for surface morphology evolution will be discussed using the results of kinetic Monte Carlo simulations.

SESSION DD6: Interfaces, Superlattices, and Thin Films
Chair: Costas Grigoropoulos
Thursday Morning, March 31, 2005
Room 3003 (Moscone West)

8:00 AM *DD6.1
Heat and Mass Transport in Nanostructures. Arun Majumdar, Department of Mechanical Engineering, Univ of California-Berkeley, Berkeley, California.

The fundamental length scales related to transport phenomena often lie in the length scale range of 1-100 nm. For thermal transport in solids, this includes the mean free path and wavelength of electrons and phonons. For liquids, in contrast, the characteristic length scales are determined by the range of intermolecular and surface forces. These include steric forces, which generally occur in the 1-3 nm range; electrostatic forces that are characterized by the Debye screening length, which fall in the 1-50 nm range; and van der Waals forces which also fall in the 1-50 nm range. Hence, it is clear that when solid and liquid and gaseous media are nanostructured in the 1-100 nm length scale range, one can expect new phenomena that is not observed in bulk media. Scientific understanding of these phenomena offers the opportunity to tailor transport phenomena in unprecedented ways, which could have significant technological implications. In this talk, we will discuss the progress in our laboratory in understand heat transport in 0, 1 and 2 dimensional nanostructured solids and liquids.

8:30 AM *DD6.2
Thermal Conductance of Interfaces. David Cahill, Materials Science, Univ of Illinois-Urbana, Urbana, Illinois.

The thermal conductance of interfaces is a key factor in controlling thermal conduction in nanostructured materials and individual nanostructures. We have recently advanced the state-of-the-art of time-domain-thermoreflectance (TDTR) measurements of thermal transport and are using TDTR to study heat transport across individual interfaces with extremely high and low thermal conductance. The thermal conductance of interfaces between similar materials, e.g., TiN/MgO, approaches the high values predicted by theory and computation; on the other hand, the conductance of interfaces between highly dissimilar materials, e.g., Bi/sapphire, greatly exceeds the so-called radiation limit and the mechanisms for interfacial heat transport in this case are not yet understood. The 3 mm spatial resolution of our TDTR measurements also enables rapid high-resolution imaging of the thermal conductivity of complex microstructures. Heat transport in suspension of carbon nanotubes and metal nanoparticles are studied by picosecond transient absorption. Most of the vibrational modes of a carbon nanotube are weakly coupled to their environment; by contrast, the thermal coupling of metal nanoparticles to surrounding water is surprisingly efficient.

9:00 AM DD6.3
Analysis of Heat Transfer Limitations in III-Nitride Thin Films Grown on Non-Native Substrates. Christian Mion[1], Ji-Soo Park[2] and John Muth[1]; [1]ECE Dept., North Carolina State University, Raleigh, North Carolina; [2]Materials Science and Engineering, North Carolina State University, Raleigh, North Carolina.

Several sources of heat transfer limitations have been identified in III-Nitride heterostructures grown on sapphire, silicon, gallium nitride, or silicon carbide. The role of buffer layers, thermal boundary resistances, and the film-substrate thermal conductivity contrast are studied using harmonic surface joule heating. To explore these issues analytical heat transfer models were compared with finite element modeling. This permitted the comparison of multilayer structures with a variety of thicknesses and thermal conductivity mismatches between layers. In the case of a high thermal conductivity thin film (GaN) on a low thermal conductivity substrate (sapphire or silicon) it was found that the temperature at the location of the heat source will slowly decrease with increasing film thickness and increasing film-to-substrate thermal conductivity ratio. In the case of low thermal conductivity thin films (AlGaN) on high thermal conductivity substrates (SiC or GaN) it was found that the analytical models can deviate significantly from the finite element modeling results, especially when the driving frequency of the surface heat sources was increased. Thermal boundary resistances were included in the analytical model and their effects on heat transfer efficiency were studied. The effects of 500nm AlGaN or AlN buffer layers were also studied. It is found that the presence of a buffer layer can increase the temperature of the surface heat source by 10%. This suggests that the presence of a buffer layer can play an observable role in lowering the thermal impedance of GaN devices. To complement the modeling results the 3 omega technique was used to characterize the thermal transfer in GaN grown on low and high thermal conductivity substrates.

9:15 AM DD6.4
Beating the Alloy Limit of Thermal Conductivity in Crystalline Solids using Embedded Nanostructures. Woochul Kim[1], Pramod Reddy[2], Joshua Zide[3], Arthur Gossard[3], Ali Shakouri[4] and Arun Majumdar[1]; [1]Mechanical Engineering, University of California at Berkeley, Berkeley, California; [2]Applied Science and Technology, University of California at Berkeley, Berkeley, California; [3]Department of Materials, University of California at Santa Barbara, Santa Barbara, California; [4]Department of Electrical Engineering, University of California at Santa Cruz, Santa Cruz, California.

Low thermal conductivity is essential for efficient operation of thermoelectric power generation devices. There have been several attempts to design materials with low thermal conductivity without sacrificing electrical transport. These approaches utilized different mechanisms of phonon scattering. However, each of these approaches scatter phonons only in a particular region of the phonon spectrum. In this paper we present experimental results of the thermal conductivity of epitaxially grown superlattices engineered to take advantage of the various scattering mechanisms to scatter phonons over the entire phonon spectrum. Epitaxially grown superlattices of ErAs/InGaAs were used in our experiments. This superlattice effectively scatters

phonons in various regions of the phonon spectrum: a) The high frequency phonons in the superlattice are scattered by the InGaAs alloy structure present in the superlattice b) the low and intermediate part of the phonon spectrum is blocked by placing ErAs islands with dimensions comparable to the phonon wavelength. Thermal conductivity of ErAs/InGaAs superlattice was measured by using the 3ω technique. For the thermal conductivity of ErAs/InGaAs, a period thickness has been fixed as 40nm to see the effects of monolayer (ML) thickness over the thermal conductivity. Incorporation of ErAs scattering islands results in a significant reduction in the thermal conductivity possibly due to suppression of low and intermediate frequency phonons in addition to alloy scattering. However, the dependency of thermal conductivity on ML thickness of ErAs is less pronounced in the case of monolayer thickness greater than 0.1ML. Thermal conductivity measurement was done on 0.1 ML with different period thickness. One has 10nm period thickness and the other has 40nm. Although the total thickness of the superlattice is not same with each other, the effect of period thickness over thermal conductivity do exist. ErAs/InGaAs superlattice with low period has less thermal conductivity. However the thermal conductivity increases again as in the case of 0.05ML with 5nm period thickness even though its low period thickness. It maybe the sizes of the ErAs islands are so a small compared with phonon wavelength, so that the scattering is now in the Rayleigh regime, where the phonon transport is already blocked by alloy scattering. The thermal conductivity suppression is most evident between around 150 K and 400K. At high temperature above 600K, Umklapp scattering dominates over other scattering process. Total composition of Er is fixed as 0.3 % for both 0.1 ML ErAs/InGaAs with 10nm period thickness and randomly distributed ErAs/InGaAs. Thermal conductivity of randomly distributed ErAs in InGaAs is lower than that of 0.1ML ErAs/InGaAs. The reason for this could be attributed to the spacing between ErAs particles, which could be smaller than 10nm.

9:30 AM DD6.5
Phonon-Hopping Thermal Conduction in Quantum Dot Superlattices. Manu Shamsa, Weily L. Liu, Yun Bao, Khan Alim and Alexander A. Balandin; Nano-Device Laboratory, Department of Electrical Engineering, University of California-Riverside, Riverside, California.

Quantum dot superlattices (QDS) have been proposed for thermoelectric and other applications [1-2]. Understanding the features of thermal transport in QDS with partially ordered quantum dots is important for the structure optimization for a specific application. In this paper we present results of our experimental and theoretical investigation of the thermal conductivity in the doped and undoped Ge/Si quantum dots superlattices. Thermal conductivity measurements carried out by the 3w technique were coupled with the Hall carrier mobility measurements over the wide temperature range [3]. The strain field in Ge/Si QDS, which affects the conduction properties, has been evaluated from the Raman spectroscopic study. We have observed an order of magnitude decrease in the room-temperature thermal conductivity compared to bulk, as well as significant shift of the thermal conductivity peak to the higher temperature values. The thermal conductivity dependence on temperature has been approximated as $K \sim T^{0.7} - T^{0.9}$ in the low-temperature region. Since the theoretical models, developed for high-quality bulk crystals, cannot describe the thermal conductivity in disordered Ge/Si QDS, we adopted the phonon-hopping approach proposed for nanocrystalline and granular materials. This model assumes that the phonons hop from one dot site to another through grain boundaries. Therefore, the interfaces between the dots and the host matrix play an important role in limiting the thermal conductivity. We simulated the effect of dot size, size dispersion and inter-grain interface conditions on the phonon hopping transport and the thermal conductivity values under various conditions. The modeling results were then fitted to the measured thermal conductivity data for Ge/Si QDS. We were able to obtain an excellent agreement between the experimental data and the model prediction in the whole temperature range. The fitting procedure allowed us to introduce an effective Debye temperature for Ge/Si QDS. This work has been supported by the NSF NER and SGER Awards to A.A.B, and through the DARPA - DMEA Center for Nanoscience Innovation for Defense (CNID). [1]. A.A. Balandin, Phonon confinement in nanostructures and its effect on thermal conductivity, Plenary Talk, 11th International Conference on Phonon Scattering in Condensed Matter, St. Petersburg, Russia, 2004; page 6. [2]. A.A. Balandin and O.L. Lazarenkova, Appl. Phys. Lett., 82, 415 (2003). [3]. Y. Bao, A.A. Balandin, et al., Appl. Phys. Lett., 84, 3355 (2004).

9:45 AM DD6.6
Thermal Conductivity of the AlxGa1-xN Thin Films: Al Mass Fraction Dependence. Weili Liu and Alexander A. Balandin; Electrical Engineering, University of California–Riverside, Riverside, California.

It is known that the operation of the high-power density AlGaN/GaN heterostructure field-effect transistors (HFETs) can be significantly hampered by temperature rise in the device active area due to poor heat conduction [1]. Optimization of GaN-based devices requires accurate knowledge of thermal conductivity of GaN thin films and AlxGa1-xN alloys used as barrier layers in HFETs. It has been previously shown that the presence of the large densities of point defects, dopants and dislocations lead to a significant variation of thermal conductivity in GaN thin films even at room temperature and above [2]. In this paper we report on experimental and theoretical investigation of thermal conduction in AlxGa1-xN alloy films. A focus of this study is on understanding the effect of the Al mass fraction and temperature on thermal conductivity in AlxGa1-xN thin films. The thermal conductivity of a set of AlxGa1-xN thin films with different Al fraction x, as well as of a pure GaN sample was measured using the differential 3w technique in the temperature range from 80K to 400K. Thermal conductivity of the examined AlGaN alloy, which is about 25 W/mK at 300 K, displays a noticeable growth with temperature up to 350 K, which is more characteristic for amorphous or completely disordered materials. Application of the virtual crystal model allowed us to elucidate the strength of the mass-difference and strain-field-difference phonon scattering in AlxGa1-xN alloy system [3]. The measured variation of the thermal conductivity with the Al fraction is in good agreement with the theory predictions. The measured values of thermal conductivity and their temperature dependencies have been incorporated within the ISE TCAD software tools for evaluating the self-heating effect in AlxGa1-xN /GaN HFETs and modeling HFET current-voltage characteristics. Obtained results can be used for the AlGaN/GaN transistor structure optimization. [1]. V.O. Turin and A.A. Balandin, Electron. Lett., 40, 81 (2004). [2]. J. Zou, D. Kotchetkov, A.A. Balandin, D.I. Florescu, F.H. Pollak, J. Appl. Phys., 92, 2534 (2002); ibid, Appl. Phys. Lett., 79, 4316 (2001). [3]. W.L. Liu and A.A. Balandin, Temperature dependence of the thermal conductivity of AlGaN thin films measured by the differential 3w technique, Appl. Phys. Lett, in print, 2004. This work has been supported by ONR Award N000140210352 to A.A.B., and through the DARPA - DMEA Center for Nanoscience Innovation for Defense (CNID).

10:30 AM *DD6.7
Interfacial Thermal Transport: Insights from Simulation. Simon Robert Phillpot[1], Taku Watanabe[1], Patrick Schelling[2] and Pawel Keblinski[3]; [1]Materials Science and Engineering, University of Florida, Gainesville, Florida; [2]Physics, University of Central Florida, Orlando, Florida; [3]Materials Science and Engineering, Rensselaer Polytechnic Institute, Troy, New York.

Experimentally, it is very difficult to probe the interfacial thermal conductivity. Therefore, over the last four years, we have developed an integrated suite of atomic-level simulation methods specifically designed to dissect the interactions of phonons with interfaces. We have applied these techniques to both individual interfaces and to multilayer systems. We explore the role of bonding at the interface by comparing the thermal-transport properties of diamond grain boundaries, in which there is a mixture of sp3 and sp2 bonding, with those of crystallographically identical silicon grain boundaries, in which all of the bonding is sp3 in nature. Finally, challenges and opportunities for more fully elucidating interfacial thermal transport by simulation are identified.

11:00 AM DD6.8
DMM Calculation of the Thermal Conductance of Interfaces without the Debye Approximation.
Pramod Reddy Sangi Reddy[1], Kenneth Castelino[2] and Arun Majumdar[2,3]; [1]Applied Science & Technology, University of California, Berkeley, Berkeley, California; [2]Mechanical Engineering, University of California, Berkeley, California; [3]Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, California.

Thermal conductance of interfaces plays an important role in the transport of thermal energy in nanometerscale devices, composites, semiconductor superlattices, thinfilm multilayers, and nanocrystalline materials. Thermal interface conductance at the interface between solid Cu and liquid He was first observed by Kapitza and subsequently explained by Khalatnikov using the acoustic mismatch model (AMM) of phonon reflection and transmission across an interface. Much of the subsequent work has focused on phonon transmission across solid-solid interfaces, which was summarized in a comprehensive review by Swartz and Pohl. In particular, it was shown that the assumption of specular (or non-diffuse) phonon reflection and transmission breaks down for high-frequency phonons (>100 GHz) because the chemical and physical roughness of an interface can become on the order of the wavelength of the dominant heat-carrying phonons. This led Swartz and Pohl to propose a diffuse mismatch model (DMM), which assumes that phonons lose their memory after reaching the interface and that the probability of transmission to

either side of the interface depends on the ratio of the phonon density of states. The calculation of thermal interface conductance using the DMM requires a detailed knowledge of the phonon dispersion relationship over the entire Brillouin zone. However, for simplicity the dispersion relationship is usually approximated by a linear dispersion relationship (Debye approximation). The Debye approximation is a good representation of the dispersion relation ship for phonon states close to the zone center but away from the zone center the dispersion relationship given by the Debye approximation deviates significantly from the real dispersion relationship. Here, we present a DMM calculation of the thermal conductance of Al-Si, Al-Ge, Cu-Si, Cu-Ge interfaces obtained by taking into account the phonon dispersion relationship over the entire Brillouin zone. The calculated thermal interface conductance for each of the cases deviates significantly (by a factor of 2 to 3) from the thermal interface conductance calculated under the Debye approximation at high temperatures (T> Debye temperature). However, at low temperatures (T< Debye temperature) the thermal conductances calculated with and without the Debye approximation do not show a significant deviation.

11:15 AM DD6.9
Interfacial Thermal Resistance of Octane-Water Interface. Harshit Patel[1], Shekhar Garde[1] and Pawel Keblinski[2]; [1]Chemical & Biological Engineering, Rensselaer Polytechnic Institute, Troy, New York; [2]Materials Science & Engineering, Rensselaer polytechnic institute, Troy, New York.

Interfacial resistance to heat flow can control the rate of thermal transport in inhomogeneous systems with nanoscale features. While a large body of work exists for thermal transport across solid-solid and solid-liquid interfaces, much less is known about heat flow across interfaces between immiscible liquids. In this work we use classical molecular dynamics simulations to study the interfacial resistance for heat flow between octane-water at room temperature. Our study demonstrate a large value of the interfacial resistance associated with weak coupling between water and octane. We identified an important role played by the soft vibration modes in heat transfer across the interface. We will also discuss the implications of our results for thermal energy transfer between water and biological molecules.

11:30 AM DD6.10
Anomalously High Thermal Conductivity in Gold-core Polymer Shell Nanoparticles. Zhenbin Ge, David G. Cahill and Paul V. Braun; MatSE, University of Illinois at Urbana-Champaign, Urbana, Illinois.

Gold-core polymer-shell nanoparticles have been investigated to study the effect of organic co-solvents on the thermal conductivity of the polymer shell using transient absorption pump-probe measurements. In pure water, the cross-linked copolymer shells provide a physical barrier that isolates the gold core from the surrounding media. The permeability of the polymer shell can be modulated by adding an organic co-solvent to the aqueous particle suspension, solvating the hydrophobic polymer block, thus altering the thermal transport from the particles to the environment. Sub-picosecond λ=770 nm optical pulses are used to heat the particles and the cooling of the nanoparticles is measured through time-resolved changes in the optical absorption of the solution. Thermal conductivities of the polymer shells are determined by fitting the data with a model of the heat flow from the particles through the polymer shell and into the surrounding fluid. The effective thermal conductivity of the shell increases from 0.25 W m^{-1} K^{-1} in pure water to 0.50 W m^{-1} K^{-1} in THF/H_2O mixtures with a threshold near 5 vol% THF; and increases from 0.25 W m^{-1} K^{-1} to 0.50 W m^{-1} K^{-1} in DMF/H_2O mixtures with a threshold near 40 vol% DMF. Below the threshold levels of organic solvent, the thermal conductivity of the shell is independent of solvent composition. The large increase in the effective thermal conductivity of the shell with swelling is unexpected based on macroscopic effective medium theory. We note that our experimental results for the thermal conductivity of the nanoscale polymer films may provide some insight on the design of nanoparticle systems for applications in photo-thermal medical therapy and drug delivery.

11:45 AM DD6.11
Crossover of Density of States and Heat Capacity in Spherical Quantum Shell Structures. Seung J. Lee[1], Tae Won Kang[1] and Gukhyung Ihm[2]; [1]QSRC, Dongguk University, Seoul, South Korea; [2]Physics, Chung-Nam National University, Taejeonl, South Korea.

Recently nanofabrication technology have made it possible to manufacture semiconductor quantum dots (nano-crystals) synthesizd in colloidal solutions and it has attracted much interests because of their small size ranging from 1 to 10nm. Those quantum dots grown in a colloidal solution have frequently spherical shapes and can be fabricated as multi-shell structures such as quantum dot-quantum wells and quantum dot-quantum barriers, which is very attractive for applications in novel optoelectronic devices. Motivated by such experimental techniques to fabricate mutli-shell structures, we study the density of electronic states in quantum dot structures (nano-crystals) formed by a thin spherical barrier. The finite thickness of the spherical barrier layer allows electrons in the quantum dot to escape to the outside of the dot. The purpose of this paper is to know how the density of states (DOS) of the quantum dot depends on the barrier thickness and the conduction band discontinuity between the core/outer-shell material and the barrier material. Another purpose is to investigate the heat capacity of such systems. It is interesting to ask how are the electron density dependence and the temperature dependence of the heat capacity influenced by the thickness of the spherical barrier. Even though the fundamental importance of the temperature and the heat capacity of small systems, the heat capacities of quantum dots have not been investigated except for the important work in which the effect of electron-electron interaction is studied in strong magnetic field. The simple analytical expression for the DOS of the nano-spherical dot covered by spherical shell is evaluated. It shows that the control of the thickness and/or height of the spherical shell barrier cause the 3D-0D direct transition in DOS. Interestingly, the presence of the 1D and 2D like crossover regime is also predicted by using our formula. We also study the heat capacity of electrons in a spherical quantum dot formed by a spherical thin barrier. The control of the spherical barrier thickness or height is found to cause the dimensional transition from the three dimensional (3D) behavior to the quasi-zero dimensional (Q0D) behavior in the heat capacity. When the barrier is thick enough such that the DOS shows the Q0D-like signature but is thin enough to allow electrons to tunnel it, the temperature dependence of the heat capacity exhibits quite distinct behavior depending on the electron density whether the shell is fully filled or half filled. Author to whom correspondence should be addressed; electronic mail: leesj@dongguk.edu

SESSION DD7: Characterization, Applications and Devices
Chair: Shriram Ramanathan
Thursday Afternoon, March 31, 2005
Room 3003 (Moscone West)

1:30 PM *DD7.1
Nanoshell-Mediated Photothermal Cancer Therapy. Naomi Halas, Department of Chemistry, Rice University, Houston, Texas.

The modification of heat transfer properties by the presence of nanostructures dispersed in fluids or embedded in dielectric media is a topic of great current interest. The photothermal analog of this effect has recently been utilized to induce localized heating in cancerous tissue both in vitro and in vivo. Plasmon resonant nanoparticles, known as nanoshells, whose resonance frequency has been tuned to the near infrared region of the spectrum provide a unique opportunity for direct resonant optical excitation of nanoparticles in biological media at wavelengths where the medium is optimally transmissive. The dramatically rapid temperature increase that occurs upon resonant illumination of the nanoparticles embedded in tumors is sufficient to effectively induce cell death in the immediate vicinity of the nanoparticles. Studies in animals have shown remarkable effectiveness of this process for the noninvasive reduction and elimination of cancerous tumors with long term survivability of the subjects under study.

2:00 PM *DD7.2
Micro and Nano Structuring of Aluminum Films with Water and Localized Heating. Andreas Stemmer, Nanotechnology Group, Swiss Federal Inst of Technology, Zurich, Switzerland.

Micro and nano structured thin metal films are widely used in micro-electronic and micro-mechanical devices. Typically, patterning is achieved via multi-step processes employing resists, UV-light or electron beam lithography, and lift-off technique. Patterning of thin (10-600 nm) aluminum films can also be achieved in a one-step process by low-power laser-thermal oxidation in water. In neutral water of pH=7 at room temperature, aluminum forms a passivation layer composed of hydrargillite. Local heating of the aluminum film due to the absorption of light inhibits this passivation process and, close to the boiling point of water (T=373K), leads to corrosion of the aluminum film in the irradiated zone. Metal ions are dissolved in water, hence no debris are deposited adjacent to the zone processed that would require additional process steps for their removal. Using standard light microscope objectives, laser light of λ = 488 nm or 532 nm, and a movable stage, line patterns can be drawn that serve as micrometer-sized aluminum electrodes on glass or polymer substrates. On very thin films (10-20 nm) the minimum line width is 'diffraction limited', i.e. determined by the size of the focused laser spot, whereas on thicker films heat conduction in the metal film and in the substrate away from the irradiated zone leads to broader lines. Similarly, for a

given film thickness, line width increases with decreasing scan speed. Furthermore, an upper limit exists for the laser irradiation power, above which the corrosion process stops because local evaporation of water and the formation of steam bubbles interrupt the oxygen supply necessary for metal oxidation. Converting the laser beam into an evanescent field at a glass-water interface creates a heat source of limited (a few 10 nm) spatial extent normal to the interface, that allows one to corrode subwavelength-sized apertures into aluminum coated pointed probes that are immersed into this evanescent field. For example, such probes can be used in optical near-field microscopy. Writing lines less than 100 nm wide in planar aluminum films of 20 nm thickness on glass substrates becomes feasible when the laser light is totally internally reflected at the glass-aluminum-water interface and generates surface plasmons in the metal film. Writing is achieved with the probe of an atomic force microscope in contact with the aluminum film. The tip acts as an optical antenna generating an enhanced electromagnetic field in the vicinity of the tip apex. Depending on the magnitude of the field enhancement, the energy density in the near field below the tip can be high enough to heat the aluminum via absorption of light and induce local corrosion. The fabrication processes and their applications will be reviewed in terms of the underlying mechanisms responsible for local heat production.

2:30 PM *DD7.3
Peltier Tip Microcalorimeter. Yoon Hee Jeong[1], Dae Hwa Jung[2] and Ilkwon Moon[2]; [1]Department of Physics and Electron Spin Science Center, Pohang Univ. of Sci & Tech, Pohang, South Korea; [2]POSVAC, Pohang, South Korea.

The well-known Peltier effect refers to the fact that heat is generated or absorbed at a thermocouple junction, that is, a junction of two dissimilar metal wires, depending on the direction of electric current. Previously we developed an ac microcalorimeter utilizing the Peltier effect of a thermocouple junction as an ac power source and another thermocouple as a sensor [1]. This Peltier calorimeter allowed us to measure the absolute value of the heat capacity of small solid samples with submilligrams of mass in the temperature range of 15-420 K. We also developed a novel calorimeter, termed as the Peltier tip calorimeter, consisting of a single thermocouple junction (Peltier tip) which is used as a heater and a sensor simultaneously. The Peltier tip calorimeter is capable of measuring the heat capacity of a small solid sample with sub-milligrams of mass, and also the heat capacity and thermal conductivity of a liquid sample [2]. It is demonstrated that the Peltier tip has a potential as a local probe for scanning thermal microscopy, and that it is capable of measuring heat conduction of a gas and therefore can be used as a sensitive vacuum sensor [3] and an acceleration sensor [4]. It is further demonstrated that because the Peltier tip can be scaled down with the MEMS technique, it offers wide applications in measuring heat transport on a nanometer scale. [1] I. K. Moon et al., Appl. Phys. Lett. 76, 2451 (2000). [2] D. H. Jung et al., Preprint. [3] Korea Patent reg. number 407815 (2003); US Patent reg. number 6727709 (2004); Japan Patent reg. number 3452913 (2003). [4] Korea Patent applied 10-2004-0061995 (2004).

3:30 PM *DD7.4
Engineering of Sub-Wavelength Photonic Meta Materials: A Route towards Nano-Scale Plasmonics and Super Imaging. Xiang Zhang, NSF Nano-scale Science and Engineering Center, University of California, Berkeley, Berkeley, California.

Recent theory predicted a new class of meta structures made of engineered sub wavelength entities - meta "atoms" and "molecules" which enable the unprecedented electromagnetic properties that do not exist in the nature. For example, artificial plasma and artificial magnetism, and super lens that focuses far below the diffraction limit. If the theory is correct and these unique properties can be realized, it will have profound impact in wide range of applications such as nano-scale imaging, nanolithography, and integrated nano photonics. These photonic "atoms" usually form highly complex structures which present a critical need in developing truly 3D micro and nano-manufacturing techniques which are not available presently. In the first part of this presentation, I willl discuss a few micro and nano fabrication technologies that we developed for engineering complex meta-structures. In the second part, I will discuss sub-l photonic "atoms" and "molecules" and the potential applications in nano-scale imaging and lithography. We demonstrated, for the first time, the high frequency magnetic activity at THz generated by artificially structured "molecule resonance", as well as the artificial plasma. Our experiment also confirmed the key proposition of super lens theory by using surface plasmon. We indeed observed preliminary superlensing at near-field. The surface plasmon indeed promises an exciting engineering paradigm of "optical frequency and x-ray wavelength". This talk will be concluded with a vision of the nano-manufacturing that will enable the new nano plasmonics and other applications.

4:00 PM DD7.5
Nanoscale Energy Transport in Information Technology Research (ITR) with an Application to High-Density Data Storage Devices and Systems. Mehdi Asheghi, [1]Mechanical Engineering, Carnegie Mellon University, Pittsburgh, Pennsylvania; [2]Data Storage System Center, Carnegie Mellon University, Pittsburgh, Pennsylvania.

By all measures, data storage is one of the most important components of the Information Technology (IT) revolution. New applications are putting increased demands on the technology upon which data storage is based. The architecture of the information infrastructure of organizations and systems is based on a certain number of well-accepted assumptions. Among these is the assumption that non-volatile mass storage is a relatively inexpensive part of the total system cost and that its storage capacity is orders of magnitude greater than the processing capacity of the system, in terms of the quantity of data operated upon, at any given time. This assumption and hence the paradigm by which IT infrastructures are designed has been maintained even as processor capabilities have increased (doubling every 18 months-Moore's Law) and cost has been reduced over time, mainly due to the fact that the magnetic hard drives have stayed on a parallel density (and data rate) improvement curve as semiconductor technologies. However, whether the storage densities will continue to increase at this rate and be able to keep up with the improvements in processor technology is under a near term threat resulting from the fundamental physics upon which hard disk drives are based. If storage systems are not able to continue to improve, to keep up with processing systems, the relative cost of mass storage will increase over time. Eventually it is conceivable that this could become the limiting cost in an information technology infrastructure. Thus the manner in which such systems are designed, what their capabilities are, and how they develop over time could be radically different from what is assumed today. It is expected that novel, more unconventional technological solutions may become necessary to overcome limitations such as the superparamagnetic effect. However, many of these technologies rely heavily on energy transport at extremely short time and length scales. This work describes three interwoven research thrusts in the following areas: (a) design of sub-continuum energy transport/delivery in data storage systems, (b) thermally induced failure in nanoscale data storage devices, and (c) fundamental measurements of sub-continuum heat transfer. The presentation will address the thermally assisted magnetic disk recording (using light); thermally assisted scanned probe recording (using tunneling electrons); and phase change data recording (using thermal point contact).

4:15 PM DD7.6
Thermal Transport of Nano-Stacked Superconducting Josephson Devices. Yonuk Chong, Paul D. Dresselhaus and Samuel P. Benz; NIST, Boulder, Colorado.

NIST has been developing nanoscale-packed Josephson junctions for advanced quantum voltage standards. The vertically stacked junction is the most promising candidate until now, and was successfully demonstrated with a dramatic increase in the junction density and the chip performance. Some of the stacked-junction devices with more than 100,000 on-chip junctions are ready to be delivered to the customers soon. As the junction density increases, self-heating becomes an issue because the high power density generates a significant amount of local power dissipation under typical operating conditions. In this report, we analyze the heating effect of these sandwich-type SNS Josephson junctions using a model to quantitatively estimate and predict thermal-transport properties of the stacked structures. This analysis turned out to be a very efficient way of measuring thermal variables at the same time, such as the thermal conductivity and the thermal boundary resistance in a thin film device. We describe several strategies that reduce the heating, and demonstrate improved properties of stacked junction devices with enhanced cooling capacity. Reference : Yonuk Chong, P. D. Dresselhaus, and S. P. Benz, "Thermal transport in stacked superconductor-normal metal-superconductor Josephson junctions", Appl. Phys. Lett. 83, 1794 (2003).

4:30 PM DD7.7
Sub-continuum Thermal Phenomena in Transistor Drains. Sanjiv Sinha and Kenneth E. Goodson; Mechanical Engineering, Stanford University, Stanford, California.

Transistors with gate lengths well below 100 nm have power densities approaching 50 W/um3 at the drain terminal. The spatial distribution of Joule heat in such devices has a full width at half maximum on the order of the electron mean free path near the peak electric field region, which is less than 10 nm. These conditions lead to two important phonon conduction phenomena in the device drain: a non-equilibrium "hot" phonon distribution at high electric fields [1], and a locally reduced thermal conductance when the size of the source is comparable to the phonon mean free path [2]. The relative importance of these two effects in silicon semiconductor devices is an

open question, particularly toward the limits of scaling. We examine these phenomena using the Boltzmann transport equation (BTE) for phonons and electron-phonon scattering theory. In investigating hot phonon effects, we follow the approach of Artaki and Price [1] but include phonon transport in our model. The phonon BTE is solved analytically using the split-flux departure function [3], and a phonon emission term that accounts for g-type inter-valley electronic transitions in silicon [4]. The results show that "hot" phonon related mobility degradation is likely at electric fields typical in sub-100 nm transistors. We discuss its impact on device characteristics using empirical relations between mobility and the lattice temperature in thin silicon films. In modeling the size effect, we use a full phonon emission spectrum computed by Monte Carlo simulations [5]. We find that the sub-continuum size effect is much less than predicted earlier, using a phonon mean free path computed from the theory of lattice thermal conductivity. When the spectral distribution of the emitted phonons is taken into account, the size effect is found to decrease due to the shorter mean free path of phonons dominating the emission spectrum. We find that though there is a size related reduction in thermal conductance at the drain, its magnitude is much less than previously reported. This work shows that the sub-continuum thermal phenomenon of interest in sub-100 nm transistors is that due to "hot" phonons rather than that due to the size of the heat source. 1. M. Artaki and P.J. Price, J. Appl. Phys., 65, 1317(1989). 2. G. Chen, J. Heat Transfer, 118, 539(1996). 3. S. Sinha, E. Pop and K.E. Goodson, Int. Mech. Eng. Cong. Expo. (IMECE), Anaheim, California, November 2004. 4. D. Long, Phys. Rev., 120, 2024(1960). 5. E. Pop, R.W. Dutton and K.E. Goodson, submitted to Appl. Phys. Lett.

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Entropic Modeling of Thermoelastic Dissipation in Microstructures. Saurabh Arun Chandorkar[1], Rob N. Candler[1], Amy Duwel[2], Matthew Varghese[2], Thomas W. Kenny[1] and Kenneth E. Goodson[1]; [1]Mechanical Engineering, Stanford, Stanford, California; [2]Charles Stark Draper Lab, Cambridge, Massachusetts.

Understanding energy loss mechanisms is critical for the design of mechanical dynamical systems. A microresonator is an example of a Micro Electro Mechanical System (MEMS) whose performance is affected by the Quality factor(Q), a measure of the energy loss that occurs in the resonating device. Wafer scale vacuum encapsulation of microresonators eliminates air damping, such that in many devices thermo elastic dissipation (TED) is the dominant loss mechanism. Zener [1] developed a model capturing the peak in the intensity of TED at a critical frequency that is comparable with the inverse heat diffusion time across the resonator. In recent years, TED has been revisited primarily because its effects are encountered in MEMS devices [2, 3, 4], and there is much interest in improving the computational approaches for resonator design, in particular the impact of TED. This paper develops a modeling approach for TED based on entropy generation, which is useful both for computations of Q and for improving understanding and design of microstructures. A statistical description of phonon populations and their entropy and energy densities is used to quantify the change in temperature due to strains applied to structures. Extension of this result to macroscopically observable variables is shown to result in a three-dimensional analog of the single-dimension equations of Zener [1]. The new computational approach is used to illustrate the ways that the geometry of structures affects the characteristic thermal modes and the temperature distribution in the vibrating structure can be mapped onto these modes to yield information about sensitivity of TED losses to variations in characteristic length scales. The paper will discuss an analytical solution for a two-dimensional vibrating beam case in which the Q variation with resonant frequency will be derived based upon aforementioned approach. A finite element method based code has been developed to obtain Q for complex geometries. Simulation results will be compared against experimental results. Entropy generation minimization will be carried out for obtaining optimal geometric parameters for specific cases of microresonators. References: 1) C. Zener, *Internal Friction in Solids*, Physical Review, Vol. 52, pp 230 - 235, Aug 1937. 2) R. N. Candler, M. Hopcroft, W.T. Park., S. A. Chandorkar, G. Yama, K. E.Goodson, M. Varghese, A. E. Duwel, A. Partridge, M. Lutz, and T. W. Kenny, *Reduction in Thermoelastic Dissipation in Micromechanical Resonators by Disruption of Heat Transport*, Proc. of Hilton Head Conference, pp 45-48, Jun 2004. 3) A. E. Duwel, J. P. Gorman, M. Weinstein, J. T. Borenstein and P. A. Ward, *Quality Factor of MEMS Gyros and the Role of Thermoelastic Dissipation*, Proc. of 15th International Conference on MEMS, pp 214-219, Jan 2002. 4) S. Srikar and S. Senturia, *Thermoelastic Damping in Fine-Grained Polysilicon Flexural Beam Resonators*, IEEE/ASME JMEMS, Vol. 11, pp 499-504, Oct 2002.