TECHNICAL DISCUSSION

REPORT OF WORKSHOP: THERMOPHYSICAL PHENOMENA IN MICROSCALE SENSORS, DEVICES, AND STRUCTURES

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The goal of this one-day workshop was to provide a cross-disciplinary forum for discussion and presentation of the latest results in the rapidly developing area of Thermophysical Phenomena in Microscale Sensors, Devices, and Structures. It

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was co-funded by the Division of Chemical and Transport Systems of the National Science Foundation as well as by the Division of Engineering of the Basic Energy Sciences in the Department of Energy. The workshop was held in the Baltimore Hilton and Towers on August 9, 1997. As shown in the program (see Appendix), the workshop consisted of 27 presentations divided into four sessions: fluidics, thermomechanic, and thermoelectric, micro- and nanostructures, and microscale experimental techniques. In addition, there was a lunch-time keynote talk on Microelectromechanical Systems given by Dr. Noel MacDonald, Director of Electronics Technology Office, Defence Advanced Research Projects Agency. The workshop was attended by approximately 100 participants including people from academia (faculty and graduate students), industry, and national laboratories. A brief description on the highlights of the each session is provided here.

FLUIDICS

The workshop started with a presentation by Prof. Ho of UCLA on control of fluid flow using micromechanical sensors and actuators. By using integrated-circuit fabrication technology, sensors and actuators on the order of 100 μ m in size can be monolithically batch-fabricated and distributed over areas of interest. Using such sensors, Prof. Ho showed that separation of flow over airfoil wings can be controlled in such a way that the maneuverability of an aircraft can be significantly increased. Such distributed sensors also can be used to study the structure of turbulence near a wall, a measurement that is crucial for drag reduction and understanding the fundamentals of turbulent flow.

Prof. Lin of the University of Michigan demonstrated that microbubbles, generated by boiling of water from small polysilicon microheaters, can be used as an efficient fluid actuator and pump. By utilizing the Marangoni effect, the position of the bubble is stabilized towards the hottest region, i.e., on the heater. By comparing it with well-established theories of nucleation, it was suggested that these bubbles undergo homogeneous nucleation. Such bubble actuators can have many applications in systems such as inkjet printers, microfluidic chemical and biochemical reactors, and so forth.

One of the problems associated with the accurate design and analysis of microfabricated fluid systems is the understanding of viscous behavior in very small geometries. This has fundamental implications in several structures; for example, the viscous damping of resonant microstructures such as accelerometers or floating element sensors, the performance of bearings in high-speed microturbomachinery and even the performance of micronozzles for use in propulsion, rocketry, and so forth. Prof. Breuer of MIT used careful measurements of gas-surface interactions in conjunction with theoretical models to determine the gas-surface tangential momentum accommodation coefficient. These results also were compared with numerical results that use the direct-simulation Monte Carlo method, which does not assume continuum flow in the microgeometry.

Prof. Maruyama of the University of Tokyo presented molecular-dynamic simulation of the formation of a liquid droplet on a single-crystal surface. By assuming Lennard-Jones potential and varying the adjustable parameters in the energy potential, it was shown that the first few layers of the liquid droplet contain a very ordered layered structure. The simulation also showed that Young's equation for the contact angle was valid even for these molecular-sized droplets. The phenomena of evaporation and condensation of these ultrasmall droplets also was simulated.

Prof. Webb of Penn State University presented experimental results of heat transfer and pressure drop for two-phase flow through very narrow channels (0.1-2.0 mm diameter). The experiments showed the data to fall far below well-established correlations that have been derived for macroscopic channels. It is unclear as to whether there is a critical channel diameter below which the correlations fail to predict the behavior. Further investigations are suggested.

Prof. Karniadakis of Brown University numerically studied rarefied gas flows in channels, pipes, and backwards-facing steps in a wide range of Knudsen numbers (Kn), with the objective of developing continuum-based simplified models. A new general boundary condition that accounts for the reduced momentum exchange with wall surfaces was proposed and its validity investigated. A universal scaling for the velocity profile was obtained that was used to develop a unified model predicting the mass flowrate with reasonable accuracy in the entire flow regime $(0 = Kn < \infty)$. The effect of rarefaction on separated flows was studied by considering the backwards-facing step geometry in the slip-flow regime.

The ability to mix fluids thoroughly and in a reasonable amount of time is fundamental to the creation of fully integrated, "on-chip" micro-electromechanical (MEMS) fluid-processing systems. Turbulence, which often is used for efficient mixing in macroscopic systems, cannot be generated in microfluidic devices because of their small size and low velocities. Diffusion is unacceptably slow in most cases because the planar nature of MEMS devices limits the interfacial area between the different species. Prof. Liepmann of the University of California, Berkeley, demonstrated that one approach to rapidly mix fluids in a planar, laminar environment is to generate a chaotic flow field. Using microfabricated bubble pumps connected with a mixing chamber, it was demonstrated that the time required for mixing of a dye with a fluid can be brought down from 30 minutes without chaotic mixing, i.e., based on diffusion, to approximately 30 seconds using chaotic mixing. Such a drastic improvement is expected to make significant impact on microfluidic devices and technology.

THERMOMECHANIC AND THERMOELECTRIC

Prof. L. H. Allen (University of Illinois, Urbana) presented results of a MEMS-based scanning calorimeter for measuring thermodynamic properties of nanoscale materials with an energy resolution of 0.2 nJ. This was used to measure the melting point of Sn nanocrystals, which decreased with crystal size; this was explained through the existence of a surface molten layer. The calorimeter also was used to study the thermodynamics of submonolayer films.

Micromechanical, chemical, physical, and biological sensors based on microcantilevers were presented by T. Thundat (Oak Ridge National Laboratory). Microcantilever sensors operate by detecting changes in resonance response or deflection caused by mass loading, surface stress variation or changes in damping conditions. A bimaterial cantilever can be used for calorimetry and infrared imaging. Arrays of such microcantilevers have been fabricated and used for distributed sensing.

Filters and sensors based on Complimentary Metal-Oxide Semiconductor thermal oscillators was presented by E. J. J. Kruglick (University of California, Berkeley). Polysilicon microheaters were modeled using SPICE to develop schemes for filtering signals and for their use as sensor systems.

Dr. A. Shakouri (University of California, Santa Barbara) presented results based on Monte Carlo simulations of current and heat transport in thermionic cooling devices using III-V and II-VI materials. These devices are based on thermionic emission of current across controlled band edges, which can be fabricated using molecular-beam epitaxy. The thermoelectric performance of these devices was better than traditional thermoelectric devices and efforts are now being devoted to fabrication of these devices.

Prof. N. C. Tien (Cornell University) presented the development of a miniature optical bench consisting of interferometers, lenses, translators, miniature mechanical systems with moving parts, and detectors micromachined on a surface. Such a miniaturized optical system was used to measure the thermal expansion of a furnace using interferometry.

Theoretical calculation for lower size limits for Stirling cycle heat engines was presented by Prof. R. B. Peterson (Oregon State University). Calculations of cycle efficiencies were based on thermal conduction through the regenerator as well as the effectiveness of the regenerator. It was demonstrated that the efficiency of Stirling engines decreased with size and that engines smaller than 1 mm are impractical because of low efficiency.

MICRO- AND NANOSTRUCTURES

Eight papers were presented in the session on micro- and nanostructures. The papers offered significant experimental and theoretical results and were well received by the audience in general.

The first paper of the session by Prof. D. Cahill (University of Illinois, Urbana) explored the principle of minimum thermal conductivity, which is of importance to the thermal management of thin film structures. It was shown that the thermal conductivity of multilayer structures is not influenced by the presence of interfaces separated by nanometer-length scales. New data on polymers showed that the thermal conductivity was lower than the minimum predicted by traditional theories.

The second paper, by Prof. G. Chen (UCLA), reported recent progress on understanding quantum effects on heat conduction in thin films. The theoretical approach has considerable implications and can contribute to controlling thermal transport at the micro- and nanoscales through phonon engineering.

The third paper, by Prof. P. Phelan (Arizona State University), showed that reduction of size in two and three dimensions has a pronounced effect on the material thermodynamic properties, i.e., the internal energy and specific heat. The analysis also showed that at small dimensions the Debye model breaks down, even for very low temperatures.

The fourth paper, by Dr. R. Bhargava (Nanocrystals Technology), presented new results on the quantum-confined atoms in nanocrystals. These nanocrystals

have unique optical properties—the absorption spectrum is determined by the nanocrystal size and the emission spectrum depends on the confined atoms. The possibility of using the unique properties of these nanostructures in applications in science and engineering, including opto-electronics, lasers, and high-density optical storage, was discussed.

The paper on the scanning laser confocal microscopy by Dr. J. Marschall (NASA, Ames) was aimed at characterizing the fiber orientation and using the information to calculate heat and mass transport modeling (such as thermal radiation and heat conduction). One critique of the paper asked whether the fiber orientation information obtained represents the true location and fiber orientation, due to the effect of scattering.

The paper on interface propagation in the processing of metal matrix composites by Prof. S. Garimella (University of Wisconsin, Milwaukee) was based on classical transport theory, but the results obtained are interesting for the processing of composite materials.

Prof. S. H. Chan (University of Wisconsin, Milwaukee) presented results on the development of novel biological inhibitors of fouling and scale formation. These molecules can be mass produced by through bioprocessing and are biodegradable. These have great economical and environmental implications for applications in heat exchangers.

The last paper, by Prof. C. Grigoropoulos (University of California, Berkeley) presents recent progress on the surface modification by pulsed laser ablation and the direct transfer of materials to form desired patterns. This interesting technique can be used for maskless patterning in a variety of applications.

MICROSCALE EXPERIMENTAL TECHNIQUES

The final session of the day consisted of six presentations featuring microscale experimental techniques. The purpose of the session was to highlight recent advancements in the application of powerful tools that have been developed by the applied physics community, including ultrafast lasers and scanning probe microscopes, to the study of microscale thermophysical phenomena. The presentations discussed the thermal physics occurring at short time and length scales and properties relevant for new electronic and opto-electronic devices. Many of the techniques discussed in this session are promising for the integrated circuit and MEMS industries, because existing thermal metrology used by companies cannot keep pace with the rapid operation and the decreasing feature sizes of devices.

Three of the presentations focused on laser-based processing techniques and metrology. M. C. Hipwell (Seagate), C. L. Tien (University of California, Berkeley), X. L. Mao, and R. E. Russo (Lawrence Berkeley National Laboratory) used a picosecond continuum technique to investigate spectral and nonlinear radiative properties of porous silicon. These authors investigated the impact of carrier confinement, the large material surface area, and the many scales of disorder on the short-timescale optical properties of porous silicon, which are important for the development of fast optical switches.

Ultrashort laser pulses were used by L. Phinney, K. Fushinobu, and C. L. Tien (University of California, Berkeley) to reduce microstructure adhesion in MEMS. These authors modeled the absorption and cooling process in silicon using

separate energy balances for free carriers and phonons. Because the predictions for the maximum carrier temperature are much higher than those for the material lattice, these authors indicated that the hot carriers may facilitate the adhesion reduction without damaging the material lattice. Y. S. Ju, K. Kurabayashi, and K. E. Goodson (Stanford University) studied thermal properties of novel organic passivation for integrated-circuit interconnects by combining Joule heating with high-spatial-resolution photothermal imaging. The optical thermometry employed by these authors makes possible measurements over a wide range of heating frequencies, which allows the thermal conductivity to be precisely determined without calibration or precise knowledge of the heat capacity of the layer.

Three of the presentations discussed high-spatial-resolution thermal imaging using the atomic force microscope (AFM). This work finds strong motivation in the decreasing dimensions of electronic and opto-electronic devices, whose temperature fields strongly influence their performance and reliability. O. Nakabeppu, M. Kajii, M. Igeta, T. Inoue, and K. Hijikata (University of Tokyo) presented data that raise questions about the calibration of the AFM thermometry and the impact of varying the ambient pressure. These authors proposed a modification to the standard thermometry approach, which heats the cantilever tip to the same temperature as the sample to avoid the influence of the tip-surface thermal conductance. J. Varesi, T. Chang, M. Igeta, S. Muenster, C. Riviera, and A. Majumdar (University of California, Berkeley) provided an overview of their ongoing work on scanning thermal microscopy using the AFM, including recent progress that uses transient thermal expansion of the sample near-surface region. Key data include the temperature distribution within a vertical-cavity surface-emitting laser, obtained by scanning a cleaved sample, and images of the expansion of individual grains on an indium tin oxide resistor. T. Boumaza described new activities in the area of microscale heat transfer at the National Physical Laboratory, United Kingdom.

APPENDIX:

WORKSHOP PROGRAM: THERMOPHYSICAL PHENOMENA IN MICROSCALE SENSORS, DEVICES, AND STRUCTURES

(NSF-4 and DOE-funded workshop) Organized by: A. Majumdar and C. L. Tien August 9, 1997, Baltimore Hilton & Towers, Baltimore, MD

7:30-8:15 Registration + Continental Breakfast (Outside Baltimore Theater)
8:15-8:20 Introduction

SESSION A: FLUIDICS

Session Co-chairs: D. Liepmann and S. Maruyama

- 8:20-8:35 "Micro-electro-mechanical Systems and Fluid Flows," C. M. Ho, UCLA
- 8:35-8:50 "Microscale Thermal Bubble Formation: Thermophysical Phenomena and Applications," L. W. Lin, U. Michigan, Ann Arbor

- 8:50-9:05 "Gas-Surface Interactions in Micromachined Devices," K. Breuer, MIT
- 9:05-9:20 "Liquid Droplet in Contact with a Solid Surface," S. Maruyama, T. Kurashige, S. Matsumoto, Y. Yamaguchi, T. Kimura, U. Tokyo
- 9:20-9:35 "Heat Transfer in Small Diameter Channels," R. Webb & M. Zhang, Penn State U.
- 9:35-9:50 "Simulations and Models for Microflows," A. Beskok, MIT & G. Karniadakis, Brown U.
- 9:50-10:05 "Rapid and Controlled Mixing in Microscale Devices," D. Liepmann, J. Evans, A. Pisano, U. C. Berkeley
- 10:05-10:25 BREAK

SESSION B: THERMOMECHANIC & THERMOELECTRIC

- Session Co-Chairs: T. Thundat and N. Tien
- 10:25-10:40 "MEMS Based Scanning Calorimeter for Thermodynamic Properties of Nanostructures," L. Allen & S. L. Lai, U. of Illinois, Urbana
- 10:40-10:55 "Microcantilever Array Sensors," T. Thundat, Oakridge Natl Lab.
- 10:55-11:10 "CMOS Thermal Oscillator Transducers as Sensors and Filters," E. Kruglick & K. Pister, U. C. Berkeley
- 11:10-11:25 "Thermoelectric Effects in Submicron Heterostructure Barriers,"
 A. Shakouri, E. Lee, D. Smith, V. Narayanamurti, J. Bowers, U. C. Santa Barbara
- 11:25-11:40 "Optical interferometric sensors using polysilicon surface micromachining," N. Tien, Cornell Univ.
- 11:40-11:55 "Size Limits for Stirling Cycle Heat Engines," R. Peterson, Oregon State Univ.
- 12:00-1:40 LUNCH BANQUET (Versailles Room), KEYNOTE SPEECH: Prof. N. MacDonald, Cornell University

SESSION C: MICRO & NANOSTRUCTURES

Session Co-Chairs: G. Chen and C. Grigoropoulos

- 1:40-1:55 "Thin Film Materials and Minimum Thermal Conductivity," D. Cahill, S. M. Lee, G. Matamis, U. Illinois, Urbana, W. Allen, United Tech.
- 1:55-2:10 "Towards Phonon Engineering in Thin Films and Superlattices," G. Chen, UCLA
- 2:10-2:25 "Size Effects on the Thermodynamic Properties of Small Structures,"
 R. Prasher and P. Phelan, Arizona State U., J. P. Longtin, SUNY Stony Brook
- 2:25-2:40 "Quantum Confined Atoms—Physics and Applications," R. Bhargava, Nanocrystals Technology
- 2:40-2:55 "Application of Laser Scanning Confocal Microscopy to Heat and Mass Transport Modeling in Porous Microstructures," J. Marschall, F. Mios, J. Fredrich, NASA
- 2:55-3:10 "Interface Propagation in the Processing of Metal Matrix Composites," S. Garimella & J. Simpson, U. Wisconsin, Milwaukee

Metal Microstructures," C. Grigoropoulos, U. C. Berkeley

3:40-4:00 BREAK

SESSION D: MICROSCALE EXPERIMENTAL TECHNIQUES

Session Co-Chairs: K. Goodson and M. C. Hipwell

- 4:00-4:15 "Picosecond Differential Transmission Measurements for Porous Silicon," M. C. Hipwell, C. L. Tien, X. L. Mao, and R. E. Russo, Seagate, U. C. Berkeley, and Lawrence Berkeley Natl. Lab.
- 4:15-4:30 "Subpicosecond laser processing of polycrystalline silicon microstructures," L. Phinney, K. Fushinobu, and C. L. Tien, U. C. Berkeley
- 4:30-4:45 "Thermal Measurement by the AFM-measurement principle and future strategy," O. Nakabeppu, U. Tokyo, M. Kajii, M. Igeta, T. Inoue, K. Hijikata, Tokyo Institute of Technology
- 4:45-5:00 "Thermal Characterization of IC Interconnect Passivation using Farand Near-Field Optics," Y. S. Ju, K. Kurabayashi, M. Asheghi, D. Fletcher, K. E. Goodson, Stanford U.
- 5:00-5:15 "Scanning Thermal and Expansion Microscopes," J. Varesi, T. Chang, M. Igeta, S. Muenster, C. Reviera, A. Majumdar, U. C. Berkeley
- 5:15-5:30 "Calibration and standards for micro-scale thermal property measurement," T. Boumaza, National Physical Lab., U.K.
- 5:30-6:10 **OPEN FORUM & DISCUSSIONS**
- 6:10-6:15 CLOSING COMMENTS