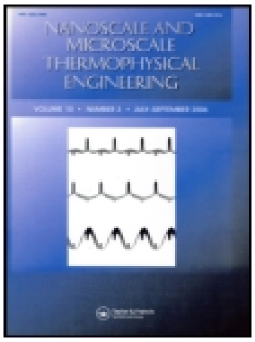

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Report on the Seventh U.S.–Japan Joint Seminar on Nanoscale Transport Phenomena—Science and Engineering

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REPORT ON THE SEVENTH U.S.–JAPAN JOINT SEMINAR ON NANOSCALE TRANSPORT PHENOMENA—SCIENCE AND ENGINEERING

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The seventh U.S.–Japan Joint Seminar on Nanoscale Transport Phenomena was held in Shima, Japan, from December 11 to 14, 2011. The goals of this joint seminar were to provide a critical assessment of the state of the art and future directions in the field of nanoscale transport phenomena and energy conversion processes, to foster U.S.–Japan collaborations, and to provide international exposure to a new generation of scientists in this field. Issues discussed in the joint seminar were organized in 10 topical sessions, including (1) nanoscale thermophysical measurements; (2) optical characterization; (3) thermal and molecular transport; (4) phonon transport modeling; (5) energy storage and conversion; (6) nanoscale fluidics and phase change phenomena; (7) biological and organic systems; (8) interfacial thermal transport; (9) novel thermoelectric and thermal management materials; and (10) nanocarbon materials and devices. In addition to these topical sessions, the joint seminar featured an opening plenary session and a closing plenary session as well as an expert panel, where leading experts provided critical assessment of the past progress and addressed future directions in the field. In addition, an evening poster session provided opportunities for graduate and postdoc students to present their latest research results. About 35 researchers from Japan and 31 researchers from the United States participated in the meeting. The meeting was organized by S. Maruyama, K. Fushinobu, L. Shi, and J. Lukes together with about 20 other participants who served as session chairs. Summaries of different sessions of the seminar were prepared by the session and conference chairs and are collected into this report.

KEY WORDS: nanoscale thermal transport, energy conversion, thermal interface conductance, carbon nanomaterials, soft matters, molecular dynamics simulations

OPENING REMARKS

In his opening remarks, A. Yabe discussed the challenges in deploying newly developed technologies. He discussed these issues by introducing a Japanese national research and development (R&D) initiative, the Eco-Energy City Project. This initiative is a package of R&D projects, and one of its major objectives is the effective use of low-quality waste heat energy to reduce total energy consumption and to mitigate global-level environmental issues. A vast amount of low-quality waste heat is produced by industry, but it is not used very effectively. However, at the same time, there is a large demand for energy from residential and business consumers. Such a mismatch of heat production and usage can be resolved by connecting industry to consumers using energy transportation systems. One such example discussed by Yabe was a seed project from the Japanese private sector. In this project, the latent heat of pumped tetra-n-butylammonium bromide clathrate slurry is harnessed to transport a large amount of low-quality thermal energy through the cooling systems of business or residential buildings.

Yabe introduced a view graph to the audience with number of commercialized equipment and/or public interest as the ordinate and year as abscissa. In the view graph, there was a clear increase in public interest during the initial phase of the project followed by a slowdown period of several years. During the slowdown period of the project, however, fundamental R&D continued in collaboration with the National Institute of Advanced Industrial Science and Technology, a national R&D institute. This R&D included investigating the economics of the system to identify avenues for cost reduction and carrying out demonstration projects for the air-conditioning systems in buildings. As pointed out by Yabe, during the slowdown period the project was continually supported by the New Energy and Industrial Technology Development Organization, a Japanese national funding agency. A company then finally developed the technology and initiated its commercial deployment. Then the technology was finally introduced to the market.

Yabe pointed out several important issues learned from this success story. Although numerous energy-related technologies have been developed, not many of them have been commercialized. There are clear obstacles to be overcome in a gap called the “Valley of Death,” including unclear application area of the seed ideas, economic feasibility, reliability, performance improvement, social acceptance, and social circumstances. Yabe termed all of the issues ranging from technological issues to the aforementioned barriers in the Valley of Death *social technology*.

Yabe concluded by remarking on two examples as challenges and opportunities for the audience: silicon carbide power electronics for energy savings and the international standardization of measurement techniques and lifetime estimations based on fundamental nanoscale research to make a difference in real-world technologies.

OPENING PLENARY LECTURE

Following Yabe’s opening remarks, A. Majumdar [1] delivered a plenary lecture to discuss global energy challenges and opportunities. Large regions of the developing world currently use very little energy per capita. As the gross domestic product in these nations increases, energy demand will skyrocket along with environmental issues associated with producing that energy. It is critical to use science and technology to develop game-changing advances that can address the energy needs of a growing world population in an affordable, sustainable way.

The two main energy sectors are energy for transportation and stationary energy. Global transportation energy demand will increase significantly as exponential growth in passenger vehicle ownership is expected in China and India over the next several decades. Because oil is the dominant transportation fuel and consumption currently exceeds production in the United States, Japan, and China, diversification of transportation fuels is essential. The challenge is that unconventional fuels such as sugarcane- and corn-derived biofuels are expensive to produce relative to conventional oil, leading to small or even negative profit margins in the absence of subsidies. However, there is much room for improvement: the conversion of sugarcane, corn, algae, and cellulose into biofuels is currently less than 1% efficient. The Plants Engineered to Replace Oil program of the Advanced Research Project Agency-Energy (ARPA-E) is aimed at increasing these efficiencies.

Two other transportation-related initiatives at ARPA-E are Batteries for Electrical Energy Storage for Transportation (BEEST) and Rare Earth Alternatives in Critical Technologies (REACT). The goal of BEEST is to enable the development of electric cars with longer range and lower subsidy-free life cycle costs than gasoline cars. The target is to achieve batteries with double the energy density and one third the cost of current batteries. Technologies under investigation include all electron, lithium–oxygen, lithium–sulfur, lithium ion, magnesium ion, metal–air, and flow batteries. REACT is aimed at developing low-cost, abundant alternatives to rare earth magnetic materials, which are used in electric vehicle motors and wind turbine generators.

The large domestic reserves of natural gas in the United States make it another potential transportation fuel. Liquefied natural gas is already used for long-haul trucking, but natural gas–fueled passenger cars, buses, and short-haul trucks are not widespread.

It would be prohibitively expensive to build a network of compressed natural gas filling stations, so the leading concept for subsidy-free natural gas–fueled transportation is to fuel at home. This will require development of high-density, low-pressure, low-cost natural gas storage systems for home refilling. Another idea is to create low-cost alternatives to the Fischer-Tropsch process for chemically converting natural gas to liquid fuel, via low-cost modular reactors rather than large, capital-intensive chemical plants.

Stationary energy systems for electrical power production were discussed next. Many states have established standards and goals for renewable energy. Consequently, a key ARPA-E goal is to enable the development of clean and inexpensive subsidy-free electricity. The present cost of electricity from natural gas combined cycle plants is 5 cents per kilowatt-hour, so other energy technologies including solar, wind, geothermal, clean coal, and nuclear must compete with this benchmark. The SunShot program is aimed at reducing solar energy installed system costs from the 2010 cost of \$3.80/W to \$1/W (equivalent to 5–6 cents/kWh) by 2017. These reductions will come not only from module efficiency improvements and module manufacturing cost reductions but also from advances in power electronics and reductions in balance of system soft costs related to installation and permitting.

Grid-level storage is required to maintain a stable electrical grid. Two major existing approaches to grid-level energy storage include pumped hydro—pumping water uphill—and underground compressed air storage. These storage modalities are only available in limited locations. Developing battery technologies suitable for grid-scale storage is desirable because batteries can be used anywhere. Current energy storage costs using batteries are two to five times higher than those from pumped hydro and underground compressed air. Flow batteries, which consist of particles of anode and cathode mixed into a conducting fluid, offer great potential for advances in this area. Another type of grid level energy storage is thermal energy storage. The High Energy Advanced Thermal Storage (HEATS) program supports approaches in which chemical reactions are used to store energy that can later be released to the grid. Materials with appropriate enthalpies of reaction can enable advanced thermal batteries. The HEATS program also supports other thermal energy storage technologies for lower temperature applications, such as cabin heating and cooling of electric vehicles.

Cooling of buildings consumes substantial amounts of energy, and emissions from refrigerants will be an increasing problem in the future. The Building Energy Efficiency Cooling System program is aimed at developing better, more energy-efficient cooling strategies for buildings. One promising strategy is to dehumidify the air before cooling using special membranes, thus eliminating the significant contribution of water heating to the energy load.

Majumdar closed his presentation by noting the link between science, systems, and society and by asking the audience to consider how our research will make a positive impact on the world.

SESSION 1: NANOSCALE THERMOPHYSICAL MEASUREMENTS

This session, chaired by Y. Taguchi and S. Shen, included five presentations that covered techniques to measure diffusion coefficients at the micro- and nanoscale, thermal conductivities of carbon nanotubes and polymer nanofibers, thermal radiation across a nanoscale gap, nanowatt heat generation, nanogram mass, and transport properties in polymer electrolyte fuel cells.

The keynote lecture of this session was delivered by Y. Nagasaka [2] from Keio University. First, he briefly introduced optical techniques developed in his laboratory for measuring the thermophysical properties such as thermal diffusivity, thermal conductivity, viscosity, surface tension, diffusion coefficients, and surface viscoelastic properties of fluids and solids at the micro- and nanoscale. He then focused his talk on measurements of mass diffusion coefficients based on the Soret forced Rayleigh scattering method. A periodic spatial concentration modulation on a sample is generated due to the periodic heating by the interference of two laser beams. Another laser beam is used to monitor the decay of the concentration modulation due to the mass diffusion and thus measure the mass diffusion coefficients. This technique provides several advantages such as noncontact measurement, high speed, and high spatial resolution.

O. Nakabeppu [3] presented thermal measurements with microelectromechanical systems (MEMS) sensors at nanometer, nanogram, and nanowatt scales. He developed various cantilever-type calorimeters with heaters, temperature sensors, and heat flow sensors. With these calorimeters, differential thermal analysis and differential scanning calorimetry (DSC) can be performed for micro- to nanogram samples at short timescales. A small mass down to the nanogram level can also be detected by measuring the mechanical resonance of the cantilever.

S. Shen [4] discussed thermal radiation measurement using atomic force microscopy (AFM). The results indicated that thermal radiation at nanoscale separations exceeded Planck's blackbody radiation law by three orders of magnitude. He suggested that surface phonon polaritons can enhance energy transfer in the near-field. In addition, the significant enhancement of thermal conductivity in nanostructured polymers was reported. Compared to bulk polymers, ultra-drawn polymer nanofibers had very high thermal conductivity.

K. Takahashi [5] reported a technique for measuring thermal boundary conductance of individual carbon nanotubes (CNTs). The thermal boundary conductance of the end of a CNT was measured by hot-film sensor technology. A CNT was bonded onto a platinum thin-film sensor and a heat sink, and the temperature change of the film was measured while the CNT contacted a target. The thermal conductance of an open-end CNT was approximately five times larger than that of a closed-end CNT.

K. Fushinobu [6] discussed an investigation of the transport reaction phenomena across the membrane electrode assembly of polymer electrolyte fuel cells. The transport properties and the potential across the electrolyte membrane, transport reaction phenomena in the multilayered catalyst layer, and the species transport between the channel and the catalyst layers were investigated.

SESSION 2: OPTICAL CHARACTERIZATION

This session was chaired by N. Fang and M. Kohno. In the keynote presentation, K. Nelson [7] reported direct measurement of nondiffusive thermal transport on small macroscopic length scales. He introduced a transient grating measurement with the use of crossed beams of picosecond excitation pulses. Such an interference pattern of crossed pulses is used to excite propagating acoustic waves from the gigahertz to terahertz frequency in a bulk material or at an interface. Nelson showed that such methods have enabled measurement of phonon mean free paths and heat transport at the nanoscale. In addition, the time-dependent diffraction of laser pulses can be applied to study nonlinear lattice vibrations and other collective effects.

Z. Zhang and N. Fang both presented optical characterization studies of photon transport and interaction with plasmonic metamaterials, with potential impact on advanced energy systems. Zhang [8] showed that obliquely aligned Ag nanorods can be used to render the spectral and directional properties of radiation. The light–material interaction of such nanostructured materials was measured using a laser scatterometer and was modeled effectively as a homogeneous uniaxial optical material. N. Fang [9] used focused electron beams to selectively excite plasmonic nanoantennas and measure photon emission with spatial resolution better than 20 nm. With this technique, it is possible to resolve the radiation spectrum associated with different photon transitions inside the nanostructures. With proper projection of dipole sources, he was able to show that the dark modes, which are usually weakly coupled to plane waves, can radiate more effectively than bright modes. This application illustrates the potential use of hotspots in plasmonic nanostructures to enhance stimulated light emission.

Y. Taguchi [10] presented a new technique for measurement of nanoscale temperature distribution based on fluorescence lifetime and polarization state measurements in the near field. To decrease autofluorescence, a critical noise source in the measurement, Taguchi proposed fabrication of new fiber probes using fusion splicing of single-mode fibers, as well as photonic crystal fibers. He also presented results on fluorescence detection of quantum dots and detection of the polarization change in the near-field.

SESSION 3: THERMAL AND MOLECULAR TRANSPORT

Chaired by A. McGaughey and M. Shibahara, this session consisted of one keynote and three contributed talks. The keynote speaker was G. Galli [11]. Motivated by a need to reduce thermal conductivity in materials for thermoelectric energy conversion, she described molecular dynamics (MD) simulations and lattice dynamics calculations on silicon- and germanium-based bulk materials and nanostructures. In the MD simulations, the techniques applied included the Green-Kubo method, the nonequilibrium direct method, and normal model projection. The lattice dynamics–based Allen-Feldman theory was applied to predict the contribution of diffusive vibration modes to the thermal conductivity of disordered structures. The materials studied were amorphous silicon, silicon–germanium alloys, silicon nanowires, and nanoporous silicon and silicon–germanium. For amorphous silicon and the silicon–germanium alloy, very large system sizes are required to approach the bulk thermal conductivity. This result highlights that careful attention must be paid when simulating disordered materials, where much longer length scales than might be expected are required. The thermal conductivity of amorphous silicon was decomposed into contributions from phonon-like modes and nonlocalized diffusive modes, with both types of vibrational entity making a significant contribution. Though the thermal conductivity of nanoporous silicon was found to be reduced by rough surfaces, that of nanoporous silicon–germanium was not due to the already disordered nature of the structure. Silicon nanowires with a diameter of 15 nm (larger than others previously modeled in MD simulations) were studied, with an objective of determining the mechanisms associated with the very low thermal conductivities measured experimentally. It was found that a combination of oxidized surfaces, internal defects, and closely spaced internal grain boundaries is needed to obtain the experimentally observed thermal conductivity. The ability to perform such large simulations (>100,000 atoms) bodes well for future simulations that can access the length scales found by experiment.

S. Inoue [12] discussed simulations that predicted how functionalizing carbon nanotubes with metal atoms can affect their mechanical and thermal properties. Using nonequilibrium MD simulations where a thermal pulse is applied to the nanotube and the evolution of the temperature field is tracked, he predicted a 10-fold decrease in thermal conductivity. As the bonding energy between the metal atoms and the nanotube increased, the thermal conductivity was predicted to decrease. This result can be understood in terms of stronger phonon scattering and reinforced the emerging knowledge that even small perturbations to the periodicity of a nanostructure can have a significant effect on thermal transport properties.

M. Shibahara [13] presented results from MD simulations designed to study liquid–solid thermal transport on nanostructured surfaces. In order to increase heat transfer, the interface thermal resistance needs to be decreased. The effects of the morphology of the stepped solid surface on the thermal resistance and the local nonequilibrium behavior of liquid molecules at the liquid–solid interface were discussed. Wetting and non-wetting surfaces were considered, as was the presence of a nanoparticle on the solid surface.

I. Kinefuchi [14] described an experimental study of how helium molecules interact with a forest of vertically aligned carbon nanotubes. Though the accommodation coefficient between helium and a single nanotube is predicted to be small, the multiple interactions that take place inside the thin film lead to excellent overall accommodation (97% for a 4-μm-thick film, compared to 40% for most metals). This result suggests strategies that could be applied to enhance heat transfer at the gas–solid interface. Through the design of a holding plate with an open back surface, the properties of the molecules both reflected and transmitted through the surface were obtained.

SESSION 4: PHONON TRANSPORT MODELING

This session was chaired by C. Dames and T. Yamamoto. In his keynote address, J. Shiomi [15] discussed numerical simulations of mode-dependent phonon transport in complex systems such as multiatomic crystals and alloys. In his simulations, by calculating anharmonic interatomic force constants from first principles using the direct method [16, 17], the phonon relaxation time was estimated by Fermi's golden rule of three-phonon scattering processes or model analyses of MD phase space trajectories. He showed that the framework can be successfully applied to thermoelectric crystals such as half-Heusler compounds [18] and lead telluride. In addition, he discussed the possibility of extending the MD framework to handle systems with alloys and interfaces, such as alloyed thermoelectric crystals and carbon nanotubes on a substrate or in a polymer matrix [19].

A. McGaughey [20] described a new model for the thermal conductivity reduction due to boundary scattering in thin films and other nanostructures. The model begins with the common assumption that the dispersion relation and phonon–phonon scattering rates in the film are well approximated by those in the bulk, which were calculated using lattice dynamics for Stillinger-Weber silicon. Then the effects of boundary scattering were incorporated using a new approach that compares the nanostructure's length scale to individual free paths statistically sampled from a Poisson distribution based on the corresponding mean free path. Results were presented for thin films and nanograined materials, including the impact of the grain size distribution having a large breadth.

T. Yamamoto [21] reported a numerical study of coherent phonon transport in isotope-disordered single-walled carbon nanotubes (SWNTs) [22]. His simulation technique is based on the nonequilibrium Green's function (NEGF) method [23], which enables fully quantum-mechanical simulation of the coherent phonon transport in nanoscale systems. Using the NEGF technique, he showed that the isotope-disordered SWNTs exhibit three transport regimes depending on the phonon frequency: ballistic, diffusive, and localization regimes. A remarkable result is that the phonon transmission exhibits a universal fluctuation, irrespective of the tube chirality, isotope concentration, or isotope mass.

C. Dames [24] presented a model for the thermal boundary conductance when one of the two materials is highly anisotropic. The model generalizes the common isotropic Debye model by using ellipsoids to approximate the anisotropy in the phonon dispersion and first Brillouin zone. The model shows that, due to phonon focusing effects, the phonon irradiation in a specific direction can be reduced if a sound velocity in an orthogonal direction is increased. When compared with published experiments for the thermal conductance between graphite and various metals [25], the new model performs approximately 10 times better than a traditional isotropic diffuse mismatch model.

SESSION 5: ENERGY STORAGE AND CONVERSION

This session was chaired by O. Nakabeppu and P. Reddy. In his keynote presentation, M. Kaviany [26] discussed the possibility of utilizing nonequilibrium atomic vibrations to achieve efficient energy conversion. He discussed the potential of converting vibrational energy into work before it is fully thermalized. Specifically, the use of phonon-assisted electronic transitions in recycling vibrational energy generated during energy conversion processes was discussed. As an example, Kaviany presented the possibility of pre-thermalization intervention using semiconductor materials to recover a substantial fraction of energy lost as waste heat during nuclear fission in reactors. Further, he discussed phonon recycling as a path to achieve improved laser efficiency and solar photovoltaic devices. Kaviany concluded his talk by pointing out to the community that phonons can be harnessed in novel ways if devices are engineered to harvest them before thermal equilibration.

The second talk in this session was by Y. Murakami [27], who discussed photochemical up-conversion using ionic fluids. Murakami described the upconversion of two photons of a lower energy into a photon of a higher energy. The mechanics of the up-conversion process was related to the triplet–triplet annihilation process of excited aromatic molecules via Dexter energy transfer. Specifically, Murakami presented results from his work where photon up-conversion was accomplished using aromatic molecules in ionic fluids. He also described the unusual stability of the nonpolar molecules in ionic liquids and proposed a mechanism for the unexpected stability of aromatic molecules in ionic liquids. Finally, an analytical model was presented to explain the observed quantum yields of the upconversion process.

The third talk of the session was presented by P. Phelan [28], who described photothermal energy conversion in liquid nanoparticle suspensions. Specifically, Phelan presented experimental results on solar collectors based on nanofluids made from a variety of nanoparticles/nanomaterials such as carbon nanotubes, graphite, and silver. Efficiency improvements of up to 5% were shown for solar thermal collectors utilizing nanofluid for optical absorption. An initial rapid increase in efficiency with volume fraction was observed, followed by a leveling off in efficiency as the volume fraction continued to increase. A study of the dynamics of rotating paramagnetic micro-/nanoparticles was also briefly discussed.

The final talk of this session was presented by K. Fumoto [29], who described his study of the thermophysical properties of nanoemulsions. The studied properties include thermal conductivity, viscosity, and density. In particular, Fumoto described the possibility of using oil-in-water emulsions as latent heat storage materials. Such emulsions were described as having low melting points, thus offering attractive opportunities for heat transfer enhancement and thermal energy transportation and storage. Specifically, milky white oil-in-water emulsions were formed using water, Tween 80, Span 80, and tetradecane using low-energy emulsification methods (e.g., the phase inversion temperature method). The relations between the component ratios of the emulsions and both the droplet diameters and the stability of the resulting emulsions were determined by dynamic light scattering and vibration viscometry. The obtained results showed that the apparent viscosity of the nanoemulsion was lower than that of an emulsion prepared with the same mixing ratio of surfactant and concentration of phase-change material (PCM). Moreover, the surfactant concentration was found to contribute to the stability of the phase-change nanoemulsion. Fumoto concluded by suggesting that phase-change nanoemulsions are promising materials for thermal storage applications.

SESSION 6: NANOSCALE FLUIDICS AND PHASE CHANGE PHENOMENA

Three presentations were given in this session chaired by H. Daiguji and D. Li, covering transport and phase change in nanopores, heat conduction in nanofluids, and nanoscale nucleate boiling. The keynote presented by Daiguji [30] covered ion transport and water adsorption–desorption phenomena in mesoporous silica. For ion transport, mesoporous silica SBA-16 thin films with highly ordered 3D cubic structures were synthesized on a silicon substrate via the dip-coating method. After these films were filled with KCl aqueous solutions, ionic current passing through the mesopores induced by an applied DC electric field was measured. At low ion concentrations, the measured *I–V* curves were nonlinear, and the current increased exponentially with respect to voltage. However, as the ion concentration increased, the *I–V* curve approached linear behavior. A theoretical analysis suggested that the nonlinear *I–V* curves could be attributed to the electric potential barrier created in nanopores and the fact that the local dielectric constant and the ion diffusion due to the concentration gradient are suppressed in comparison to those in bulk liquid. For water adsorption–desorption, the reduction in freezing–melting temperature was discussed. It is well known that the melting and freezing point of water confined in hydrophilic mesopores is lower than that of bulk water, which was confirmed by thermograms obtained by DSC during the melting and freezing of water in mesopores. However, the DSC measurements are typically performed after the mesopores are filled with water. If mesoporous materials are exposed to water vapor below 273 K, it is possible that the water vapor adsorbs on the outer surface of the materials as well as the inner surface of the mesopores. The adsorption–desorption isotherms of water vapor on Zr-doped mesoporous silica with highly ordered 2D hexagonal structures were measured in the temperature range of 263–298 K. The Zr-doped mesoporous silica sample, which had uniform pores with a diameter of approximately 3.8 nm, adsorbed water vapor without freezing at 263 K. Theoretical analysis suggested that the thickness of the adsorbed non-freezable water layer was about 0.7 nm and that the layer thickness for capillary condensation was slightly larger than that for capillary evaporation. The transport and phase change phenomena in nanopores are strongly related to the structural and dynamic properties of the ions and molecules involved. It is a major challenge to clarify the transport and phase change phenomena in nanopores with nanoscale precision.

G. Chen [31] presented a study of electrical and thermal conductivities of nanofluids, which are liquids containing suspensions of nanoparticles. First, he summarized the controversy regarding whether nanofluids can effectively enhance thermal conductivity and the various proposed mechanisms for thermal conductivity enhancement in nanofluids. He then discussed insights obtained by his group through freezing the nanofluids. They found that graphite flakes can be used as additives to form stable graphite suspensions with large thermal conductivity enhancement. Combined optical and AC impedance spectroscopy studies indicated that nanoparticle clustering is the key contributor to the thermal conductivity enhancement. His group also demonstrated reversible tuning of electrical and thermal conductivities during freezing–melting of the nanofluids, which could have significant technology impacts.

M. Matsumoto [32] discussed how nucleate boiling starts on smooth surfaces. The initial stage of nucleate boiling of a Lennard-Jones model liquid on an ideally smooth surface was investigated with MD simulation. The results showed that as the temperature of the liquid increased, the liquid thermally expanded, leading to a decrease in pressure and the formation of atomic-scale bubble nuclei through cavitation. When the surface was hydrophobic and the heating area was small, a size oscillation of the generated bubbles was observed. Matsumoto attributed this behavior to the balance among the heat flux from the wall, thermal diffusion into the surrounding liquid, and latent heat consumption during the phase change.

SESSION 7: BIOLOGICAL AND ORGANIC SYSTEMS

Five presentations were given in this session chaired by K. Pipe and T. Zolotoukhina, covering a range of topics from biomedical applications to organic semiconductor devices. Keynote speaker J. Bischof [33] gave a presentation on the use of gold nanoparticles (GNPs) to deliver heat energy or drugs to cancer cells. In this talk, Bischof summarized the current state of the art in the field, as well as several topics currently under study in his laboratory. One example involved combining GNPs with a vascular targeting agent that enhances thermal therapies. Another example involved heating of the GNPs by laser absorption and subsequent killing of cancer cells. General challenges were discussed, such as how to image the location of GNPs, how to increase specificity, how to increase optical absorption, how to tailor thermal response, and how to measure temperature. Because many of these topics fall within the range of expertise of the U.S.–Japan seminar, this application of nanoscale heat transfer is of great interest and could potentially be expanded in future seminars.

Zolotoukhina [34] presented on the use of force field spectroscopy to identify DNA nucleobases in nanopore sensor films at the time of translocation. The choice and parameters of the sensor film were discussed from the point of view of the force signal resolution in the presence of thermal noise from atomic motion during the measurement. The force dependence on the electronic structure of the bases was accounted for by use of MD simulation. A hydrogenized Si film of 5 atomic layer thickness with 1.6 nm pore diameter was utilized as the force sensor. Preliminary evaluation showed a difference of one to a few piconewtons in the force signals between the different bases; the measurement of such a difference, which is in the range measurable by existing scanning tunneling microscopy (STM) and AFM instruments, was further discussed.

D. Leitner [35] gave a presentation on the anomalous diffusion of vibrational modes in proteins. Quantum mechanical effects were considered in modeling thermal conduction through proteins of various geometries; these models were then compared with experimental data, showing good agreement. Proteins represent an interesting regime of thermal conduction in which very discrete vibrational modes propagate with strong anharmonic coupling.

K. Miyazaki [36] discussed the fabrication of nanoporous polymer thin films. Hexagonally periodic nanosized pores were formed in the presence of humid air at the time of polystyrene film formation from a polymer solution. During solvent evaporation, cooling of the polymer solution surface led to simultaneous water droplet condensation and subsequent pore formation at the droplet locations after polymer drying. The relationship between the speed of the drying process of the separated water droplets and the droplet and pore sizes was demonstrated. A polystyrene film with pores smaller than 200 nm in diameter was made by controlling the substrate temperature to ensure a fast drying process. The depth and diameter of the pores were explained by the force balance of surface tension and water flotation.

Pipe [37] gave a presentation on heat transfer at organic–inorganic interfaces. Applications in organic semiconductor devices and thermal interface materials were discussed, and recent measurements of thermal boundary resistance and adhesion at metal–copper phthalocyanine interfaces using 3-omega and optical pump-probe techniques were presented. In particular, the effects of interface mixing and adhesion on thermal boundary resistance were highlighted through both models and experiments. Thermoelectric measurements in pentacene thin films were also presented, demonstrating how measurement of the Seebeck coefficient and electrical conductivity can be used to study mobility in bulk organic semiconductors (rather than the field-effect geometry typically used for mobility measurements). Finally, the concept of a resonant heat sink that captures ballistic phonons emitted by a device was discussed, and an example was given for an AlGaN-GaN high electron mobility transistor.

SESSION 8: INTERFACIAL THERMAL TRANSPORT

Six presentations on interfacial thermal transport were given during this session chaired by B. A. Cola and G. Kikugawa. The topics of the presentations were diverse, ranging from studies of transport at interfaces modified with self-assembled monolayers to interfaces between individual nanostructures in contact. The presentations mostly focused on fundamental aspects of interfacial transport with both experimental and modeling work. The work presented has broad applicability to emerging biological, thermoelectric, and thermal management technologies.

Kikugawa [38] presented on interfacial transport at solid–liquid interfaces modified with self-assembled monolayers (SAMs). He and collaborators used MD simulations to show that the overall thermal boundary resistance at a gold–SAM–toluene interface is significantly lower than that of a gold–toluene interface. They used methyl ($-CH_3$) and hydroxyl (-OH) SAM terminal groups to demonstrate the effect of interface spacing on thermal conductance in a SAM–water solvent system. Their results revealed a smaller interface spacing and higher conductance at the OH-terminated SAM interface. Van der Waals rather than Coulombic interactions were found to be the dominant contribution to thermal energy transfer; this was a point of discussion with the audience.

J. Lukes, P. Norris, and K. Goodson gave presentations on thermal transport at solid–solid material interfaces. Lukes [39] discussed the use of phonon scattering functions analogous to those employed in radiative heat transfer as a technique to explore the effects of nanoparticle size and roughness on phonon scattering in bulk materials. She discussed how multiple length scales affect phonon scattering at interfaces and presented results showing the effect of geometry on scattering by modeling nanoparticles of various shapes and size inside a crystal matrix with MD. Phonon scattering properties from the particle were analyzed in detail.

Norris [40] showed with MD and experimental results that interstitial layers can be applied as vibrational bridges to increase interface conductance between two vibrationally mismatched materials. Several parameters such as vibrational spectrum, atomic disorder, film thickness, and temperature were varied to show their effect on conductance. The importance of atomic mixing in the interface region on thermal interface transport was demonstrated and highlighted.

Goodson [41] discussed basic interface problems in several emerging technologies in electronics such as phase change random access memory and memory on 3D logic chip stacks. The thermal penetration depth in a time-domain thermoreflectance technique was varied to extract interface resistances embedded in a multilayer interconnect structure. The same technique was used in combination with a technique that employs a cantilever to measure in-plane mechanical properties to make simultaneous thermal and mechanical measurements on aligned CNT films. Goodson stressed the importance of developing techniques to measure properties of interfaces and interface materials under representative device operating conditions.

The topics discussed by Cola [42] and D. Li [43] were related to thermal transport at solid–solid interfaces with weak van der Waals bonding. Cola discussed the application of aligned polythiophene (PTh) nanotube arrays as filler-free, polymer-based thermal interface materials (TIMs). Enhanced thermal conductivity in PTh nanostructures was demonstrated and related to improved alignment of constituent chains. PTh nanotube arrays were shown to produce large surface contact (∼80%) in an interface. The total thermal resistance of PTh nanotube array interfaces was measured to be as low as approximately 15 $\mathrm{mm^2K/W}$, which compares favorably to existing polymer TIMs with conductive fillers. Nanoscale conformal coatings of poly(3-hexylthiophene) were applied to CNT arrays and shown to bond the free tips to metal surfaces and reduce thermal resistance by 70%. The resistance reduction was attributed to increased contact size at the nanoscale.

Li [43] discussed the importance of understanding thermal transport through van der Waals contacts with individual nanostructures used to make microfibers, thin films, and bulk composites. A custom microfabrication technique was used to isolate and place two CNTs or nanoribbons in contact for thermal measurements. The measured thermal resistances compared well with results from MD simulations. Thermal resistance was reduced at the van der Waals contacts by soaking the interface in solvent and allowing it to dry, because the capillary forces bring the nanostructures closer.

SESSION 9: NOVEL THERMOELECTRIC AND THERMAL MANAGEMENT MATERIALS

Four presentations were given in this session chaired by J. Malen and K. Takahashi, covering a range of topics including approaches to improve thermoelectric efficiency by tuning electronic band structure, thermal transport in nanocrystal superlattices, and synthesis of high-quality hexagonal boron nitride.

The keynote presentation was given by J. Heremans [44] and was split equally between resonant electronic band structure for enhanced thermoelectric performance and recent studies of the spin Seebeck coefficient. Following a review of successful approaches to reduce thermal conductivity, Heremans described how resonant impurity levels can be used to concurrently increase the Seebeck coefficient (S) and electrical conductivity (σ) in many conventional thermoelectric materials. Two mechanisms that cause this improvement are (1) increased density of states from resonant levels that increases S in a nearly temperature independent way and (2) resonant scattering that causes a large energy (E) dependence in mobility (μ); that is, high $d\mu/dE$, which can improve S at low temperature. In general, these effects can be accurately predicted with electronic structure calculations. Heremans then contrasted the behavior of Tl:PbTe with Ti:PbTe to further clarify the origin of the thermopower enhancement in Tl:PbTe, which was reported in Heremans et al. [45]. Finally, he reviewed resonant levels in a wide range of materials, offering hope for efficient thermoelectric conversion by electronic band structure engineering.

In the second part of the talk, Heremans described the spin Seebeck coefficient, which is a spin redistribution generated by thermal gradients in both semiconductors and spin-polarized metals. His group has experimentally observed this effect in the ferromagnetic semiconductor GaMnAs [46, 47]. By comparing temperature-dependent thermal properties (heat capacity and thermal conductivity) with the temperature dependence of the spin Seebeck coefficient, they concluded that it is driven by phonons [46]. They were able to quantitatively describe this effect using a phonon–magnon drag–based model.

P. Reddy [48] gave the second talk, which focused on a new approach to thermoelectric energy conversion using molecular junctions. Molecular junctions describe small organic molecules sandwiched between inorganic (usually metal) contacts. Reddy pioneered measurements of thermoelectricity in molecular junctions [49–52] that spurred predictions of high ZT in such systems from other authors [53–55]. He is now pursuing an experimental method to confirm the legitimacy of these predictions using gated molecule junctions. Reddy described that high ZT may result from a sharply peaked density of states in the junction that can concurrently give high electronic conductivity and thermopower if it is well aligned with the Fermi energy of the contacts. His new experiments [48], based on capturing molecules in electromigrated rather than STM-based nanogaps, will use back gating to tune the Fermi energy so that it is well aligned with the density of states peak. A first step toward this challenging experimental setup involves establishing a temperature gradient over the nanogap, such that a Seebeck voltage is established by the molecular junction. To verify this temperature gradient, Reddy has built a scanning thermal microscope with custom-built thermocouple AFM tips inspired by Shi and Majumdar [56]. In a vacuum environment, these tips showed a temperature resolution of 15 mK, with spatial resolution of 10 nm, and were adequate to verify the temperature difference in Reddy's nanogaps.

Malen [57] gave the third talk, which focused on thermal transport in nanocrystal superlattices (NCSLs). NCSLs are 3D arrays of inorganic spheres spaced by organic molecules. This class of organic–inorganic hybrid materials has already attracted attention for applications in electronics, photonics, and energy conversion because unique collective properties emerge at the organic–inorganic interface [58–61]. Though several groups have suggested that the organic–inorganic interface will yield new thermal phenomena, few experimental studies have probed these systems, and none have addressed NCSLs [52, 62–65]. Malen described his group's effort to measure thermal conductivity in NCSLs synthesized by Dmitri Talapin's lab at the University of Chicago. Measurements were made using the frequency domain thermoreflectance technique (FDTR). Malen noted that his group has recently achieved modulation frequencies in excess of 200 MHz, which is an order of magnitude higher than time domain thermoreflectance, indicating that FDTR may hold promise for mean free path spectroscopy. His measurements of NCSLs showed that their thermal conductivity is dominated by the organic molecules and that the magnitude of thermal conductivity depends on the alignment between vibrational levels of the molecules and the phonon density of states in the nanocrystals. Malen presented complementary MD results from Alan McGaughey that supported these points.

T. Taniguchi [66] gave the final talk that focused on the synthesis and applications of hexagonal boron nitride (h-BN). His introduction pointed out the analogy between carbon in the form of graphene and h-BN. Though h-BN, a by-product of cubic boron nitride (c-BN), is known primarily as an ultra-hard material like diamond, it has also attracted interest from many researchers because of its wide bandgap in the ultraviolet. In addition, this novel material may have high thermal conductivity because of its structural similarity to graphene. To obtain high-quality crystalline h-BN, selection of the solvent is key issue. The Ba-BN solvent has been successfully used in high-pressure and high-temperature synthesis and the Ni-base solvent can be used for high pressure and atmospheric pressure. Taniguchi's h-BN samples have been provided to many collaborators in the United States and are now being investigated from many aspects. Taniguchi finished by introducing the most exciting current h-BN topic—its application as a substrate for graphene. He mentioned that the atomistic flatness of graphene on the h-BN substrate is important for its performance.

SESSION 10: NANOCARBON MATERIALS AND DEVICES

This session, chaired by S. Inoue and S. Kumar, included one keynote presentation and three contributing presentations. The focus of these presentations was thermal actuation and electrothermal transport in carbon-based devices and new synthesis and controlled growth techniques for carbon nanotubes.

Photo-induced thermal actuation of the graphene and CNT cantilevers was presented by S. Akita [67] in his keynote speech. These cantilevers provide unique opportunities as high-frequency mechanical resonators. The method for extraction of thermal relaxation time using the frequency response of the system was discussed. The motion of nano-cargo inside a CNT was demonstrated using both transmission electron microscopy and MD simulations. A small piece of CNT acts as nano-cargo, which can move back and forth inside the outer CNT. The competing effect between thermal energy and van der Waals energy between nano-cargo and CNT determines the nano-cargo motion. Akita concluded that the thermal energy is crucial for the actuation of nanomechanical systems.

Kumar [68] discussed the effect of self-heating on carbon nanotube network thin-film transistors (CNT-TFTs). TFTs are very promising for performance improvements in various applications such as liquid crystal displays, chem-bio sensors, and flexible and shape-conformable antennae and radars. Kumar developed a computational model to couple electrical and thermal transport in CNT networks self-consistently for accurate predictions of both electrical and thermal characteristics [68]. A network breakdown analysis of the CNT-TFTs was performed to elucidate the effect of thermal resistances at CNT interfaces on device reliability. This investigation concluded that the CNT-to-substrate thermal contact resistance can severely diminish device performance and reliability, but the CNT-to-CNT thermal contact resistance has relatively less effect on the device temperature increase and breakdown.

The last two presentations in this session focused on the selective synthesis of CNTs. M. Kohno et al. [69] sought a way to control the diameter and length of CNTs using a newly built differential mobility analyzer (DMA) apparatus in their chemical vapor deposition (CVD) setup. Their study was inspired by the idea that the CNT diameter is closely correlated to the catalyst size. They succeeded in controlling the diameter distribution following this idea. They also changed the partial pressure of the source gas and showed that the growth rate is linearly correlated with the partial pressure. They concluded that this corresponds to a first-order reaction. They could not synthesize SWCNTs, because it required the fine selection of catalyst nanoparticles for the DMA analyzer. However, they anticipate success in the near future.

S. Chiashi et al. [70] attempted to control the diameter and growth direction of CNTs. They employed commercially available diamond nanoparticles as catalysts to control the CNT diameter. By oxidizing the nanoparticles, they controlled the catalyst size, resulting in CNT diameter control. Because diamond is stable at high temperature, it does not aggregate at the temperature of CVD synthesis, leading to success in selective synthesis. R-cut quartz substrates were used for experiments on the growth direction control. Under appropriate conditions such as slow growth rates, synthesized SWCNT showed good alignment on the substrate. They concluded that the atomic structure of the (101) crystallographic surface affected the growing direction. On the other hand, for synthesis conditions with very high growth rates, SWCNTs crossed each other and did not follow the surface direction. These last two presentations suggest that the diameter-selective synthesis of CNTs requires well-controlled catalyst particle size and supply of the source gases at a controlled rate.

EXPERT PANEL

The expert panel was moderated by Lukes and Fushinobu. The Japanese panelists were Matsumoto, Miyazaki, Shiomi, and Murakami. The U.S. panelists were Goodson, Norris, Phelan, and Shi.

Matsumoto discussed the physics of fluids at different length scales. He stated that fluid behavior at micro-/nanoscales is well described by macroscopic (empirical) constructs such as the Young-Laplace equation and classical instability analyses. He pointed out that surfaces, interfaces, and boundaries become more important as the length scale is decreased and that some of the coefficients important in transport phenomena, such as surface tension, depend on the length scale. In addition, dimensionless quantities often approach limiting values. He remarked that new physics rarely appears even down to the atomic scale and introduced several examples to this effect. He suggested nanofluids as a new frontier of research.

Miyazaki summarized the essence of previous research topics and achievements in the U.S.–Japan seminar series from the discipline of thermal science and engineering. He focused on micro- and nanoscale regimes, where heat conduction, thermal radiation, convection, and phase change are investigated from a microscopic point of view. Specifically, he focused on phonon and electron transport in conduction, photon transport in radiation, and nanofluids and solid–liquid interface problems in convection. Major interests of the speakers in the seminar series have been functional devices, such as thermoelectric and thermophotovoltaic devices, and device fabrication processes. Miyazaki listed possible challenges to be addressed by the community, ranging from fundamental phenomena to global needs and demands, especially new challenges in food and water. He commented on new opportunities such as conventional heat transfer improvement and pointed out that few Japanese students have come to study in the United States in recent years.

Shiomi raised two issues in his talk. The first is the issue of atomistic modeling of thermal interfaces and the role of theoretical modeling. He mentioned the increasing accuracy of bulk phonon transport analyses and the remaining challenges in linking thermal interface modeling at the atomistic scale to transport across the real engineering interfaces between two materials. He also discussed the effectiveness of NEGF approaches for treating harmonic interfaces. He then pointed out, for what he termed "the third generation" of this U.S.–Japan collaboration, the importance of this seminar series and the resulting interactions across the Pacific Ocean. He named several key U.S. institutions that have hosted Japanese researchers. He also noted that few students come from the United States to Japan and suggested that a bidirectional exchange of students between the United States and Japan would be important and helpful for future growth of the field.

Murakami introduced opportunities in ionic liquids. Ionic liquids are room-temperature molten salts, have negligible vapor pressure, are nonflammable, and are largely different from conventional liquids. The number of research papers associated with ionic liquids has rapidly increased in the past decade, and Murakami introduced their key characteristics, including that mass transport in ionic liquids is higher than that estimated by Stokes-Einstein theory. A wide variety of applications have been proposed for ionic liquids, such as biomass, fuel cells, solar cells, secondary batteries, and other energy and industrial applications. However, their fundamental transport mechanism is still unclear. Murakami concluded his talk by stating that energy and mass transport phenomena in ionic liquids are an interesting future research direction.

In summary, the Japanese panelists discussed fundamental issues in various material phases and suggested future directions in nanofluids, ionic liquids, interface thermal transport, and heat transfer enhancement. They emphasized the need for and benefit of the bilateral exchange of next-generation researchers in this field.

Among the U.S. panelists, Goodson spoke on opportunities for advancements in metrology in engineering systems. Single property measurements on idealized systems with carefully controlled interfaces are the focus of much experimental work in this field. The data from these measurements are regarded with some skepticism in industry because real systems formed by integrating multiple components have many imperfect interfaces, leading to much different behavior. It is important to develop new techniques for performing multiproperty measurements on the same sample and to incorporate humidity and other real-world conditions into the measurements. MEMS-integrated temperature and pressure sensors are one example of such techniques.

Norris discussed thermal transport at interfaces. The diffuse mismatch model does not do a good job of predicting interfacial thermal conductance at room temperature, and substantial research has been performed to improve our theoretical understanding in this area. One key advance in the field in recent years has been the inclusion of inelastic scattering effects. Inclusion of elastic effects alone underpredicts interface conductance but including three- and four-phonon effects brings the calculations much closer to experimental values. Advances have also been made in investigating the role of optical phonons, which are typically assumed unimportant for transport but comprise the largest number of phonons in newly emerging complex materials. The role of electron–phonon coupling at interfaces between dielectric and metallic materials has also been clarified. Recent studies on the physical aspects of the interface indicate that different methods used to prepare an interface—for example, as-cleaved versus electron cleaned versus ion cleaned—all give very different values for interfacial conductance. Interfacial bonding energy has also been found to correlate strongly with conductance. Even soft interfaces such as transfer-printed interfaces can enhance conductance due to their large area. Norris concluded by stating that there is still progress to be made, because there are future directions for clarifying interfacial thermal transport identified in the 2003 nanoscale thermal transport paper by Cahill et al. [71] that are still not fully resolved, including employing spectral methods and observing the interaction of individual phonons with interfaces.

Phelan spoke on recent progress in heat transfer in nanofluids. Regarding convection, experimental data in the laminar regime give mixed results: some show heat transfer enhancement and some do not. For turbulent flow the consensus is that nanofluids are not desirable. The article by Buongiorno [72] provides a good description of thermal conduction mechanisms in nanofluids. Nanofluids have potential as solar thermal fluids, and it is important to understand their radiative properties. Volumetric absorption rather than surface absorption is desirable to enable maximum heating of the fluid. Looking ahead, the key challenges are in how to control fluid properties by controlling particle distribution, aggregation, motion, and functionalization. Effective procedures for driving particle motion include redox reactions that induce electric fields in the vicinity of bimetallic nanorods and magnetic fields that align particles into chains.

Shi discussed research opportunities in energy. For large-scale implementation, it is important to consider system requirements such as materials availability and system cost and not just lab-scale efficiencies. Improved energy storage as well as charging and discharging mechanisms are an important future direction. Graphene foam composites provide a promising direction for improving the power capacity of both thermal and electrochemical energy storage devices. For thermal energy storage, water/ice is the state-of-the-art PCM for low-temperature applications. The ARPA-E HEATS program is promoting research into improved thermal storage materials. Other types of energy storage and conversion mechanisms have been little explored for practical systems but deserve more research attention. These include thermochemical energy storage and pyroelectric and magnetocaloric energy conversion. Finally, new types of energy carriers and energy conversion mechanisms should be investigated, including spin waves, magnons, and charge density waves. One example is the recently discovered spin Seebeck effect [73–75] discussed by Heremans in the seminar.

After the panel presentations, an open discussion was held among the panelists, audience, and moderators in which open questions and future directions were identified. McGaughey discussed that there is still uncertainty in determining when exactly specular and diffuse scattering at interfaces should be considered. Shiomi and Norris mentioned that a big challenge related to this is the lack of repeatability of experimental interfaces, which can lead to order of magnitude variation in the interface conductance. Carefully controlled and prepared interfaces are needed for direct comparison of theory and experiment. Cola questioned the perceived emphasis in modeling and simulation research on validation rather than prediction. Lukes replied that there has to be some level of confidence in the models before they can be used for prediction. Galli emphasized that it is very important to have a clear picture of what the limitations are in the models and that careful ties to experiment are needed for validation. Heremans said that the main role of the models should be to provide intuition and insight, not exact quantitative prediction. Factor of two or even order of magnitude agreement is acceptable; the critical task is to identify the trends and point out which directions the experiments should be heading. Chen mentioned that near-field optical radiation is an important area that is “low-hanging fruit” that is easier to analyze than phonon transport because the Maxwell equations are linear. Nanoscale transport in metamaterials is a field ripe for exploitation but is only beginning to be explored. Chen also mentioned as a future direction the identification of the transition between conduction and radiation at small separations. Pipe pointed out that many people are working on thermoelectrics and questioned whether we as a community should expand our efforts to other, more conventional energy sources or other directions of research. Shi responded that some other topics are also being investigated actively by the community in addition to solid-state thermoelectric conversion—for example, electronics cooling and electrothermal transport effects in devices—and agreed that there are other new interesting future directions. In closing, Bischof remarked that it seems that only a few topics are being investigated actively by this community and that our skill set both in experimentation and modeling could be applied to challenging issues in nanoscale transport processes in biological systems.

CLOSING PLENARY LECTURES

The closing plenary lectures were given by T. Ohara and Chen and moderated by Fushinobu and Shi. Ohara [76] addressed the challenges and opportunities of nanoscale transport phenomena in soft matter. Ohara began by introducing the research trends in Japan and the United States. Japan generally focuses more on fluids, whereas the United States focuses more on solids. Ohara suggested that something in between, soft matter, will be a promising future direction.

Soft matter is condensed matter that easily deforms at room temperature. Soft matter has very unique features such as highly ordered structures formed through self-organization, a wide variety of designed structures, only short-range order, and tailor-made surfaces. Many types of soft matter such as polymer mono-/bilayers, micelles, and liquid crystals are categorized in this group.

Ohara discussed several examples of prior research in soft matter, including biomembranes, polymer brushes, polymer nanosheets, the layer-by-layer assembly technique, and some other related materials, such as polymer nanocomposites, confined polymer liquids, and single molecular chains. The thermal, mass, and momentum transport in such soft materials, particularly thermal transport, have been little investigated and are not well understood. The key issue is the anomalous transport characteristics associated with their unique (e.g., heterogeneous) structures. Understanding of the transport mechanisms can lead to the design of unique thermal properties in such materials.

Ohara further discussed several research activities in this area. The first example is the fundamental physics in the formulation of the conduction heat flux in soft matter. Ohara extended the idea introduced in 1950 that is based on the migration of molecular energy. He proposed adding the effect of accumulation of kinetic energy transfer between individual molecules. Energy transfer analysis was then extended to polymers, from simple alkanes to complex biomolecules. It was shown that the multibody potentials for deforming molecules must be properly treated and that the contribution of intramolecular energy transfer along covalent bonds should also be considered. Results of MD heat conduction simulations in bulk alkane liquids have demonstrated good agreement for various liquids and have revealed the composition of the energy transfer mode for each molecule. Anisotropic thermal conductivity of a lipid bilayer membrane has also been considered using MD.

Ohara also pointed out that about a dozen presentations in this seminar were either directly or indirectly related to soft matter and noted the increasing focus on this topic in the community. He summarized that soft matter has great potential for material design in a wide range of applications but that there is much still to be understood. Transport properties, especially thermal transport properties, need further investigation. He advised the community to keep in mind several key issues in future research on soft matter: there is much to learn from both solids and liquids, transport properties are determined by material structures, precise measurements are critical, and the concept of soft interfaces is also important.

Chen [77] reviewed two decades of micro-/nanoscale thermophysics and heat transfer research in his closing presentation. He began with a slide that summarized different topics presented by Japanese and U.S. participants during this and the previous six Japan–U.S. meetings. This series of joint seminars focused on transport phenomena at micro- and nanoscales was initiated by late Professors C.-L. Tien, K. Hijikata, and others in the early 1990s, a decade before the National Nanotechnology Initiative was launched in the United States. During the earlier joint meetings, some of the topics were addressed by only U.S. or Japan participants. One notable example is MD simulation of transport processes, which was presented only by Japanese participants in the 1993 and 1996 meetings. After being exposed to the Japanese colleagues' presentations in this joint seminar, the U.S. participants started to report increasing efforts in MD simulations after 1999. Because of the opportunities provided by the joint seminars to exchange information between participants from the two countries, in the 7th Joint Japan–U.S. seminar participants from both countries presented a wide range of fundamental studies of nanoscale transport topics, which are relevant to applications in energy storage and conversion, biomedical devices, materials processing and manufacturing, and information technologies.

Chen provided a critical assessment of the achievements made over the past two decades in this field. The first one in the area of conduction is the engineering of material thermal conductivity, which has been one area of focus in this joint seminar series. The past investigations of a variety of nanostructured materials, including disordered layered thin films, nanocomposites, aligned polymer chains, carbon nanotubes, and graphene, have extended the thermal conductivity limits of solids. In many cases, particle transport theories such as the Casimir limit of diffuse interface scattering of phonons can be used to understand the mechanisms for thermal conductivity suppression in nanocomposites and nanowires. On the other hand, coherent wave effects including coherent scattering by interfaces and defects, phonon localization phenomena, and thermal conductivity divergence with length in low-dimensional systems have been suggested in the literature and a better understanding is still necessary. A transition from 3D phonon transport, where the thermal conductivity decreases with the characteristic size, to 1D phonon transport, where an opposite size dependence is expected, has been identified. Chen further used the results from the ultrafast laser reflectance measurements presented in Nelson's keynote presentation to highlight another achievement in the improved understanding of heat transfer outside a nanostructure.

Though these types of ultrafast measurements are becoming powerful tools for phonon mean free path spectroscopy, Chen also summarized other achievements over the past two decades in experimental tools to characterize thermal transport at the nanoscale. He highlighted microfabricated platforms, the 3-ω method, and pump-probe techniques as three notable examples. He further listed a number of other experimental techniques for nanoscale or ultrafast temperature measurements based on scanning probe microscopy, photothermal reflectance, photoluminescence, Raman spectroscopy, and near-field scanning optical microscopy for heat flux measurements based on AFM cantilevers and microfabricated suspension and for calorimetry based on microfabricated platforms. Among them, he pointed out that nanoscale temperature measurement remains a challenge.

Chen further examined the progress made in multiscale simulation. At the atomic scale, progress has been made in density functional theory, equilibrium, nonequilibrium, and ab initio MD and the Green's function approach. The results from these atomic-scale simulations can be used in numerical or Monte Carlo solutions of the Boltzmann transport equation to predict the effective medium properties or those of the continuum. He was optimistic that this community will be able to accomplish multiscale phonon transport in the next decade and suggested creating a database of phonon mean free path as a function of wavevector. He further suggested that we cannot predict interfacial transport yet and that the potential tools to overcome this challenge include Green's function approach and MD, especially equilibrium MD.

In the area of convection, Chen reviewed research in single- and multiphase flow and heat transfer in microchannels; superhydrophilic and superhydrophobic surfaces; electrokinetic flow, heat, and mass transfer; and thermal conductivity and radiative coupling of nanofluids. He emphasized that there is limited understanding of thermal transport in fluids, although knowledge of gas flow in the Knudsen regime has been well established. He agreed with Ohara that there is a lot of room for research on soft materials.

In the area of photons and radiation transport, Chen elaborated on his comments made in the open discussion that near-field optical radiation is an important area and that radiation transport in photonic crystals and metamaterials has not received much attention. He listed four possible future directions, including spectral control for solar thermal processes, high-temperature photonics, convergence of radiation and conduction, and convergence of interfacial energy and bonding.

Chen concluded his presentation by responding to Majumdar's emphasis on the connection between science, systems, and societal needs. He suggested that one important impact of the efforts in the past two decades is in workforce development, evidenced in the training of a new generation of researchers for universities, industries, and government labs. He used vehicle and industrial waste heat recovery, solar energy utilization, sensors, and other examples to illustrate the existing and potential impact of the research in this field on applications ranging from micro- to gigawatt scales. He further used examples of desalination, directional solvent extraction, and high thermal conductivity plastics to illustrate future research opportunities that can make a positive impact on society.

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