

SYMPOSIUM S

Nanoscale Thermal Transport: From Fundamentals to Devices

April 22 – 23, 2003

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* Invited paper

SESSION S1: NANOSTRUCTURED MATERIALS
AND COMPOSITES

Chair: David G. Cahill
Tuesday Morning, April 22, 2003
Concordia (Argent)

8:30 AM *S1.1

THERMAL CONDUCTIVITY IN NANOSTRUCTURED MATERIALS. J.A. Eastman^a, Ho-Soon Yang^{a,b}, G. Skandan^c, L.J. Thompson^a, and G.-R. Bai^a; ^aMaterials Science Division, Argonne National Laboratory, Argonne, IL; ^bDepartment of Physics, Pusan National University, Pusan, KOREA; ^cNanopowder Enterprises Inc., Piscataway, NJ.

This talk will describe recent thermal conductivity studies in which significant effects of nanostructuring on thermal transport rates have been observed. Compared to the thermal conductivity of single-crystal or coarse-grained polycrystalline yttria-stabilized zirconia (YSZ), the thermal conductivity of nanocrystalline YSZ with an average grain size of 10 nm is observed to be reduced by more than a factor-of-two. This reduction is believed to be due to grain boundary (Kapitza) resistance to heat flow. The expected variation in the magnitude of the Kapitza resistance in different materials will be discussed. In contrast with the reduction in thermal transport that arises when grain size is reduced in solids, the effective thermal conductivity of heat-transfer fluids such as water or ethylene glycol can be increased substantially through the suspension of nanoparticles to create what are called nanofluids. Increases in effective fluid thermal conductivity of more than 40% have been observed in nanofluids containing only a few volume per cent dispersed nanoparticles. Recently, we have observed that the modification of nanoparticle surfaces with surfactants can have a strong influence on the thermal conductivity of nanofluids. The mechanisms believed responsible for the observed behavior will be discussed. Implications for possible future thermal management applications of nanostructured materials will also be described.

9:00 AM *S1.2

ON THE IMPORTANCE OF NANOSCALE THERMAL TRANSPORT TO LARGE SCALE INTEGRATED CIRCUIT DEVELOPMENT AND MANUFACTURING. Wayne K. Ford, Intel Corporation, Hillsboro, OR; Humphrey J. Maris, Brown University, Providence, RI.

Future generations of integrated circuit technology is being increasingly constrained by the nanoscale thermal transport properties of the materials and device geometries employed. Traditional silicon process scaling and ever higher performance objectives lead to thermal transport related challenges, increasingly on the nanometer length scale, involving the transistor, interconnect system, and package design that must be addressed and overcome in each process generation. Some common examples include loss of carrier mobility, self-heating, and electromigration. The planned use of more complex devices employing new materials and process methods, such as Si alloys, novel polymers, and 3D structures, presents technology researchers with new, relatively unexplored contexts in which to address the consequent thermal energy transport problems. Finally, the rapid incursion of large scale integrated devices into a wider range of market applications, driven by the convergence of communications and computing, the rush to highly mobile computing platforms, and the expanded deployment of high speed networks, requires that the products employed be engineered over a wider range of sometimes uncertain thermal and use conditions. This paper provides first an overview of some of these salient issues. Then a detailed example is presented of our recent work involving the thermal conductivity of thin film dielectrics, studied primarily using time domain thermal reflectance.

9:30 AM S1.3

RESISTIVITY-DEPENDENT POWER LAW THERMAL CONDUCTIVITY FOR POROUS SILICON. Jennifer R. Lukes, University of Pennsylvania, Dept of Mechanical Engineering and Applied Mechanics, Philadelphia, PA; Ming-Hong Lee, KLA Tencor, Santa Clara, CA; Costas P. Grigoropoulos, Chang-Lin Tien[†], University of California, Berkeley, Dept of Mechanical Engineering, Berkeley, CA. [†]deceased 10-29-02.

Porous silicon is a special form of the semiconductor silicon characterized by a complex structural network of nanometer-scale silicon crystallites and voids and an extremely high surface area. Reported thermal conductivity values for this material span four orders of magnitude, ranging from 0.025 to 140 W/m-K. It is not clear how much of this variation stems from real structural differences among the porous silicon samples and how much results from the different fabrication procedures and thermal conductivity measurement techniques used by the various groups. To clarify such ambiguities, the present experiments use a single technique, modulated laser thermoreflectance, on a significant number of samples

that are fabricated in a consistent manner. The results suggest that a simple power law model depending only on porous silicon solid fraction and starting wafer resistivity can be used to estimate the thermal conductivity of p-type, (100) oriented, as-anodized porous silicon. In this model, the exponent of the solid fraction is linearly proportional to resistivity. Although empirical, the model reflects important features of porous silicon structure, is consistent with theoretical predictions of size effects, fits literature data well over a wide range of resistivities, and compares favorably with power law models of other porous materials.

9:45 AM S1.4

THERMAL TRANSPORT IN PYROCHLORES USING MOLECULAR-DYNAMICS SIMULATION. P K. Schelling, S.R. Phillpot, Materials Science Division, Argonne National Laboratory, Argonne IL; R.W. Grimes, Department of Materials, Imperial College, London, UNITED KINGDOM.

Pyrochlore materials with composition A₂B₂O₇ are known to exhibit very low thermal conductivities (~1W/mK), and are important candidate materials for thermal barrier coatings. To elucidate the importance of the choice of A and B ions on the thermal conductivity, we have used molecular-dynamics simulation to study the thermal conductivity of pyrochlores for 50 different combinations of A and B cations. We analyze the results using the computed sound velocity and specific heat, and show that we can explain the observed trends. We also find that some pyrochlores exhibit some disorder in the oxygen sublattice, resulting in a yet lower thermal conductivity. Work at Argonne National Laboratory supported by the U.S. Department of Energy, Basic Energy Science-Materials Sciences under Contract #W-31-109-ENG-38.

10:30 AM *S1.5

NANO-FLUID: THE HEAT TRANSFER FLUID FOR THE FUTURE. Sarit K. Das, Department of Mechanical Engineering, Indian Institute of Technology, Madras, INDIA.

Ever shrinking size of electronic components and ever rising energy density in LASER, computing and opto-electronic devices has given rise the need for cooling far more efficient than that with present conventional strategies. The inherent weakness of the common fluids in the form of low thermal conductivity is proposed to be overcome in the recent times by suspending nano particles in fluids known as nano-fluids. An unusual increase of thermal conductivity of nano-fluids has been reported in a number of recent publications [1, 2]. The present paper brings out results showing the strong temperature dependence of thermal diffusivity of oxide based nano-fluids using a novel temperature oscillation method of measurement. The direct measurement of thermal diffusivity is found to be more accurate since it need not know a priori the conductivity of a reference layer which is required for measurement of thermal conductivity. The paper also reports results for nano-fluids with particles of gold and silver metal clusters in organic liquids such as toluene. The effects of parameters such as particles size coupled with temperature as well as particle material on thermal conduction have been investigated. The temperature effects clearly indicate that the Brownian type motion is not a likely cause of the enhancement of conductivity. However, it is felt that micro-convection around particles as well as non-Fourier conduction effect can go a long way in explaining this behaviour. [1] Lee, S., Choi, U.S., Li, S., Eastman, J.A., 1999, "Measuring Thermal Conductivity of Fluids Containing Oxide Nanoparticles," ASME Journal of Heat Transfer, Vol. 121, pp. 280-289. [2] Eastman, J.A., Choi, U.S., Li, S., Yu, W and Thompson, L.J., 2001, "Anomalous Increased Effective Thermal Conductivities of Ethylene glycol-based nanofluids containing copper nanoparticles," Applied Physics Letter, Vol. 78, No. 6, pp. 718-720.

11:00 AM S1.6

HEAT TRANSFER IN NANOFUIDS—A PERCOLATION PERSPECTIVE. Shiu-Wing Tam, Steven U.S. Choi, and Yung Y. Liu, Argonne National Laboratory, Energy Technology Division, Argonne, IL.

Nanofluids are solid/liquid suspensions developed primarily for heat transfer applications. Carbon nanotube-based nanofluids have been shown to exhibit significant enhancement in thermal conductivity relative to the matrix fluid used with addition of low concentrations of nanotubes (up to 1 vol %) [1]. Similar conductivity enhancement has been observed in carbon nanotube composites [2]. These experimental results cannot be understood with the traditional effective medium theory. We have analyzed the conduction process from the perspective of highly shape-dependent percolation. The results indicate that, due to the large aspect ratio of the nanotubes, the concentration regime of these experiments is already beyond the critical percolation threshold. Substantial overlap of the nanotubes occurs despite the apparently low nanotube concentration. This finding is consistent with the observed conductivity enhancement. Because of this overlap, modeling

of the single-nanotube thermal conductivity needs to be modified to include contact resistance, which is a major heat conduction barrier. We have applied this modification to a virial-like expansion of the thermal conductivity in terms of the nanotube concentration to describe recent experimental data [1]. The result indicates that the conductivity enhancement, while significant (125-160 percent), is nowhere near what the huge single-nanotube conductivity (3000-6000 W/m-K) would seem to suggest [1,2]. Since a similar observation is applicable to the viscosity of nanofluids, one expects a comparable enhancement in the nanofluid viscosity. Viscosity is important because heat transfer fluids are usually used in a circulating mode. Employing the theoretical methodology outlined above, we will assess the competing contributions from the thermal conductivity and viscosity enhancements to the heat transfer capability of nanofluids. 1. S.U.S. Choi et al., Appl. Phys. Lett. 79, 2252 (2001). 2. M.J. Biercuk et al., Appl. Phys. Lett. 80, 2767 (2002).

11:15 AM S1.7

TWO REGIMES OF THERMAL RESISTANCE AT A LIQUID-SOLID INTERFACE. L. Xue and P. Keblinski, Rensselaer Polytechnic Institute, Dept. of Materials Science and Engineering, Troy, NY; S.R. Phillpot^a, S. U.-S. Choi^b, and J.A. Eastman^a. ^aMaterials Science Division; ^bEnergy Technology Division, Argonne National Laboratory, Argonne, IL.

Using non-equilibrium molecular dynamics simulations in which a temperature gradient is imposed, we determine the thermal resistance of a model liquid-solid interface. Our simulations reveal that the key factor controlling interfacial thermal resistance is the strength of the bonding between liquid and solid atoms, rather than bulk properties of the solid and liquid themselves. The functional dependence of the thermal resistance on the strength of the liquid-solid interactions exhibits two distinct regimes: (i) exponential dependence for weak bonding (non-wetting liquid) and (ii) power law dependence for strong bonding (wetting liquid). The identification of the two regimes of the Kapitza resistance has profound implications for understanding and designing the thermal properties of nanocomposite materials. The effect of liquid layering at the solid liquid interface on the thermal conductivity is also discussed.

This work was supported by U.S. Department of Energy, Office of Basic Energy Sciences, Division of Materials Sciences and Engineering, under Contract No. W-31-109-Eng-38. LX and PK were also supported by the Petroleum Research Fund, Grant No. PRF 36305-G9.

11:30 AM S1.8

NANOSCALE THERMAL TRANSPORT IN COLLOIDAL SUSPENSIONS. Scott Huxtable, Orla Wilson, Blaise Hilton, Giles Siddons, David G. Cahill, Moonsub Shim, and Paul V. Braun, Department of Materials Science and Engineering, University of Illinois at Urbana-Champaign, Urbana, IL.

While thermal transport across solid-solid interfaces has received significant attention in recent years, there has been comparatively little work done on solid-liquid interfaces. We examine nanoscale thermal transport across solid-liquid boundaries using colloidal suspensions of metal nanoparticles and suspensions of single-walled carbon nanotubes. The nanoparticles and nanotubes are heated using subpicosecond optical pulses from a Ti:sapphire mode-locked laser and their thermal decay is measured by examining time resolved changes in optical absorption. Using this pump-probe measurement technique it is possible to determine approximate values of the thermal conductance G across the solid-liquid interfaces. Initial results indicate $G \approx 5 \text{ MW m}^{-2} \text{ K}^{-1}$ for alkanethiol-terminated $\text{Au}_{0.94}\text{Pd}_{0.06}$ nanoparticles in toluene while Au nanoparticles with alkanethiol termination exhibit $G > 20 \text{ MW m}^{-2} \text{ K}^{-1}$. Citrate-stabilized Pt nanoparticles in water were found to possess $G \approx 130 \text{ MW m}^{-2} \text{ K}^{-1}$. These measured values of the interface thermal conductance are within a factor of ≈ 2 of estimates from the diffuse-mismatch model. Initial experiments on the thermal decay of carbon nanotubes in water give a time constant of $\approx 65 \text{ ps}$.

11:45 AM S1.9

IN SITU THERMOOPTICAL STUDIES ON NANO-ALUMINA. Lia A. Stanciu and Joanna R. Groza, Chemical Engineering & Materials Science Department, University of California at Davis, Davis, CA; Friedrich Raether, Ronald Springer, Fraunhofer Institute for Silicate Research (ISC), Wuerzburg, GERMANY.

Recently, a thermo-optical measuring device (TOM) has been developed to in-situ monitor the thermal diffusivity, shrinkage and light scattering of materials during sintering. The initial stage of sintering is difficult to study by conventional methods (e.g., dilatometry) since no shrinkage is detected before the second sintering stage. Densification of nanosize particles indicated enhanced phenomena during early sintering stages. The goal of the present work is to systematically investigate, by in-situ thermo-optical

measurements, the mechanisms involved in the initial stages of sintering of alpha nano-alumina powders. The initial alpha-alumina nanopowders were characterized for particle size by the TEM method, using a Phillips CM-12 microscope, operating at 120kV. The nanocrystalline powders were in-situ measured for thermal diffusivity by TOM, in a temperature range between room temperature and 1300°C, with heating rates of 10 and 15°C/min. The beginning of thermal diffusivity increase started around 250°C. The increase in thermal diffusivity corresponds to the formation of the sintering necks. The thermal diffusivity is proportional with the diameter of the sintering necks, which could be this way calculated. The samples obtained by interrupted sintering experiments under an electric field (FAST method) at 500, 800 and 900°C have been measured for the thermal diffusivity, followed by TEM observation to confirm the indirectly calculated diameter of the sintering necks.

SESSION S2: LATTICE VIBRATIONS OF NANOSTRUCTURES

Chair: Simon R. Phillpot
Tuesday Afternoon, April 22, 2003
Concordia (Argent)

1:30 PM *S2.1

OPTICAL, ELECTRICAL, MECHANICAL, AND THERMAL PROPERTIES OF NANOSTRUCTURES: THE ROLE OF PHONONS IN QUANTUM CONFINED GEOMETRIES.

Michael A. Stroschio, Departments of Bioengineering, Electrical and Computer Engineering, and Physics, University of Illinois at Chicago, Chicago, IL; Mitra Dutta, Departments of Electrical and Computer Engineering, and Physics, University of Illinois at Chicago, Chicago, IL.

This talk will describe how selected optical, electrical, mechanical, and thermal properties of nanostructures are determined by confined phonons and the interactions of these phonons [1]. The talk will highlight the utility of the dielectric and elastic continuum models for describing phonons in nanostructures. In view of their potential device applications, the confined phonon modes in Si-Ge structures will be discussed. As will be discussed, the properties of confined, interface and propagating modes in wurtzite quantum-confined structures may be described theoretically in terms of the dielectric continuum model and Loudons model for uniaxial semiconductors. Moreover, dimensionally-confined acoustic phonon modes in carbon nanotubes and fullerenes may be described in terms of the elastic continuum models. This talk will also describe how the confined optical phonon modes in carbon nanotubes may be modeled in terms of these continuum models. The talk will illustrate how continuum models may be used to describe selected properties in a variety of nanostructures and nanodevices. The work was supported, in part, by AFOSR under grant F49620-021-1-0224.

1. Michael A. Stroschio and Mitra Dutta, Phonons in Nanostructures (Cambridge University Press, Cambridge, 2001).

2:00 PM *S2.2

ANISOTROPIC THERMAL TRANSPORT IN CARBON NANOTUBE ARRAYS. Theodorian Borca-Tasciuc and Claudiu Liviu Hapenciu, Rensselaer Polytechnic Institute, Dept. of Mechanical, Aerospace and Nuclear Engineering, Troy, NY; Bingqing Wei, Robert Vajtai, and Pulickel M. Ajayan, Rensselaer Polytechnic Institute, Dept. of Materials Science and Engineering, Troy, NY.

This work presents experimental measurements of the temperature dependent anisotropic thermophysical properties of aligned carbon nanotube arrays. The multiwalled carbon nanotube films are grown on silicon dioxide membranes deposited on silicon substrates. The thermal characterization technique employs a modulated laser beam incident to one side of the sample to create a thermal wave. The generated thermal wave is detected on the other side by a fast responding temperature sensor. 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. Moreover, the work will explore the effect of carbon nanotube length and annealing temperature on the anisotropic thermal transport properties.

3:00 PM *S2.3

ATOMISTIC SIMULATIONS ON THERMAL CONDUCTIVITY OF NANOSTRUCTURED CARBON BASED MATERIALS. Jianwei Che, Tahir Çağın, William A. Goddard, III, California Institute of Technology, Materials and Process Simulation Center, Pasadena, CA.

We present molecular dynamics studies on the thermal conductivity of carbon based nanostructures. Using the corresponding Green Kubo relation of linear response theory, we evaluated the classical thermal conductivity for various carbon based system, diamond, graphite and nanotubes. We have examined the role of quantum correction to

classical thermal conductivity, and we have found this effect small for these systems. Furthermore, we investigated the isotope effects and influence of vacancy concentration in diamond. Thermal management in nanoscale devices are crucial in nanoscale device design. As a step towards this goal we will report our studies on various nanostructured diamond like systems and carbon nanotubes.

3:30 PM S2.4

ATOMISTIC SIMULATION OF PHONON HOTSPOTS IN SILICON DEVICES. Sanjiv Sinha, Stanford Univ., Dept of Mechanical Engineering, Stanford, CA; Patrick K. Schelling, Simon R. Phillpot, Argonne National Lab, Materials Science Division, Argonne, IL; Kenneth E. Goodson, Stanford Univ., Dept of Mechanical Engineering, Stanford, CA.

As semiconductor devices shrink to scales well below the phonon mean free path, heat generation and transport in the active region of the device exhibit behavior that departs more substantially from simple diffusion theory [1, 2]. Device simulations of short-channel MOSFETs indicate a sharply peaked electric field with increased densities of phonons generated in the drain, a significant fraction being slow optical modes [3]. These factors, along with the disparity in the electron and phonon mean free paths, are expected to cause phonon hotspots in MOSFETs. In this work, we compare the time evolution of non-equilibrium optical and acoustic wavepackets. The wavepacket is constructed from the normal modes obtained using the Stillinger-Weber potential [4, 5]. We model the spatial confinement of the hotspot in an actual device by a Gaussian spread of the wavepacket energy in space such that the energy density corresponds to that in the transistor drain. The initial phonon is chosen such that it has a high scattering probability with conduction electrons in silicon [6]. Molecular dynamics is used to evolve the wavepackets in time. Due to computational constraints, we simulate the dynamics of the wavepacket in a one-dimensional system with $2 \times 2 \times 2000$ cells. Normal mode analysis of the evolved system yields the spread of energy amongst various phonon modes. The initial simulations, carried out in the absence of any background phonons, show that such non-equilibrium phonons essentially disperse without any scattering on the picosecond time scale. Heat generated through optical modes will dissipate slower than that generated through acoustic modes, in direct proportion to their respective group velocities. This behavior is likely to be modified at room temperature that is closer to the actual thermal environment in a device. We intend to explore this regime in our future work and compute scattering rates for the non-equilibrium wavepackets. 1. P.G. Sverdrup, S. Sinha, M. Ashegi, S. Uma, and K.E. Goodson, "Measurement of ballistic phonon conduction near hotspots in silicon," *Appl. Phys. Lett.*, v. 78, pp. 3331-3333, 2001b. 2. S. Sinha and K.E. Goodson, "Phonon heat conduction from nanoscale hotspots in semiconductors," *Proceedings of the 12th International Heat Transfer Conference*, pp. 573-578, Grenoble, France, 2002. 3. E. Pop, S. Sinha, and K.E. Goodson, "Monte Carlo modeling of heat generation in electronic nanostructures," *IMECE*, New Orleans, LA, Nov. 2002. 4. F.H. Stillinger and T.A. Weber, "Computer simulation of local order in condensed phases of silicon," *Phys. Rev. B*, v. 57, pp. 5262-5271, 1985. 5. P.K. Schelling and S. R. Phillpot, "Phonon scattering at a semiconductor interface by molecular-dynamics simulation," *Appl. Phys. Lett.* 80 [14] 2484 (2002) 6. D. Long, "Scattering of conduction electrons by lattice vibrations in silicon," *Phys. Rev.* v. 120, p. 2024, 1960.

3:45 PM S2.5

THERMAL EQUILIBRIUM AND TRANSPORT PROPERTIES OF NANOCRYSTALLINE FCC METALS. P. M. Derlet and H. Van Swygenhoven, Paul Scherrer Institut, Villigen-PSI, SWITZERLAND.

The equilibrium thermal properties of nanocrystalline (nc) materials using molecular dynamics have recently been investigated via the Fourier transform of the velocity-auto-correlation-function (*Phys. Rev. Lett.* 87 205501 (2001)). It was found that the vibrational density of states (VDOS) of the grain boundary region is responsible for the enhanced low and high frequency phonon modes, thus elucidating on the anomalous nc-VDOS previously observed by incoherent thermal neutron scattering experiments. In the present work, we investigate in more detail the nc phonon properties, by directly calculating the onsite and inter-site phonon Greens function derived from large-scale computer generated atomic nc configurations. We investigate this as a function of local grain boundary environment and grain size, and consider the effect of the grain boundary structure on general phonon scattering and the thermal conductivity properties of nc materials.

4:00 PM S2.6

STRAIN EFFECT ON THERMAL CONDUCTIVITY IN NANOSTRUCTURES. Catalin Picu, Theodorian Borca-Tasciuc, Mihai Pavel, Rensselaer Polytechnic Inst, Dept of Mechanical Engineering, Troy, NY.

The relative role of the residual strain and dimensional scaling on the

size effect of lattice thermal conductivity measured in nanostructures is investigated by means of computer simulations. Dimensional reduction down to the nanoscale is typically associated with a marked reduction of the thermal conductivity. At the same time, nanostructures carry elastic strains much larger than those usually found in the bulk material. It is observed that tensile (compressive) strains lead to a reduction (enhancement) of the lattice thermal conductivity. This effect is controlled by the variation of the stiffness tensor, and therefore of the phonon group velocity, with strain. Furthermore, strain influences the lattice anharmonicity and the phonon mean free path. A non-hydrostatic strain induces thermal conductivity anisotropy in the material. However, the strain-induced effect is seen to be much weaker than that due to the reduction of specimen dimensions.

4:15 PM *S2.7

TOWARD CALORIMETRY AND THERMAL TRANSPORT AT THE QUANTUM LIMIT. M.L. Roukes, Department of Physics, Applied Physics, & Bioengineering, California Institute of Technology, Pasadena, CA.

I will describe our investigations with freely-suspended, nanometer-scale semiconductor devices, which enable direct thermal conductance measurements and calorimetry on nanostructures. The ultimate limits of sensitivity for such structures are intriguing, they promise energy resolution at the level of individual phonons. Calorimetry at the single-phonon level has analogs in classical and quantum optics - intriguing possibilities such as phonon shot noise, phonon bunching, anticorrelated electron-phonon relaxation. I will describe the challenges to reaching this regime, and the progress we have made to date, and interesting near-term experiments that can be done along the way. Work in collaboration with Warren Fon, Wonhee Lee, Keith Schwab, and John M. Worlock.

SESSION S3: ELECTRONS AND PHONONS IN NANOSTRUCTURES

Chair: Pawel Koblinski

Wednesday Morning, April 23, 2003

Concordia (Argent)

8:30 AM *S3.1

PHONON DRAG IN CARBON NANOTUBES. Gerald D. Mahan, Dept. of Physics and Materials Research Inst., Penn State University, University Park, PA.

Measurements of the temperature dependence of the Seebeck coefficient in carbon nanotubes shows large values. These large values can be divided into two contributions: (i) a term linear in temperature ($S \sim T$) due to impurity resonances in the density of states, and (ii) a low temperature peak about $T \sim 100$ K. The latter peak was originally identified as a Kondo resonance, due to electron scattering from transition metal impurities used as catalysts in the growth process. Recently we have proposed that the peak is due to phonon drag. The traditional theory of Bailyn has been adopted to the one-dimensional subband structure of the carbon nanotubes, and compared to the experimental measurements of Eklund's group. 1) V.W. Scarola and G.D. Mahan, "The phonon drag effect in single-walled carbon nanotubes", *Phys. Rev. B* 66, 2054XX (2002) 2) H.E. Romero, G.U. Sumanasekera, G.D. Mahan, and P.C. Eklund, "Thermoelectric power of single-walled carbon nanotube films", *Phys. Rev. B* 65, 205410 (2002).

9:00 AM *S3.2

ELECTROTHERMAL PHENOMENA IN NANOTRANSISTORS. Kenneth Goodson, Eric Pop, Sanjiv Sinha, David Campion, and Robert Dutton, Departments of Mechanical and Electrical Engineering, Stanford University.

Modeling heat generation at nanoscales in semiconductors is of great interest and particularly relevant to the heating and reliability of nanoscale transistors [1]. While the phonon Boltzmann Transport Equation (BTE) has been used at such scales, there are complexities associated with the phonon generation and transport that remain unresolved [2]. These are related electron ballistic transport and branch- and polarization-specific phonon generation, as well as the strong departure from equilibrium of the phonon system. This talk summarizes progress on coupled electro-thermal Monte Carlo simulations of nanotransistors, and related measurements of hotspot formation in semiconductors. In the simulations, electrons accelerated by the electric field scatter strongly with optical phonons and heat transport occurs predominantly through acoustic phonons. We account for differing energy transfer rates from electrons to each phonon branch and polarization and use analytical expressions for electron energy bands and the phonon dispersion relationships. This approach focuses on computational efficiency and is applied initially

to a 10 nm fully depleted dual-gate transistor structure. The MC method developed here is extended to 2-dimensional systems, where heat generation rates from the interaction between confined electrons and phonons are analyzed. The method described here is useful for transport situations with high spatial or temporal non-equilibrium between electrons and phonons and particularly facilitates careful microscopic analysis of heating in the drain of a nano-transistor. This talk also summarizes recent work on measuring the sub-continuum thermal resistance near a sub-continuum hotspot in silicon. Measurements at low temperature indicate large deviations from diffusion theory predictions, induced mainly by the departure from equilibrium within the phonon system at lengthscales below the mean free path. The experiments are compared with analytical sub-continuum model derived from the energy moments of the phonon Boltzmann transport equation. Parameters in the model such as the non-equilibrium scattering time of non-zone-center optical phonons are calculated from atomistic simulations. The most recent measurements near room temperature are using heaters and temperature sensors fabricated using electron-beam lithography. The small dimensions are necessary to provide heat generation at dimensions comparable with the room temperature phonon mean free path. The measurements and analysis in this study are assisting with the development of electrothermal simulation tools for advanced semiconductor devices. We appreciate the support of the Semiconductor Research Corporation. [1] E. Pop et al, "Localized Heating Effects and Scaling of Sub-0.18 Micron CMOS Devices", International Electron Devices Meeting 2001 [2] P. Sverdrup et al, "Sub-continuum simulations of heat conduction in silicon-on-insulator transistors", J. Heat Transfer, v. 123, Feb. 2001.

10:00 AM *S3.3

THERMAL TRANSPORT AND THERMOELECTRIC MEASUREMENTS OF NANOTRANSISTORS, NANOWIRES AND SUPERLATTICES. Li Shi, Department of Mechanical Engineering & Center for Nano and Molecular Science and Technology, Texas Materials Institute, The University of Texas at Austin, Austin, TX.

Nanoscale devices and materials exhibit unique thermal and thermoelectric transport properties. For example, ballistic electron and phonon transport phenomena influence device characteristics of nanotransistors and raise intriguing questions regarding the heat dissipation mechanisms. In addition, enhancement of thermoelectric figure of merit has been predicted for low dimensional materials including superlattices of quantum wells, wires, and dots. Recent experimental works have supported the theoretical predictions and generated tremendous interest in this field. We have developed various nanoscale characterization methods based on scanning probe microscopy (SPM) and MEMS fabrication techniques. These methods include scanning thermal microscopy (SThM) for mapping surface temperature distribution of nanoelectronic devices, ultra-high-vacuum (UHV) scanning thermoelectric microscopy (SThEM) for profiling Seebeck coefficient of superlattices, and a suspended micro device for measuring thermal conductivity, electrical conductivity, Seebeck coefficient of various nanotubes, nanowires, and nanobelts. Recent measurement results using these methods will be discussed.

10:30 AM *S3.4

NANOSCALE HEAT CONDUCTION IN GIANT MAGNETORESISTIVE (GMR) TECHNOLOGY. Yizhang Yang^a, Shu Zhang^a, Katayun Barmak^b, Mehdi Asheghi^a; ^aDepartment of Mechanical Engineering; ^bMaterials Science and Engineering Department, Carnegie Mellon University, Pittsburgh, PA.

GMR technology makes use of multilayer metallic films, comprising for example Co, Cu, and FeCo, with repeat thicknesses of less than 1 nm. The focus of the present work is the study of nanoscale heat conduction in two areas of GMR technology namely in sensors for magnetic read heads, and in magnetoresistive random access memory (MRAM). The former is a well-established commercial technology, in which nanoscale thermal transport not only affects reliability - through electrostatic damage (ESD), but also performance. In MRAM, a more nascent technology, thermal transport clearly limits ultimate device performance, but may in fact present an opportunity for thermally assisted switching. Thus, GMR technology can significantly benefit from a more in-depth understanding of thermal transport in GMR multilayers. In this paper, we present the first comprehensive thermal characterization of Cu/CoFe_n GMR multilayers (10 < n < 40 repeated bi-layers) as a function of temperature (4-450 K) and thickness (50-100 nm). The experimental data will be examined using the semi-classical approach.

SESSION S4: IN-ROOM POSTER SESSION

Chair: Pawel Keblinski
 Wednesday Morning, April 23, 2003
 11:00 AM
 University (Argent)

S4.1

EFFECTS OF INTERFACE SCATTERING AND OPTIC PHONON DRAG ON THE THERMAL CONDUCTIVITY OF SELECTED SEMICONDUCTORS. Alexander I. Chervanyov, Pittsburgh Univ., Dept. of Chemical Engineering, Pittsburgh, PA.

The effects of boundary scattering and normal phonon collisions on the lattice thermal conductivity of a semiconductor slab of rectangular cross-section are investigated. The approximate kinetic equation for acoustic phonons is derived from the exact kinetic equations for the binary phonon gas in a confined geometry. Both effects of the interface phonon scattering and the optic phonon drag are taken into account. It is shown that a proper account of these effects gives rise to a violation of Matthiessen's rule. The derived kinetic equation is solved rigorously with the diffuse boundary conditions. The obtained solution is used to calculate the coefficient of thermal conductivity for some model phonon energy-momentum relations. The obtained results are used to calculate the effect of normal phonon collisions on the thermal conductivity of GaAs, Si, Ge and the GaAs/AlAs superlattice. It is found that this effect gives rise to a significant increase in the thermal transport of the considered materials. It is also shown that the neglectance of the normal phonon collisions in the conventional theories leads to the overestimation of the phonon mean free path. This, in turn, causes the underestimation of the role of the bulk scattering in thermal conductivity of quantum well structures. The proper simultaneous treatment of the interface scattering and the drag effect leads to a new understanding of the considered phenomena in the framework of the developed approach. A comparison with the experimental results and former theories is presented.

S4.2

QUANTUM DOT CRYSTALS AS PERSPECTIVE MATERIALS FOR THERMOELECTRIC APPLICATIONS. Olga L. Lazarenkova and Alexander A. Balandin, Nano-Device Laboratory, Department of Electrical Engineering, University of California-Riverside, Riverside, CA.

Under certain conditions quantum dots (QDs) may form highly regimented three-dimensional (3D) quantum dot arrays characterized by unique carrier and phonon spectra [1-2]. We refer to such novel nanostructured materials as quantum dot crystals (QDC). By changing the size of QDs, inter-dot distance and dot regimentation one can tune both electron [1] and phonon [2] spectra of QDC. In this presentation we demonstrate that thermoelectric properties of such structures can also be significantly enhanced. The thermoelectric figure of merit improves when electrical conductivity and thermoelectric power increase while thermal conductivity decreases. In this work we numerically calculate both carrier and phonon spectra, which determine the thermoelectric characteristics of the material. The interaction between regimented quantum dots leads to splitting of discrete electron energy levels of single QD and formation of the mini-bands. It results in nonlinear electrical conductivity and electron part of thermal conductivity as well as sign switching of the thermoelectric power. The latter means that the same material can be utilized for both legs of the thermoelectric device. On the other hand, the existence of 3D periodic scatters, e.g. QDs, leads to folding of acoustical phonon modes, formation of mini-gaps, and emergence of the low-energy quasi-optical modes. This results in reduction of the phonon part of thermal conductivity. These factors lead to the enhancement of thermoelectric figure of merit. Together with an additional benefit of using the same type of QDC for both legs of thermoelectric device it makes QDC very attractive as perspective materials for thermoelectric applications. This work has been supported by the NSF Nanoscale Exploratory Research project ECS-0210282 and NSF CAREER Award to A.A.B. [1]. O.L. Lazarenkova and A.A. Balandin, J. Appl. Phys., 89, 5509 (2001). [2]. O.L. Lazarenkova and A.A. Balandin, Phys. Rev. B (to appear, 2002).

S4.3

STRUCTURAL ASPECTS OF HEAT FLOW MONITORING IN NON-METALLIC NANOMATERIALS. Valery Shklover, Laboratory of Crystallography, Swiss Federal Institute of Technology, Zuerich, SWITZERLAND; Leonid Braginsky, Institute of Semiconductors, Novosibirsk, RUSSIA; Heinrich Hofmann, Laboratory of Powder Technology, Swiss Federal Institute of Technology, Lausanne, SWITZERLAND.

Using literature and original data, the structural regularities of nanomaterials and nanodevices, designed for heat monitoring are discussed. At first, the design of nanomaterials for phonon propagation in the disordered media at a high temperature (about the Debye temperature or higher) is considered. Scattering on the grain boundaries is assumed to be the main mechanism restricting heat conductivity. The use of the model for structure monitoring of the heat conductivity is suggested (change of grain size and its dispersion, sintering, pore diameter and their volume concentration, and intergrain interface structure). The numerical results obtained using

our model are compared with experimental results on heat conductivity in nanocrystalline alumina. The extension of the model to medium and low temperatures is discussed, when the wavelength of the phonons, responsible for the heat transport, is about or exceeds the particle size. The new applications may include ordered anisotropic multilayered nanoarrays and nanoarrays immersed in selected matrix. The structure conditions of formation of sandwich superlattice structures built of alternating layers and possessing anisotropic heat conductivity and "mini-zones" in direction normal to the layers are considered. The structural peculiarities and phonon spectra of high-heat conductivity low-dimensional nanomaterials (graphite, carbon nanotubes and others) are discussed. Carbon nanotubes may exhibit metallic or semiconducting properties, depending on the crystal structure. The thermal and topographic STM images of electrically heated both multiwall and single wall carbon nanotubes have revealed the temperature profile along the carbon tubes, characteristic of electron transport. Our own data on precision structural studies of nanomaterials with potential for phononic applications will be reported.

S4.4
FEATURES OF ELECTRON TRANSPORT IN Bi-NANO AND MICROBRIGES. Albina Nikolaeva^a, Dmitrii Gitsu, Alexandr Burchakov, Institute of Applied Physics, Academy Sciences of Moldova, Chishinau, MOLDOVA. ^aInternational Laboratory of High Magnetic Fields and Low Temperatures, Wroclaw, POLAND.

Conductivity of low-dimensional structures, at low temperatures is connected to effects of weak localization and interelectron interaction. Increase of interelectron interaction at diffusive movement of electrons leads to appearance of a peculiarity in the density of states at the Fermi level and to the conductivity change connected to this. In the work current-voltage characteristics (CVC) and the resistance temperature dependences $R(T)$ of micro- and nanobridges based on bismuth were studied. Bismuth based micro- and nanobridges were obtained by local heating of thin ($1\mu < d < 5\mu$) glass-covered single crystal bismuth wire by a laser beam. The length and thickness of the bridge was regulated by intensity and velocity of the laser beam displacement. The resistance of the structure microbridge-single crystal Bi wire being "shores" of the microbridge was 5-15 kOhm. In the low temperature region the resistance was $R_T/R_{300} < 1$. On the dependences of the differential conductivity $\Delta G = dI/dV$ at 4.2 K the minimum at the displacement voltage $V=0$ was found. The zero anomaly had symmetrical form, and in the initial region of voltages $\Delta G \sim \ln V$ with transition to the root dependence $\Delta G \sim V^{1/2}$ with the displacement voltage increase. The region of the transition from the logarithmic to the root dependence corresponded to the predictions of the theory of interelectron interaction at transition from the quasi-one-dimensional 1d to the three-dimensional 3d case. This work is support by Civilian Research and Development Foundation for the Independent States of the Former Soviet Union (CRDF) # MP2 - 3019.

S4.5
ELECTRON TRANSPORT IN Bi-0.02Sn WIRES BY ELASTIC ELONGATION. Tito E Huber, Department of Chemistry, Howard University, WA; Albina Nikolaeva, Dmitrii Gitsu and Leonid Konopko, Institute of Applied Physics, Academy of Sciences of Moldova, Chishinau, MOLDOVA.

The work is devoted to investigation of electric and thermoelectric properties of Bi-0.02at%Sn wires with $d \geq 100$ nm under elastic stretch up to $\xi = 2-3\%$ relative elongation. The wires were high quality glass-coated single crystals, their axis make up angle $\sim 19.5^\circ$ with the bissector axis C° in bissector trigonal plane. In the undeformed state at 4.2 K the ShdH oscillations were registered, this allowed to find that the Fermi level is located in the band gap e_{gL} , i.e. the Fermi surface consists of one hole ellipsoid in T. Under elastic stretch, in the result of the hole ellipsoid L_1 rising above the Fermi level followed by lowering of electron ellipsoids $L_{2,3}$ below e_F , the electron topological transition occurs. The current - voltage characteristics, magnetoresistance $R(H)$, thermopower, $\alpha(T)$, resistance $R(T)$ at the electron topological transition depending on the wire diameter d were investigated. The peculiarities shown in the absence of the Longitudinal Magnetoresistance maximum in initial magnetic field, at $\xi=0$ and its appearance at $\xi=2,3\%$, growth of the LM non-characteristic of metal with one type of carriers, the thermopower sign inversion with temperature and stretch, anomalous dependence of the resistance $R(T, \xi)$ are explained by both the size effect manifestation and actuality of the intervalley scattering processes and the electron topological transition. This work is support by Civilian Research and Development Foundation for the Independent States of the Former Soviet Union (CRDF) # MP2 - 3019.

S4.6
APPLICATION OF DIAMOND THIN FILMS FOR THERMAL MANAGEMENT IN Si-BASED ELECTRONICS. N. Govindaraju,

S.D. Wolter, F. Okuzumi and Z. Sitar, North Carolina State University, Dept of Materials Science and Engineering, Raleigh, NC; J.T. Prater, Army Research Office, Research Triangle Park, NC.

Diamond has many alluring thermal, electronic and optical properties. Although the epitaxial growth of diamond proves elusive, thereby stifling full fledged electronic applications, the high thermal conductivity and breakdown voltage make it attractive for application as a heat sink and insulator in microelectronic circuits. Steady state thermal conductivity measurements are performed on diamond samples of various microstructures by employing an array of thin film thermocouples along with a thin film heater. The experimental set up is calibrated by performing measurements on substrate materials of known thermal conductivity. Experimental results are presented for polycrystalline, textured, and highly oriented diamond (HOD) films grown on silicon by Microwave Plasma Chemical Vapor Deposition (MPCVD) using bias enhanced nucleation. In addition, polysilicon resistors and field effect transistors are fabricated on these diamond films to compare thermal properties with respect to similar devices on silicon on insulator (SOI) employing silicon oxide.

SESSION S5: INTERFACES AND SUPERLATTICES
 Chair: Arunava Majumdar
 Wednesday Afternoon, April 23, 2003
 Concordia (Argent)

1:30 PM *S5.1
THERMAL TRANSPORT AND PHONON DYNAMICS IN SEMICONDUCTOR NANOSTRUCTURES. P.K. Schelling and S.R. Phillpot, Materials Science Division, Argonne National Laboratory, Argonne, IL.

As the physical dimension of electronic devices continues to shrink, thermal management is becoming an increasingly important issue. To understand thermal transport in nanostructures, it is necessary to consider the regime where the phonon wavelength and mean free path are comparable to the system dimensions. Due to such phonon confinement and wave interference effects, thermal transport in semiconductor nanostructures is very different from bulk systems. To describe thermal transport in semiconductor nanostructures, we have developed molecular-dynamics simulation methods to determine the Kapitza conductance of interfacial and grain boundary systems. Moreover, we have developed methods that use phonon wave packet dynamics to elucidate the fundamental processes of phonon scattering at interfaces and grain boundaries. This allows us to develop a deeper understanding of scattering and thermal transport in interfacial systems. We have also used phonon wave packet dynamics in a multiscale approach to thermal transport. In this approach, phonon wave packet dynamics are used to obtain information on phonon scattering that is then used to parameterize a particle-type approach to thermal transport, where the particles represent phonon wave packets. We have also demonstrated that standard particle type approaches that neglect wave interference effects often cannot be used to describe thermal transport in semiconductor nanostructures. To address this shortcoming, we have developed a simple approach to incorporate interference effects in a particle model.

2:00 PM *S5.2
EXPLORING NANOSCALE HEAT TRANSFER EFFECTS FOR ENERGY CONVERSION. Gang Chen, Massachusetts Institute of Technology, Mechanical Engineering Department, Cambridge, MA.

Nanostructures have profound impacts on the transport of heat and energy carried by phonons, electrons, and photons. In this paper, we will discuss some of the nanoscale heat transfer effects on the phonon and photon transport and their implications for thermoelectric and thermophotovoltaic energy conversion technologies. For example, low thermal conductivity materials with good electrical properties are required in solid-state refrigerators and power generators for high energy-conversion efficiency. Size effects on phonon transport in nanostructures can be utilized to engineer new structures with improved energy conversion efficiency. Thermal conductivity of superlattices will be used to illustrate the phonon transport characteristics in nanostructures. In another example, we will discuss some nanoscale thermal radiation phenomena, such as interference, tunneling, and surface waves, that can potentially be exploited to improve the efficiency of thermophotovoltaic power generation devices.

2:30 PM S5.3
THERMAL CONDUCTANCE OF EPITAXIAL INTERFACES. Ruxandra Costescu, Marcel Wall, David Cahill, Department of Materials Science and Engineering, Coordinated Science Laboratory and Materials Research Laboratory, University of Illinois, Urbana, IL.

To better understand thermal transport across solid-solid interfaces -

a significant issue for nano-devices and nanostructures – we investigated the thermal conductance of interfaces between epitaxial TiN and single crystal oxides. We measured TiN/MgO(001), TiN/MgO(111) and TiN/Al₂O₃ at temperatures between 79.4 and 294 K using the picosecond thermoreflectance technique with a highly efficient optical design. For more accurate data analysis, we employed a new method that relies on the ratio of the in-phase and out-of-phase signals of the lock-in amplifier. The validity of this approach was verified by measuring the thermal conductivity of 6.5, 11.8, and 25 nm thick thermally oxidized SiO₂ on Si. The thermal conductances of TiN/MgO(001), TiN/MgO(111) and TiN/Al₂O₃(0001) are essentially identical despite expected differences due to the varying degree of misfit dislocations and stacking faults present at these interfaces. Significantly, the conductance data is in good agreement with predictions based on lattice dynamics and diffuse mismatch models with a four-atom fcc unit cell. Near room temperature, our experimental thermal conductance is $\sim 700 \text{ MW m}^{-2} \text{ K}^{-1}$, ~ 5 times larger than the highest values reported previously for any individual interface.

3:15 PM S5.4

THERMAL RESISTANCE OF GRAIN BOUNDARY SUPER-LATTICES: A MOLECULAR DYNAMICS SIMULATION. L. Xue, P. Keblinski, Materials Science and Engineering Department, Rensselaer Polytechnic Institute, Troy, NY; P.K. Schelling, and S.R. Phillpot, Materials Science Division, Argonne National Laboratory, Argonne, IL.

Using non-equilibrium molecular dynamics simulations and an empirical Tersoff potential parameterized for carbon, we studied heat flow across multiple planar grain boundaries (GBs) in crystalline diamond. For systems involving equally spaced GBs we observed an increase of GB thermal resistance with increasing number of GBs. However, once the number of GB became larger than ~ 5 , additional GBs led to very little increase of the overall resistance of the superlattice. We discuss the effect of GB spacing on thermal resistance and differences between microstructures involving equally and randomly spaced GBs.

LX and PK acknowledge support from the Petroleum Research Fund, Grant No. PRF 36305-G9. PS and SP are supported by the U.S. Department of Energy, under Contract No. W-31-108-Eng-38.

3:30 PM S5.5

ACOUSTIC PHONON SPECTRUM MODIFICATION IN NANOSTRUCTURES AND ITS EFFECT ON LATTICE THERMAL CONDUCTIVITY. A.A. Balandin and O.L. Lazarenkova, Univ of California, Nano-Device Laboratory, Department of Electrical Engineering, Riverside, CA.

The feature size of conventional electronic devices has already fallen below the acoustic phonon mean free path (MFP) in silicon, which is estimated to be 50 nm - 300 nm at room temperature. The lateral dimensions of nanowires and the size of quantum dots in quantum dot superlattices (QDS) fabricated by different self-assembly techniques are approaching the wavelength of a dominant phonon mode, which is on the order of 1 nm - 2 nm at room temperature. As the feature size of nanostructures that consist of elastically dissimilar materials becomes smaller than MFP and approaches the length scale of the thermal phonon wavelength one can expect a significant modification of the acoustic phonon spectrum, e.g. flattening of dispersion branches and mini-band formation. This modification, in its turn, affects the lattice thermal conductivity via enhanced phonon relaxation rates [1] or reduction of phonon density of states in the relevant frequency range. In this talk we theoretically investigate phonon spectrum modification in arrays of semiconductor nanowires and three-dimensional regimented arrays of quantum dots, e.g. quantum dot superlattices (QDS). We present new results for QDS obtained without simplifying assumptions of free- or clamped surface boundary conditions [2]. We argue that phonon spectrum for nanostructures that consists of regimented and closely spaced quantum dots deviates significantly from the predictions based on Lamb's model. It is shown that strong modification of acoustic phonon spectrum is accompanied by the decrease of the phonon group velocity and corresponding decrease of the lattice thermal conductivity. For model validation, we calculate Raman peak positions for QDS and compare them with available experimental data. This work was supported by the NSF CAREER Award to A.A.B. and AFOSR subcontract F49620-02-0002. [1]. A. Balandin and K.L. Wang, Phys. Rev. B, 58, 1544 (1998). [2]. O.L. Lazarenkova and A.A. Balandin, Phys. Rev. B (to appear, 2002).

3:45 PM S5.6

CONCURRENT COMPUTATIONAL AND EXPERIMENTAL INVESTIGATION OF THERMAL ENERGY TRANSPORT BY PHONONS. Edward Piekos, Samuel Graham, C. Channy Wong, Sandia National Laboratories, Albuquerque, NM.

A concurrent computational and experimental investigation of thermal transport is undertaken with the goal of elucidating transport behavior in phonon-phonon and phonon-boundary scattering through manipulation of test conditions. The computational component involves Monte Carlo simulation of phonon transport. In these simulations, all acoustic modes are included and their properties are drawn from a realistic description of the dispersion relation. Phonon-phonon and phonon-boundary scattering events are treated independently. A new set of phonon-phonon scattering coefficients are proposed that reflect the elimination of assumptions present in earlier analytical work. The experimental component involves steady-state measurement of thermal conductivity on single-crystal silicon films as thin as 340 nm at a range of temperatures. Initial agreement between simulation and experiment is excellent. In the future, more complex materials will be tested and sub-models will be added to the simulation, each guiding the other to build understanding of the underlying physical phenomena.

4:00 PM S5.7

ANALYSIS OF RADIATIVE HEAT TRANSFER BETWEEN PERIODICALLY PLACED EMITTERS AND RECEIVERS. Arvind Narayanaswamy and Gang Chen.

Photon thermal radiation exchange between closely spaced surfaces can be significantly altered due to various proximity effects such as interference, tunneling, and surface wave coupling. These effects have been studied in the past for radiation heat transfer between closely spaced planar surfaces. In this work, we explore the effects of periodicity, in addition to the proximity effects, on the radiation heat transfer. Photon thermal radiation exchange between periodic, closely spaced emitters and receivers are considered. Appropriate periodic arrangement of dielectrics (or metallic material) into a photonic crystal can result in forbidden regions in the electromagnetic spectrum within the structure. In addition, by spacing the emitters and receivers in the near field, we can enhance the transfer due to tunneling and surface mode coupling. Fluctuation and dissipation theorem, coupled with the Green function method, is used to simulate the photon radiation exchange. Results of this study have interesting implications for developing high efficiency thermophotovoltaic energy converters.

4:15 PM S5.8

THERMAL DIFFUSIVITY EVALUATION IN STRONTIUM COMBINATORIAL LIBRARY COMPRISING La_{1-x}Sr_xCoO₃ USING TRANSIENT GRATINGS CONFIGURATION OF NANOSCALE. Yoshiaki Takata, Hajime Haneda, Yutaka Adachi, Yoshiki Wada, Takefumi Mitsuhashi, Advanced Materials Laboratory, NIMS, Tsukuba, JAPAN; Makoto Ohtani, Tomoteru Fukumura, Masashi Kawasaki, Tohoku University, Sendai, JAPAN; Hideomi Koinuma, Tokyo Institute of Technology, Yokohama, JAPAN.

Composition spreads of La_{1-x}Sr_xCoO₃ (LSCO) were synthesized as thermo-electric transducer material by means of combinatorial material synthesis, and information on their thermal diffusivity throughout the specimens was obtained by transient gratings configuration space-time of nanoscale with spatially and temporally higher resolving power. Meanwhile, the most important problem which confronts this study is to make interference fringes by matching properly timing of two pumping pulses (wavelength; 266 nm) on the surface of a sample specimen, wherein the focused size of the pumping beam is a few tens of micrometer if visible. We succeeded in making interference fringes on the surface of SrTiO₃ substrate in this study at last. Our results showed that the value of thermal diffusivity of SrTiO₃ surface was 0.05 cm²/s close to 0.04~0.026 cm²/s, reference value by Laser Flash technique. Furthermore, the values of thermal diffusivity of the library changed at between 0.3 < Sr content < 0.7, similar to our former results.