8th US-Japan Joint Seminar on Nanoscale Transport Phenomena
- Science and Engineering -

Sponsored by
National Science Foundation, USA
Japan Society for the Promotion of Science

With additional support from
Western Digital Corporation
Seagate Corporation

July 13-16, 2014

Chaminade Resort, Santa Cruz, CA, USA

Co-Chairs

US: Chris Dames, University of California, Berkeley
Pramod Reddy, University of Michigan, Ann Arbor

Japan: Yuji Nagasaka, Keio University
Hirofumi Daiguji, The University of Tokyo

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Program Overview

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8.00 – 9.40	**Opening Session & Plenary Talks**
9.50 – 11.00	**Thermal Transport**
11.10 – 12.35	**Thermal Transport**
12.35 – 14.00	**Lunch** buffet in the Sunset Restaurant, included for all conference participants
14.00 – 15.40	**Thermal Transport in 1D and 2D Structures**
15.50 – 17.15	**Radiative Heat Transfer**
17.30 – 18.30	**Expert Panel/Discussion** (Industry, Academia, Funding Agencies)
18.30 – 19.15	**Dinner** buffet in the Sunset Restaurant (free to participants lodging at the Chaminade)
19.15 – 21.00	**Poster Session**

Tuesday, July 15th

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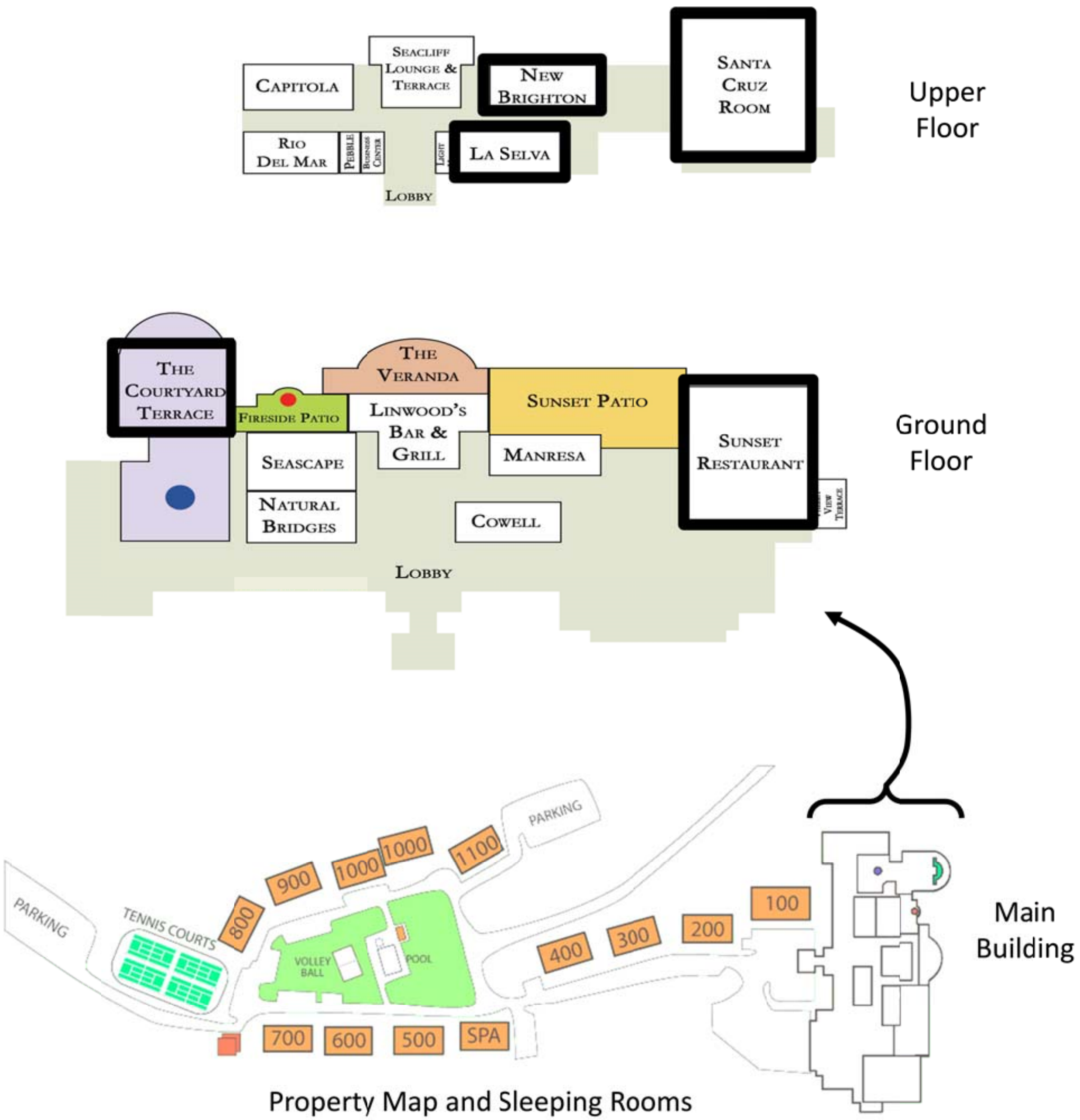
9.35 – 11.00	**Nanoscale Heat Transfer**
11.10 – 12.30	**Thermal Management**
12.30 – 14.00	**Lunch** buffet in the Sunset Restaurant, included for all conference participants
14.00 – 15.25	**Experimental Techniques**
16.00 – 20.00	**Excursion & Conference Dinner** (included for all participants)

Wednesday, July 16th

7.00 – 8.00	**Breakfast** buffet in the Sunset Restaurant. Free to participants lodging at Chaminade.)
8.00 – 9.35	**Nanoscale Transport Phenomena**
9.45 – 11.10	**Energy Conversion**
11.20 – 12.30	**Applications**
12.30 – 13.00	**Closing Remarks**
13.00 – 14.15	**Lunch** buffet in the Sunset Restaurant, included for all conference participants
	End of the Seminar

Map of the Chaminade Hotel

Main Venue: Santa Cruz Room
Poster Session: New Brighton & La Selva Rooms
Buffet Meals: Sunset Restaurant
Banquet: Courtyard Terrace
Address: 1 Chaminade Lane, Santa Cruz CA 95065. Front Desk Phone: 831-475-5600



Sunday, July 13th

17.30 - 21.00 **Buffet dinner in the *Sunset Restaurant*** (free to participants lodging at the Chaminade).

17.00 - 22.30 Dinner available at *Linwood's Bar & Grill Restaurant* (not included with lodging).

Monday, July 14th

(7.00 - 8.00 **Breakfast** buffet in the Sunset Restaurant. Free to participants lodging at the Chaminade.)

8.00 - 9.40 **Opening Session & Plenary Talks**

8.00 – 8.05 **Welcome Remarks by the Chairs**

8.05 – 8.20 Introductory remarks by **A. Majumdar**

8.20 – 9.00 Plenary Talk 1 **G. Chen** (Ballistic, coherent, and quantum heat conduction)

9.00 – 9.40 Plenary Talk 2 **S. Maruyama** (Carbon nanotube-Si heterojunction solar cells)

(9.40 - 9.50 Break)

9.50 – 11.00 **Thermal Transport**

Chair: **Jon Malen**

9.50 – 10.15 **Keynote: M. Nomura (**From photonic to phononic-thermal conduction control by phononic crystal nanostructures**)**

10.15 – 10.30 **J. Shiomi (**Phonon transport calculations of crystals with strong anharmonicity, disorders, interfaces, and nanostructures**)**

10.30 – 10.45 **P. Norris** (Alloys and amorphous materials: the microstructure and thermal conductivity)

10.45 – 11.00 **I. Kinefuchi (**New formulation of dissipative particle dynamics: Non-Markovian models**)**

(11.00 - 11.10 Break)

11.10 – 12.35 **Thermal Transport**

Chair: **M. Kohno**

11.10 – 11.35 **Keynote: D. Cahill** (Coupling of heat and spin currents in cuprates and metallic multilayers)

11.35 – 11.50 **C. Dames (**Heat Transfer in Non-Linear and Highly Anisotropic Systems**)**

11.50 – 12.05 **G. Kikugawa (**Molecular dynamics viewpoint on heat transfer characteristics of self-assembled monolayers and polymeric substances**)**

12.05 – 12.20 **R. Yang (**Thermal conductivity of polymer and hybrid organic-inorganic thin films**)**

12.20 – 12.35 **T. Shiga** (Anomalous lattice dynamics of lead telluride arising from strong anharmonicity)

12.35 – 14.00 **Lunch**. Buffet in the Sunset Restaurant, free to all conference participants.

14.00 – 15.40 **Thermal Transport in 1D and 2D Structures**

Chair: **K. Miyazaki**

14.00 – 14.25 **Keynote: L. Shi (**Phonons in higher manganese silicides of complex Nowotny chimney ladder phases**)**

14.25 – 14.40 **A. Narayanaswamy (**Measurement of heat flow though polymeric nanostructures using the dual cantilever technique: Thermo-mechanical response and teasing out the thermal part**)**

14.40 – 14.55 **D. Li (**Non-intrinsic Sharvin resistance between nanostructures**)**

14.55 – 15.10 **E. Pop** (Ballistic to diffusive thermal transport in two-dimensional materials and devices)

15.10 – 15.25 **A. McGaughey (**Thermal transport across organic-inorganic interfaces**)**

15.25 – 15.40 **R. Chen (**Thermal and thermoelectric transport in nanostructures**)**

(15.40 - 15.50 Break)

15.50 – 17.15 **Radiative Heat Transfer**

Chair: **J. Shiomi**

15.50 – 16.15 **Keynote: Z. Zhang (**Near-field radiative transfer enhanced by Graphene covered nanostructures**)**

16.15 – 16.30 **K. Hanamura (**Spectral control of near-field radiation transfer using pillar array structured surface**)**

16.30 – 16.45 **P. Reddy (**Effect of film thickness on near-field thermal transport**)**

16.45 – 17.00 **J. Duda (**Nanometer-scale thermal phenomena in heat-assisted magnetic recording**)**

17.00 – 17.15 **M. Morelli** (Nano-thermal consideration for heat assisted magnetic recording (HAMR)

(17.15 - 17.30 Break)

17.30 – 18.30 **Expert Panel/Discussion** (Industry, Academia, Funding Agencies).

18.30 – 19.15 **Dinner.** Buffet in the Sunset Restaurant (free to participants lodging at the Chaminade).

19.15 – 21.00 **Poster Session**

Tuesday, July 15th

(7.00 - 8.00 **Breakfast** buffet in the Sunset Restaurant. Free to participants lodging at the Chaminade.)

8.00 – 9.10 **Nanofluidics**

Chair: **A. Schmidt**

8.00 – 8.25 **Keynote: Y. Kazoe** (Spatially-resolved measurement of nanochannel flows by evanescent wave-based particle tracking**)**

8.25 – 8.40 **P. Phelan (**The effective latent heat of aqueous nanofluids**)**

8.40 – 8.55 **H. Daiguji (**Adsorption and transport of water in mesoporous silica**)**

8.55 – 9.10 **K. Fushinobu (**On the oxygen transport in cathode catalyst layer of PEFCs**)**

9.10 – 9.25 **D. Irima (**Self-generated chemical gradients guide the migration of cancer cells**)**

(9.25 – 9.35 Break)

9.35 – 11.00 **Nanoscale Heat Transfer**

Chair: **A. Minnich**

9.35 – 10.00 **Keynote: T. Tokumasu (**Study on Transport Phenomena of Reaction Materials in Fuel Cell by Quantum/Molecular Dynamics Method**)**

10.00 – 10.15 **J. Massen (**Novel Approach to Ballistic Phonon Transport**)**

10.15 – 10.30 **T. Yabuki (**MEMS Measurements of boiling heat transfer with a single bubble**)**

10.30 – 10.45 **J. Bischof (**Nanoparticle heat transfer for biomedical applications**)**

10.45 – 11.00 **K. Takahashi (**Experimental investigations of nanodroplets and nanobubbles**)**

(11.00 – 11.10 Break)

11.10 – 12.30 **Thermal Management**

Chair: **K. Takahashi**

11.10 – 11.35 **Keynote: K. Goodson (**Nano thermal management beyond 50 kW/cm2**)**

11.35 – 11.50 **J. Lukes** (One-way phonon isolation in acoustic waveguides)

11.50 – 12.15 **Keynote 2: K. Uchida (**Thermal-aware device design of advanced nanoscale electronic devices**)**

12.15 – 12.30 **M. Kohno (**Reduction in thermal conductivity of silicon processed by high-pressure torsion**)**

12.30 – 14.00 **Lunch.** Buffet in the Sunset Restaurant, free to all conference participants.

14.00 – 15.25 **Experimental Techniques**

Chair: **M. Nomura**

14.00 – 14.25 **Keynote: D. Reis (**Fourier transform inelastic x-ray scattering: a new tool for measuring phonon dispersion and more with a free-electron laser**)**

14.25 – 14.40 **O. Delaire (**Investigations of microscopic energy transport with Neutron and X-Ray Scattering (IA)**)**

14.40 – 14.55 **Y. Nagasaka (**Accurate instrument for measuring the surface tension, viscosity and surface viscoelasticity of liquids using ripplon surface laser-light scattering with tunable wavelength selection**)**

14.55 – 15.10 **J. Malen (**Analytical solutions to the BTE, to interpret MFP spectroscopy in FDTR and TDTR**)**

15.10 – 15.25 **A. Minnich (**Uncovering and engineering the thermal phonon spectrum**)**

(15.25 – 16.00 Break)

16.00 – 20.00 **Excursion & Conference Dinner** (free for all participants).

Meet Buses at 16.00 by the main Chaminade lawn (by spa and outdoor pool), for a group tour of the Soquel-Bargetto Winery. After returning to Chaminade, the Conference Banquet will be held at the Courtyard Terrace in the main building.

Wednesday, July 16th

(7.00 - 8.00 **Breakfast** buffet in the Sunset Restaurant. Free to participants lodging at the Chaminade.)

8.00 – 9.35 **Nanoscale Transport Phenomena**

Chair: **H. Daiguji**

8.00 – 8.25 **Keynote: A. Shakouri (**Superdiffusive heat transport in semiconductors**)**

8.25 – 8.50 **Keynote 2: R. Matsuda (**Selective gas adsorption in the nanospace of flexible metal-organic frameworks**)**

8.50 – 9.05 **S. Shen (**Thermal and elastic properties of crystalline polymer nanostructures**)**

9.05 – 9.20 **A. Endo (**Synthesis and characterization of mesoporous materials for energy-efficient adsorption systems**)**

9.20 – 9.35 **A. Schmidt (**Thermal property measurement of nanoscale films with frequency-domain thermoreflectance**)**

(9.35 – 9.45 Break)

9.45 – 11.10 **Energy Conversion**

Chair: **Y. Murakami**

9.45 – 10.10 **Keynote: P. Allen** (Size effects in thermal conduction by phonons)

10.10 – 10.25 **D. Broido (**Phonon thermal transport in BAs nanowires from first principles**)**

10.25 – 10.40 **K. Miyazaki (**Printable thermoelectric materials**)**

10.40 – 10.55 **S. Sinha (**Parsing the Seebeck coefficient: The effect of Non-equilibrium)

10.55 – 11.10 **S. Inoue (**Mass spectroscopy of intermediates observed in carbon nanotube synthesis**)**

(11.10 – 11.20 Break)

11.20 – 12.30 **Applications**

Chair: **S. Shen**

11.20 – 11.45 **Keynote: Y. Murakami (**Kinetics of triplet-sensitized photon upconversion in ionic liquids for utilizing wasted solar photons**)**

11.45 – 12.00 **C. Hogan (**Microscopy based inference of nanoscale aggregate morphologies: Applications in nanomedicine and aerosol science**)**

12.00 – 12.15 **T. Zolotoukhina (**Vibrational spectra in the study of molecular interactions in transient molecular dynamics simulation. Application to the van der Waals interaction of nucleobases with graphene**)**

12.15 – 12.30 **S. Chiashi (**Fabrication of semi-conducting single-wall carbon nanotube array**)**

12.30 – 13.00 **Closing Remarks (Li Shi)**

13.00 – 14.15 **Lunch.** Buffet in the Sunset Restaurant, free to all conference participants.

End of the seminar.

Oral Presentation Abstracts

In Chronological Order

Ballistic, Coherent, and Quantum Heat Conduction

Gang Chen[1]

[1]*Mechanical Engineering Department*
Massachusetts Institute of Technology, Cambridge, MA 02139

In this talk, I will start with a discussion on ballistic transport in both bulk materials and nanostructures, and move on to discuss signatures of coherent and quantum heat conduction. We develop phonon mean free path spectroscopy techniques by exploring quasi-ballistic heat transfer around nanoscale heat sources. We measure the thermal conductivity of short-period superlattices and observed that their thermal conductivity increased linearly with increasing total superlattice thickness over a temperature range from 40 to 300 Kelvin. We interpret this trend as a result of the coherent phonon heat conduction process. This interpretation is supported by first-principles and Green's function based simulations. Accessing the coherent heat conduction regime opens a new venue for phonon engineering for an array of applications. We will show that how that breaking the phonon coherence can further reduce thermal conductivity of superlattices. I will also discuss some recent work in understanding the quantum nature of heat transport processes.

This material is based upon work supported as part of the "Solid State Solar-Thermal Energy Conversion Center (S^{3}TEC), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number: DE-SC0001299/DE-FG02-09ER46577.

Carbon Nanotube-Si Heterojunction Solar Cells

Shigeo Maruyama, Kehang Cui, Takaaki Chiba, Shohei Chiashi

Department of Mechanical Engineering, The University of Tokyo, Japan

Single-walled carbon nanotubes (SWNTs) with outstanding electronic, optical, mechanical and thermal properties are expected to be the most promising materials for next-generation energy conversion devices as well as optical and electronic ones. Highly transparent-conductive SWNT films from controlled bundle-diameter and long bundle length were synthesized by floating catalyst CVD [1]. The SWNT films with a sheet resistance of 134 Ω/sq. at the 81.5% transparency were dry-transferred onto Si substrate to form a diode. The power conversion efficiency (PCE) of the solar cell is 11% and is stable after 1 year [1], which is attributed to the high purity pristine SWNTs. Moreover, the solar cell performance under different light intensities is investigated to evaluate both the series and shunt resistance of the device. The interfacial oxide layer between the SWNT film and the Si substrate is also discussed.

In order to further improve the performance of the solar cell, we investigated the effect of the SWNT morphology. As shown in Fig. 1, using the vertical-aligned SWNT arrays synthesized by alcohol catalyst CVD method, we have obtained a hierarchical 3D honeycomb-like architecture of SWNTs using the breath figure technique, where water vapor condenses on the surface of vertical-aligned SWNT and forms hexagonal pattern [2]. The micro-honeycomb network consists of vertical aggregated SWNT walls and a buckypaper bottom. This hierarchical structure exhibits lower sheet resistance and higher optical transmittance compared with the buckypaper. The honeycomb networked SWNT film was transferred onto the 3 mm by 3 mm n-type silicon substrate by hot water thermocapillary method. The pristine SWNT-Si solar cell shows a record-high fill factor of 72% as well as a PCE of 6%. The PCE remains stable for months in ambient condition. A PCE exceeding 10% is achieved in the dry state after dilute nitric acid treatment [2]. Through modeling, the honeycomb-networked SWNT film shows much smaller series resistance than random-oriented SWNT film.

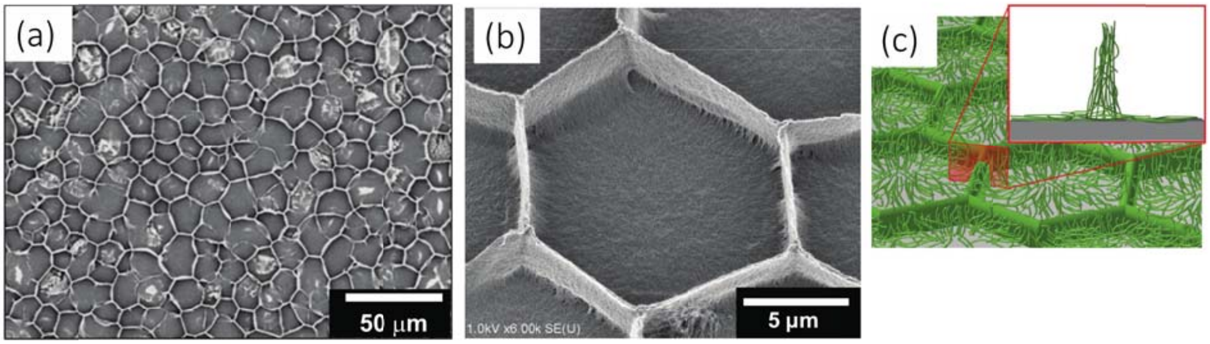


Fig. 1: Self-assembled honeycomb structure of single-walled carbon nanotubes.
(a) SEM image, (b) magnified SEM image, (c) illustration of the structure.

[1] K. Cui, A. S. Anisimov, T. Chiba, S. Fujii, H. Kataura, A. G. Nasibulin, S. Chiashi, E. I. Kauppinen, S. Maruyama, *J. Mater. Chem. A*, (2014), DOI: 10.1039/C4TA01353K.

[2] K. Cui, T. Chiba, S. Omiya, T. Thurakitseree, P. Zhao, S. Fujii, H. Kataura, E. Einarsson, S. Chiashi, S. Maruyama, *J. Phys. Chem. Lett.* **4**, 2571 (2013).

Thermal conduction nanoengineering by Si phononic nanostructures

Masahiro Nomura[1,2] *and Jeremie Maire*[3]

[1] *Institute of Industrial Science, Univ. of Tokyo, Komaba, Meguro-ku, Tokyo, Japan*
[2] *Nanoquine, Univ. of Tokyo, Komaba, Meguro-ku, Tokyo, Japan*
[3] *LIMMS-CNRS, Univ. of Tokyo, Komaba, Meguro-ku, Tokyo, Japan*

Nanostructuring is effective technology to control thermal conduction in solid. Many groups have been investigating characteristic thermal conduction in various nanostructures such as nanowires, holey, grained, and phononic structures. We are interested in the analogy between phonons and photons to coherently control their transport by the band-engineering. Thermal conduction nanoengineering by phononics [1] is our current main interest, and we use Si phononic crystal (PnC) nanostructures fabricated by electron beam lithography to investigate characteristic heat transport in nanostructures [Figs. (a) and (b)].

Air-suspended Si nanowires with various widths between 60 and 150 nm and a one-dimensional (1D) PnC nanostructures were fabricated on a 145-nm-thick SOI wafer by top-down approach using electron beam lithography, and their thermal conductivities were investigated at room temperature. The thermal conductivity was obtained by measuring time-domain thermoreflectance signal using a micro metal pad, which is attached to the nanostructures, and simulation by finite element method. Larger reduction in thermal conductivity, compared with that of a thin membrane (70 W/mK), was observed for thinner nanowires (60 nm wide, 47 W/mK) due to more frequent surface scattering of phonons. This result indicates that the phonon transport is ballistic in the investigated systems. The 1D phononic crystal showed smaller thermal conductivity compared with a nanowire with the averaged width (30 W/mK).

Theoretical investigation, by collaboration with Shiomi group, of this further reduction in the thermal conduction in 1D PnC clarified that phonons scattering is mixture of specular reflection and diffusive scattering with nearly the same ratio. We think that the observed reduction in thermal conductivity mainly stems from the chaotic billiard system, not from the phononic effect. We are currently trying to observe phononic effect at lower temperature and/or with smaller structures.

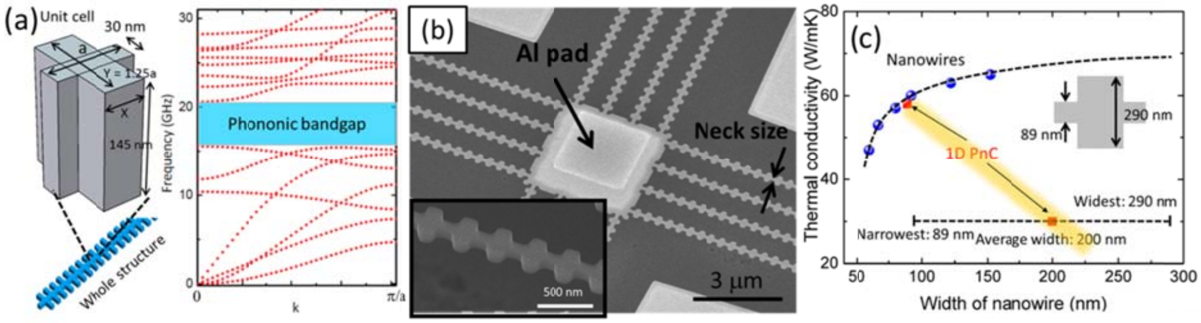


Fig. 1: (a) Phononic crystal nanostructure and the calculated phononic band diagram of the structure. (b) Fabricated air-suspended Si PnC nanostructures for thermal conductivity measurement. (c) Obtained thermal conductivities for nanowires and 1D PnC.

[1] M. Maldovan, “Sound and heat revolutions in phononics,” Nature, **503**, 209 (2013).
[2] J. Maire and M. Nomura, “Reduced Thermal Conductivities of Si 1D periodic structure and Nanowires,” to be published in Jpn. J. of Appl. Phys. (2014).

Phonon transport calculations of crystals with strong anharmonicity, disorders, interfaces, and nanostructures

J. Shiomi[1,2], *T. Murakami*[1], *T. Hori*[1], *T. Shiga*[1]

[1] *The University of Tokyo, 7-3-1 Hongo, Bunkyo, Tokyo, Japan*
[2] *Japan Science and Technology Agency, PRESTO, 4-1-8 Honcho, Kawaguchi, Saitama 332-0012, Japan*

Over the last several years, there has been a significant progress in the methodology to calculate phonon transport in crystals. This includes development in first-principles calculations of anharmonic interatomic force constants, which now allows us to accurately obtain lattice thermal conductivity of crystals through lattice dynamics or molecular dynamics. To make the analysis more useful for material development, we have extended the method to account for various complexities that are commonly present in actual materials: (1) strong anharmonicity[1], (2) alloy disorders[2-4], and (3) interfaces[5]. Here, molecular dynamics is particularly useful to capture effects beyond the perturbation theory, such as atom displacements far from equilibrium and local variation of mass and force fields. With these, we have identified (1) the origin of anomalous anharmonic lattice dynamics of lead telluride, (2) the large contribution of local force-field variation to the thermal conductivity reduction in lead-chalcogenide solid solutions, and (3) the contribution of the inelastic phonon transmission to the thermal boundary conductance across bonded crystal interfaces. Combined with the Monte Carlo simulations of phonon Boltzmann transport[6], mutual adoptability of the effects can be investigated in terms of phonon spectrum. The capabilities and limits of the current framework for designing thermoelectric materials will be discussed.

[1] T. Shiga, T. Murakami, T. Hori, O. Delaire, and J. Shiomi, *Appl. Phys. Express* **7** 041801 (2014).
[2] T. Hori, T. Shiga, and J. Shiomi, *J. Appl. Phys*., **113**, 203514 (2013).
[3] T. Shiga, T. Hori, and J. Shiomi, *Jpn. J. Appl. Phys*, **53**, 021802 (2014).
[4] T. Murakami, T. Shiga, T. Hori, K. Esfarjani, and J. Shiomi, *Europhys. Lett*., **102**, 46002 (2013).
[5] T. Murakami, T. Hori, T. Shiga, and J. Shiomi (to be submitted).
[6] T. Hori, G. Chen, and J. Shiomi, *Appl. Phys. Lett*., **104**, 021915 (2014).

Alloys and Amorphous Materials: the Microstructure and Thermal Conductivity

C.H. B aker[1], L.S. Larkin[2], W.A. Soffa[3] and P.M. Norris[1]

[1] *University of Virginia, Dept. Mech. and Aero. Eng., Charlottesville, VA, USA*
[2] *University of Virginia, Engineering Physics, Charlottesville, VA, USA*
[3] *University of Virginia, Dept. Materials Science and Eng., Charlottesville, VA, USA*

Alloys and amorphous materials have applications in a variety of thermal technologies, including heat assisted magnetic recording, phase change memory, and thermal barrier coatings, among many others. Yet, in comparison to crystalline materials, little is known about energy transport in these disordered materials, especially on the micro- and nanoscales. To this end, we present recent experimental and computational investigations that link the transport properties of this class of materials to the microstructure.

The microstructure of an alloy is defined by its composition and order parameter. The order parameter takes on values between zero and one, with a value of zero corresponding to complete disorder, and a value of one corresponding to the crystalline phase. We varied the order parameters of $Fe_{0.5}Pd_{0.5}$ alloys by subjecting them to different heat treatments and we measured the resulting thermal conductivities with TDTR. The alloys showed increased thermal conductivity with order parameter over the tested range. To better understand the observed relationship between order parameter and thermal conductivity, we performed calculations on simulated $Si_{0.5}Ge_{0.5}$ alloys. We systematically generated alloys with independent long-range and nearest neighbor (short-range) order parameters and tested them using molecular dynamics simulation to calculate the thermal conductivity and mode relaxation times. By decoupling the short- and long-range order parameters, we found that the short-range order parameter is the dominant factor, accounting for nearly the entire change in mode relaxation times. This suggests that the long-range order parameter of a real alloy, as probed by X-ray diffraction, determines the thermal properties insofar as it changes the short-range order parameter of the alloy.

Just as we seek to connect alloy transport properties to the microstructure, and ideal model of transport in amorphous materials would depend on its microstructure, as defined by the radial distribution function. We generated simulated samples of amorphous silicon with various methods and potentials to measure the impact on the thermal properties. Using a transient and localized heat pulse, in combination with wavelet analysis, we were able to measure the frequency dependent thermal diffusivity of the simulated amorphous silicon. Our results corroborate the Allen-Feldman theory of thermal transport in amorphous materials and efforts are underway to translate the theory's concepts into an analytical model incorporating the microstructure, aiding device engineers.

New formulation of dissipative particle dynamics: Non-Markovian models

I. Kinefuchi[1]*, Y. Yoshimoto*[1]*, T. Mima*[1]*, A. Fukushima*[2]*, T. Tokumasu*[2]*, and S. Takagi*[1]

[1] *Department of Mechanical Engineering, The University of Tokyo*
[2] *Institute of Fluid Science, Tohoku University*

The dissipative particle dynamics (DPD) method is one of the powerful tools for simulating mesoscale flows because the DPD simulation can be extended over larger domains and longer time scales compared with molecular dynamics (MD) simulation. The conventional DPD method is based on a top-down coarse-graining approach since the DPD parameters are designed to recover macroscopic properties such as compressibility and diffusivity. However, such a simple matching procedure may not be applicable to a complex fluid system involving the matching of multiple properties.

In the present study, we derive the equation of motion for non-Markovian dissipative particle dynamics (NMDPD) by introducing the history effects on the time evolution of the system [1]. Our formulation is based on the generalized Langevin equation [2], which describes the motions of the centers of mass of clusters comprising microscopic particles (**Fig. 1a**). The mean, friction, and fluctuating forces in the NMDPD model are directly constructed from an underlying MD system without any scaling procedure. For the validation of our formulation, we construct NMDPD models from high-density Lennard-Jones systems (**Fig. 1b**), in which the typical time scales of the coarse-grained particle motions and the fluctuating forces are not fully separable. The NMDPD models reproduce the temperatures, diffusion coefficients, and viscosities of the corresponding MD systems more accurately than the DPD models based on a Markovian approximation. Our results suggest that the NMDPD method is a promising alternative for simulating mesoscale flows where a Markovian approximation is not valid.

[1] Y. Yoshimoto, I. Kinefuchi, T. Mima, A. Fukushima, T. Tokumasu, and S. Takagi, *Phys. Rev. E* **88**, 043305 (2013).
[2] T. Kinjo and S. Hyodo, *Phys. Rev. E* **75**, 051109 (2007).

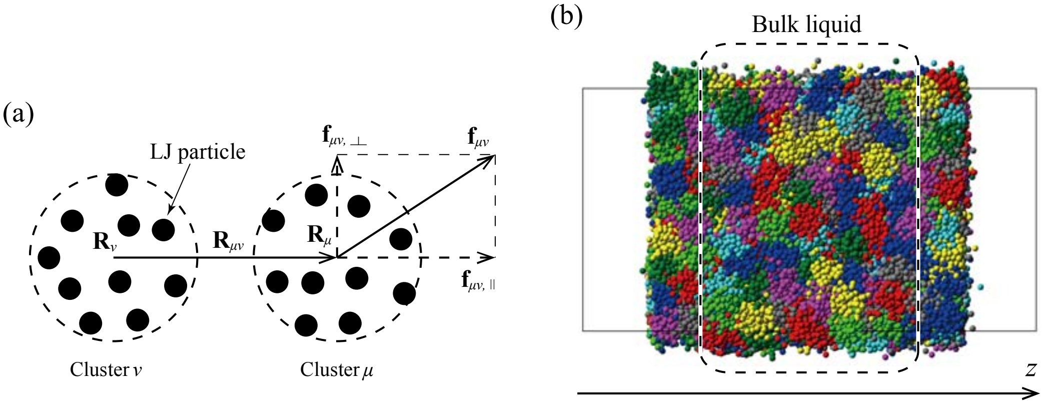


Fig. 1: (a) Schematic of clusters containing LJ particles. The center of mass of each cluster is regarded as a coarse-grained particle. (b) MD system employed for the construction of the NMDPD model. The clusters are tinted in eight colors for easy identification.

Coupling of heat and spin currents in cuprates and metallic multilayers

David G. Cahill, Greg Hohensee, and Gyungmin Choi

Department of Materials Science and Engineering and Materials
Research Laboratory, University of Illinois, Urbana, Illinois 61801

I will discuss two aspects of the coupling of spin and heat transport that we are probing using time-domain thermoreflectance (TDTR) and time-domain magneto-optic Kerr effect (TR-MOKE). Low-dimensional quantum magnets based on copper oxides (Sr14Cu24O41, La2CuO4, CaCu2O3), demonstrate that electrons and phonons are not the only significant carriers of heat in materials. Near room temperature, the magnon thermal conductivity is comparable to the electronic thermal conductivities of metal alloys. At high modulation frequencies, the thermal conductivity is suppressed by non-equilibrium between phonons and magnons on short length scales. We extract the effective strength of magnon-phonon coupling from the TDTR data using a two temperature model. In metallic multilayers, we are studying the generation of ultrafast spin currents using fast temperature excursions and strong temperature gradients. Thermally-driven demagnetization of ferromagnetic layer with perpendicular magnetization produces a transient spin current with duration of ~1 ps. In addition, a heat current passing through a ferromagnetic layer generates a spin current due to the spin-dependent Seebeck effect. We directly observe spin accumulation in the time domain using TR-MOKE and an optically opaque Cu layer as a transducer. We calibrate the size of the spin currents by quantifying the spin transfer torque applied to an in-plane ferromagnetic layer.

Heat Transfer in Non-Linear and Highly Anisotropic Systems

C. Dames[1,2] & Z. Chen[1]

[1] Department of Mechanical Engineering, UC Berkeley, USA
[2] Materials Sciences Division, Lawrence Berkeley National Laboratory, USA

Various modern devices involve materials and structures that are highly anisotropic and/or non-linear. Here I will briefly summarize two examples from our recent work.

First, the Cahill-Pohl / Einstein model of the minimum phonon thermal conductivity, k_{Min}, has been generalized for layered materials with highly anisotropic bonding (soft cross-plane and stiff in-plane). The resulting anisotropic Debye model [1] shows how the already low cross-plane conductivity is further reduced by phonon focusing caused by the stiff in-plane bonding [2]. As a result, k_{Min} of a layered material with anisotropic bonding is lower than k_{Min} of a corresponding isotropic material based on the weakest bonding available in the original anisotropic material [3]. These observations help explain the ultra-low thermal conductivity measured in WSe_2 and other highly anisotropic layered materials [4].

Second, we present experimental results for a ballistic thermal rectifier based on anisotropic reflections of photons by pyramidal mirrors. Control experiments verify recent theoretical predictions that this mechanism also requires a non-linear thermal collimator element, due to a fundamental constraint of the 2nd Law of Thermodynamics. Experiments confirm both effects: With pyramids and collimator the thermal rectification is 10.9% ± 0.8%, while without the collimator no rectification is detectable (< 0.3%) [5].

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Molecular Dynamics Viewpoint on Heat Transfer Characteristics of Self-Assembled Monolayers and Polymeric Substances

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Recently, heat conduction through the organic substances attracts a great attention due to the capability of controlling thermal conductance by molecular chain alignment or molecular organization, ranging from low thermal conductivity in a usual disordered polymer bulk to high thermal conductivity in a elongated polymer wire or highly aligned alkyl thin films. Therefore, soft matters comprised of organic molecules and polymeric materials, for example, are promising candidates for heat transfer materials applied particularly to nanoscale devices. In this study, we performed molecular dynamics (MD) simulations on two kinds of organic substances: self-assembled monolayer (SAM) and crosslink polymers, in order to examine heat transfer characteristics inside the alkyl chains and over the SAM–solvent interfaces. To analyze thermal energy transfer in detail, we executed the decomposition of energy transfer modes in a real-space description from the molecular dynamics perspective, i.e., total heat flux was decomposed into the internal energy transfer associated with molecular motions and the energy exchange by molecular interactions like covalent-bond interactions and intermolecular interactions [1].

As for the SAM–solvent interface systems, we showed that an alkanethiolate SAM modification on the gold substrate enables to increase the overall thermal boundary conductance (TBC) at the SAM–toluene interface as compared with the bare gold interface [2]. Furthermore, the detailed energy carriers inside the SAM were examined by using energy decomposition techniques. We found that most of the thermal energy is transferred by the covalent-bond interactions inside the alkyl chains of SAM due to a highly-ordered alignment of SAM molecules along the heat transfer direction and the SAM layer consequently exhibits significantly high thermal conductivity. The effects of terminal groups or adsorption density of SAM on TBC was investigated as well. It was found that the affinity between SAM terminal and solvent greatly affects local TBC at the SAM–solvent interface.

In the context of energy transfer inside polymer chains, the variation of thermal conductivity with changing internal molecular-scale structure in the typical amorphous polymers was investigated. Here we measured thermal conductivity of cross-linked polyethylene (PE) and polystyrene (PS) for a range of crosslink concentration [3]. Crosslink formation increased conductivity more or less linearly with the crosslink concentration for PE. On the other hand, in the PS case, the magnitude of change in thermal conductivity was insignificant. This striking difference is presumably attributed to highly heterogeneous PS based network including phenyl side groups. In order to elucidate the mechanism for the increase of thermal conductivity in the PE case, the decomposition scheme monitoring energy transfer modes was also applied. As a result, it was found that the rise of conductivity is mostly dominated by the covalent-bond interaction which is introduced by crosslink bonds between polymer chains. Our analyses of heat transfer phenomena could shed light on the microscopic mechanisms of the heat conduction particularly in soft matters or organic substances.

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Thermal Conductivity of Polymer and Hybrid Organic-Inorganic Thin Films

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Comparing to the understanding of thermal conductivity of inorganic materials, the exploration on structure-thermal conductivity relationship in nanostructured polymers is still in its nascent stage. In this talk, we will show two examples of our study on thermal conductivity of nanostructured polymers using the ultrafast laser-based frequency-dependent time-domain thermoreflectance method: 1). Ultrathin polymers have recently been shown to exhibit different chain dynamics and physical properties, as compared to their bulk counterparts. Our measurement shows that the effective thermal conductivity of PS films increase with decreasing film thickness when the thickness of the PS film is comparable to or smaller than the radius of gyration of bulk PS. By correlating the effective thermal conductivity with the ratio of the film thickness to radius of gyration, we find that this increase is mainly due to the increase of interfacial thermal conductance between PS thin film and the substrate, which likely results from the changing chain structure near the PS/substrate interface. 2). Atomic layer deposition (ALD) and molecular layer deposition (MLD) techniques with atomic level control enable a new class of hybrid organic–inorganic materials with improved functionality. The cross-plane thermal conductivity and volumetric heat capacity of three types of hybrid organic–inorganic zincone thin films fabricated by molecular layer deposition (MLD) and alternate atomic/molecular layer deposition (ALD/MLD) processes were measured. We revealed the critical role of backbone flexibility in the structural morphology and thermal conductivity of MLD zincone thin films by comparing the thermal conductivity of MLD zincone films with an aliphatic backbone to that with aromatic backbone. Much lower thermal conductivity values were obtained in ALD/MLD-enabled hybrid organic–inorganic zincone thin films compared to that of the ALD-enabled W/Al2O3 nanolaminates reported by Costescu et al. [*Science* **2004**, *303*, 989–990], which suggests that the dramatic material difference between organic and inorganic materials may provide a route for producing materials with ultralow thermal conductivity.

Anomalous lattice dynamics of lead telluride arising from strong anharmonicity

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Lead Telluride (PbTe) has been a popular material for studying lattice anharmonicity because it exhibits intrinsically low lattice thermal conductivity (2.0-2.2 $Wm^{-1}K^{-1}$ at room temperature) [1]. We have recently revealed that the strong lattice anharmonicity causes the coupling between longitudinal acoustic (LA) and transverse optical (TO) phonons, and it inhibits heat conduction of LA phonons [2,3]. Further anomalous anharmonic characteristic of PbTe lattice dynamics have been observed by neutron scattering experiments [4,5]. The radial distribution function (RDF) for the nearest neighboring Pb and Te atoms obtained from neutron diffraction experiments [4] was found to deviate from a symmetric Gaussian profile. In addition, inelastic neutron scattering (INS) experiments [5] have found a peak emerging at zone center is different from the longitudinal optical (LO) phonon (*double peak*) [5]. In this work, by performing classical molecular dynamics simulation with non-empirical force field, we have investigated the peak asymmetry in the RDF, and the double peak in the phonon spectra. The calculated RDF between Pb and its nearest neighboring Te atoms exhibit an non-Gaussian profile with the distortion increasing with temperature, while RDFs for Pb(Te)-Pb(Te) atoms remain Gaussian. As for the phonon spectra, by calculating the dynamical structure factor, we identified the double peak of TO modes with the magnitude also increasing with temperature. By parameterizing the anharmonic interatomic force constants (a-IFCs), the origin for non-Gaussian RDF and double peak of TO modes was clarified to be the cubic a-IFCs of nearest neighboring Pb and Te atoms along [100] direction, which are much larger than the other cubic a-IFCs.

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Phonons in Higher Manganese Silicide of a Complex Nowotny Chimney Ladder Structure

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Higher manganese silicide (HMS) has been studied for several decades as a p-type thermoelectric material that is made of non-toxic and earth-abundant elements. Among its attractive properties for high-temperature thermoelectric power generation, HMS is characterized with good chemical, thermal, and mechanical stability at elevated temperatures and in reactive gases. Moreover, the complex Nowontny Chimney Ladder (NCL) crystal structure of HMS gives rise to already very low and anisotropic thermal conductivity even in HMS crystals. Although the thermoelectric properties of HMS materials of different impurity doping have been obtained from past studies, there is a lack of fundamental understanding of the phonon dynamics including the phonon dispersion in the complex NCL structure, and it is unclear whether the already low lattice thermal conductivity of HMS can be suppressed much further. Here I will review the recent efforts of my co-workers in obtaining the phonon dispersion of HMS crystals from inelastic neutron scattering measurements and density functional theory calculation, and in suppressing the HMS thermal conductivity by elemental substitution and in nanostructures. These studies suggest the presence of numerous low-lying optical phonon branches in the complex NCL structure, especially a very low-lying twisting polarization of the Si ladder in the Mn chimney. The twisting polarization undergoes several avoided crossing with the three acoustic branches, and is expected to scatter the acoustic phonons. In addition, the anisotropic thermal conductivity found in HMS crystals is mainly caused by the anisotropy in the group velocity. The obtained phonon dispersion is further used to suggest that glass-like thermal conductivity can be obtained in nanostructured HMS with a grain size of about 10 nm without reducing the thermoelectric power factor. While this prediction is being examined by experiments with both individual HMS nanostructures and nanocrystalline bulk HMS, partial substitution of Mn with heavier Re has been used to obtain a thermal conductivity approaching the amorphous limit at high temperatures.

Measurement of heat flow though polymeric nanostructures using the dual cantilever technique: Thermo-mechanical response and teasing out the thermal part

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Bi-material microcantilevers, with their high sensitivity to thermal stimuli, are ideally suited sensors for investigating nanoscale heat transfer. We have designed and fabricated low thermal conductance bi-material microcantilevers by minimizing their width and thickness. Using such cantilevers, we have demonstrated heat flux resolution of less than 1 picowatt. A pair of such cantilevers is proposed as a configuration for measuring thermal conductance of a nanostructure suspended between the two. In our cantilever technique, two lasers are focused, one on each cantilever. One laser is modulated to vary the temperature at the end of one cantilever, while the second laser senses variation in heat flow through the second cantilever due to thermal conduction along the nanowire. We have measured the stray conductance between the cantilevers, i.e., the spurious conductance measured when no object is suspended between the two cantilevers, to be less than 0.05 nW/K.

Segments of electrospun polymeric nanowires are suspended between the two cantilevers and the heat flow through such nanowires is quantified by measuring the deflection of the sensing cantilever for a known, laser-induced deflection of the sensing cantilever. Results of measurements from polystyrene nanowires will be presented. The deflection of the sensing cantilever is influenced by two factors: (1) heat flow through the nanostructure, and (2) deflection because of mechanical coupling. We will discuss the effects of mechanical deflection and techniques to eliminate it.

Non-intrinsic Sharvin resistance between nanostructures

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In thermal transport, Sharvin resistance denotes the contact resistance when the phonon mean free path is much larger than the contact size, which is also known as the ballistic contact resistance. The Sharvin resistance between two bulk materials forming a point contact has been derived as the ratio of the phonon mean free path to the product of the thermal conductivity of the materials and the contact area. As such, the contact conductance per unit area is independent of the contact size, which can be regarded as an intrinsic value. With the rapid development of nanotechnology, it is common to encounter situations with individual nanostructures forming point contacts, as can be seen in various nanocomposites such as those with carbon nanotubes (CNTs) and various polymers. After extensive efforts of using CNTs to tune the thermal conductivity of polymers, the enhancement is still far below the predicted values based on the particle mixing theory, which has been attributed to the contact resistance between CNTs and between CNTs and host materials. However, to date, a good understanding of the contact thermal resistance between two CNTs is still lacking. Through systematic measurements of contact thermal conductance between different diameter individual multi-walled CNTs, we show that the normalized contact conductance per unit area still linearly proportional to the tube diameter, which is surprising. Further analyses indicate that the contact thermal conductance is Sharvin type in nature because of the unexpectedly long phonon mean free path in the cross-plane direction for graphite. In this case, phonon reflection from nearby free surfaces modulates the Sharvin resistance, renders it non-intrinsic and dependent on the nanostructure size even after normalized with the contact area.

Ballistic to Diffusive Thermal Transport in Two-Dimensional Materials and Devices

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Two-dimensional (2D) materials like graphene, h-BN, and transition-metal dichalcogenides (TMDs like MoS_2) have shown promising applications in electronics [1]. In this context, their thermal properties remain an area of active investigation, particularly with respect to their anisotropic thermal conductivity, the thermal conductance of their interfaces, and the heat flow in nanoscale samples comparable in size to the phonon or electron mean free paths.

We have found that despite its great intrinsic thermal conductivity, heat dissipation can be a challenge in graphene transistors, where heat flow is limited by interfaces with adjacent materials (Fig. 1a) and thermal transients are dominated by the surrounding layers [2]. In addition, when devices are scaled below ~1 μm, experiments and theory show that the intrinsic graphene thermal properties become dependent on the system size [3].

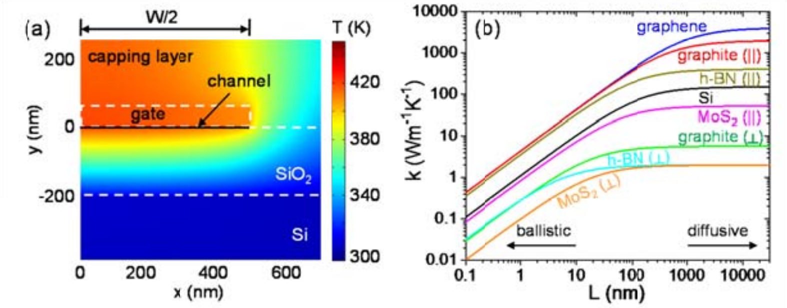

Fig. 1. (a) Simulated temperature distribution in a graphene transistor including its top gate [2]. Cross-section showing one-half of device width ($W/2$) by symmetry considerations. (b) Ballistic-to-diffusive transition of thermal conductivity as a function of length for various layered 2D materials, including in-plane (||) and cross-plane (⊥), compared with Si, at 300 K [3-6].

We also investigated the in-plane and cross-plane ballistic thermal conductance of other 2D materials and stacks based on full phonon dispersions (Fig. 1b). For a given material, monolayers and multilayers have similar in-plane ballistic thermal conductance per cross-sectional area (G_b) above ~100 K, but monolayers show higher G_b at low temperature due to the contribution of flexural phonons. Cross-plane G_b values are approximately one order of magnitude lower than those for in-plane due to weak van der Waals interactions between layers. Based on the calculated G_b, we estimate the phonon mean free path of these materials, given the diffusive thermal conductivity [3,4]. The size-dependent thermal conductivity shows the ballistic to diffusive transition for a variety of anisotropic layered 2D materials in Fig. 1b [4]. It is clear that most sub-micron devices and *all* sub-100 nm devices exhibit some degree of quasi-ballistic heat flow.

Besides size effects, grain boundaries in chemical vapor deposition (CVD) grown 2D materials will also affect thermal transport. We investigated thermal conduction across grain boundaries in graphene by non-equilibrium Green's functions and obtained the dependence of thermal conductivity on grain size [5]. The results are in good agreement with our recent measurements of substrate-supported layers of CVD-grown graphene [6]. We also measured suspended graphene devices, obtaining thermal transport properties up to device breakdown (T > 1000 K) [7]. Such results broaden our understanding of thermal transport in 2D materials, and help us explore their applications for devices and thermal management.

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Thermal transport across organic-inorganic interfaces

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A self-assembled monolayer (SAM) junction is a periodic monolayer of organic molecules that bridges two metallic or semiconducting contacts. A nanocrystal array (NCA) is a periodic, three-dimensional array of metallic or semiconducting nanoparticles decorated with organic molecules. The electronic structure of these low-cost organic-inorganic hybrid materials can be carefully tuned, making them attractive alternatives to semiconductors in thermoelectric, photovoltaic, and electronic applications. While the electronic properties of SAM junctions and NCAs have been extensively studied, their thermal properties have received less attention.

To address this knowledge gap, we use molecular dynamics simulations and lattice dynamics calculations to predict the thermal conductance of SAM junctions of the thermal conductivities of NCAs. The modeling predictions are directly compared to experimental measurements. For the SAM junction, we resolve a long-standing discrepancy between measurements and predictions by considering the imperfect contact due to surface roughness. We find that the degree of vibrational overlap between the two contacts can be used to tune the junction thermal conductance. For the NCA, we examine the effects of nanoparticle size and composition on thermal conductivity. The organic-inorganic interfaces are found to be an important source of thermal resistance.

Thermal and Thermoelectric Transport in Nanostructures

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During the last decade we have witnessed tremendous advancement in characterization and understanding of thermal transport in nanostructures, particularly in the 'phonon boundary scattering' regime where the characteristic size of nanostructures is comparable to phonon mean free path. However, there is little experimental work on thermal transport in nanostructures when the size is even smaller, approaching to that of phonon wavelength, which for most semiconductors ranges from 1 to 10 nm. For instance, it is not clear if the phonon spectra will be modified due to the spatial confinement effect, and if so, what would be the effect on thermal transport properties. In this presentation, I will discuss our recent work on using rationally designed nanostructures to study nanoscale thermal and thermoelectric transport phenomena in this regime, i.e., with sub-10 nm characteristic size. I will describe the instrumentation we developed that enables the characterization of thermal transport and related properties of these nanostructures and discuss and interpret the measurement results.

Near-Field Radiative Transfer Enhanced by Graphene Covered Nanostructures

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Tunneling of evanescent modes enables the radiative heat flux to be several orders of magnitude higher than that between far-field blackbodies, especially when surface plasmon polaritons (SPPs) are excited. Due to its unique characteristics, graphene can support surface plasmons with low loss and excellent tunability ranging from near-infrared to terahertz frequencies. Graphene has been reported for tailoring the near-field heat transfer and improving the efficiency of TPV cells. However, the near-unity photon tunneling probability occurs only in narrow wavevector or *k*-space where coupled SPPs are excited. This study explores hybridized modes based on graphene-covered nanostructured materials, such as doped-silicon nanowires (D-SiNWs) and periodic grating structures. For D-SiNWs, the dielectric functions have opposite signs for orthogonal electric field directions; therefore, the isofrequency contour is hyperbolic and evanescent waves in vacuum become propagating waves in the medium. Therefore, the tunneling probability can be improved with hyperbolic metamaterials in a broad frequency region. By combining graphene plasmons and hyperbolic modes, it is shown that photon tunneling with near-unity probability across a broad frequency range and large *k*-space for enhancing near-field heat transfer. As a result, the near-field heat transfer coefficient between doped-silicon-nanowire hyperbolic metamaterials can be further improved by several folds when covered by a graphene sheet, leading to near-field blackbody behavior.

Spectral control of near-field radiation transfer using pillar array structured surface

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Near-field radiation transfer between pillar-array-structured surfaces as shown in Fig.1 was enhanced through an interference of SPP (Surface Plasmon-Polariton) compared with that between plane surfaces. Even in nano-scaled channels between the pillars, the SPP could propagate, and then, a kind of interference and resonance took place based on the depth of the channel between pillars. With decreasing pillar-height, the frequency at the maximum radiation transfer was shifted to a high-frequency side. That is, the spectral control of near-field radiation could be achieved using the pillar-array-structured surfaces. The pillar array structure was made on the surface of tungsten metal using an Electron Beam lithography method for a resist and a Reactive Ion Etching method, as shown in Fig.2. The size of channel between pillars was around 100nm. In the case of the large width, such as 100nm and 200nm, there were two kinds of radiation transfer peaks corresponding to the short distance and the long distance propagating modes corresponding to the angular frequency. Moreover, in a higher angular frequency range, there was another radiation transfer peak originated from SPP resonance between top surfaces of emitters 1 and 2.

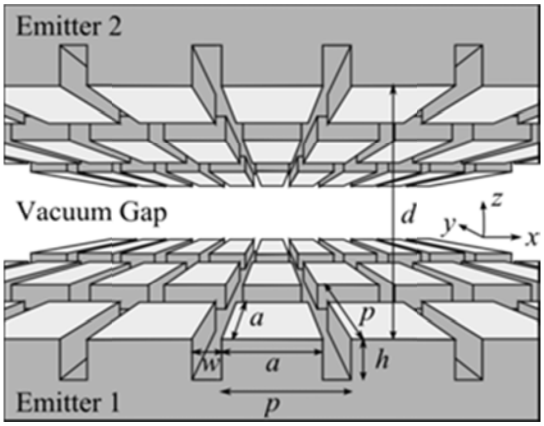

Fig.1 Schematic diagram of pillar array structured surfaces

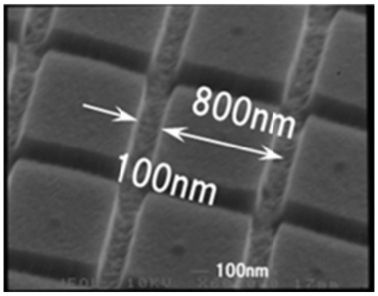

Fig.2 SEM image of pillar array structured surfaces made of tungsten

Effect of film thickness on near-field radiative transport

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Near-field radiative thermal transport has attracted increasing attention recently, with orders-of-magnitude heat transfer enhancement already demonstrated between bulk materials. Using a novel custom-built experimental platform, we conducted a systematic investigation of the effect of film thickness on the near-field heat transport properties. By studying thermal radiation between a hot silica microsphere and thin silica films of varying thicknesses (50 nm to 3 microns), at different gap sizes (30 nm to 10 microns), we found substantial enhancements in heat transport properties due to near-field effects, even for the thinnest films when the gaps size was comparable to the film thickness. Further, we find that at larger separations (~1 micron), the thicker films show substantially larger near-field enhancement than thinner films. These results provide the first direct evidence of a distance dependent penetration depth in thin films.

Nanoscale Thermal Phenomena in Heat-Assisted Magnetic Recording

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Heat-Assisted Magnetic Recording (HAMR) uses a near-IR laser to heat a small area of a magnetic recording medium in order to reduce its coercivity below that of the magnetic field generated by the recording head. This enables writing of data in only the small heated region. Confinement of optical energy delivered to the magnetic recording medium, and the resulting thermal response, are critical to HAMR's ability to deliver high-density, reliable data storage. The focusing of laser energy is achieved using a gold near-field transducer (NFT) that creates a 50 nm-wide heated region, well below the diffraction limit of the laser light. The laser excitation of the NFT and the near-field energy transfer create intense heat fluxes, on the order of 1 TW/m^2, and temperature gradients with magnitudes in excess of 10 GK/m.

In this presentation we will introduce thermo-optical models employed to study the thermal response of an NFT and recording media during HAMR operation. Within these models a collection of nanoscale thermal phenomena can be accounted for, including experimentally determined size-dependent thermal conductivities, measured metal-dielectric and metal-metal interface resistances, two-carrier electron-phonon transport, and the ballistic transport of hot electrons. Even with these effects, the models ultimately rely on the heat diffusion equation, and the validity of such will be open for discussion.

Nano-thermal consideration for heat assisted magnetic recording (HAMR)

M. Morelli

Western Digital Corporation

Spatially-resolved measurement of nanochannel flows by evanescent wave-based particle tracking velocimetry

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The field of nanofluidics for single molecule analysis, ultra filtration and energy conversion has been expanded with recent micro/nanotechnology. Since liquids in nanospace with dominant surface effects are in a transitional regime from single molecules to continuum, specific fluid properties different from bulk can be expected. Previously, our group has revealed unique properties in size-regulated 10-1000 nm spaces such as higher viscosity, lower dielectric constant and higher proton mobility [1]. However, fluid flow in nanochannels is still unknown owing to lack of measurement method because nanochannel is smaller than light wavelength. For breaking through the limitation, evanescent wave light, which penetrates from the surface within 100 nm-order distance, is a key optical phenomenon. In this study, we developed evanescent wave-based particle tracking method for measuring flow profile in nanochannel.

Carboxylate-modified fluorescent polystyrene particles of 64 nm diameter were used as flow tracer and seeded into water at volume fraction of 0.002%. The particles flowing through a fused-silica nanochannel of 50 μm width and 410 nm depth were illuminated by the evanescent wave of 532 nm wavelength generated at a glass-liquid interface. Since the evanescent wave exponentially decays from the interface, the position of nanoparticle in the nanochannel was determined by using the fluorescent intensity detected by an EMCCD camera. From sequential images of fluorescent particles, the velocity distribution was obtained.

Velocity profiles of pressure-driven flow in the nanochannel were successfully measured for the first time. The velocities show parabolic profiles with approximate agreement with Hagen-Poiseuille flows. However, the results show slip velocities at the wall even in the fused-silica nanochannel, which is considered to have strong interaction between water molecules and hydrophilic surface. A possibility of appearance of nanoscale molecular behavior in the fluid flow can be considered. Further development of the method with much smaller tracer is required for detailed understanding.

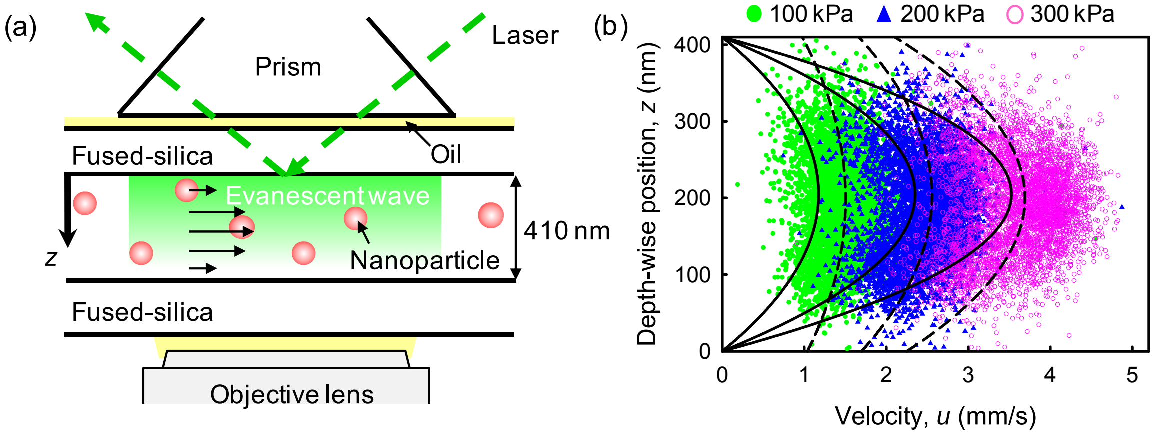

Fig. 1: (a) Schematic of a measurement system. (b) Velocity profiles of pressure-driven flow by 100-300 kPa pressure in the nanochannel (solid line: Hagen-Poisseuille equation, dotted line: fitting).

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The Effective Latent Heat of Aqueous Nanofluids

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Nanoparticle suspensions, popularly termed “nanofluids,” have been extensively investigated for their thermal and radiative properties. Such work has generated great controversy, although it is (arguably) generally accepted today that the presence of nanoparticles rarely leads to useful enhancements in either thermal conductivity or convective heat transfer. On the other hand, there are still examples of unanticipated enhancements to some properties, such as the specific heat of molten salt-based nanofluids reported by Shin and Banerjee (2011). Another largely overlooked example is the reported effect of nanoparticles on the effective latent heat (h_{fg}) of aqueous nanofluids, as reported by Ameen et al. (2010). Through molecular dynamics (MD) modeling supplemented with limited experimental data they found that h_{fg} increases with increasing nanoparticle concentration, for Pt nanoparticles (MD) and Al_2O_3 nanoparticles (experiments). Here, we extend those exploratory experiments in an effort to determine if h_{fg} of aqueous nanofluids can be manipulated, i.e., increased or decreased by the addition of graphite or silver nanoparticles. Our results to date indicate that, yes, h_{fg} can be substantially impacted, by up to ± 30% depending on the type of nanoparticle.

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Adsorption and Transport of Water in Mesoporous Silica

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The adsorption–desorption isotherms and relaxation rates of water in Zirconium-doped two-dimensional hexagonal mesoporous silica with pore diameters of 3.8 nm were measured at 283–298 K using a gravimetric method. A type V adsorption–desorption isotherm with significant hysteresis was obtained. The adsorption layer was formed on the pore surface at low relative pressure of water vapor, capillary condensation was initiated at around 0.4–0.6 relative humidity, and then pore filling was completed near the saturated vapor pressure. Regarding to the kinetics, the relaxation rate of water uptake in the capillary condensation state was much lower than that in the layer-adsorption state or pore-filling state. The isotherms and relaxation rates during desorption had a similar trend. Effects of the hydrophilicity of mesopores and temperature on the adsorption–desorption kinetics suggest that the water transport mechanism in mesopores includes activated processes. The activation energy for water transport in the mesopores estimated by the temperature dependence of the relaxation rate ranged from 20 to 50 kJ mol^{-1} and the activation energy decreased with increasing the relative humidity. When capillary condensation and evaporation occur, the relaxation curve could be estimated by the Fickian diffusion equation at a small stepwise change in relative humidity. The relaxation curves at large stepwise change in relative humidity suggest that the transport mechanism could be liquid-water flow due to capillary action [1, 2, 3].

In order to investigate the kinetics of water uptake into mesoporous silica in detail, canonical ensemble molecular dynamics simulations were performed using a model of mesoporous silica thin film [4, 5, 6]. The calculation results showed that the kinetics of water uptake depended on the number of water molecules and there were two different transport mechanisms in the pore. One was diffusion of water along the pore surface, and the other was capillary rise of liquid water. The transport mechanism at small stepwise change in relative humidity could be surface diffusion, while that at the large stepwise change could be liquid-water flow due to capillary action.

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On the oxygen transport in cathode catalyst layer of PEFCs

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PEFC (polymer electrolyte fuel cells) is a promising energy conversion device for stationary, portable, and automobile applications. Fuel cell based cogeneration system for households have been deployed over fifty thousands units in Japanese households and are increasing the number. Major automobile companies are targeting their FCV (fuel cell vehicle) sales from in near future.

One of the recent issues associated with the nanoscale transport phenomena in PEFCs is the transport process of oxygen molecules in the cathode catalyst layer. PEFC consists of polymer electrolyte, catalyst layers on both sides of the polymer electrolyte, gas diffusion layer and the gas channels. Supplied oxygen gas from the gas channel diffuses across the gas diffusion layer and the catalyst layer to take place the charge transfer reaction process to produce electricity. Therefore the enhancement of the oxygen transport in the catalyst layer is crucial to improve the performance of the PEFCs.

The authors have investigated the oxygen transport characteristics in the cathode catalyst layer of PEFCs. One of the major factors to govern the oxygen transport is the water uptake in the catalyst layer and the associated structural issue of the catalyst layer. Effect of the equivalent weight and the supply gas relative humidity are controlled to examine the effect of the water uptake in the catalyst layer.

Partial pressure of the oxygen in the cathode gas is controlled in order to discriminate the Knudsen diffusion in the cathode catalyst layer from the bulk diffusion process. Porosimetry is conducted to evaluate the pore structure of the catalyst layer and a simple mathematical model is developed to evaluate the experimental results. The results showed the impact of various parameters.

Self-generated chemical gradients guide the migration of cancer cells

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Cancer cells often migrate away from the primary tumor to form distant metastases which are the cause of death in 90% of cancer patients. Blocking or delaying the migration of cancer cells could extend the life of cancer patients. However, our current understanding of the conditions that favor cancer cell migration is very limited. Research using animal models is relevant to disease but complicated by the variability of many microenvironment factors. Research using *in vitro* assays has better control of the conditions but its relevance is frequently questioned. To circumvent these limitations, we built a series of microfluidic assays in which cancer cells have to migrate through microscopic mazes of channels that are uniformly pre-filled with standard cell culture media. Surprisingly, cancer cells from patients can exit the maze along the shortest path in the absence of any external cues. More than 80% of cells exit, two orders of magnitude more than expected from random migration through the maze. This unexpected result, in conjunction with biophysical models and additional microscale engineering tools, helped us uncover a novel, self-guidance strategy during which cancer cells generate their own guiding cues. This strategy does not require pre-existing chemical gradients, is not bound by the spatial limits of any gradient, and locks the cells into a self reinforcing loop of persistent migratory phenotype. Overall, our findings could lead to new therapeutic approaches for delaying cancer cell invasion and stopping cancer metastasis.

Study on Transport Phenomena of Reaction Materials in Fuel Cell by Quantum/Molecular Dynamics Method

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These days Polymer Electrolyte Fuel Cell (PEFC) is expected to be the next generation power supply system. It is very important to understand the flow phenomena of reaction materials in PEFC to increase the efficiency of PEFC. The flow field, however, is made of very fine materials, whose characteristic length is of the order of from nanometer to micrometer. The flow field cannot be analyzed by conventional fluid dynamics based on continuum theory.

Molecular simulations are very effective tools to analyze such flow fields. In the flow fields, however, quantum feature of molecule, such as dissociation and recombination, affects much on transport phenomena. Moreover, the fine materials construct agglomerate and therefore there are many characteristic scale in the flow fields. The flow fields should be analyzed by considering such quantum phenomena and the structure of materials.

We analyze some transport phenomena of reaction materials which affects much on the efficiency in some parts of PEFC, that is, Polymer Electrolyte Membrane (PEM), Catalyst Layer (CL) and Micro Porous Layer (MPL)[1]. The schematic diagram of our simulation is shown in Fig. 1. I will introduce the results of our simulations and discuss about the characteristics of nanoscale transport phenomena of reaction materials in PEFC.

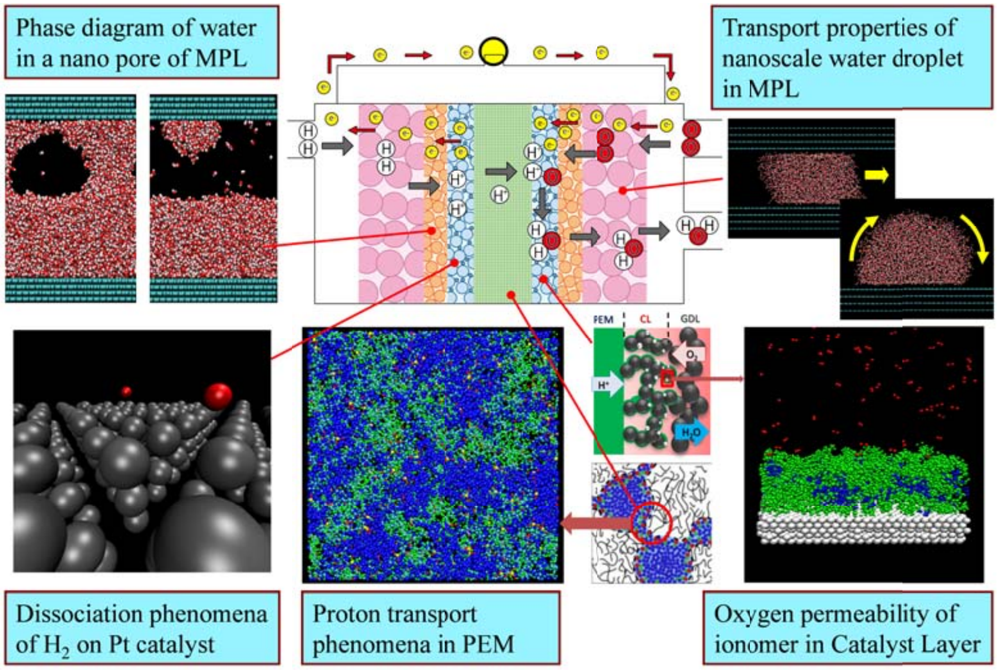

Fig. 1: Schematic diagram of our simulation of transport phenomena in PEFC

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Alternative Approach to Ballistic Phonon Transport

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In recent years, the importance of understanding the nature of heat transport on short length- and time-scales, where ballistic effects can be significant, has become evident from both scientific and engineering standpoints. From a scientific viewpoint, there is interest in: i) understanding how ballistic transport can reduce the contribution of long mean-free-path phonons in nano-structures and how this can be exploited to determine the mean-free-path distributions of materials; and ii) providing a detailed explanation of the role of ballistic phonons in the observed change in thermal conductivity as a function of a frequency-dependent power input. From an applications standpoint, size- and time-dependent variations in thermal transport properties can impact (negatively or positively) important technological issues including: i) self-heating and power dissipation in high-frequency nano-scale electronic devices; and ii) the design of state-of-the-art thermoelectric materials with multiple-scale defects intended to scatters phonons of different wavelengths and effectively reduce the thermal conductivity.

In this talk, I will present an alternative approach, an extension of the McKelvey-flux method, to study heat transport phenomena at all length- and time-scales. This approach readily spans ballistic, quasi-ballistic and diffusive phonon transport regimes, and can thus provide clear insight into the detailed role of ballistic effects. It is relatively easy to implement numerically and even permits analytical solutions for important, special cases. I will show how the McKelvey-flux method is connected to, and can even go beyond, other common approaches such as the Landauer formalism, Fourier's law, the heat equation and the Cattaneo equation. Interestingly, it is found that one can capture ballistic transport effects by solving the traditional heat equation, or Fick's law, and simply implementing the right physical boundary conditions. There is a clear connection and analogy to electron transport, for which the McKelvey-flux method was originally developed that will be discussed. This predictive theory relies solely on fundamental physical parameters, such as the phonon band velocity and mean-free-path, which can be extracted or calculated for bulk materials. Finally, I will present recent results, using the McKelvey-flux method, to problems where ballistic effects are important, including a solution of heat current and temperature in the case of a frequency-dependent power input.

MEMS Measurements of Boiling Heat Transfer with a Single Bubble

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Nucleate boiling has numerous industrial applications (e.g. cooling of CPUs and semiconductor power devices of electric vehicles and steam generation in electric power plants) because of its high heat transfer performance. Since the boiling includes phase change, solid-liquid-vapor interactions and micro- & nano-scale heat transfer phenomena, it's very difficult to accurately measure the boiling heat transfer. Thus, there have been unclear points in physical boiling mechanisms yet. On the other hand, the development of high-resolution diagnostics such as MEMS sensors and high-speed infrared cameras enables to measure fundamental heat transfer phenomena in nucleate boiling precisely [1].

In this study, a MEMS thermal measurement technique was applied to elucidate heat transfer mechanisms in the single bubble boiling of water. The MEMS sensor shown in **Fig. 1** has thirteen micro temperature sensors and an electrolysis trigger on the upper surface, and two thin film heaters on the bottom surface. The electrolysis trigger consisting of two nickel electrodes can supply a tiny hydrogen bubble serving as a boiling bubble nucleus by electrolysis of water. So, we can generate a boiling bubble from the intended position (the gap of the trigger electrodes) at an intended timing. **Fig. 2** indicated a local wall temperature beneath an isolated boiling bubble recorded at the sampling frequency of 50kHz. The measured temperature clearly indicates the local and fast heat transfer phenomena under the bubble, such as evaporation and dry-out of microlayer and rewetting of the dry-patch. The highly resolved wall temperature must be useful to verify the results of direct numerical simulations of boiling. The heat transfer characteristics of single bubble boiling were investigated by a quantitative heat transfer evaluation using the measured temperature data, such as features of the spatiotemporal distribution of the local heat flux, the contributions of each fundamental heat transfer phenomenon to the overall wall heat transfer, the contribution of microlayer evaporation to bubble growth, and the spatial distribution of the initial microlayer thickness. The microlayer evaporation was found to be the dominant heat transfer mechanism in the wall heat transfer, and the contribution of microlayer evaporation to bubble growth was about 50%.

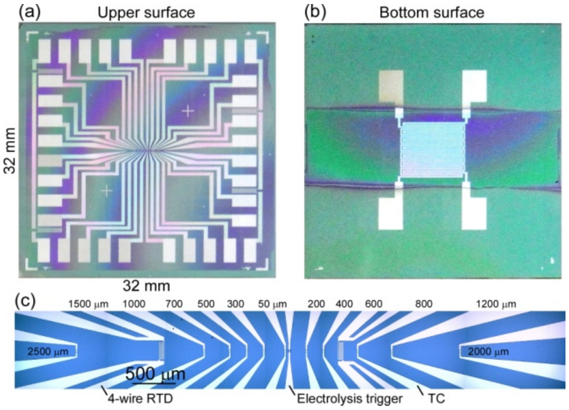

Fig. 1 MEMS sensor for pool boiling research.

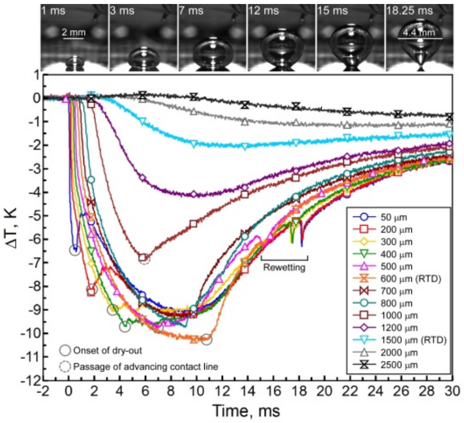

Fig. 2 Local wall temperature beneath a single bubble.

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Nanoparticle Heat Transfer for Biomedical Applications

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Unique physical characteristics and properties of nanoparticles (1 – 100 nm) are supporting new opportunities for diagnostics and therapeutics in the field of nanomedicine. For example, gold and iron oxide nanoparticles have unique and tunable properties that allow transduction of optical (light), or radiofrequency (RF) electromagnetic fields to affect heating of biomaterials at multiple scales. This talk will explore the underlying physics and relative advantages of each form of nanoparticle heating and then introduce several applications. Specifically, optical excitation of gold is dramatically more efficient than radiofrequency heating of iron oxide and can be designed based on size and shape, as well as proper selection of the wavelength and fluence of incident light. However, properly selected RF fields can penetrate far more deeply into tissues than optical sources. This allows RF excitation of properly designed and deployed iron oxide (i.e. size, composition, distribution and aggregation state) to affect heating more deeply and uniformly than gold within biomaterials. After discussing these general capabilities, several applications are highlighted. First, laser heating of gold nanoparticles has demonstrated improvement of a common diagnostic assay (i.e. a lateral flow immunoassay or LFA) by creating a "thermal" vs. visual contrast. Further, RF heating of iron oxide has shown capabilities for improved cancer hyperthermia and regenerative medicine applications (i.e. rapid thawing of vitrified systems). In summary, this talk demonstrates the growing opportunity for nanoparticle heating in biomedical applications.

Experimental Investigations of Nanodroplets and Nanobubbles

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Boiling and condensation have been studied by numerous researchers for more than a century but their initial stages are not well understood. For example, we frequently observe nucleation of vapor bubble at unexpected spots on a heated surface in water as well as the condensation on a complicated surface. Their mechanism is desired to be investigated in submicron or nanoscale while the number of atoms/molecules to be considered is much more than the calculation capability of the newest computers for obtaining reliable data. Thus, there is a strong demand of submicron/nanoscale experimental techniques for phase change phenomena. Fortunately, equipments for nanotechnology have been dramatically improved in a few decades and their targets are expanding even into the "wet" systems. In this presentation, SEM observation of nanodroplets and AFM measurement of nanobubbles are introduced for water-air two-phase on HOPG substrate and their limitations are also discussed. By using an ESEM, we investigate the relationship between non-uniform surface wettability and water condensation and propose an extended nucleation theory considering the absorbed water molecules on hydrophilic portions. The coalescence of 100nm-order droplets was clearly observed and the line-tension effect on the three-phase contact line is discussed. Peak-force tapping mode of AFM and frequency modulation AFM enable us to investigate the initiation of nanobubbles on solid/liquid interface (**Fig. 1**). For example, adhesion force mapping on HOPG substrate in water unveils the interactive mechanism between gas molecules and substrate atoms in the sub-nanoscale near field.

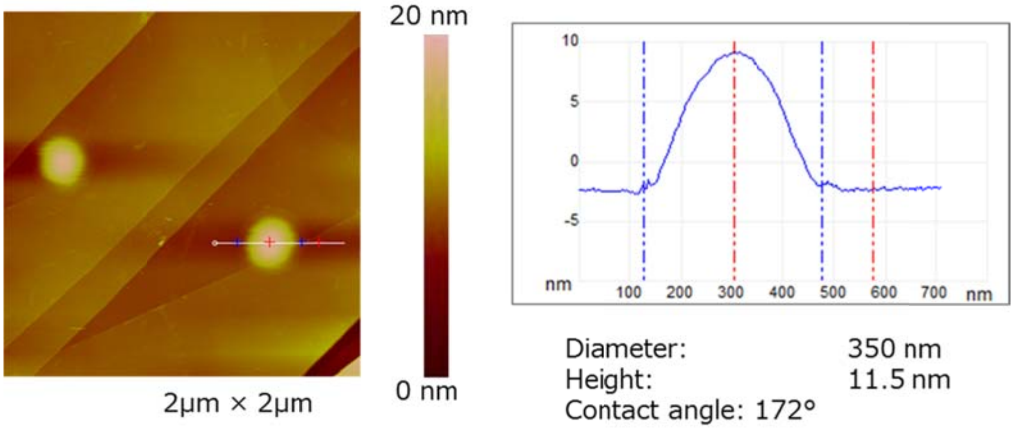

Fig. 1: Nanobubbles on HOPG surface measured by peak-force tapping mode of AFM

Nano Thermal Management beyond 50 kW/cm^2

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The peak heat generation rates that can be sustained in the highest power electronic devices – such as GaN radar amplifiers, monolithic 3D circuits, and vehicle power converters - are limited by a hierarchy of conduction and convection resistances from the junction to the ambient.

We are working on conduction and convection technologies – based mainly on nanostructured materials and nanoscale materials integration - that extend fundamental cooling limits beyond 50 kW/cm^2. Examples include the integration of synthetic diamond within nanometers of active junctions and the reduction of defects and phonon scattering in the key interfacial region. Two-phase heat exchangers include graded nanoporous metal bilayers and a hydrophobic capping region for improved stability. Also for heat exchangers, we are integrating these technologies with three-dimensional hierarchical routing for the liquid and vapor phases to strongly reduce the pressure drop and increase the system efficiency.

Through continued attention to near-junction resistances and extreme flux convection, power densities that may exceed 100 kW/cm^2 – depending on gate width and hotspot dimension – are feasible within 5 years.

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One-way phonon isolation in acoustic waveguides

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Using analytical methods and numerical simulations, we demonstrate the possibility of one-way phonon isolation in thin plate waveguides and double layer graphene nanoribbons. This isolation is enabled via spatio-temporal modulation of the waveguide material properties, which permits symmetry breaking such that a vibrational mode entering the waveguide from one direction is converted into a different vibrational mode while the same mode entering from the other direction propagates unchanged. Possible experimental implementation and applications for on-chip signal isolation in MEMS and NEMS devices will be discussed.

Thermal-aware Device Design of Nano-scale MOS Transistors and Graphene ReRAM Formed by Joule-Heating in Nano-dimensions

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[Thermal Aware Device-Design of Advanced FETs] In order to suppress the short-channel effects (SCE) in aggressively scaled MOS transistors, three-dimensional transistor structure such as fin-type FETs (FinFETs) is now becoming a main-stream technology. In FinFETs fabricated on bulk Si substrate, sub-10-nm silicon slab is utilized as a channel layer [1] to realize good controllability of channel potential through gate voltage. However, because of worse thermal conductivity of silicon nano-structures, heat generated by Joule-hearing during transistor operation tends to stay around the channel and raises the channel temperature of transistors. The increased channel temperature degrades electron/hole mobility. Since carrier mobility is important for both analog and logic applications of transistors, the understanding of thermal properties of advanced MOS transistors is critically important. In this work, experimental data on the evaluation of thermal properties of advanced MOS transistors in operation will be shown. Moreover, strategies to enhance transistor performance by thermal-aware device design will be discussed.

The thermal properties of MOS transistors are evaluated by AC conductance method and pulsed IV method [2]. The channel temperature is directly evaluated in MOSFETs with four-terminal gate electrode [3]. In particular, short-channel bulk and SOI (silicon-on-insulator) MOSFETs with various SOI and BOX (buried oxide) thicknesses are characterized through four-terminal gate electrode methods. Even in bulk MOSFETs and SOI MOSFETs with thin BOX significant increase in channel temperature is observed [4]. By utilizing device simulator, it is shown that traditional optimization methods such as resolving the trade-off between parasitic resistance and capacitances are not enough to achieve maximum performance in the case of three-dimensional transistors but consideration for device thermal property is a key. It is demonstrated that the power consumption can be reduced by thermal-aware device design.

[Graphene ReRAMs] Another topic is the realization of two-terminal mono- and multilayer graphene nanoribbon resistive random access memories (ReRAMs) by utilizing Joule-heating in nano graphene. After the fabrication of graphene transistors, the graphene was electrically broken with high drain voltages. However, with adopting proper bias schemes, the broken graphene show ReRAM characteristic; broken graphene films recover/loose the resistivity. TEM observation after the electrical break-down reveals that the temperature of graphene becomes higher than the melting temperature of SiO_2. The origin of ReRAM effects is investigated through physical analysis.

[Conclusion] In nano-scale electronic devices, the understanding of thermal properties is important not only to achieve high performance and/or low power consumption but also to realize new-type of devices where high temperature by Joule-heating in nano structure is utilized. The collaboration between specialists on nano thermal engineering and electronic device engineers will be critically important.

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Reduction in Thermal Conductivity of Silicon Processed by High-Pressure Torsion

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Materials with length scales on the order of few nanometers exhibit unique abilities to control thermal transport[1]. Tailoring the thermal properties of nanostructured systems have a promising application n dimensionless figure of merit, $ZT = S^2 \sigma T k^{-1}$, where S is the Seeback coefficient, σ is the electrical conductivity, T is the temperature and k is the thermal conductivity[2]. To achieve higher ZT, the lattice thermal conductivity of the thermoelectric system needs to be reduced without compromising the charge carrier mobility. Significant work has been done in recent years by using chemically distinct secondary phases either in the bulk form, or in the form of thin films, to reduce lattice thermal conductivity[3]. The introduction of nanostructured interfaces to scatter phonons more efficiently than electrons and thereby reduce the thermal conductivity of the material has yielded high ZT in thermoelectric devices[4].

From an engineering perspective, a practical thermoelectric device requires a significant volume of material. To realize that objective, nano structuring using ball milling followed by hot pressing was shown to have an order of magnitude reduction in the thermal conductivity of doped silicon[5] and mechanical deformation using high pressure have shown improved Seebeck coefficient in Bi_2Te_3 and PbTe respectively. In this work, we demonstrate a novel technique using high-pressure torsion (HPT) to create a high density of lattice defects such as dislocations and grain boundaries on nanometer length-scales[6]. Although crystalline silicon is not a good thermoelectric material due to its intrinsically high thermal conductivity, we use silicon as a model system to study the effect of HPT processing on thermal conductivity. We report a dramatic reduction in the thermal conductivity of bulk crystalline silicon when subjected to severe plastic strain under a pressure of 24 GPa at room temperature using HPT. Thermal conductivity of the HPT-processed samples were measured using pico-second time domain thermoreflectance. Thermal conductivity measurement shows that the HPT-processed samples have a reduction in thermal conductivity by a factor of ≈20 (from intrinsic single crystalline value of 142 $Wm^{-1}K^{-1}$ to ~7.6 $Wm^{-1}K^{-1}$). The reduction in thermal conductivity is attributed to the formation of nanograin boundaries and metastable body centered cubic Si-III and rhombohedral Si-XII phases which act as phonon scattering sites and because of a large density of lattice defects introduced by HPT processing. Subsequent annealing at 873 K shows a reverse transformation from metastable phases to Si-I cubic diamond phase and a nominal increase in thermal conductivity due to the reduction of the density reduction of secondary phases and nanocrystalline defects.

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Fourier transform inelastic x-ray scattering: a new tool for measuring phonon dispersion and more with a free-electron laser

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There is a long and productive history of using inelastic scattering to measure lattice dynamics. Typical experiments use extremely high-resolution monochromators and analyzers to measure small shifts in the energy of the scattered particles under equilibrium conditions. Under appropriate conditions, time-domain measurements can yield much better resolution and provide access to transient non-equilibrium dynamics. We discuss potential opportunities for studying low-lying excitations using recent results using the LCLS x-ray free-electron laser as examples. In both cases we perform high-resolution inelastic x-ray scattering in the time-domain using a femtosecond optical laser to prepare broadband two-phonon coherences in the sample. In the first case, we extract the transverse phonon dispersion in the prototypical semiconductor germanium with sub-meV resolution--- without the use of an analyzer. In the second case, we use this same method to investigate the strongly anharmonic lattice dynamics in PbTe and present evidence for strong photo-induced mode-coupling spanning the Brillouin zone.

Investigations of Microscopic Energy Transport with Neutron and X-Ray Scattering

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A microscopic understanding of heat transport is of broad interest for the design of efficient energy materials, and relies on a detailed knowledge of phonon dispersions and mean-free-paths to establish reliable atomistic models of thermal conductivity. Inelastic neutron scattering instruments can map excitations throughout reciprocal space efficiently, and measurements with single-crystals provide quantitative accounts for different phonon scattering mechanisms, including anharmonicity, electron-phonon coupling, and scattering by defects or nanostructures. X-rays enable complementary phonon measurements at high pressures, and also reveal details of the nanostructure. In addition, first-principles simulations of the dynamical structure factor, including anharmonic effects, enable the rationalization of complex experimental datasets. We present investigations of several important thermoelectric materials, establishing a microscopic picture of their thermal conductivity. These new insights suggest avenues to improve the performance of thermoelectric materials.

We acknowledge funding from the US DOE, Office of Basic Energy Sciences, Materials Science and Engineering Division, and as part of the S3TEC EFRC.

Accurate instrument for measuring the surface tension, viscosity and surface viscoelasticity of liquids using ripplon surface laser-light scattering with tunable wavelength selection

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We describe our new accurate instrument that simultaneously measures the surface tension, viscosity and surface viscoelasticity of liquids (**Fig. 1**). The instrument works on the ripplon surface-laser light scattering principle and operates with an automatically tunable selection of ripplon wavelength from 4 to 1500 μm, which corresponds to the frequency range of observing surface phenomena from approximately 400 Hz to 3 MHz in the case of water. The heterodyne technique instrument uses a reference laser beam which intersects at an arbitrarily adjustable angle with a vertically directed probing beam. For the determination of the wavelength of selected ripplons we substituted with the interference fringe spacing, measured using a high-resolution beam profiler. To extract reliable surface tension and viscosity data from the experimentally obtained spectrum shape for a selected wavelength of ripplon, we developed an algorithm to calculate the exact solution of the dispersion equation. The uncertainties of surface tension and viscosity measurement were confirmed through the measurement of seven pure Newtonian liquids at 25°C measured with the selected wavelength of ripplon from 40 μm to 467 μm. To verify the genuine capability of the tunable wavelength selection of ripplon, we measured the surface elasticity of soluble surface molecular layers spread on pentanoic acid solutions (**Fig. 2**).

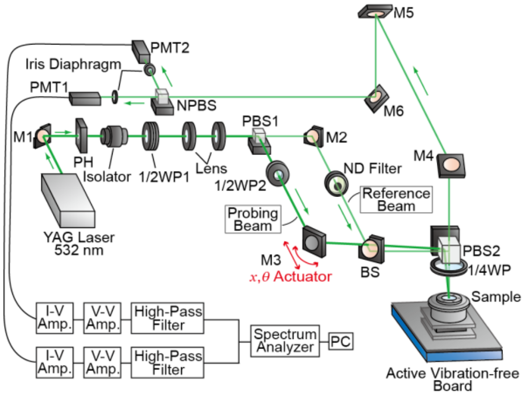
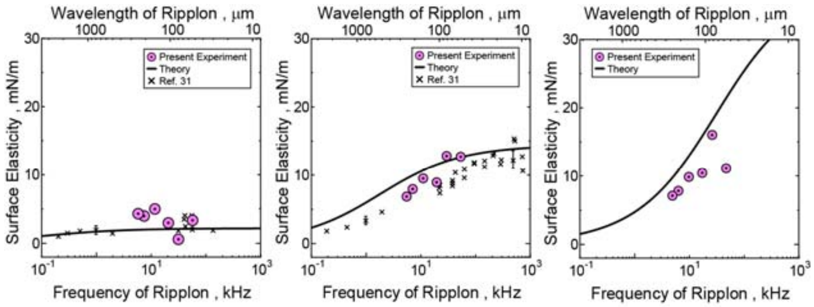


Fig. 1: Ripplon surface laser-light scattering apparatus.



(a) 3 mM/L (b) 12 mM/L (c) 50 mM/L

Fig. 2: Frequency dependence of the surface elasticity for solutions of pentanoic acid solutions.

Analytical interpretation of non-diffusive phonon transport in thermoreflectance thermal conductivity measurements

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We derive an analytical solution to the Boltzmann transport equation (BTE) to relate non-diffusive thermal conductivity measurements by thermoreflectance techniques to the bulk thermal conductivity accumulation function, which quantifies cumulative contributions to thermal conductivity from different mean free path energy carriers (here, phonons). Our solution incorporates two experimentally-defined length scales: thermal penetration depth and heating laser spot radius. We identify two thermal resistances based on the predicted spatial temperature and heat flux profiles. The first resistance is associated with the interaction between energy carriers and the surface of the solution domain. The second resistance accounts for transport of energy carriers through the solution domain and is affected by the experimentally-defined length scales. Comparison of the BTE result with conventional heat diffusion enables a mapping of mean-free- path-specific contributions to the measured thermal conductivity based on the experimental length scales. In general, the measured thermal conductivity will be influenced by the smaller of the two length scales and the surface properties of the system. The result is used to compare non-diffusive thermal conductivity measurements of silicon with first principles-based calculations of its thermal conductivity accumulation function.

Uncovering and engineering the thermal phonon spectrum

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California Institute of Technology

Recent works have demonstrated that the thermal phonons responsible for heat conduction possess a broad spectrum, yet this spectrum remains unknown for most materials and is not always accounted for in simulations due to computational cost. In this talk, I will describe our efforts to directly measure and engineer the thermal phonon spectrum using computation and experiment. Experimentally, I will describe a new experimental technique that has enabled the first direct measurements of phonon mean free paths in a wide range of crystalline solids. Computationally, I will show how our use of novel, efficient algorithms to solve the Boltzmann transport equation is advancing our understanding of phonon transport in complex materials.

Superdiffusive heat transport in semiconductors

A. Shakouri, B. Vermeersch, A.S. Mohammed, and Y. Koh

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A wide distribution of phonon mean-free-paths contribute to thermal conductivity of semiconductors at room temperature. Changing the modulation frequency in time domain thermoreflectance (TDTR) has been used to extract the contribution of ballistic phonons as phonons with mean free path larger than the thermal penetration depth don't contribute to the "apparent" thermal conductivity of the material. This explanation is based on quasi-ballistic description that considers "ballistic" heat transport near the metal transducer and a transition to pure "diffusive" transport at larger distances. An alternative explanation is based on truncated Lévy flight where ballistic "jumps" and Brownian "diffusion" are mixed (see Fig. 1a) [1,2]. This gives rise to a fractional diffusion at early times or short distances. This has important implications about the extent of the temperature field at different times or frequencies. We show that the superdiffusive exponent is given by the dominant scattering mode for phonons and it is almost constant for several alloys [1]. While modified Fourier and truncated Lévy can both explain the top transducer temperature profile accurately, their prediction for internal temperature distribution inside the semiconductor alloy can be significantly different (see Fig. 1b) [2]. This can lead to improved thermal characterization of nanoscale devices and Kapitza interface thermal resistance.

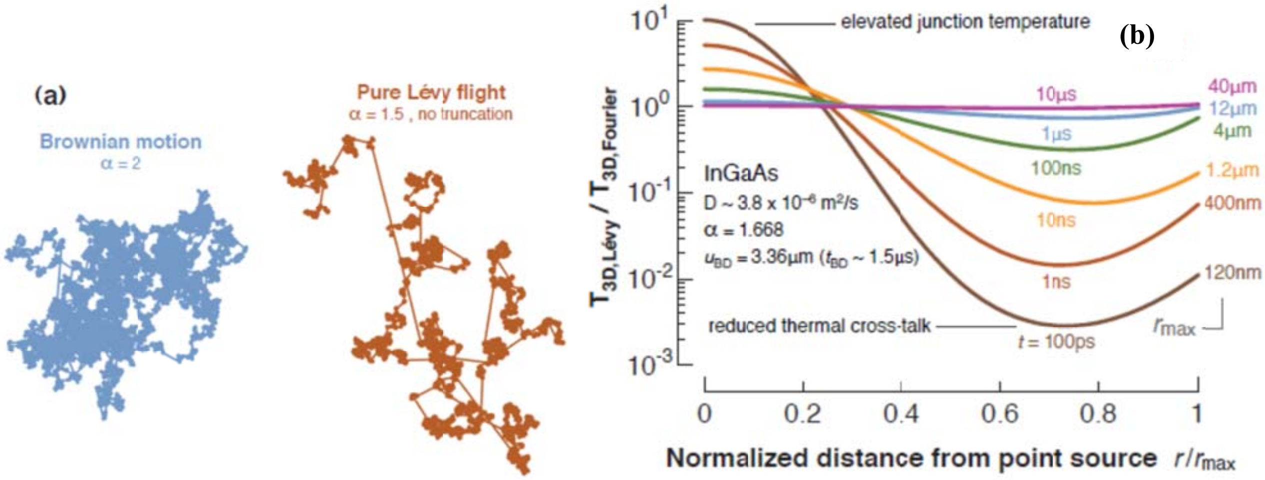

Fig. 1: Stochastic energy transport in solid media. (a) Example of random walk trajectories. (b) Ratio of truncated Lévy and Fourier 3D single pulse responses on semi-infinite InGaAs at room temperature. Listed parameters were determined from TDTR experiments.

[1] B. Vermeersch, J. Carrete, N. Mingo, and A. Shakouri, Superdiffusive heat conduction in semiconductor alloys -I. Theoretical foundations. Submitted to *Phys. Rev. B.* (2014) Preprint available online at arXiv.

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Selective gas adsorption in the nanospace of flexible metal-organic frameworks

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The discovery of a new nanoporous compound that has unique porous properties is scientifically and technologically topical. In particular, the creation of a porous compound that possesses a switchable pore surface and channel structure is currently a major challenge in material science. This has not yet been realized with currently available materials. The recent advent of porous coordination polymers (PCPs) or metal–organic frameworks (MOFs) as new functional crystalline microporous compounds, has attracted the attention of scientists because of the great practicality of regular nano-sized spaces prepared by simply mixing their organic and inorganic molecular components which result in their finding unusual porous functions[1].

Here we report new flexible PCPs that show large structural transformation in response to the adsorption of specific guest molecules or external stimuli such as light[2], resulting in high selectivity for guest inclusion or step adsorption behaviors[3−4]. Dynamic effects can arise either locally from flexible ligands and/or flexibility of the coordination geometry of the metal ions, or from the global cooperative movement of the framework on a periodic scale. We will also report new soft MOFs that selectively adsorb CO with adaptable pores. The high selectivity toward CO was achieved by the synergetic effect of the local interaction between CO and accessible metal sites and a global transformation of the framework, which was elucidated by various techniques including in-situ X-ray powder diffraction/sorption experiments. The transformable crystalline materials realized the separation of CO from a mixture with nitrogen (N_2), a gas that is the most competitive to CO (**Fig. 1**). The dynamic and efficient molecular trapping and releasing system so-called self-accelerating CO sorption is reminiscent of sophisticated biological systems such as heme proteins[5].

Fig. 1: Schematic representation of the mechanism of highly cooperative CO adsorption so-called self-accelerating CO sorption.

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[3] J. Seo, C. Bonneau, R. Matsuda, M. Takata, S. Kitagawa. *J. Am. Chem. Soc*. 133, 9005 (2011).
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[5] H. Sato, W. Kosaka, R. Matsuda, A. Hori, Y. Hijikata, R. V. Belosludov, S. Sakaki, M. Takata, S. Kitagawa. *Science* 343, 167 (2014).

Thermal and Elastic Properties of Crystalline Polymer Nanostructures

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Polymers play an essential and ubiquitous role in everyday life due to their extraordinary range of properties. However, bulk polymers generally have low stiffness and low thermal conductivity. In this talk, I will present thermal and mechanical characterizations of two crystalline polymer structures: polyethylene nanofibers and polysilsesquioxane hybrid crystal fibers. Polyethylene nanofibers with diameters between 50 and 500 nm are characterized using atomic force microscope (AFM) based techniques, and we find that their Young's modulus and thermal conductivity can be as high as 326 GPa and 100 W/m·K, respectively. The Young's modulus of polymer nanofibers reported is comparable with the best Young's modulus of metal alloys. Their thermal conductivity is higher than most of metals. For polysilsesquioxane hybrid crystal fibers, molecular dynamics simulations show significant enhancement of thermal transport in the hybrid crystals due to the strong hydrogen bonding. The thermal conductivity of polysilsesquioxane hybrid crystal fibers is measured using micro-fabricated thermal devices in the temperature range of 10-350 K.

Synthesis and characterization of mesoporous materials for energy-efficient adsorption systems

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Ordered mesoporous silica (MPS) is expected to provide an adsorbent for energy-efficient air-conditioning systems, such as desiccant cooling systems, humidity control systems, and adsorption heat pumps. These systems can contribute to the reduction of CO_2 emissions because they offer the possibility of recovery at temperatures as low as 50℃.

Many papers have been published on the sysnthesis, characterization and application of mesoporous materials for adsorptions systems[1]. Recently, we reported the synthesis of mesoporous silica materials using the block copolymer supramolecular assembly[2]. It is well known that block copolymers containing two chemically dissimilar blocks can form periodically ordered structures via the microphase separation. When some additive is attached to one block of a block copolymer with non-covalent interactions, the resulting supramolecular complex also forms similar ordered structures. In our synthesis method, it is possible to control the mesostrucure of obtained mesoporous silicas. The results of scanning electron microscopy (Fig. 1) revealed that SiO_2 formed various structures including cylindrical, spherical, and lamellar. Different SiO_2 nanostructures formed via the microphase separation of siloxane/polymer complexes are prepared simply by varying solvent mixtures without changing the polymer chain.

When these materials are used as adsorbents, the mass transfer of adsorbates is very important and strongly influenced on the surface and inner structure. The detailed characterization of pore structure on obtained mesoporous silicas by high-resolution FE-SEM and gas/vapor adsorption measurements were carried out. In the presentation, the comparision with conventional mesorous silicas will be discussed, especially for cylindrical pore structures.

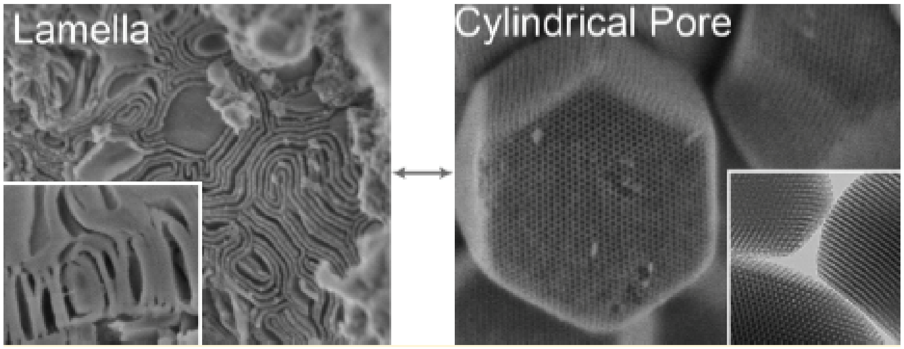

Fig. 1: High-resolution FE-SEM/TEM images of obtained mesoporous silica strucure

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Thermal property measurement of nanoscale films with frequency-domain thermoreflectance

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Frequency-domain thermoreflectance is an optical technique for measuring thermal properties of bulk materials and thin films, where a periodically modulated laser beam locally heats a sample while a second beam monitors the surface reflectivity. This talk will describe how this technique can be used to determine thermal properties of nanoscale films as thin as one atomic layer. Topics will include sensitivity analysis, the optimization of experimental parameters such as the laser spot size and modulation frequency range, and the determination of experimental uncertainty. Measurements of thin-film superlattices and subsurface graphene multilayers will be used as examples.

Size effects in thermal conduction by phonons

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Heat transport in nanoscale systems has been hard to measure and to interpret. Ballistic and diffusive flow coexist, adding complication. Therefore, it is worth studying an over-simplified case, not achievable experimentally. This is a nanoscale crystal repeated periodically. Both structure and heat flow are constrained by periodic boundary conditions. No primary distinction is made between ballistic and diffusive transport. Fourier's law $J = -\kappa\nabla T$ is non-local, $J(x) = -\int dx'\kappa(x,x')\nabla T(x')$. The thermal conductivity $\kappa(x - x')$ can be analyzed by a straightforward extension of the standard quasiparticle gas theory (*i.e.* Peierls-Boltzmann theory) of bulk solids. One-dimensional flow is studied in a three-dimensional supercell of length *L*, conceptually divided into *N* parallel planar segments ℓ. External heat enters chosen segments uniformly at rates $\dot{e}(\ell)$, and leaves other segments. Microscopic information is encoded in the non-local response function $\kappa(\ell - \ell')$. Such geometries are popular for simulation of bulk heat transport using classical molecular dynamics (MD). Unfortunately, phonon carriers of heat have mean free paths comparable to the computational scale of the heating and cooling. Thus, undesirable nanoscale aspects affect bulk answers, unless eliminated by extrapolation. The reverse point of view is that nanoscale effects are seen here in their simplest form. An analysis based on the Peierls-Boltzmann equation, using a generalized Debye model, shows that extrapolation requires fractional powers of *1/L*. It is also argued that heating could be imposed sinusoidally, $\dot{e}(\ell) \propto \cos(2\pi\ell/L)$, to improve convergence. The analysis has implications about finite size effects that may be extended to nanoscale systems of less physical simplicity.

Phonon thermal transport in BAs nanowires from first principles

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Recently the thermal conductivity of zinc blende boron arsenide (BAs) has been predicted to be exceptionally high, exceeding 2000W/m-K at room temperature, comparable to those of the carbon crystals, diamond, graphite and graphene and far higher than those of other non-carbon compounds [1, 2]. Here we examine the thermal conductivity of BAs nanowires as a function of the wire diameter and compare this to the thermal conductivity of diamond nanowires. Striking reductions in the BAs nanowire thermal conductivity compared to those in diamond are shown to result from much larger phonon mean free paths in BAs as demonstrated from thermal conductivity accumulation curves. The underlying reasons for the large BAs mean free paths will be discussed.

Support for this work has been provided primarily from the S3TEC, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award No. DE-FG02-09ER46577, and also from the National Science Foundation under Grant No. CBET 1066634.

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Printable thermoelectric materials

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Thermoelectric generator can convert low grade waste heat into electricity, making it a key technology to contribute to sustainability through the scavenging of waste heat or heat source.[1] Practical use of thermoelectric devices spread, both improvement in device performance and reduction of a manufacturing cost are required[2,3]. Generally, thermoelectric devices are fabricated by vacuum-processing particularly for thin film applications. Thermoelectric thin films with high thermoelectric properties can be made by thin film deposition process mentioned above, but these processes require manufacturing cost, owing to longer takt time of the vacuum processing. Printing processes such as screen- and inkjet printings are attractive to reduce the manufacturing cost of thermoelectric devices. We fabricated flexible printed thermoelectric thin films containing thermoelectric particle, conductive polymer and several additives. We prepared mixture of thermoelectric Bismuth telluride particle, a conductive polymer (PEDOT:PSS), poly(acrylic acid) (PAA), and several organic additives to fabricate thermoelectric films. In the mixture, the organic components (PEDOT:PSS, PAA, and an additive) act as a binder to connect Bismuth Telluride particles mechanically and electrically. Among employed organic additives, glycerol drastically enhanced electrical conductivity. The $Bi_{0.4}Te_{3.0}Sb_{1.6}$ films fabricated by a spin-coating of the mixture showed thermoelectric figure of merit (ZT) = 0.3 at 300 K when $Bi_{0.4}Te_{3}Sb_{1.6}$ particle diameter was 5 μm and its concentration in the elastic films was 95 wt%.

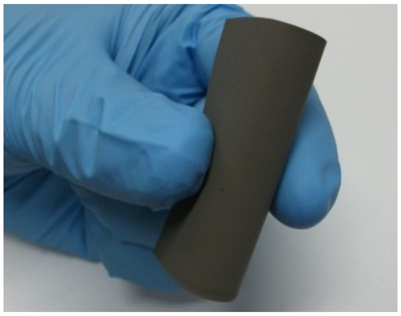

Fig. 1: Photograph of a printed flexible thermoelectric thin film

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Parsing the Seebeck Coefficient: The Effect of Non-Equilibrium

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The ability to reduce thermal conductivity through nanostructures has attracted interest in silicon and other materials for thermoelectric applications. In particular, the boundary scattering of phonons has been exploited to report significant enhancement in the figure of merit. It is implicitly assumed that the introduction of crystal boundaries or other defects does not affect charge transport provided there is a difference in the mean free paths of electrons and phonons. However, in a non-equilibrium picture of transport with simultaneous and self-consistent transport of electrons and phonons, phonon boundary scattering can indeed alter momentum transfer between electrons and phonons, with significant impact on the Seebeck coefficient. Here, we discuss experiments and theory to better understand the Seebeck effect from a non-equilibrium perspective.

Evaluation of catalysts employed in CVD synthesis of carbon nanotube

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Chemical vapor deposition (CVD) process is considered to be one of the most efficient processes. Unlike laser ablation process and arc discharge process, CVD process proceeds accompanied with pyrolysis of materials; therefore, its growth mechanism is still unclear. So far some reports related to precursors synthesized during CVD process are reported, but there is no quantitative discussion about catalyst ability. There are a lot of reports about catalysts combination and their qualitative discussion using Raman spectroscopy, PL, thermo gravimetric analysis, and so on is reported. In this study we developed high vacuum CVD apparatus directly connected to mass spectrometer and measured reaction products and their temperature dependence. Assuming first-order reaction and the reaction follows Arrhenius equation; we estimated activation energy of dissolving source gases.

Figure 1 indicates our experimental apparatus. The back ground pressure is less than 2×10^{-4} Pa. Source gasses are introduced through variable leak valve. The reactor is made by quartz glass and its temperature is controlled to be 500 °C to 1100 °C. Before introducing source gases, catalysts were reduced by argon/hydrogen mixture. In quadrupole mass spectrometer, molecules are ionized by electron impact method. The energy of electron impact is 50 eV. This energy is much higher than ionization energy, so that a lot of fragments originated from the source gas, which is not reacted or decomposed, are produced by the excess energy. We carefully compared with the fragment pattern, which was usually apparatus dependent, and derived the actual mass spectra by subtracting the fragments. Figure 2 shows Arrhenius plots of two cases of 'with iron' catalyst and 'without catalyst'. As the slope becomes smaller, activation energy decreases from 1.0 eV to 0.66 eV. We also examined cobalt, molybdenum, and nickel. Compared with synthesis of carbon nanotube, there still remains contradiction but generally preferred catalysts decreased activation energy.

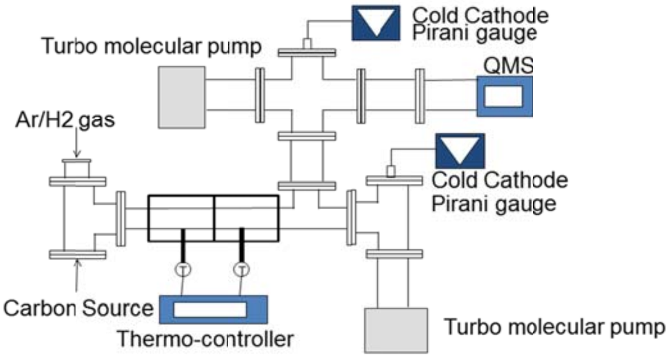

Fig. 1: Experimental apparatus.

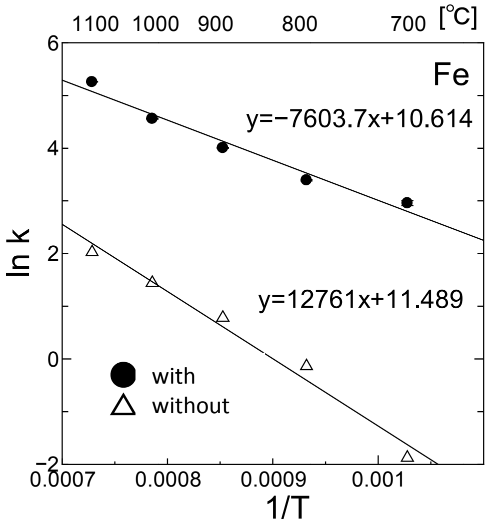

Fig. 2: Arrhenius plot.

Kinetics of triplet-sensitized photon upconversion in ionic liquids for utilizing wasted solar photons

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In solar conversion systems such as photovoltaic, photo-catalysis, and natural/artificial photo-syntheses, the efficiencies are largely limited by an existence of system-dependent threshold energy E_g for incident photon (or threshold wavelength λ_g). Any photons with the energy below E_g, which are the *sub-bandgap* solar photons, cannot be utilized by a system and this aspect has presently caused irreversible loss of solar energy. One strategy often taken to cope with this problem is to reduce E_g (i.e., to increase λ_g), but since this is tantamount to a lowering of electron free energy, this strategy always accompanies some negative side-effects, often perceived as a reduction in the output voltage and/or reaction quantum yield.

Photon upconversion (UC) is a technology that converts presently wasted sub-bandgap photons into less-number of utilizable photons of $E > E_g$ to increase the overall efficiency of the conversion system *without requiring the reduction of* E_g *to a system*. For a long time such UC had only been possible for intense, coherent, and linearly-polarized light (i.e. laser light), and UC for low-power, non-coherent, and randomly-polarized light (e.g. sunlight) had not been possible. Recently, a new strategy of UC that is applicable to the latter type of light has been proposed [1]. Since this method utilizes both diffusion and inter-molecular collision of organic molecules in spin-triplet state, the medium has to be fluidic in order to allow for the energy-carrying organic molecules to perform the inter-molecular energy transfer.

We have been studying this UC strategy for past several years, started from the development of new class of UC samples that are made with *ionic liquids* as the medium for the molecular transport [2,3]. While volatile organic solvents such as benzene and toluene had mostly been used in the preceding studies [4], the use of ionic liquids has successfully imparted several important properties to the samples, such as non-volatility and non-flammability which are advantageous for application. Since ionic liquids are novel *organic* fluids, virtually infinite number of types are possible due to the high design flexibility of organic synthesis [5]. Interestingly, we found that the UC quantum efficiency (Φ_{UC}) in ionic liquids is highly dependent on the type of ionic liquid used [2]. To elucidate the mechanism, we have been carried out several kinetics studies by means of photophysical experiments [6,7]. So far, some important interplay between the energy-carrying solute molecules and ionic liquids has been found out as to how the molecular kinetics (partly relevant to the molecular dynamics) governs the magnitude of Φ_{UC} [6-8]. In this talk, our recent results as well as the interpretations obtained through the investigations will be presented.

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Microscopy Based Inference of Nanoscale Aggregate Morphologies: Applications in Nanomedicine and Aerosol Science

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A common issue which arises in the study of transport processes in nanomaterial laden media in biological and environmental systems is that nanoparticles readily collide with and stick to one another, aggregates. Thermal transport through aggregate laden media is dependent not only on aggregate material properties, but aggregate morphology. In this presentation, a method to infer aggregate three-dimensional structures from cryo-electron micrographs of aggregates in suspensions is discussed, which can be used to provide boundary conditions for numerical examination of thermal transport in aggregate laden media. In the proposed method, aggregates are modeled as quasifractal aggregates, in which their geometries are described by the number of primary particles per aggregate, the fractal dimension (which varies between 1.0 and 3.0), a pre-exponential factor, and the average primary particle size. The most probable quasifractal geometric descriptors are inferred from images by direct calculation of observable two-dimensional properties, namely, the projected area, longest end-to-end distance, radius of gyration, and perimeter, and comparison of these four parameters to those tabulated for more than 50,000 computationally generated quasifractal aggregates with prescribed geometric descriptors. This comparison enables determination of the weighted average quasifractal descriptors for each imaged aggregate. Application of this technique to the analysis of titania aggregates synthesized in gas phase reactors (with comparison of predicted to measured drag coefficients for imaged particles) and the examination of iron oxide nanoparticle aggregation in intracellular and extracellular matrices will be discussed.

Vibrational spectra in the study of molecular interactions in transient molecular dynamics simulation. Application to the van der Waals interaction of nucleobases with grapheme.

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The study of vibrational characteristics in the several types of molecular interactions or bonding in order to define the possible pathways of energy transfer and influence of thermal environment on the transfer process has been studied. The calculation was performed by molecular dynamics method (MD). Recent studies of ultrafast phenomena by IR spectroscopy showed possibility of some induced proton transfer reactions and set a ground for coherent control in condensed phases. Starting from the study of vibrational relaxation in a model proton transfer reaction that are present in the range of oxidation reactions of cold ignition we tested vibrational frequencies defined by the Fourier transformed velocity autocorrelation function (ACF) for the proton transfer bonds at the time of reaction. Due to the limited reaction time and non-equilibrium character of bond switching process, the transient correlation was taken in the time interval approximately corresponding to the experimentally confirmed reaction time of few ps. The bond switching model has been utilized in the description of proton transfer inside MM2/MM3 force field potential. The bond part of potential was modified from harmonic one to anharmonic in order to bring potential closer to the quantum potential energy surface defining this type of reactions. The calculated vibrational spectrum in the n-heptane+ OH reaction has shown high sensitivity to the potential anharmonicity by substantial deviations in the frequencies of reacting bonds C-H and O-H responsible for the proton transfer up to 30-to 40 cm^{-1} in the bond stretching vibrations that have experimental range of ~3000 cm^{-1} frequencies. In the present reaction model no dependence of stretching vibrational frequencies on temperature was presently found in the temperature range 400-700 K. However, vibrational relaxation along the proton transfer bond was registered at an approximate amount of 26 J, with supposed energy transfer from stretching and bending modes to heptane rocking in nonequilibrium MD calculations.

The obtained sensitivity of the transient velocity ACF analysis to the variations in bonding potential allows us to suppose that above vibrational frequency analysis might be applicable to the dynamics of small biomolecules interacting by Van der Waals forces with sensors at the time scale of several vibrational periods. The graphene nanopore could be utilized as one type of such sensor. Our previous studies has shown that interaction forces between small biomolecules such as nucleobases and graphene pore edge can be sensitive to small variations in biomolecule structure, but the period of sensing is limited by the time of the molecule passing through the nanopore. Experimental measurement of dynamic force field are still not available in such a limited time and considerations on time resolution of IR spectroscopy has lead us to study vibrational frequencies of interacting with graphene nucleobases.

The atoms of graphene pore edge and base molecule are graded by the magnitude of interaction force. For atoms with the largest values, the vibrational frequency analysis has been carried out separately for graphene and nucleobase. Graphene has shown a range of frequencies between out of plane Z modes and up to G modes close to 50 THz that were not much affected by interaction with the base. The base molecules passing at the fixed distance from the pore edge exhibited a range of frequencies depending on the molecule structure and orientation. We compared obtained modes with the experimentally available modes from IR spectroscopy. A possibility of molecular selection by frequency analysis can be estimated from obtained data.

Fabrication of Semi-conducting Single-wall Carbon Nanotube Arrays

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Single-walled carbon nanotube (SWNT) is a rolled-up graphene and it is one of the most important materials in nano-technology, owing to the excellent physical, chemical and mechanical properties. Forward many SWNT applications, the control of the electric conductivity (metallic or semiconducting), which depend on the atomic structure (so-called chirality), is quite important. However, it is difficult to synthesize only semi-conducting SWNTs in the growth stage so far, and the separation or purification techniques are necessary. Here, we synthesized horizontally-aligned SWNTs (HA-SWNTs) and performed selectively removal of metallic SWNTs based on electrical breakdown method. The resulting structure (semi-conducting SWNT arrays) is preferred for the fabrication of integrated circuits using SWNTs.

HA-SWNTs were synthesized on crystal quartz substrates (R-cut) by using alcohol catalytic CVD method [1, 2]. After the substrates with iron nano-particles was heated at 800 °C, ethanol vapor was supplied with Ar/H_2 buffer gasses. Ethanol molecules decomposed and SWNTs were grown from the iron nano-particles. SWNTs interacted with the substrate surface and they were aligned along the x-axis of crystal quartz. Figure 1 shows SEM image of HA-SWNTs, which are highly oriented. The as-grown SWNTs were mixture of metallic or semi-conducting SWNTs. HA-SWNTs were coated with polymer thin-film (PMMA) and they were Joule-heated. Figure 2(A) shows metallic and semiconducting SWNTs, which were connected with a pair of electrodes. During Joule-heating, SWNT temperature increased and only metallic SWNTs exhibited breakdown, owing to high current density. A part of metallic SWNT were removed, as shown in Fig. 2(B). While the removal length is generally 100 nm without polymer coating, the polymer thin film clearly enhanced the removal length. It suggests that the polymer film affects the temperature distribution of SWNTs and the heat of chemical reaction during breakdown.

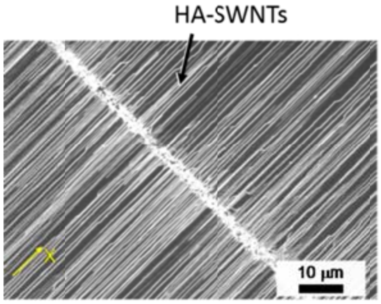

Fig. 1: SEM image of HA-SWNTs grown on crystal quartz substrates.

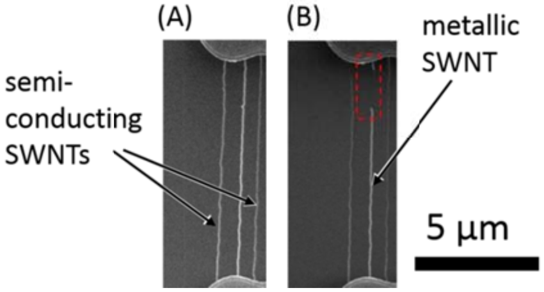

Fig. 2: SEM image of (A) as-grown SWNTs and (B) after polymer film-assisted electrical breakdown.

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[3] K. Otsuka, T. Inoue, S. Chiashi, and S. Maruyama, *Nanoscale*, (2014) to be published.

Poster Abstracts

Alphabetical by Presenter’s First Name

Anisotropic and Nonhomogeneous Thermal Conduction in Few m Thick Nanocrystalline Diamond Films

Aditya Sood[1,2], Jungwan Cho[2], Karl Hobart[3], Tatyana Feygelson[3], Bradford Pate[3], Mehdi Asheghi[2], Kenneth E. Goodson[2]

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[2] Department of Mechanical Engineering, Stanford University, USA
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Diamond has emerged as a promising candidate heat sink material in several niche applications involving high heat-flux hot spots, due to its extremely large thermal conductivity in bulk, single crystalline form. Commercial applications however typically involve diamond that is grown using processes such as chemical vapor deposition (CVD). CVD is a nucleation and growth process that results in films with a polycrystalline grain structure, and complex morphology. Nucleation and coalescence create near-interfacial regions of small grain size and low thermal conductivity, while grain growth results in higher quality regions away from the interface with larger conductivity. Moreover, impingement of grains in the lateral direction during growth results in a highly columnar grain structure, causing the thermal conductivity to be strongly anisotropic with a lower conductivity in-plane as compared to through-plane. We present an experimental study of thermal conduction in few μm thick CVD diamond films by time-domain thermoreflectance (TDTR), an optical pump-probe technique. The samples are unique in that portions of the growth substrate are etched away leaving regions of free-standing diamond membranes. This configuration allows us to measure directly the thermal properties of both the high-quality top region and lower conductivity bottom region by performing measurements from both sides. More importantly, due to their suspended nature, heat injected into the films by the pump pulses is forced to conduct laterally, causing the thermal decay profile to be highly sensitive to the anisotropy. Our TDTR methodology utilizes the information present in both the amplitude and phase response of the system at the modulation harmonic of the pump laser, enabling us to separate out the effects of the transducer-diamond boundary conductance from the intrinsic in-plane and through-plane conductivity of diamond. To the best of our knowledge, these are the first measurements of the anisotropy and nonhomogeneity of the intrinsic thermal conductivity in diamond films as thin as 1 m. We find that the films have a strong anisotropy, with the in-plane conductivity lower than the through-plane conductivity by a nearly a factor of 6-8.

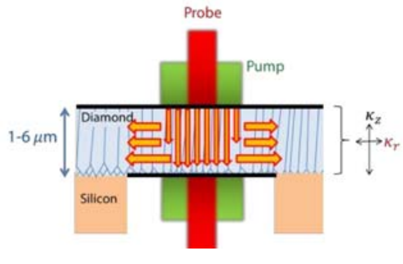

Fig. 1: Schematic of sample configuration and measurement technique for measuring the intrinsic anisotropy and nonhomogeneity of free-standing diamond films

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Spin-Dependent Molecular Motion of Oxygen Adsorbed in Nanoporous Metal−Organic Frameworks

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Among homonuclear diatomic molecules, only the oxygen molecule (O_2) exhibits magnetism (spin quantum number $S = 1$). Since notable characteristic of O_2 in intermolecular interaction are that magnetic exchange interactions have a similar magnitude of interaction as electric quadrupole moments, the molecular arrangement is affected by their competition. In a model system of an O_2–O_2 dimer confined in the nanopores of Cu-1,4-cyclohexanedicarboxylic acid, the molecular orientation associated with the spin state was observed by precise synchrotron radiation structure analysis. The obtained charge density level structures revealed that the significant change of molecular orientation particularly occurred by changing temperature, coupling with the spin states of O_2–O_2 dimer. The temperature dependence of magnetic susceptibility and the magnetization process characterized by the absence of half-plateau ($S_{\mathrm{dimer}} = 1$) were both consistent with the theoretical model for dimer spin states in terms of molecular orientation [1]. Our findings, therefore, proved that the molecular orientation could cause various spin state, i.e., the rectangular parallel H-geometry for the singlet ground state ($S_{\mathrm{dimer}} = 0$) and the shifted parallel S-geometry for the thermally excited quintet state ($S_{\mathrm{dimer}} = 2$), which has not been found for solid O_2. In this present study, we perform the Raman scattering measurement and discuss on the molecular motion, coupling with the spin states of the O_2–O_2 dimer.

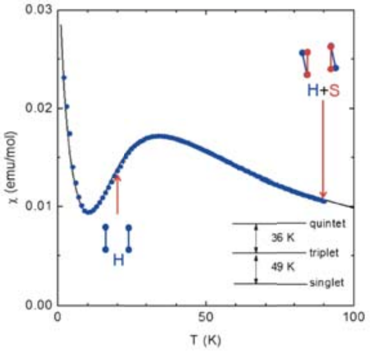

Fig. 1: Temperature dependence of susceptibility of O_2 adsorbed in Cu-1,4-cyclohexanedicarboxylic acid. The solid curve is the susceptibility calculated using the O_2–O_2 dimer model taking into account the thermally excitation from the H-geometry with $S_{\mathrm{dimer}} = 0$ to the overlap of the S-geometry with $S_{\mathrm{dimer}} = 2$ and the H-geometry with $S_{\mathrm{dimer}} = 1$ and 0 in heating process [1].

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Observation of Nonlinear Peltier Coefficient in Low-doped Semiconductors at Room and Cryogenic Temperatures

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We report the first room and low temperature experimental observation of Peltier effect in thin film microrefrigerators. Nonlinear (current-dependent) Peltier coefficient of low-doped n-type InGaAs and its associated Peltier cooling are extracted from electrical and thermal imaging characterization techniques. The idea of utilizing current-dependent peltier coefficient for cooling application was first proposed by Mona Zebarjadi, et. al. in [1]. At high electric fields the linear relation between Peltier cooling/heating with current is no longer valid. Peltier coefficient depends nonlinearly on current and rises significantly as current increases. Nonlinear Peltier coefficient was calculated using Monte Carlo simulation. It is indicated that this coefficient is temperature independent, proportional to the effective mass, and inversely proportional to the square of carrier concentration in the semiconductor. Although the non-linear term is temperature independent, significant cooling at low temperature due to weaker electron-phonon coupling is predicted. In an effort to measure the Peltier coefficient and Peltier cooling in nonlinear thermoelectrics, we designed and fabricated a set of nonlinear microrefrigerators. A 5µm thick low-doped n-type InGaAs was grown by the molecular beam epitaxy. A highly-doped InGaAs contact layer was grown on top of the active layer for low metal/semiconductor contact resistance. Devices of various sizes ranging from $10x10\mu m^2$ to $150x150\mu m^2$ were fabricated on the wafer by creating 0.8 micron deep square mesas of different sizes using the inductive-coupled plasma etch. The devices act as a Metal-Semiconductor-Metal structure due to presence of two back to back Schottky diodes.

We employed thermoreflectance thermal imaging to obtain the temperature profile of the microrefrigerators under forward and reverse biasing conditions at different current densities ranging from $100A/cm^2$ to $1500A/cm^2$. Temperature profiles as well as DC electrical measurements are input to a hybrid analytical-numerical model, based on the full heat balance equation in order to extract the current-dependent Peltier coefficient of the thin film. The calculated current dependent coefficients at room temperature are in agreement with the Monte Carlo simulation results at biases lower than punch-through voltage in the thin film. Beyond the punch-through, Peltier coefficient saturate as we further increase the applied voltage and in turn the current density. We compare the experimental and the Monte Carlo results at the two regimes and discuss about the differences. Additionally, we conducted measurements at cryogenic temperatures (30K, 50K, 70K). In this regime, due to the strong current and temperature non-uniformity at the top surface of the microrefrigerators, one can extract a coarse estimate of the Peltier coefficient. Stronger nonlinearity as a function of current density is observed. Further analysis are being performed to accurately quantify the nonlinear thermoelectric transport.

We exploited the extracted Peltier coefficient, both at room and low temperature, to determine temperature changes due to Peltier cooling/heating at different interfaces and Joule heating. About 7-8 degrees Peltier cooling is achieved at a current density of about $1200A/cm^2$ at room temperature. Due to excessive Joule heating, the overall cooling performance of the device is not significant. We will discuss design requirements for a nonlinear thermoelectric device to achieve large coolings.

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Investigation of the Wiedemann-Franz law in the conducting polymer PEDOT

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The conducting polymer PEDOT (Poly-3,4-ethylenedioxythiophene) has been studied as a promising polymer thermoelectric material, with a reported ZT on the order of 0.3 at room temperature. Previous measurements of the thermal conductivity using the 3ω method have reported an in-plane thermal conductivity less than the estimated electronic contribution from the theoretical Sommerfeld value of the Lorenz number. The validity of the Wiedemann-Franz law in these systems has remained an open question, as the charge transport mechanism can be different than in inorganic materials. However, no previous studies have directly measured all three thermoelectric properties of PEDOT films in the same transport direction and on the same sample, as the 3ω method requires different processing between thermal and electrical measurements. This poster will present results on the in-plane thermoelectric properties of PEDOT:Tosylate thin films measured with the use of suspended devices. The value of the Lorenz number and its temperature dependence for this conducting polymer system are discussed.

Penetration depth of near-field radiative heat transport in dielectrics

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Thermal radiative emissions are of crucial importance to a variety of energy conversion and thermal management applications. Recent experimental studies have demonstrated orders-of-magnitude heat transfer enhancement between closely spaced bulk materials, where near-field contributions to thermal transport are dominant. Using a novel experimental platform, we conducted a systematic investigation of the effect of film thickness on the near-field heat transfer properties. By measuring radiative heat flow between a hot silica microsphere and a set of thin silica films of various thicknesses (50 nm to 3 µm) as a function of gap size ranging from ~20 nm to ~10 µm, we found substantial enhancements in heat transport properties due to near-field effects, even for the thinnest films when the gap size was comparable to the film thickness. Further, we found that at larger separations (~1 µm), the thicker films show significantly larger near-field enhancement than thinner films. These results provide the first direct evidence of a distance-dependent penetration depth of near-field radiative energy transport.

Long-range communication by thermally excited graphene plasmons

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As one emerging plasmonic material, graphene can support surface plasmons at infrared and terahertz frequencies with unprecedented properties due to the strong interactions between graphene and low frequency photons. Since graphene surface plasmons exist in the infrared and terahertz regime, they can be thermally pumped (excited) by the infrared evanescent waves emitted from an object. Here, we show, for the first time, that thermal graphene plasmons can be excited with a remarkable efficiency and have monochromatic and tunable spectra, thus paving a way to harness thermal energy for graphene plasmonic devices. We further demonstrate that we can potentially realize "thermal information communication" via graphene surface plasmons by effectively harnessing thermal energy from various heat sources, e.g., the waste heat dissipated from nanoelectronic devices. These findings open up a new avenue of thermal plasmonics based on graphene for different applications, ranging from infrared emission control, to information processing and communication, and to energy harvesting.

Metrology for Thermal & Electrical Transport

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Although numerous measurement techniques have been developed for investigating thermal transport in thin films and nanowires, high accuracy, high throughput measurements of nanostructured materials are still challenging. Beyond single property measurements, simultaneous measurement of multiple properties (*e.g.* thermal and electrical conductivity) is advantageous for fully characterizing materials for specific applications such as thermoelectric devices. For characterization of thermoelectric mateirals, a combined measurement structure [1] is optimized using numerical Comsol simulations to determine the accuracy of the thermal conductivity measurement (see Fig. 1). In these structures, the thermal conductivity is measured using the 3ω technique with heater lines patterned on the top surface of the sample. Electrical conductivity and Seebeck coefficient are characterized using integrated electrodes. The heater design is optimized to minimize the uncertainty in the 3ω measurement and for uniformity of the heat flux for thermoelectric characterization. Although originally designed for thermoelectric materials such as bismuth telluride, these devices are easily adapted to study a variety of materials including organic electrically conducting polymers. The versatile structure provides a simple platform for combined property characterization.

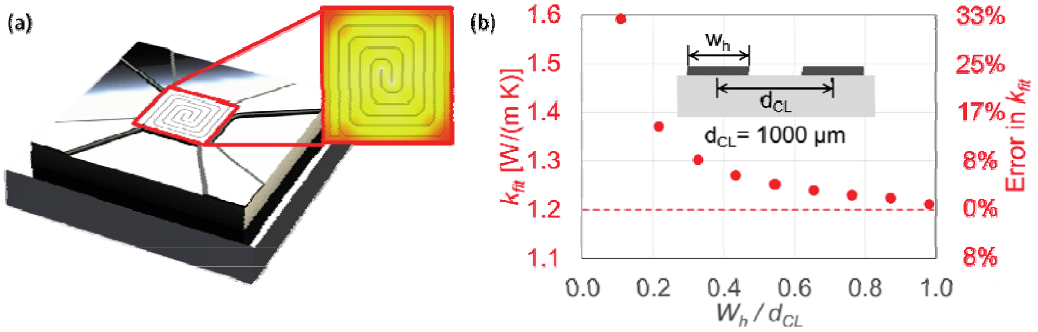

Fig. 1(a): Scalable device for simultaneous characterization of thermal and electrical properties. **(b)** Impact of heater line width (w_h) on the fitted thermal conductivity of a sample material with nominal thermal conductivity of 1.2 W/(m K). The value extracted from 1-D diffusive thermal transport model approaches the input value as the heater line width approaches the heater spacing (d_{cl}) and the thermal transport becomes more one-dimensional.

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Obtaining Localized Phonon Spectra from Molecular Dynamics Simulations using the Wavelet Transform

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A molecular dynamics simulation implicitly contains everything there is to know about the simulated system, including most types of phonon scattering. The difficulty lies in how to extract spectral information that furthers understanding of transport in the system. We discuss the wavelet transform as a flexible technique to obtain spatially or temporally localized vibrational spectra from a simulation trajectory and we apply the method to two case studies. In the first study, we use the wavelet transform to measure the frequency dependent intrinsic diffusivity of simulated amorphous silicon. In the second study, we calculate the localized phonon population near an interface in a typical non-equilibrium molecular dynamics measurement of thermal boundary conductance for a 1D chain. These studies illustrate how molecular dynamics simulation in concert with the proper analysis framework can contribute to the theoretical understanding of nanoscale thermal transport in diverse material systems.

Phase Separation Microfluidics

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High power density GaN HEMT technology can increase the capability of defense electronics systems with the reduction of CSWaP. However, thermal limitations have currently limited the inherent capabilities of this technology where transistor-level power densities that exceed 10 kW/cm^2 are electrically feasible. This work introduces the concept of an evaporative microcooling device utilizing some of the current two-phase vapor separation technologies currently being developed for water and dielectric liquids.

Dimensional scaling and corresponding exponential increase in transistor density has been accompanied by a significant increase in power density in microchips and the heat flux for high performance chips in the 14 nm generation is projected to be greater than 100 W/cm^2 with a junction-to-ambient thermal resistance <0.2°C/W [1]. High power density GaN high-electron-mobility transistor (HEMT) technology can increase the capability of defense electronics systems however, thermal challenges arise due to transistor-level power densities that can exceed 10 kW/cm^2. This has motivated research on liquid cooling, both direct [2] and indirect [3], have been well with an emphasis on addressing challenges for high power electronics.

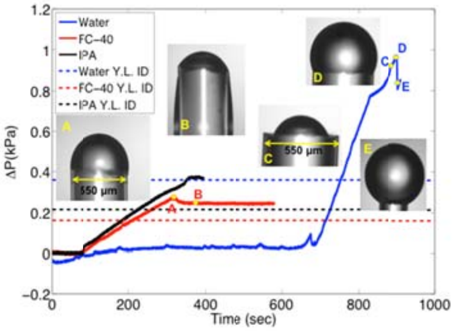

Fig. 1. Glass capillary bursting pressure results for (a) water, (b) IPA, (c) FC-40.

In this work, we focus on developing vapor phase separation technology designed for an evaporative microheat exchanger, designed to target heat fluxes exceeding 5 kW/cm^2 with a temperature rise of less than 5K. To achieve these aggressive targets, three essential goals must be met: 1.) Obtaining a stable, ultra-thin evaporating liquid film at the walls of the microcooling device that remains wetted even at extreme heat fluxes and does not flood at low heat fluxes. 2.) Providing adequate liquid delivery and vapor extraction while maintaining small pressure drops (to minimize elevation of saturation temperature and required pumping power). 3.) Ensuring the lowest possible thermal conduction and convection resistances from heat generation volumes to the phase change surface including conduction along extended surfaces. We address these issues with a tightly integrated combination of porous material design, surface engineering, intricate microfluidic phase management, and application of available materials with exceptional thermal properties but major integration challenges. In this poster, we describe chemical and geometric surface engineering techniques being applied for robust and finely controlled phase separation including advances in fundamental understanding of effects of geometrically optimized surfaces for retaining completely wetting liquids, such as dielectric refrigerants (see Fig. 1) [4].

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An analytical solution to Boltzmann transport equation from diffusive to ballistic regime and its application to frequency domain thermoreflectance measurement

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Fourier's law breaks down when the periodic heating frequency is comparable to or higher than the phonon frequency (reciprocal of mean free time <MFT> or relaxation time) which lead to a heating frequency dependent thermal conductivity. Recent experiments find that [1], for semiconductor alloys such as SiGe, the heating frequency of starting to observe heating frequency dependent thermal conductivity, could be even order of magnitude lower comparing to Si.

To explain this dependence and also designing possible data analysis method for thermal conductivity measurement in the ballistic regime, the phonon transport process of planar heating source on a semi-infinite body is investigated analytically by the Boltzmann transport equation (BTE). The solution is obtained using two flux model with gray MFT approximation and extended to non-gray regime. The non-gray solutions are consistent with Koh and Cahill's observation that the single crystal SiGe alloy has stronger heating frequency dependence on effective thermal conductivity than the natural Si [1]. Basing on this BTE solution, a virtual experiment for interpreting the frequency domain thermoreflectance (FDTR) data is designed [2], which fits the phase difference between surface temperature and heat flux to obtain the effective thermal conductivity and accumulation function over MFT.

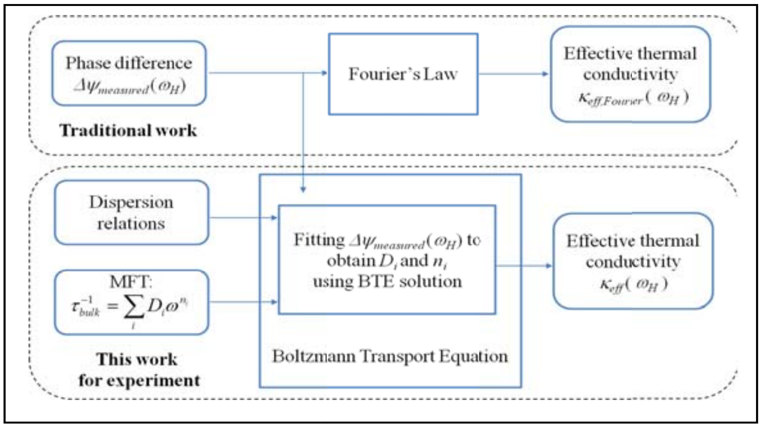

Fig. 1: Comparison between Fourier and BTE method for interpreting FDTR temperature-heat flux phase lag data

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Thermal Transport in Chirality-Sorted Carbon Nanotube Networks

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Recent advances have led to sorting of single-wall carbon nanotubes (SWNTs) into chirally purified (e.g. all-semiconducting or all-metallic) solutions and networks [1,2]. However, until now, studies have only focused on the electrical and optical properties of such sorted SWNT films, without reports of their thermal properties to the best of our knowledge.

In this work, we use infrared (IR) thermal imaging to simultaneously study thermal and electrical transport in chirality-sorted SWNT networks for the first time. SWNTs are sorted by density gradient ultracentrifugation [1] to assemble SWNT films through a vacuum filtration method. We suspend the films between two Pd-coated copper blocks that serve as both electrical contacts and heat sinks. We use Joule heating and IR microscopy to obtain the temperature profiles of the suspended SWNT films [3]. We use the transfer length method to obtain the electrical contact resistance, and a finite element model to extract the thermal conductivity of the film and the thermal boundary conductance between the film and Pd/Cu contacts.

We characterized the thermal and electrical properties of 90% semiconducting, 90% metallic, and unsorted (66% semiconducting) SWNT films. The electrical conductivity of these films ranges from 8.5×10^4 to 1.3×10^5 S/m. For the semiconducting films the thermal conductivity is ~180 $\mathrm{Wm^{-1}K^{-1}}$ and the thermal contact conductance is 2700 $\mathrm{WK^{-1}m^{-2}}$ between the film and the Pd/Cu contacts. The metallic films have thermal conductivity of ~140 $\mathrm{Wm^{-1}K^{-1}}$ and a contact conductance of 3000 $\mathrm{WK^{-1}m^{-2}}$. Finally, the unsorted films have a thermal conductivity of 290 $\mathrm{Wm^{-1}K^{-1}}$ and a thermal contact conductance of 1500 $\mathrm{WK^{-1}m^{-2}}$. We uncover that metallic films have lower thermal conductivity but higher electrical conductivity due to greater SWNT junction density and greater mass density (~2 $\mathrm{g/cm^3}$ instead of ~1 $\mathrm{g/cm^3}$ for the other networks). In addition, we find that chirality plays a lesser role on thermal properties than the individual SWNT lengths and overall junction density. Our results are in good agreement with mesoscopic models relating the SWNT film thermal conductivity to mass density [4].

The thermal conductivity of the materials studied here is comparable to that of metals like Al while having one-half the mass density, making SWNT films attractive as lightweight thermal and electrical conductors. In addition, unlike metals, the SWNT film thermal properties can be tuned over several orders of magnitude by varying the SWNT length and junction density [4,5].

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Tailoring thermal radiative properties with film-coupled concave grating metamaterials

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Spectral control of thermal radiation has numerous applications in energy harvesting, thermal management, spacing cooling, and optical sensing. Over last decade, various micro/nanostructures have been demonstrated to tailor thermal radiative properties based on different physical mechanisms. Among them, the metal-insulator-metal, or so-called film-coupled metamaterials have drawn much attention. Perfect absorbers and coherent emitters made of film-coupled metamaterials with different geometries such as one-dimensional (1D) grating [1,2], 2D patch arrays [3,4], disk arrays [5], cross bars [6], and nanoparticles [7] have been studied, in which magnetic polaritons (MPs) and surface plasmon polaritons (SPPs) can be excited, resulting in exotic radiative properties. MP refers to the coupling between incident electromagnetic fields and magnetic resonance inside the structures, while excitation of SPP is due to the oscillation of charges at the interface of different media whose real parts of permittivity have opposite signs. However, the photon transport with film-coupled concave gratings made of subwavelength mesh-like patterns is little investigated. There have been discussions about the optical properties of photonic crystals and fishnet structures with similar geometries, but the effects of MP and SPP in controlling the radiative properties of film-coupled concave grating micro/nanostructures are not well understood so far.

This work numerically investigates the radiative properties of film-coupled metamaterials made of a 2D metallic concave grating on a continuous metal film separated by an ultrathin dielectric spacer. Spectrally-selective absorption is demonstrated in the visible and near-infrared regime, and underlying mechanisms are elucidated to be either localized MPs or SPPs excited inside the metamaterial. The unique behaviors of MPs and SPPs are explained with the electromagnetic field distributions at respective resonance frequencies. Geometric effects such as ridge width and grating period on the resonance absorption peaks are discussed. An inductor-capacitor model is utilized to further confirm the excitation of MP, while dispersion relation is used to understand the behaviors of different SPP modes. Directional radiative properties of the proposed metamaterial structure are also studied for different polarization states as well.

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Phonons transport in a film with asymmetric pores

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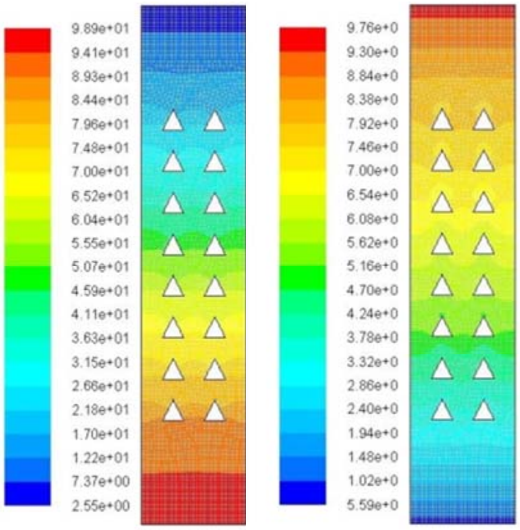
In recent years, development of fine processing technology enables to control physical properties by using a micro- and nano- structure. The size effect on heat conduction due to phonon boundary scattering in films have been well discussed. A thermal rectifier can be made by using asymmetric micro-structures with the ballistic transport of phonons [1,2]. Here, we intend to realize the thermal rectifier by using a thin film with asymmetric pores. We calculated heat conduction in a thin film with asymmetric pores by using radiative heat transfer calculation of ANSYS Fluent based on Boltzmann transport theory [3, 4]. The ballistic transport of phonons in a thin film was numerically calculated for high Knudsen number. The phonon transport was suppressed by the asymmetric pores as shown in Fig. 1 (a). The effective thermal conductivity for forward is lower than that for backward. The thermal rectification was confirmed in the numerical simulation.

The free-standing Si thin films with triangle pores were fabricated from SOI wafer by using standard micro-fabrication processes. The effective thermal conductivities of the films were measured by a periodic laser heating method. The effects of triangle pores on the effective thermal conductivities will be discussed with the numerical simulation results.



(a) (b)

Fig. 1 Calculated temperature distribution based on Kn=0.5, (a)forward (b)backward

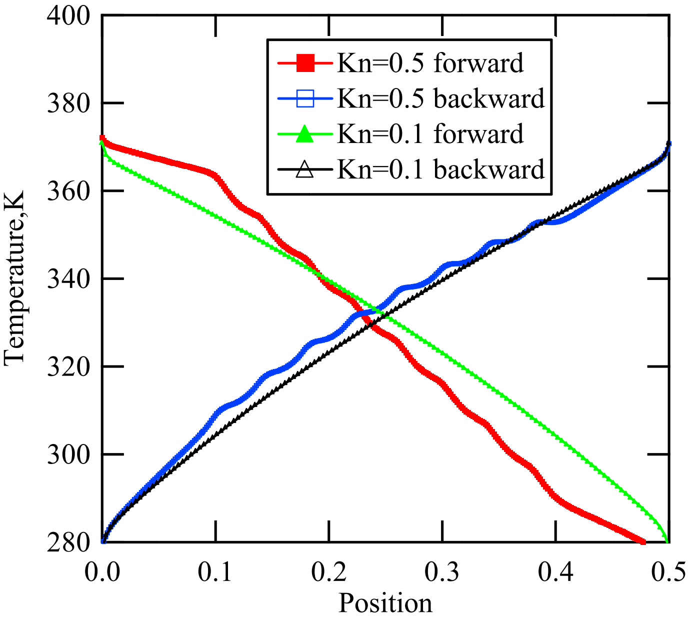


Fig. 2 Calculated temperature distribution at center line.

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Thermal Conduction in Gallium Nitride Composite Substrates

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GaN-based high electron mobility transistors (HEMTs) are promising for next generation radar applications due to their wide band gap, high electron velocity, and high breakdown field [1]. However, due to the high power density in GaN HEMT devices, localized self-heating can be a critical issue. HEMT self-heating can degrade device performance and impair reliability and stability [2]. Thus, in terms of thermal management, efficient heat removal from active semiconducting regions is a key task, which is often limited by the material quality of the GaN composites [3],[4].

For the epitaxial growth of high-performance GaN/AlGaN HEMT structures, SiC is commonly used as a substrate material because SiC offers much higher thermal conductivity (~400 W m^{-1} K^{-1}) than conventional Si (~142 W m^{-1} K^{-1}) and sapphire (~35 W m^{-1} K^{-1}). An AlN transition film is commonly used as an interlayer material in the heteroepitaxial growth of GaN on SiC substrates to minimize the lattice mismatch stress and enable the growth of a high-quality GaN buffer layer. But due to significant mechanical strain present in the AlN transition film, a high density of microstructural defects exist within the volume of the transition film and near its interface, which impedes heat transport into the substrate [5]. Substrates containing CVD diamond can be a viable material solution due to their potentially high thermal conductivity (as much as 5 times higher than that of SiC). However, the current GaN on diamond technology often incorporates a low thermal conductivity transition layer at the interface of the GaN and the diamond, which can partly offset the benefit of using the high conductivity materials [6].

This poster presentation will describe our experimental and theoretical investigation of thermal conduction in GaN composite substrates containing Si, SiC, and diamond [3], [5]-[7]. We measure the thermal resistance of the transition layer between the GaN buffer layer and the substrate as well as the thermal conductivity of the GaN, using picosecond time domain thermoreflectance (TDTR). We theoretically examine the relevant phonon scattering mechanisms responsible for the temperature trend of the transition layer resistance. The best available data in literature are also presented in comparison with our thermal modeling as well as our data.

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Contribution of Phonon Drag to the Thermopower in Bulk and Nanoscale Silicon

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The Seebeck effect, a property governing the thermoelectric energy conversion, is enhanced by the phonons which exert drag on the charge carriers that diffuse along a temperature gradient [1]. Amidst the difficulty in experimentally quantifying phonon drag, its contribution to the Seebeck coefficient is often considered negligible in highly doped semiconductors. This assumption forms the central premise of nanostructured thermoelectrics where the phonon scattering at nanoscale boundaries only reduces thermal conductivity without any apparent effect on the Seebeck coefficient [2]. In this work, we correct the existing notions by comparative measurements of the Seebeck coefficient of silicon nanowires and the bulk of equivalent doping. We deduce that phonon drag is a substantial contributor in bulk silicon both at room temperature and at high doping, and completely vanishes in nanowires of 100 nm diameters due to phonon boundary scattering. The annihilation of drag reduces the Seebeck coefficient of nanowires as much as ~27% at 300K and thermoelectric power factor at least by ~48%. We explain our findings by considering the recently emerging knowledge of mean free path spectrum of the phonons [3]. These results motivate a rethinking of the widely pursued approach of enhancing the figure of merit in thermoelectric conversion.

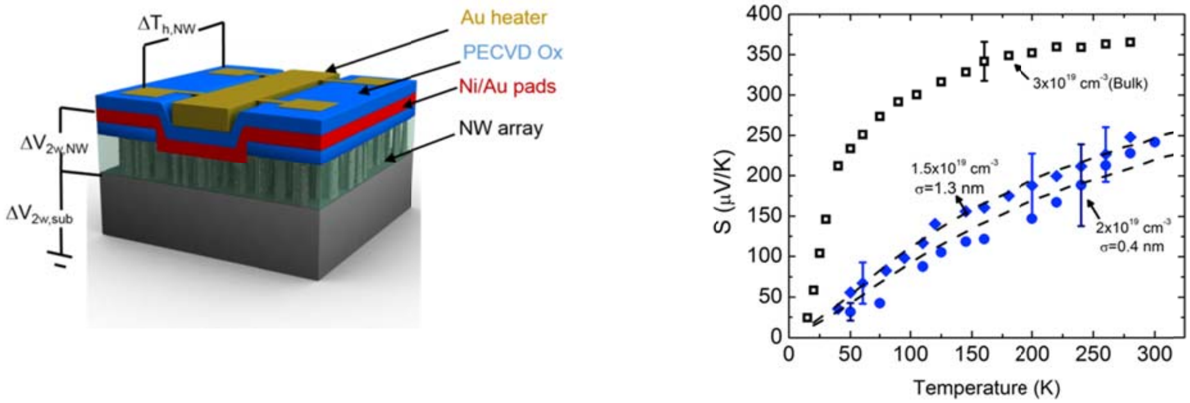

Figure 1: (a) Schematic showing the platform for the simultaneous measurement of Seebeck coefficient and thermal conductivity on the nanowire arrays. (b) The Seebeck coefficient of NW arrays.

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Novel Thermoelectric Transport in Correlated Vanadium Dioxide

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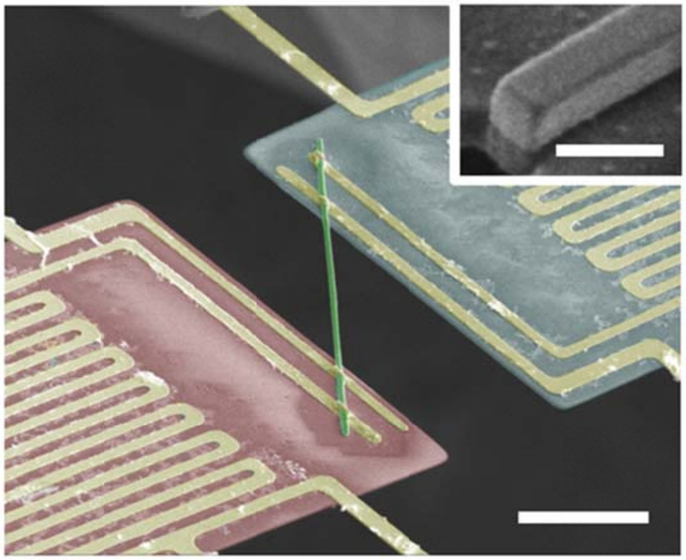
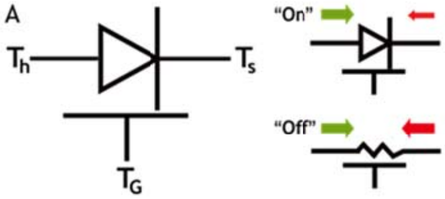
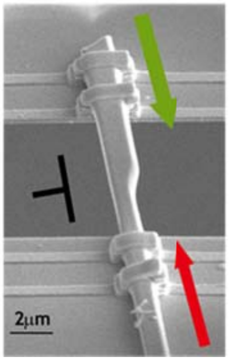
Vanadium Dioxide is a correlated material and undergoes an electronic and structural phase transition at 340K. Below 340K, it is an insulator and the transition can be induced by voltage, temperature as well as light. We perform thermal and electrical conductivity, and Seebeck measurements to study coupled electro-thermal transport in this fascinating material. We demonstrate the first achievement of an all-thermal active device, where single-crystal VO_2 beams behave as rectifiers in the insulating phase with a rectification as large as 28%. Once above the phase transition temperature, the rectification is turned off and the beam behaves as a thermal resistor exhibiting symmetric transport. Additionally, metallic VO_2 is a correlated electron system; we analyse the electrical contribution to thermal transport at the transition temperature and observe a possible violation of the Weidemann-Franz Law. The total measured thermal conductivity does not change across the phase transition, while the electrical conductivity increases by 4 orders of magnitude. Finally, we observe the phases of VO2 using a scanning Near-Field Optical Microscope and correlate the insulating and metallic phases to the observed experimental data. Understanding thermal transport in this novel system allows us to control heat and charge flow in unprecedented ways.







Analytical interpretation of non-diffusive phonon transport in thermoreflectance thermal conductivity measurements

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The thermal conductivity accumulation function describes spectral contributions to the bulk thermal conductivity of a solid from different mean free path energy carriers. Experimentally, the accumulation function is obtained by measuring the thermal conductivity of the solid as a function of a variable experimental length scale. In recent work, these measurements are converted into an accumulation function by assuming that energy carriers with mean free paths larger than the characteristic experimental length scale do not contribute to the measured value of thermal conductivity and energy carriers with mean free paths less than the characteristic experimental length scale fully contribute. However, this conversion function (known as the suppression function) is not as straightforward as originally proposed and has a more complicated functional dependence on the characteristic experimental length scales, which are different for different techniques.

In this work, we derive a suppression function for frequency-domain thermoreflectance (FDTR). In FDTR, there are two characteristic length scales: the thermal penetration depth, which arises from temporally sinusoidal laser heating, and the diameter of the laser spot. We account for both of these length scales in our derivation of the suppression function and obtain an analytical expression by solving the Boltzmann transport equation for phonons in spherically symmetrical geometry under the relaxation time approximation. The result can be used to effectively convert thermal conductivity measurements by FDTR (which are functions of both thermal penetration depth and laser spot diameter) to the thermal conductivity accumulation function in non-metallic, crystalline materials.

Thin film thermal transport via high-repetition-rate, time-resolved x-ray diffraction

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We utilized time-resolved x-ray diffraction to monitor heat flow through thin film materials and across subsequent interfaces in the near-equilibrium regime. A 1 MHz, 500 fs optical laser was used at moderate to low fluences (200-25 μJ/cm^2) to excite strain waves in nanoscale films of BiFeO3, Pb(Zr,Ti)O3, and Bi very close to equilibrium. The laser-induced strain in these films was directly studied via a change in the center of mass of the diffraction peak of the thin films using short (15 ps and 60 ps) x ray pulses from a synchrotron at a 1 MHz repetition rate, a subtle measurement enabled by the high stability and repetition rate of the synchrotron.

Through this same technique, we measured the delayed transit of this strain wave from the thin film into another layer (either the substrate itself or another thin layer), thereby directly probing thermal transport processes across solid/solid interfaces. Moreover, we indirectly explored thermal transport across an interface by examining recovery times for the excited thin film. The majority of these results are discussed in Ref. [1].

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Molecular dynamic simulations of water uptake into a silica nanopore

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Canonical ensemble molecular dynamics (*NVT*-MD) simulations were performed to investigate the kinetics of water uptake into mesoporous silica. In this sturdy, mesoporous silica was modeled as a thin film of a crystalline structure with a finite cylindrical pore normal to the film surfaces. The crystal structure was sliced by two parallel planes (top and bottom planes) and a finite cylindrical pore was aligned normal to the two parallel planes. Initially, two water liquid thin films were placed on the upper and lower surfaces of mesoporou silica thin film, and then, *NVT*-MD simulations were performed with different number of water molecule *N* and temperature *T*. At first, in order to gain insight into the water transport mechanism, *NVT*-MD simulations were performed with varying *N* at 300 K. As a result, the kinetics of water uptake depends on *N* and there were two different water transport mechanisms in the pore. One was diffusion of water along the inner surface of the pore (surface diffusion), and the other was capillary rise of liquid water accompanying the formation of meniscus at the pore entrance (capillary rise) (see Fig. 1). Next, the relaxation rate constant was investigated by varying *T* for each *N*. For surface diffusion, the temperature dependence of relaxation rate shows that the activation energy was affected by the thickness of water layer. This is due to water molecule in the outer adsorption layers could move more easily. On the other hand, the water uptake rate of capillary rise was much greater than that of surface diffusion, and the temperature dependence of water uptake rate could be expressed by the viscosity of water. Finally, from the molecular point of view, radial profile of velocity and density of water were examined. As a result, the translational motion of water in the first layer was obviously restricted. For the case of surface diffusion, the velocity profile was correlated with layered distribution of density, whereas, Poiseuille-like flow was observed for capillary rise case. These results suggest water-silica interaction is dominant for surface diffusion, while water-water interaction is dominant for capillary rise.

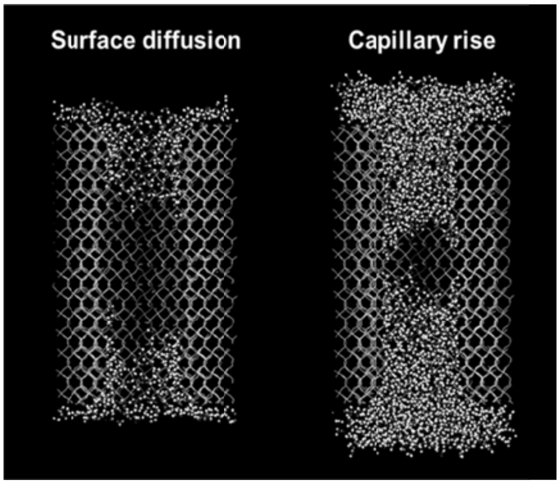

Fig. 1: Snapshot of *NVT*-MD simulations.

Probing Radiative Heat Transfer in the Extreme Near-Field

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Fluctuational electrodynamics based calculations predict significant enhancements in radiative heat transfer as the spatial separation between an emitter and a receiver is reduced to the nanoscale. Previous experiments performed with a microsphere and a planar surface yielded results that were in good agreement with theoretical predictions for gaps as small as 30 nm [1]. In order to understand near-field radiative heat transfer in the extreme near-field regime (gaps of 1 – 10 nm) we recently performed systematic studies using atomic force microscope (AFM) based scanning probes, with integrated nanoscale thermocouples as a thermal sensor, which were coated with metals/dielectrics. Our experiments of heat transport between the scanning probes and a flat substrate coated with a metal/dielectric, performed in an UHV environment, suggest that heat transport is dramatically enhanced in the near-field. The measured heat flows between both dielectric surfaces and metallic surfaces were found to be in reasonable agreement with theoretical predictions [1-3]—thus establishing the validity of using fluctuational electrodynamics in modeling near-field heat transport even at single-digit nanometer separations.

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Thermal Radiation Control by Using Gold Coated Micro-Particle Array

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Spectral thermal radiative properties can be controlled by the microstructure on the surface of the materials. Spectral controls of thermal radiation have been intensively investigated as a simple emitter by using structured metal surfaces, such as open-end resonance [1,2], surface plasmon polariton [3,4], and spoof surface plasmon [5,6]. We investigated thermal radiation properties of gold coated micro-particle array numerically and experimentally. We numerically calculated the emittance of the gold coated micro-particle array by using rigorous coupled wave analysis (RCWA). The periodic structures were made by micro-spheres of SiO_2, which diameters were 2μm, 3μm and 5μm. The surfaces of the structures were coated by gold thin film with10nm thickness. The Fourier harmonics is set to 10, and the calculation mesh size was 0.15nm. The numerically calculated spectral normal emittances were shown in Fig.1. The strong enhancement of the emittance was calculated in the wavelength vicinity to the period of the micro-structures due to plasmonic effects on the emission.

The micro-periodic structures were fabricated by using Convective Self-Assembly and gold deposited thin film on the micro-periodic structures surface. The gold thin film was deposited on the flat Si wafer simultaneously, and the measured thickness of the gold film was 50nm. The measured spectral normal emittance of a surface modified structure with 5μm micro-spheres were shown in Fig.2. The enhancement of the emittance around 5μm was confirmed. On the other hand, any enhancement of absorptance was not measured in the flat surface with a gold thin film. The results were roughly agreed with the numerically calculated results.

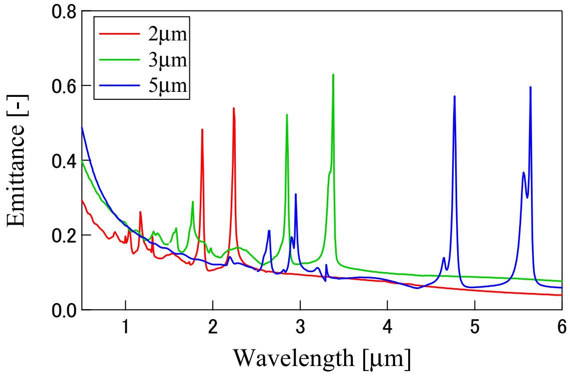

Fig. 1: Numerically calculated spectral normal emittances of the periodic structures with 2μm, 3μm, and 5μm period.

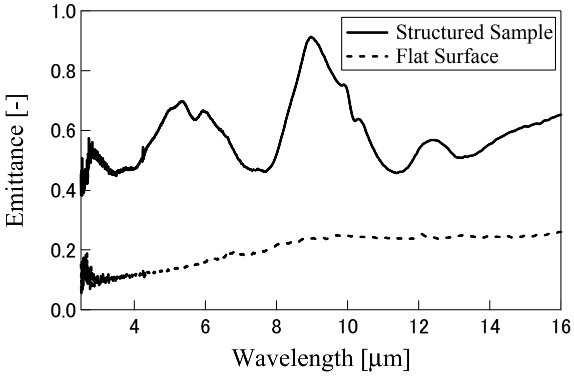

Fig. 2: Measured spectral normal emittances of surface modified micro-particle array (5 μm period), and flat gold thin film.

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High-resolution thermal bridge method and its applications to one-dimensional nanostructures

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Advances in nanoscale thermometry, particularly for one-dimensional nanostructures, are necessary for extending our understanding of nanoscale thermal transport phenomena. We have developed a high-resolution thermal bridge method based on the widely-used suspended device platform, which allows us to measure thermal conductance with sub-pW/K resolution. First, we have demonstrated that the addition of an on-chip bridge circuit for common-mode noise rejection can provide noise-equivalent temperatures below 1 mK and a minimum conductance of 10 pW/K [1]. Second, by using a modulated heating scheme akin to the 3-omega technique along with the bridge circuit, temperature and conductance resolutions of ~50 μK and ~0.25 pW/K, respectively, can be achieved [2]. Furthermore, the parasitic background thermal conductance can be effectively eliminated using the on-chip bridge setup. With the achieved increases in resolution from these thermometry techniques, we have measured the thermal properties of organic and inorganic nanostructures with low thermal conductance. These studies have included measurements on: sub-20 nm semiconductor nanowires with greatly reduced thermal conductivity [3], size effects in thin-shelled semiconductor nanotubes, and thermal conductivity and its correlation with mechanical properties of polymer nanofibers [4]. These advances in thermometry and the ability to measure small-diameter and low-conductance nanostructures will enhance our understanding of nanoscale thermal transport phenomena.

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Thermal Transport in Nanocrystal Superlattices

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We use multiscale computational models to study thermal transport in nanocrystal superlattices (NCSLs). NCSLs are formed by assembly of nanocrystals into organized structures with interesting and tunable properties. They present new phononic behaviors by combining dissimilar materials structured on the nanometer scale. We study thermal transport in these materials by calculating phonon dispersion curves and thermal conductivity. The low thermal conductivity of these materials makes them potential candidates for thermoelectric applications. Such computational models provide a complement to experiments for understanding the behavior of NCSLs, and help us modify their design to achieve better properties.

Thermal Conductivity of Metallic Nanostructures Synthesized via Template-assisted Electrodeposition

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Metallic nanostructures leverage the high thermal conductivity of bulk metal while gaining additional advantageous functions through nanostructuring, such as flexibility derived from the high aspect ratio of nanowires and fluid-permeability that is an intrinsic property of inverse opals. In the present work, we develop a synthesis route to produce these two different nanostructured metals based on template-assisted electrodeposition and a corresponding thermal characterization methodology based on the 3ω method to measure the effective thermal conductivity of the resulting films.

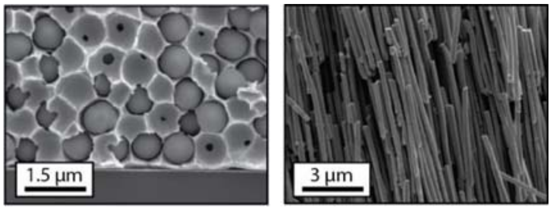

Fig. 1: Scanning electron microscopy images depicting (left) a copper inverse opal and (right) a vertically-aligned array of copper nanowires.

Template-assisted electrodeposition is a simple, scalable, and inexpensive avenue to synthesize large-area nanomaterials. This technique begins with the fabrication of a sacrificial template containing the inverse geometry of the final nanostructure. Metal is then electrodeposited into the interstitial spaces of the template, which is subsequently dissolved. This leaves behind the freestanding metallic nanostructure with the inverse geometry of the template. In this work, we specifically explore the thermal conduction properties of copper inverse opals and nanowire arrays grown by this method. Metal inverse opals are synthesized by using electrodeposition to infiltrate the interstitial spaces of a sacrificial opal template (see Fig. 1, left) [1]. The opal is formed by self-assembling silica nanospheres with diameters as small as ~200 nm into a close-packed crystalline structure. The inverse opal then contains large pores that have the same diameter as the nanospheres along with narrow, fluid-permeable windows between adjacent pores. This structure can be used for high heat flux microfluidic cooling applications owing to its high thermal conductivity and large available surface area, which leads to a low total thermal resistance pathway. Vertically-aligned metal nanowire arrays (see Fig. 1, right) are synthesized using a nanoporous membrane as the sacrificial template [2]. Both polycarbonate track-etched membranes and anodized aluminum oxide membranes are commonly used for this due to their high degree of aligned pores with tunable properties without the need for lithographic processing. These nanowire arrays preserve the high axial thermal conductivity of metal while gaining the mechanical compliance derived from the individual nanowires, which are necessary requirements for high-performance, long-lifetime thermal interface applications. A 3ω methodology is presented to measure the effective thermal conductivity, where the film is synthesized onto an electrically-passivated heater-on-substrate device. Finally, we present preliminary modeling and experimental results to predict and measure the effective thermal conductivity of these two classes of nanomaterials.

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Hydrodynamic phonon transport in suspended graphene

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The transport of phonons, which are the dominant heat carriers in non-metallic solids, is usually diffusive and described by Fourier's law of heat conduction. There are, however, some extraordinary cases where Fourier's law is known to fail. Regimes where Fourier's law breaks down, such as ballistic and hydrodynamic phonon transport, were discovered in bulk three-dimensional materials more than 50 years ago, but these phenomena were observed only at extremely low temperatures [1,2]. The recent development of low-dimensional and nanostructured materials, however, has highlighted the practical importance of ballistic phonon transport in applications such as thermoelectric and electronic devices. In this work, we discuss how hydrodynamic phonon transport as well as ballistic phonon transport can be significant in a low-dimensional material, particularly in graphene.

The main feature of hydrodynamic phonon transport is macroscopic motion of phonons with a drift velocity just like drift motion of molecules in fluid flow. The drift motion causes two representative phenomena of hydrodynamic transport: phonon Poiseuille flow and second sound which are analogous to fluid Poiseuille flow and ordinary sound in fluid, respectively. Our first principles calculation shows that the drift motion of phonons, phonon Poiseuille flow, and second sound occur in suspended graphene at 100 K, much higher than the temperature (~15 K) reported for bulk three-dimensional materials [3]. The significant hydrodynamic phonon transport in suspended graphene can be associated with graphene's two-dimensional features including flexural acoustic phonon modes. Our report on the hydrodynamic phonon transport in suspended graphene will stimulate new approaches beyond those from diffusive or ballistic pictures to understand and manipulate heat flow in two-dimensional materials.

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Acknowledgements

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A New Technique for Measuring Thermal Conductivity of Sub-Millimeter Biological Tissues

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Biomedical thermal therapies are used to treat a variety of diseases such as cardiovascular disease and cancer, and to accomplish cryogenic preservation for transplants and skin grafts. Safe implementation of these techniques requires building a reliable thermal model of the biological system, which requires accurately knowing the associated thermal conductivities, *k*. Unfortunately, traditional techniques for measuring *k* require biological samples to be at least 10 mm thick, rendering many important thin tissues immeasurable, and are susceptible to errors from thermal contact resistance and parasitic heat losses to the environment. In this work, we adapt the "3-Omega" technique [1, 2]—traditionally used for rigid inorganic solids—to overcome all of these limitations. We demonstrate that with this "Supported 3-Omega" technique [3, 4] we are able to measure the thermal conductivity of both frozen and thawed mouse liver. This technique naturally gives rise to a conveniently reusable sensor, and has the potential to measure samples less than 100 microns thick. We measure 9 separate samples ranging from 3 mm thick down to 0.5 mm, at both frozen and thawed temperatures. The measured *k* values of thawed tissue samples around 27 ºC have a spread of 7% (sd), and the frozen tissue samples around -23 ºC have a spread of 2% (sd), demonstrating that the measured *k* values are independent of the thickness of the sample used.

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Measurement of Thermophysical Properties for Latent Heat of Vaporization in Aqueous Nanofluids

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Nanofluids are submicron size nanoparticles suspended in fluids. Recent studies indicate that by adding nanoparticles, it is possible to significantly change thermophysical properties of pure fluids, such as thermal conductivity, critical heat flux, mass diffusivity, surface tension, specific heat, viscosity, and latent heat. Although the latent heat of vaporization (h_{fg}) is an important thermal property, few researchers have studied the variation of h_{fg}. Among them, the enhancement of the latent heat of vaporization in nanofluids is reported by Ammen et al. (2010) using molecular dynamics (MD) simulation and experiments. The co-authors, Lee et al. (2014), demonstrated that h_{fg} can be increased with graphite nanoparticles and decreased with silver nanoparticles. The results show that by adding a small amount (0.1% by volume) of graphite or silver nanoparticles in pure water, the latent heat of vaporization can be varied up to ± 30%. In this paper, we report a conceptual analysis of h_{fg} for aqueous nanofluids based on the Clausius-Clapeyron equation, using measured thermophysical properties, such as density and surface tension. This approach can be used for understanding the details about the variation of h_{fg} in nanofluids.

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Effective phonon mean free path prediction in nanostructures by using numerical transmission model

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Evaluation of thermal conductance in nanostructured semiconductor is of great interest for many applications such as thermoelectrics. Classically, the size effect on lattice thermal conductivity is interpreted in terms of boundary scattering of phonons, limiting phonon mean free path [1]. The effective mean free path Λ_{eff} in nanostructures here involves two different scattering mechanisms: intrinsic phonon scattering and boundary scattering, which have been often expressed as $\Lambda_{\mathrm{eff}}^{-1} = \Lambda_{\mathrm{bulk}}^{-1} + \Lambda_{\mathrm{bdy}}^{-1}$ using Matthiessen's rule [2]. Here Λ_{bulk} is the bulk mean free path only due to intrinsic phonon scattering, and Λ_{bdy} is the mean free path associated with the scattering by material boundaries. While the experimental and numerical studies [3,4] have identified the distribution of Λ_{bulk} and its influence on lattice thermal conductivity, the work on Λ_{bdy} is limited.

In this work, we calculate the effective mean free path in nanostructures, in particular, polycrystalline nanostructures. A numerical transmission model was developed based on the kinetic theory and the Landauer's formula to obtain Λ_{bdy} in the nanostructures. The difference of the effective mean free path in simple and complex shape structures is discussed.

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Thermoelectric Power of Carbon-Nanotube Bucky Paper: Simulation and Experiment

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Development of highly-efficient thermoelectric devices is of great importance to utilize huge amount of waste heat. A single-walled carbon nanotubes (SWNT) is a one-dimensional material and in expected to be a ubiquitous thermoelectric material with large thermoelectric power [1,2]. Recent experiments reported that the temperature effects and doping dependence of Seebeck coefficient (thermoelectric power) of an SWNT buckypaper is essentially different from those of an individual SWNT [3]. However, such unusual behavior of Seebeck coefficient of an SWNT buckypaper has not been understood yet. We speculate that the above-mentioned unusual behavior originates from the contacts between SWNTs. To clarify the validity of this idea, we set a simulation model consisting of the laterally contacted SWNTs as shown in Fig 1.

As a typical example, the (8,0) semiconducting SWNTs are used in our simulations. The Seebeck coefficient of the laterally contacted (8,0) SWNTs was calculated using the density functional theory combined with Landauer theory [5,6].

We also show experimental measurements of Seebeck coefficients of SWNT thin film, which is in excellent agreement with the simulation results [7]. In addition, we produced the world's first all carbon thermoelectric devices. We succeeded to generate about 10-mV power from body temperature using these devices as shown in Fig2.

In the presentation, we explain our simulation results based on Mott's formula of Seebeck coefficient and show that these unusual behavior originates from the resonant tunneling at the contact between the SWNTs.

Fig. 1: **(a)** The laterally-contacted SWNTs. **(b)** Demonstration of an SWNT thermoelectric device. [7]

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A 3 omega method to Measure an Arbitrary Anisotropic Thermal conductivity Tensor

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The 3 omega method is one of the major electrothermal methods for probing thermal conductivity at small scales. This method has been adapted for anisotropic multilayer substrates[1], [2] and attempts have been made to develop closed form solutions for substrates with small anisotropy ratios[3]. These previous works have been restricted to substrates whose anisotropic principal conductivities are aligned parallel and perpendicular to the heater line and sample surface. In this work, we solve the 3 omega problem for the general case of a semi-infinite substrate with anisotropic thermal conductivity having arbitrarily oriented principal conductivities. An exact closed form solution for surface temperature has been found for the case of an ideal finite width, infinitely long 3 omega heater line deposited on an anisotropic substrate.

Following upon the analytical result, an experimental scheme is proposed to isolate the thermal conductivity tensor elements. Using only one heater line and a known volumetric heat capacity, the 2-dimensional anisotropic thermal conductivity tensor in the aligned case can be measured with a low frequency sweep. A total of four heater lines would be required to extend this method to measure all 6 unknown elements of the complete non-diagonal 3-dimensional anisotropic thermal conductivity tensor. Anisotropic mica sheets, appropriately machined to ensure arbitrary principle conductivity direction, are being used as a test sample for these experiments.

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Energy transport in molecular junctions

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Charge transport properties of metal-molecule-metal junctions (MMMJs) have been extensively studied due to their promise in molecular electronics and thermoelectrics. Although pioneering work has studied various charge transport phenomena in MMMJs, the ability to probe energy transport in molecular junctions has remained elusive due to major experimental challenges. In order to overcome these barriers, we developed two novel experimental platforms—NTISTPs (Nanoscale thermocouple integrated scanning tunneling probes) and EBJIHs (Electromigrated break junctions with integrated heater), which were extensively leveraged to study the effect of electronic structure of MMMJs on their heat dissipation and thermoelectric properties, respectively.

The experimental results obtained using these platforms clearly highlight the dependence of heat dissipation and thermoelectric properties of MMMJs on their charge transmission characteristics. Specifically, we found that if junctions have charge transmission characteristics that are strongly energy dependent, heat is dissipated asymmetrically in the electrodes and is dependent on both the bias polarity and the identity of the majority charge carriers. Further, by tuning the electronic structure of molecular junctions, we found that their thermoelectric properties were significantly enhanced. It is expected that the platforms established here will enable testing various energy transport phenomena including Peltier effects at the atomic scale and efficient molecular scale thermoelectric energy conversion—an important and challenging goal in nano-science and technology.

Graphene-assisted near-field heat transfer between silica gratings

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Graphene has attracted much attention in the fields of nanoscale thermal radiation, but previous studies only consider the cases of graphene on simple planar substances while radiative heat transfer analysis of non-planar structures is becoming more necessary due to the high power dissipation requirement of current NEMS/MEMS devices. Silica is one of the best well known thermal emitters due to its two narrow band thermally excited surface phonon polariton (SPhP) modes. Unfortunately, corrugated silica can hardly have a better performance than bulk silica since the radiative transfer is local due to the short lateral propagation length of SPhPs. In this work, the near-field radiative heat transfer between graphene-covered corrugated silica is investigated based on exact scattering theory. Graphene is demonstrated to improve the radiative heat flux between silica gratings by more than one order of magnitude and alleviate the performance sensitivity to lateral shift. The underlying mechanism is mainly attributed to the improved photon tunneling of modes away from phonon resonances. Besides, coating with graphene leads to nonlocal radiative transfer that breaks Derjaguin's proximity approximation and enables corrugated silica to outperform bulk silica in near-field radiation. Similar observations can be expected for other polar materials supporting narrow band SPhP, such as SiC and MgO. In addition, the near-field radiative heat transfer between graphene ribbons with silica as the substrate is also discussed focusing on the interplay between graphene plasmons and SPhP. This work suggests possibilities for more efficient and robust contactless thermal management and photon energy harvesting based on graphene-covered metamaterials.

Thermal Conductivity of Two-Dimensional Transition Metal Dichalcogenides

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Two-dimensional (2-D) materials such as graphene have attracted a lot of interest due to their extraordinary optical, electrical, and mechanical properties for various technological applications. While most previous work focused on graphene, the thermal transport in many other emerging 2-D materials is not well understood. In this work, we apply the phonon Boltzmann transport equation approach with interatomic force constants from first-principles calculations to predict the thermal conductivity of a variety of 2-dimensional transition metal dichalcogenides (TMDCs) with 2-H structure and 1-T structure. The thermal conductivities of 2-H TMDCs, MX2 (M=Mo, W and X=S, Se) are found in the range of 50 to 200 W/mK at room temperature. While thermal conductivity MS2 is usually larger than MSe2, the effect of M atom is found to be abnormal. The thermal conductivity of WS2 is significantly larger than MoS2, though heavier elements in the same column in the periodic table are usually believed to give lower thermal conductivity. We find that this is due to a large phonon frequency gap between acoustic branches and optical branches that makes the acoustic-optical phonon-phonon scattering inefficient. Detailed scattering channel analysis further shows that the weak Umklapp scattering in WS2 also contributes to the high thermal conductivity. Compared with 2-H TMDCS, the thermal conductivities of 1-T TMDCs, MX2 (M=Zr, Hf and X=S, Se) are much smaller and in the order of 10W/mK.

Near-field vacuum thermal transistor made of graphene-covered silicon carbide plates

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Tremendous progress has been made during last decade in advancing the fundamental understanding of phonon transport at the nanoscale to manipulate heat flow in an exotic way, which has promising applications in thermal management, thermal circuits, and even "thermal computers". On the other hand, photon-based heat modulation might offer some unique advantages over phonon transport such as much faster speed due to the inherent difference in the energy carriers. Very recently, radiation-based thermal rectification [1-3] has been studied. The only design of a vacuum thermal transistor reported so far was by Ben-Abdallah and Biehs through modulating the radiative heat transfer upon phase transition of VO_2 [4]. However, active and continuous tuning of radiative heat transfer is quite limited when VO_2 changes between metal and dielectric phases.

In the present work, we propose a near-field vacuum thermal transistor made of two graphene-covered silicon carbide plates separated by a nanometer vacuum gap of 10 nm. Thick SiC plates serve as the thermal "source" and "drain", and are maintained at 400 K and 300 K, respectively. Identical (i.e., symmetric) or different (i.e., asymmetric) "gate" voltages are applied to the graphene sheets and thus control respective chemical potentials, which in turn tune the optical properties of graphene. Recent studies have shown that, near-field thermal radiation could be modulated by different chemical potentials due to the coupling of graphene plasmon across the vacuum gap between suspended graphene sheets, or between graphene covered dielectric [5] or doped silicon plates. With fluctuational electrodynamics, we theoretically show that, near-field radiative heat flux between two graphene-covered SiC plates is actively modulated by varying chemical potentials from 0 to 0.5 eV. Interestingly, two spectral radiative heat flux peaks around the Restrahlen band of SiC exist due to four coupled graphene plasmon modes. This unique photon transport behavior across the nanometer vacuum gap, which is not observed in previous studies, can be explained by the significant variation of the dielectric behavior of SiC upon its strong phonon absorption. Thermal amplification factors, defined as the ratio of differential radiative heat flux to the differential chemical potential, are found as high as 24.5 MW/(m^2 eV) for the symmetric case, and 59.2 MW/(m^2 eV) with asymmetric chemical potentials. The ratio of the maximum to the minimum radiative heat fluxes is 0.93 when varying chemical potentials of the source and drain graphene separately, indicating strong thermal switching effect to turn on or off the radiative heat transport at the nanoscale.

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Rational Design and Control of Nanoscale Thermal Transport

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Currently, around 60% of total energy consumption in the US is lost as waste heat, far below the 2nd law limit, leaving plenty of room for research and innovation. Recent advances in energy technologies, from solar and thermoelectrics to batteries and fuel cells, have heavily explored nanoscale physics and materials. Yet, there are still many challenges in the fundamental understanding and characterization of nanoscale energy transport where classical theories fail. There are ample opportunities to explore the unique structures, interfaces, operating principles, and integrating methodologies to achieve efficiency improvements and cost reductions in existing and emerging energy technologies. My research efforts will be focused on two folds: On one side, to develop high-performance and energy-efficient building blocks through rational design, chemical synthesis and integration of materials and devices. On the other side, to develop unique characterization platforms to measure thermal spectra, interfacial electron dynamics, and multicarrier non-equilibrium transport. The combination will provide unique platforms to study heat, electron, and ion transport, with a particular focus on multicarrier transport and energy conversion. I will apply the developed platforms for a wide range of applications in thermal management, energy conversion and storage systems.

Micro/Nanostructured Phase Separation Heat Exchangers for High Power Density Electronics

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The high power densities achieved by GaN high electron mobility transistor (HEMT) technology can dramatically increase the performance of radar systems, but increasing power will require improved heat removal technologies. Here we explore the dramatic enhancements in cooling (approaching fundamental limits) made possible with advanced thermal management technologies including engineered structures.

The peak power density of GaN HEMT technology is limited by a hierarchy of thermal resistances from the junction to the ambient. Here our work utilizes evaporation to remove large heat fluxes while minimizing thermal resistances between junction and evaporation surface by using highly conductive materials (e.g. diamond and copper) to spread heat over larger areas and transmit heat to the phase change interface. The use of copper microporous structures, as shown in **Fig. 1**, allows delivery of liquid coolant, minimizes thermal resistance by producing ultra-thin liquid films to support evaporation, and increases effective heat transfer coefficient due to their small feature size. In combination with engineering of surface nanostructure and chemistry, microporous structures can also enable control of phase separation, which decreases the total pressure drop of the system. State of the art manufacturing technology using a templated electrodeposition method can produce structures with tightly controlled pore size (from < 1 um to 30 um) and thickness as well as extreme ordering in pore placement. Also, this template method can integrate porous liquid transport layers on the interior surfaces of microchannels. To understand the physics behind the porous structures produced and their performance in devices, characterization methods of the bilayer structures are required. Therefore, we implement image analysis to quantify morphological information and measure thermal conductivity, mechanical modulus, permeability, and burst pressure as a function of porous structure geometry [1-3]. Pore-level and channel-level VOF simulations are performed to estimate the heat transfer coefficient and to understand fundamental aspects of two-phase flow in engineered porous media.

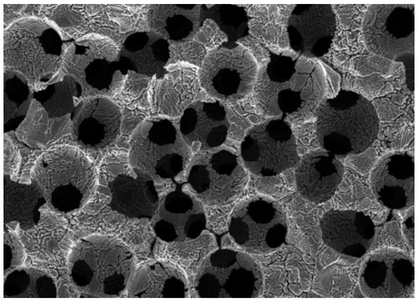

Fig. 1: Micrograph of porous copper structure produced by templated electrodeposition and electroetching process.

This poster includes key factors of recent DARPA-sponsored progress on the translation of electron kinetic energy in GaN HEMTs to fluid enthalpy through nanoengineered heat sinks (ICECool Fundamentals and ICECool Applications). This work is collaborated with multiple industries, including Raytheon, Boeing, IBM, and Nuvotronics.

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Development of New Simulation Method for Thermoelectric Responses of Large Scale Systems and Its Application

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According to the social demand for developing the energy harvesting technologies, enhancement of thermoelectric performance of materials have been attracted much attention for the device applications. Because of the proposition, offered by Hicks and Dresselhaus, that the low-dimensional materials can provide significant enhancement of thermoelectric performance due to their high density of states [1], one-dimensional materials, e.g. various types of nanowires, have been intensively studied experimentally so far [2-3]. On the other hand, similar to the electrical and thermal transport studies, theoretical approaches can work as a possible strong tool to investigate the thermoelectric properties for nanoscale materials. There are, however, still no adequate standard method dealing with the nanoscale materials particularly considering a large-scale system, interactions, and so forth.

In this study, we would like to discuss a new simulation method for thermoelectric responses based on linear response theory [4] and wave-packet dynamics [5]. We have developed the applicable form of Seebeck coefficient from the correlation function between electrical current and energy current, which can calculate from the diffusion of the wave-packet. Our new method contains the potential to apply the large-scale calculation even though we will take account of the electron-phonon interaction. In the presentation, we will discuss the theoretical derivation of our new simulation method and the results of its application.

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Experimental Demonstration of a Photon Thermal Diode

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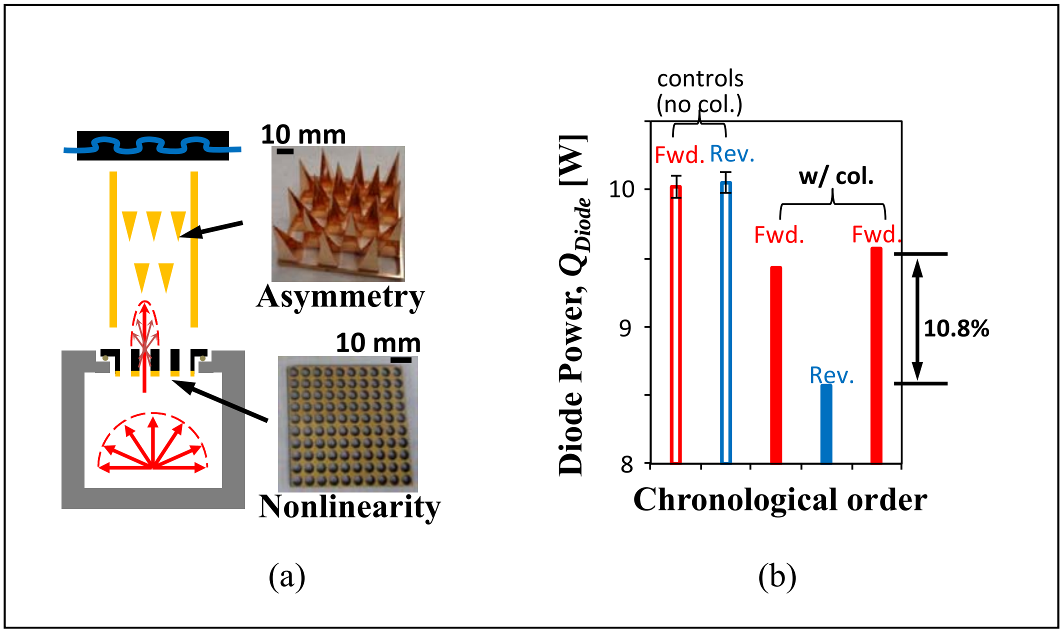
A thermal diode is an analogue to the familiar electrical diode in the heat transfer domain [1]. Effective thermal rectifiers could benefit thermal engineering greatly. However, experimental demonstrations have lagged far behind theoretical proposals [2-3].

Here we experimentally demonstrate a ballistic thermal rectification mechanism for the first time. The device exploits the asymmetric scattering of photons by pyramidal reflectors. Control experiments verify recent theoretical predictions [4-5] that this mechanism also requires a non-linear thermal collimator element, due to a deep requirement of the 2nd Law of Thermodynamics. Experiments confirm both effects: With pyramids and collimator the thermal rectification is 10.9 ± 0.8%, while without the collimator no rectification is detectable (< 0.3%) [6].



(a) (b)

Fig. 1: (a) Experimental setup and the two key ingredients: Asymmetry (polished copper) & nonlinearity (Au on graphite). (b) Experimental results: rectification needs both ingredients.

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Exploring Heat Transfer at the Atomistic Level for Thermal Energy Conversion and Management

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Heat transfer at the scales of atoms plays an important role in many applications such as thermoelectric energy conversion and thermal management of microelectronic devices. While nanoengineering offers unique opportunities to manipulate heat to our advantages, it also imposes challenges on the fundamental understanding of nanoscale heat transfer. As the characteristic lengths of the system size become comparable to the mean free paths of heat carriers, macroscopic theories based on heat diffusion are no longer valid due to size effects. Atomistic level simulation can provide powerful insights into the microscopic processes governing heat conduction.

In this poster, we first introduce atomistic techniques to investigate phonon transport in bulk crystals. We start with normal mode analysis within the classical molecular dynamics framework to estimate the spectral phonon transport properties. Although it can provide the detailed phonon properties adequately, classical molecular dynamics with empirical potentials do not always yield accurate predictions. Then, we move to first-principles density functional theory (DFT) to compute mode-dependent phonon properties. Such simulations can well reproduce experimental values of phonon dispersion and thermal conductivity with no adjustable parameters, establishing confidence that such an approach can provide reliable information about the microscopic processes. These detailed calculations not only unveil which phonon modes are responsible for heat conduction in bulk crystals, but also expand our fundamental understanding of phonon transport, such as the importance of optical phonons. Next, we study thermal transport across single and multiple interfaces via the atomistic Green's function method, especially the impact of interface roughness on phonon transmission across a single interface and coherent phonon transport in superlattices. Both the DFT and Green's function techniques provide fundamental parameters that then can be used to understand mesoscale transport. This paves the way for multiscale modeling from first-principles. Through these multiscale modeling efforts, we are able to obtain a comprehensive understanding of heat transfer from the atomistic to the macroscale, with important implications for energy applications.

Complementary to the theoretical work, we measure the interface thermal conductance using ultrafast time-domain thermoreflectance experiments, examining thermal transport across solid-liquid interfaces modified by self-assembled monolayers. We find that an extra molecular layer can enhance the thermal transport across solid-liquid interfaces.

In summary, theoretical, computational and theoretical approaches have been applied to study heat transfer at the atomistic level. These findings have improved our fundamental understanding of phonon transport properties with important implications for energy applications and beyond, and build a foundation for multiscale simulation of phonon heat conduction at the mesoscale.

Acknowledgement: Z. T. would like to thank K. Esfarjani, J. Garg, J. Shiomi, T. Shiga, A. Henry, A. Marconnet, K. Collins, and M. Luckyanova for their contribution to this work. This work is supported by the S3TEC, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-FG02-09ER46577.

Ballistic Thermal Conductance in Layered Two-Dimensional Materials

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The thermal properties of two-dimensional (2D) materials like graphene, h-BN, MoS_2 and WS_2, as well as their stacks are uniquely anisotropic, characterized by high in-plane but very low out-of-plane thermal conductivity. Here we provide a comparative study of the ballistic limits of heat flow in 2D layers and stacks. Based on full phonon dispersions from density functional theory, we calculate the in-plane and cross-plane ballistic thermal conductance of 2D materials and stacks. For a given material, we find that monolayers and multilayers have similar in-plane ballistic thermal conductance per cross-sectional area (G_b) above ~100 K, but monolayers show higher G_b at low temperature due to the contribution of flexural phonons. At room temperature (RT), graphene has the highest $G_b \sim 4.3$ $GWK^{-1}m^{-2}$, about 17% higher than h-BN and five times higher than MoS_2 and WS_2. Cross-plane G_b values are roughly one order of magnitude lower than those for in-plane due to weak van der Waals interactions. Based on the calculated G_b, we can obtain the effective phonon mean free path (mfp) of these materials, given the diffusive thermal conductivity [1]. For instance, at RT the in-plane phonon mfp of bulk h-BN is ~70 nm while the cross-plane mfp is ~3 nm. These results are important because they establish the length scales of the ballistic-to-diffusive transition of thermal transport in these materials, and the non-classical regime where thermal conductivity depends on the size of the system.

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For the 2014 meeting, we are aiming for a more critical perspective on selected topics which are part of the US-Japan meeting. Therefore, after discussions with the Editor-in-Chief of *NMTE*, Prof. Li Shi, we are soliciting both *Opinion Papers* and *Original Research Articles* to be published in a special *NMTE* issue to highlight the research topics discussed in the 8th US-Japan joint seminar.

Scope and Coverage

Opinion Papers or Topical Reviews: These are forward-looking reviews of timely and important research topics. These reviews often contain some significant aspect of the authors' own analysis and opinions, so that they are essentially opinion papers. Each article should offer a critical perspective, and should *not* be restricted to purely summarizing some number of conference presentations. The articles can comment on the themes of research and what was presented, but also other related work outside of the conference.

Original Research Papers: Related to work presented at the US-Japan meeting, or on similar topics, are also invited.

Peer Review

All articles will undergo peer review prior to publication in *NMTE*.

Publication Timeline & Rapid Dissemination

October 1 is the targeted submission date for all manuscripts, to enable rapid publication in early 2015.

To promote rapid and broad dissemination, *NMTE* has implemented an accepted manuscript online (AMO) publication model of Taylor & Francis, the publisher of *NMTE*. It now takes less than 4 months between original manuscript submission and AMO publication for papers that do not require significant changes from the authors' side. The publisher now offers free open access to noteworthy articles specified by the

NMTE Editorial Board, and allows authors to post the authors' version of the accepted manuscripts on other websites as long as the DOI of the accepted paper is included. In addition, the *NMTE* Editorial Office can help the authors to send a free electronic copy of the published paper to the email addresses of up to fifty other researchers identified by the authors.

Examples of Possible Themes

These are just a few ideas, and interested authors are specifically encouraged to propose any topic or set of topics they are most interested in.

Conduction
  Modeling advances (1st principles, MD, BTE, ...)
  MFP Spectroscopy: Modeling and Experiments
  1D (CNT, nanowire, ...)
  2D (graphene and beyond)
  Nanobulk
  Polymers / Hybrids
  Interfacial Effects
  Spin & Magnon Effects (beyond electrons & phonons)
  Coherence Effects

Radiation Heat Transfer

Nanofluidics, Nanofluids, Phase Change

Biology and Nanoscale Transport

Reacting Systems. Fuel cells, etc.

Measurement Advances
  Scanning probe microscopy
  Mean free path spectroscopy
  Calorimetry

Translation of academic advances into practical applications

Technology Drivers
  Energy Conversion (PV, TE, ...)
  Information Technology (HAMR, Transistors, Phase Change Memory, ...)

Historical perspective on the US-Japan seminar series