

## 2005 Listing of Material Science PI Publications

Mukherjee, S., H.-G. Kang, **W. L. Johnson**, and W.K. Rhim, "Noncontact measurement of crystallization behavior, specific volume, and viscosity of bulk glass-forming Zr-Al-Co-(Cu) alloys," *Phys. Rev. B*, 70, 174205 (6 pages), 2004.

*The authors are at California Institute of Technology, where Professor Johnson is the Principal Investigator on the ground-based project "Thermodynamic and Transport Properties of Glass Forming Alloy Liquids Using the Caltech High Vacuum Electrostatic Levitator Platform."*

Crystallization behavior, specific volume, and viscosity are investigated using the noncontact electrostatic levitation technique for metallic glass-forming alloys in the Zr-Al-Co-(Cu) system. The compositions investigated are  $Zr_{55}Al_{20}Co_{25}$ ,  $Zr_{55}Al_{22.5}Co_{22.5}$ , and  $Zr_{55}Al_{19}Co_{19}Cu_7$ . Free radiative cooling in the electrostatic levitator could vitrify all the three alloys. This allowed, for the first time, the determination of time-temperature-transformation (TTT) curves for ternary metallic alloys by isothermal annealing over a wide temperature range between the liquidus and glass transition temperatures. While the TTT curve for  $Zr_{55}Al_{22.5}Co_{22.5}$  shows the expected "C" shape with a single "nose," the TTT curves for the other two alloys show two noses. X-ray diffraction study shows that the double-nose structure for  $Zr_{55}Al_{20}Co_{25}$  and  $Zr_{55}Al_{19}Co_{19}Cu_7$  is caused by the overlap of TTT curves for two different crystalline phases. For  $Zr_{55}Al_{22.5}Co_{22.5}$ , however, the same crystalline phases are formed over the temperature range of the entire TTT curve, which is supported by the single nose. The average critical cooling rate for glass formation of the Zr-Al-Co-(Cu) alloys estimated from the measured TTT curves is about 17 K/s. This value of critical cooling rate is supported by the trends in specific volume and dynamic viscosity of these alloys compared to other bulk metallic glass-forming alloys.

Nakhmanson, S. M., M. Buongiorno Nardelli, and **J. Bernholc**, "Ab initio Studies of Polarization and Piezoelectricity in Vinylidene Fluoride and BN-Based Polymers," *Physical Review Letters*, 92, 115504 (4 pages), 2004.

*The authors are from North Carolina State University where Professor Bernholc is the Principal Investigator on the ground-based project "Growth and Properties of Carbon Nanotubes."*

Highly piezoelectric and pyroelectric phases of boron-nitrogen-based polymers have been designed from first principles. They offer excellent electrical and structural properties, with up to 100% improvement in the piezoelectric response and an enhanced thermal stability with respect to polyvinylidene fluoride (PVDF). Since methods for their synthesis are readily available, these polymers are extremely promising for numerous technological applications, rivaling the properties of ferroelectric ceramics and superseding PVDF-based material in high-performance devices.

Kershner, Ryan J., Joseph W. Bullard and **Michael J. Cima**, “The role of electrochemical reactions during electrophoretic particle deposition,” *Journal of Colloid and Interface Science*, 278, 146-154, 2004.

*The authors are at Massachusetts Institute of Technology, where Professor Cima is Principal Investigator on the ground-based project “Forces during manufacture and Assembly of Microscale Discrete Electronic Components.”*

Platinum microelectrodes were fabricated on a sapphire substrate by lithographic patterning and used to manipulate 1.58  $\mu\text{m}$  silica particles in the plane of the substrate. A digital video system captured the motion of particles far from the electrodes and their deposition onto the working electrode during application of a DC potential. The role of electrode reversibility was investigated by comparing as-deposited electrodes with electrodes modified by electrolytic plating of platinum. Particles were also observed adhering to the substrate before reaching the electrode. The  $\zeta$  potential of the particles and substrate was measured. The differing surface chemistry of the two systems and a local reduction in pH due to the production of hydrogen ion at the anode can explain the adhesion phenomena. Force distance curves were recorded using a colloid probe atomic force microscopy technique to directly measure the interaction of the silica particles with the sapphire substrate. These data validated the observed adhesion at the electrode and provided further support for the temporal and spatial reduction in pH. The role of Faradaic processes and the diffusion of potential determining ions in electrophoretic deposition were also considered.

Kershner, Ryan J., Joseph W. Bullard and **Michael J. Cima**, “Zeta Potential Orientation Dependence of Sapphire Substrates,” *Langmuir*, 20, 4101-4108, 2004.

*The authors are at Massachusetts Institute of Technology, where Professor Cima is Principal Investigator on the ground-based project “Forces during manufacture and Assembly of Microscale Discrete Electronic Components.”*

The zeta potential of planar sapphire substrates for three different crystallographic orientations was measured by a streaming potential technique in the presence of KCl and  $(\text{CH}_3)_4\text{NCl}$  electrolytes. The streaming potential was measured for large single crystalline C-plane (0001), A-plane (11-20), and R-plane (1-102) wafers over a full pH range at three or more ionic strengths ranging from 1 to 100 mM. The roughness of the epi-polished wafers was verified using atomic force microscopy to be on the order of atomic scale, and X-ray photoelectron spectroscopy (XPS) was used to ensure that the samples were free of silica and other contaminants. The results reveal a shift in the isoelectric point (iep) of the three samples by as much as two pH units, with the R-plane surface exhibiting the most acidic behavior and the C-plane samples having the highest iep. The iep at all ionic strengths was tightly centered around a single pH for each wafer. These values of iep are substantially different from the range pH 8-10 consistently reported in the literature for  $\alpha\text{-Al}_2\text{O}_3$  particles. Particle zeta potential measurements were performed on a model powder using phase analysis light scattering, and the iep was confirmed to occur at pH 8. Modified Auger parameters (MAP) were calculated from XPS spectra of a monolayer of iridium metal deposited on the sapphire by electron beam deposition. A shift in MAP consistent with the observed differences in iep of the surfaces confirms the effect of surface structure on the transfer of charge

between the Ir and sapphire, hence accounting for the changes in acidity as a function of crystallographic orientation.

Schroers, Jan, Chris Veazey, Marios D. Demetriou, and **William L. Johnson**, "Synthesis method for amorphous metallic foam," *Journal of Applied Physics*, 96, 255506 (4 pages), 2004.

*The authors are at California Institute of Technology where Professor Johnson is Principal Investigator on the flight project "Properties of Undercooled Glass-forming Metallic Alloys."*

A synthesis method for the production of amorphous metallic foam is introduced. This method utilizes the thermodynamic stability and thermoplastic formability of the supercooled liquid state to produce low-density amorphous metallic foams in dimensions that are not limited to the critical casting thickness. The method consists of three stages: the prefoaming stage, in which a large number of small bubbles are created in the equilibrium liquid under pressure; the quenching stage, in which the liquid prefoam is quenched to its amorphous state; the foam expansion stage, in which the amorphous prefoam is reheated to the supercooled liquid region and is processed under pressures substantially lower than those applied in the prefoaming step. Results from a dynamic model suggest that the foam expansion process is feasible, as the kinetics of bubble expansion in the supercooled liquid region are faster than the kinetics of crystallization. Within the proposed synthesis method, bulk amorphous foam products characterized by bubble volume fractions of as high as 85% are successfully produced.

Y. Y. Khine, Y. Y., and **R. M. Banish**, "3-D Simulations of Diffusivity Measurements in Liquids with an Applied Magnetic Field," *International Journal of Thermophysics*, 25, 1763-1773, 2004.

*The authors are at University of Alabama in Huntsville, where Dr. Banish is the Principal Investigator on the ground-based project "Temperature and Composition Dependence of mass and Thermal Diffusion in Liquid Metals and Compound Semiconductor Alloys."*

The effect of convective contamination in self-diffusivity experiments of liquid metals is predicted via a three-dimensional (3-D) model that includes an applied magnetic field. A uniform heat flux is applied at the sidewall of the cylindrical ampoule, and heat losses are allowed at the top and bottom walls of the ampoule. A wide range of a uniform, steady, axial magnetic field (from moderate to very strong) is considered in the model. Since the thermal Peclet number,  $Pe$ , is very small for the parameters of interest, convective heat transfer is neglected. A large interaction parameter,  $N$ , suggests that the flow is inertialess. The temperature and flow problems are solved at steady state while the time-dependent concentration problem is determined for various mass Peclet numbers,  $Pe$ . In all cases, the output  $D$  (i.e., with convective contamination) increases with an increase in the temperature non-uniformity  $\Delta T_0$ . The radial and azimuthal velocities are much smaller than the axial velocity in each case. A stronger magnetic field can tolerate a higher temperature non-uniformity  $\Delta T_0$ , but  $\Delta T_0$  is still less than 0.025 K with a 5 T magnetic field for convective contaminations to be less than 5% of the total mass flux.

Cui, X, and **B. Q. Li**, “A parallel Galerkin boundary element method for surface radiation and mixed heat transfer calculations in complex 3-D geometries,” *International Journal for Numerical Methods in Engineering*, 61, 2020-2024, 2004.

*The authors are at Washington State University where Professor Li is the PI on the ground-based project “Study of magnetic field effects on convection and solidification in normal and microgravity.”*

This paper presents a parallel Galerkin boundary element method for the solution of surface radiation exchange problems and its coupling with the finite element method for mixed mode heat transfer computations in general 3-D geometries. The computational algorithm for surface radiation calculations is enhanced with the implementation of ideas used for 3-D computer graphics applications and with data structure management involving creating and updating various element lists optimized for numerical performance. The algorithm for detecting the internal third party blockages of thermal rays is presented, which involves a four-step procedure, i.e. the primary clip, secondary clip and adaptive integration with checking. Case studies of surface radiation and mixed heat transfer in both simple and complex 3-D geometric configurations are presented. It is found that a majority of computational time is spent on the detection of foreign element blockages and parallel computing is ideally suited for surface radiation calculations. Results show that the decrease of the CPU time approaches asymptotically to an inverse rule for parallel computing of surface radiation exchanges. For large-scale computations involving complex 3-D geometries, an iterative procedure is a preferred approach for the coupling of the Galerkin boundary and finite elements for mixed mode heat transfer calculations.

Shu, Y., **B. Q. Li**, and B. R. Ramaprian, “Convection in modulated thermal gradients and gravity: experimental measurements and numerical simulations,” *International Journal of Heat and Mass Transfer*, 48, 145-160, 2005.

*The authors are at Washington State University where Professor Li is the PI on the ground-based project “Study of magnetic field effects on convection and solidification in normal and microgravity.”*

This paper presents an investigation on natural convection in a cavity with imposed modulated thermal gradients or modulated gravity forces. Numerical computations are presented, which are based on the finite element solution of the transient Navier–Stokes and energy balance equations, along with appropriate thermal boundary conditions or time-varying gravity forces. In parallel with numerical development, an experimental system is setup where oscillating wall temperatures are prescribed to produce modulated temperature gradients and the velocity fields are measured by a laser-based particle image velocimetry (PIV) system. Computed results compare well with experimental measurements for various conditions. With the mathematical model, so

verified by experimental measurements, numerical simulations are carried out to study the effects of modulation frequency and Prandtl number on the fluid flow. Results show strong non-linear interaction in a fluid with a relative high Prandtl number within the intermediate range of modulated frequency. It is also found that for a fluid with a small Prandtl number typical of molten metals and semiconductor melts, modulated gravity and thermal gradients produce almost the same flow field both in structure and in magnitude.

Kar, P., J. C. Lacombe, and **M. B. Koss**, "Velocity and radius transients during pressure mediated dendritic growth of succinonitrile," *Materials Science and Technology*, 20, 1273-1280, 2004.

This study was part of a larger effort called the transient dendritic solidification experiment (TDSE), which uses the well known Clapeyron effect to study transient effects in dendritic solidification. The transient behavior was studied between well defined steady states using pressure mediated changes since it is almost impossible to study the transient behavior during growth of a dendrite from initial to steady state. The time constants calculated for the velocity and radius transients are of the same order of magnitude. The velocity starts changing immediately after the pressure changes. The radius also changes rapidly but the change starts after an initial lag. This is attributed to its 'geometric memory' and the fact that the change in velocity results from a change in the thermal field ahead of the tip, whereas a change in radius also entails a change in the lateral thermal field. These results affirm that pressure changes affect the growth behavior and interfacial morphology of dendrites, which can be used for controlling solidification microstructure.

*Professor Koss is at College of the Holy Cross, and is the Principal Investigator on the flight experiment "Transient Dendritic Solidification Experiment (TDSE)." Mr. Kar is at UC Berkeley, and Dr. LaCombe is at University of Nevada.*

Hyers, R.W., R.C. Bradshaw, J.R. Rogers, T.J. Rathz, G.W. Lee, A.K. Gangopadhyay, and **K. F. Kelton**, "Surface Tension and Viscosity of Quasicrystal-forming TiZrNi Alloys", *Int. J. of Thermophysics*, 25, 1155-2004.

Recent X-ray scattering measurements show that icosahedral short-range order in Ti-Zr-Ni alloys is responsible for a change in phase selection from the stable C14 Laves phase to the quasicrystalline icosahedral phase, and that icosahedral short-range order increases at deeper undercoolings. This change in short-range order should be reflected in changes in the thermophysical properties of the melt. The surface tension and viscosity of quasicrystal-forming Ti-Zr-Ni alloys were measured over a range of temperature, including both stable and undercooled liquids by an electrostatic levitation (ESL) technique. ESL is a containerless technique which allows processing of samples without contact, greatly reducing contamination and increasing access to the metastable undercooled liquid. The measured viscosity is typical of glass-forming alloys of similar composition to the quasicrystal-forming alloys studied here; however, the surface tension shows an anomaly at deep undercoolings.

*Professor Kelton, the PI on the flight project “Studies of Nucleation and Growth, Specific Heat and Viscosity of Undercooled Melts of Quasicrystals and Polytetrahedral-Phase-Forming Alloys,” is at Washington University, St. Louis, as are Dr. Gangopadhyay and Dr. Lee. Dr. Rogers and Mr. Rathz are at MSFC, while Dr. Hyers and Dr. Bradshaw are at University of Massachusetts.*

Coimbra, C. F. M., D. L’Esperance, R. A. Lambert, **J. D. Trolinger**, and R. H. Rangel, “An experimental study on stationary history effects in high-frequency Stokes flows,” *Journal of Fluid Mechanics*, 504, 353-363, 2004.

We report results of a series of detailed experiments designed to unveil the dynamics of a particle of radius  $a$  moving in high-frequency, low-Reynolds-number oscillatory flow. The fundamental parameters in the problem are the Strouhal ( $Sl$ ) and the particle Reynolds numbers ( $Re_p$ ), as well as the fluid-to-particle density ratio  $\alpha$ . The experiments were designed to cover a range of  $SlRe_p$  from 0.015 to 5 while keeping  $Re_p < 0.5$  and  $Sl > 1$ . The primary objective of the experiments is to investigate stationary history effects associated with the Basset drag, which are maximized when the viscous time scale  $\alpha^2/\nu$  is of the same order of the flow time scale  $9/\Omega$ , where  $9$  is a geometrical factor for the sphere,  $\nu$  is the kinematic viscosity and  $\Omega$  is the angular frequency of the background flow. The theoretically determined behaviour of stationary history effects is confirmed unequivocally by the experiments, which also validate the fractional derivative behaviour (of order  $1/2$ ) of the history drag for the range of parameters under study.

*L’Esperance and Trolinger are with Metrolaser Incorporated, where Dr. Trolinger is the Principal Investigator on the flight experiment “Spaceflight Holography Investigation in a Virtual Apparatus.” Professor Coimbra is at University of Hawaii-Manoa, and Professor Rangel is at University of California, Irvine.*

Wang, Jingbo and **Nicholas Zabar**, “Using Bayesian statistics in the estimation of heat source in radiation,” *International Journal of Heat and Mass Transfer*, 48, 15-29, 2005.

An unknown transient heat source in a three-dimensional participating medium is reconstructed from temperature measurements using a Bayesian inference method. The heat source is modeled as a stochastic process. The joint posterior probability density function (PPDF) of heat source values at consecutive time points is computed using the Bayes’ formula. The errors in thermocouple readings are modeled as independent identically distributed (i.i.d.) Gauss random variables. ‘Maximum A Posteriori’ (MAP) and posterior mean estimates of the heat source are then computed using a Markov chain Monte Carlo (MCMC) simulation method. The designed MCMC sampler is composed of a cycle of symmetric MCMC kernels. To increase the sampling speed, a model-reduction technique is used in the direct computation of temperatures at thermocouple locations given a guessed heat source, i.e. in the likelihood computation. Two typical heat source profiles are reconstructed using simulated data to demonstrate the presented methodologies. The results indicate that the Bayesian inference method can provide accurate point estimates as well as uncertainty quantification to the solution of the inverse radiation problem.

*The authors are with Cornell University where Professor Zabarav is PI on the ground-based project "On the control of the effects of gravity on the solidification microstructures using optimally designed thermal boundary fluxes and electromagnetic fields."*

Wang, Xianghong, and **Nancy Ma**, "Strong Magnetic Field Asymptotic Model for Binary Alloyed Semiconductor Crystal Growth," *Journal of Thermophysics and Heat Transfer*, 18, 476-480, 2004.

This paper presents an asymptotic model for the unsteady species transport during bulk growth of alloyed semiconductor crystals with a transverse magnetic field. During growth of alloyed semiconductors such as germanium-silicon (GeSi), the solute's concentration is not small, so that density differences in the melt are very large. These compositional variations drive compositionally driven buoyant convection, in addition to thermally driven buoyant convection. These buoyant convections drive convective transport, which produces nonuniformities in the concentration in both the melt and the crystal. This transient model predicts the melt motion and the distribution of species for a crystal grown in a strong transverse magnetic field.

*The authors are at North Carolina State University where Professor Ma is the Principal Investigator on the ground-based project "Models of Mass Transport during Microgravity Crystal Growth of Alloyed Semiconductors in a Magnetic Field."*

Tangeman, Jean A., Brian L. Phillips, Paul C. Nordine, and **J. K. Richard Weber**, "Thermodynamics and Structure of Single- and Two-Phase Yttria-Alumina Glasses," *Journal of Physical Chemistry B*, 108, 10663-10671, 2004.

Yttria-alumina (YA) glasses containing 59.8-75.6 mol %  $\text{Al}_2\text{O}_3$  were synthesized in the form of 1-3.5mm diameter spheroids using containerless techniques. The glasses formed at cooling rates ranging from <70 K/s at compositions near 72 mol %  $\text{Al}_2\text{O}_3$  and up to 300 K/s at the ends of the composition range. Samples with compositions from 59.8 to ~69.0 mol %  $\text{Al}_2\text{O}_3$  contained two glass phases, with an immiscible droplet (~1-20 $\mu\text{m}$  diameter) phase in the matrix glass. A single glass phase was formed at greater alumina concentrations. Glasses near the alumina- and yttria-rich ends of the compositional suite also contained ~5-20% and 1-2% crystals, respectively. Heat capacities ( $C_p$ ) of the glasses and supercooled liquids, glass transition temperature ( $T_g$ ), configurational heat capacities at  $T_g$  ( $\Delta C_p(T_g)$ ), and glass structures were investigated using differential scanning calorimetry (DSC) and  $^{27}\text{Al}$  MAS NMR spectroscopy. The  $T_g$  increases slightly with alumina content from 1146 to 1156 K. The  $C_p$  increases ~60% at  $T_g$  to form a highly fragile supercooled liquid. The concentrations of 4-, 5-, and 6-coordinate  $\text{Al}^{3+}$  ions in a single phase glass with 71.5 mol %  $\text{Al}_2\text{O}_3$  (Y71.5A) are ~68%  $\pm 4$ , 27%  $\pm 3$ , and 6%  $\pm 2$ , respectively. A minimum 6- and maximum 5-coordinate  $\text{Al}^{3+}$  concentration occurs near the Y71.5A composition, which is one of the best glass formers. In the context of the structural and thermodynamic properties reported herein, the formation mechanism and coordination of polyamorphic YA glasses are discussed.

*Ms. Tangeman, Dr. Nordine and Dr. Weber are with Containerless Research, Inc, where Dr. Weber is the Principal Investigator on the ground-based project "Microgravity Studies of Liquid-Liquid Phase Transitions in Undercooled Alumina-Yttria Melts." Mr. Phillips is at State University of New York at Stony Brook.*

Kar, P., J. C. Lacombe, and **M. B. Koss**, "Velocity and radius transients during pressure mediated dendritic growth of succinonitrile," *Materials Science and Technology*, 20, 1273-1280, 2004.

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*Professor Koss is at College of the Holy Cross, and is the Principal Investigator on the flight experiment "Transient Dendritic Solidification Experiment (TDSE)." Mr. Kar is at UC Berkeley, and Dr. LaCombe is at University of Nevada.*

Coimbra, C. F. M., D. L'Esperance, R. A. Lambert, **J. D. Trolinger**, and R. H. Rangel, "An experimental study on stationary history effects in high-frequency Stokes flows," *Journal of Fluid Mechanics*, 504, 353-363, 2004.

We report results of a series of detailed experiments designed to unveil the dynamics of a particle of radius  $a$  moving in high-frequency, low-Reynolds-number oscillatory flow. The fundamental parameters in the problem are the Strouhal ( $Sl$ ) and the particle Reynolds numbers ( $Re_p$ ), as well as the fluid-to-particle density ratio  $\alpha$ . The experiments were designed to cover a range of  $SlRe_p$  from 0.015 to 5 while keeping  $Re_p < 0.5$  and  $Sl > 1$ . The primary objective of the experiments is to investigate stationary history effects associated with the Basset drag, which are maximized when the viscous time scale  $a^2/\nu$  is of the same order of the flow time scale  $9/\Omega$ , where  $9$  is a geometrical factor for the sphere,  $\nu$  is the kinematic viscosity and  $\Omega$  is the angular frequency of the background flow. The theoretically determined behaviour of stationary history effects is confirmed unequivocally by the experiments, which also validate the fractional derivative behaviour (of order  $1/2$ ) of the history drag for the range of parameters under study.

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Tangeman, Jean A., Brian L. Phillips, Paul C. Nordine, and **J. K. Richard Weber**, "Thermodynamics and Structure of Single- and Two-Phase Yttria-Alumina Glasses," *Journal of Physical Chemistry B*, 108, 10663-10671, 2004.

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*Ms. Tangeman, Dr. Nordine and Dr. Weber are with Containerless Research, Inc, where Dr. Weber is the Principal Investigator on the ground-based project "Microgravity Studies of Liquid-Liquid Phase Transitions in Undercooled Alumina-Yttria Melts." Mr. Phillips is at State University of New York at Stony Brook.*

Schroers, Jan, Sven Bossuyt, Won-Kyu Rhim, Jianzhong Li, Zhenhua Zhou, and **William L. Johnson**, "Enhanced temperature uniformity by tetrahedral laser heating," *Review of Scientific Instruments*, 75, 4523-4527, 2004.

Temperature profile on a spherical sample that is heated by laser beams in various geometries while processed in vacuum is analyzed. Sample heating by one or four laser beams was considered. An analytical expression was derived for directional sample heating cases. It suggests an enhanced temperature uniformity over the samples when heated with four diffuse laser beams arranged in a tetrahedral geometry. This was experimentally verified by heating a spherical stainless steel sample by laser beams. Both the calculated and experimentally determined temperature variations over the sample suggest that the use of diffuse four beams arranged in tetrahedral geometry would be effective in reducing temperature variation to within 1 K. The enhancement in the temperature uniformity for four diffuse beams arranged in tetrahedral geometry by a factor of 50 over a single focused beam is promising to accurately measure of thermophysical properties. This drastic improvement in temperature uniformity might even enable atomic diffusion measurements in the undercooled liquid states of the bulk glass forming alloys since Marangoni and gravity driven convection will be substantially reduced.

*Dr. Bossuyt is at Vrije Universiteit, Brussel. The other authors are at California Institute of Technology, where Professor Johnson is the Principal Investigator on the ground-based project "Thermodynamic and Transport Properties of Glass Forming Alloy Liquids Using the Caltech High Vacuum Electrostatic levitator Platform."*

Ramirez, J. C. and **C. Beckermann**, "Examination of binary alloy free dendritic growth theories with a phase-field model," *Acta Materialia*, 53, 1721-1736, 2005.

Two-dimensional phase-field simulations are used to test standard theories for free dendritic growth of alloys. While the transport of heat and solute in the melt is predicted well by the theories, the selection criterion for the operating state of the dendrite tip is found to break down in several respects. The selection parameter,  $\sigma^*$ , computed from the phase-field simulations varies strongly with alloy composition, Lewis number, and imposed undercooling, whereas the theories assume  $\sigma^*$  to be independent of these parameters. While the computed  $\sigma^*$  is the same for purely thermal and solutal dendrites, it experiences a minimum at a small but finite solute concentration where thermal and solutal effects are both important. A pronounced growth velocity maximum at this composition is therefore not found in the simulations. The high Péclet number corrections of the LKT theory are found to be ineffective for the present range of undercoolings.

*The authors are at The University of Iowa, where Professor Beckermann is the Principal Investigator on the ground-based project "Microstructure Evolution in Free Dendritic Growth."*

Giummarra, C. , J. C. LaCombe, M. B. Koss, J. E. Frei, A. O. Lupulescu and **M. E. Glicksman**, "Sidebranch characteristics of pivalic acid dendrites grown under convection-free and diffuso-convective conditions," *Journal of Crystal Growth*, 274, 317-330, 2005.

This work investigates the sidebranch characteristics of pivalic acid dendrites grown under convection-free (cf) and diffuso-convective (dc) conditions for supercoolings over the range of 0.1–1.0 K. Results indicate that the distance from the dendrite tip to the first detectable sidebranch and to the first detectable coarsening event normalized by the tip radius,  $\underline{R}$ , are independent of the supercooling. The sidebranch spacing in the uniform region near the dendrite tip, and the spacing in the coarsening region when normalized by  $\underline{R}$ , do not appear to have a significant dependence on convection or supercooling. When the envelope enclosing all sidebranches from the tip to the end of the coarsening region was fitted to a power law as a function of distance from the tip, we found that the pre-exponential and exponential terms were significantly different for the convection-free and diffuso-convective results. This supports the observation that the absence of convection seems to alter the size of the sidebranches. Lastly, the predictions from theoretical models of sidebranch spacings are much lower than experimental observations, while the predicted sidebranch amplitudes were larger than those observed.

*Professor Glicksmann, Principal Investigator for the Flight Project 'Isothermal Dendritic Growth Experiment,' is at Rensselaer Polytechnic Institute, as are Drs Guimmarra, Frei and Lupulescu. Dr. LaCombe is at University of Nevada, Reno, while Dr. Koss is at College of the Holy Cross.*

Khine, Y. Y. and **R. M. Banish**, "Electromagnetic damping of convective contamination in self-diffusivity experiments with periodic heating conditions," *Materials Science and Engineering A*, 393, 338-343, 2005.

Accurate mass diffusivity values are important in mass transfer processes. Diffusion experiments conducted on earth are typically convectively contaminated due to either thermal or solutal gradients. Liquid metals and semiconductors have high electrical conductivities, and applied magnetic fields may suppress buoyant convection in these liquids. In this paper, an axisymmetric self-diffusivity model is considered in the presence of a steady, strong, uniform axial magnetic field with liquid indium. An isopycnic (radioisotope) tracer is used so that only thermal differences drive the convection. Five different combinations of a steady, uniform heat flux and a steady, periodic heat flux are imposed along the vertical wall while uniform heat loss is allowed through the top and bottom walls of the cylinder. The addition of periodic heat flux with the reduced uniform heat flux has a positive impact on the output diffusivity results for the same applied magnetic field of 5.24 T.

The authors are at University of Alabama in Huntsville, where Dr. Banish is the Principal Investigator on the ground-based project "Temperature and Composition Dependence of Mass and Thermal Diffusion in Liquid Metals and Compound Semiconductor Alloys."

Shen, Junwu, Lou Campbell, Pavin Suri, and **Randall M. German**, "Quantitative microstructure analysis of tungsten heavy alloys (W-Ni-Cu) during initial stage liquid phase sintering," *International Journal of Refractory Metals & Hard Materials*, 23, 99-108, 2005.

Microstructure analysis plays an important role in studying liquid phase sintering process. In the current study, quantitative microstructure analysis was performed on tungsten heavy alloys with different Ni:Cu ratios using an advanced image analysis system. The measured microstructural parameters include grain size, neck size, pore size, porosity, connectivity, contiguity, neck size ratio, mean curvature and more importantly, their statistical distributions. Various statistical distribution functions were used to fit the measured data, and the model parameters were obtained. The effect of alloy composition and the corresponding effective sintering time on microstructure was discussed. The analysis results are important for studying the fundamental mechanisms of sintering, modeling and predicting liquid phase sintering process.

*Messrs. Shen and Campbell are The Pennsylvania State University where Professor German is the Principal Investigator on the Flight Project "Gravitational Effects on Distortion in Sintering." Dr. Suri is with Matsushita Electric Works, Osaka, Japan.*

Kershner, Ryan J., Joseph W. Bullard, and **Michael J. Cima**, "The role of electrochemical reactions during electrophoretic particle deposition," *Journal of Colloid and Interface Science*, 278, 146-154, 2004.

*The authors are at Massachusetts Institute of Technology, where Professor Cima is the Principal Investigator on the ground-based project “Forces during Manufacture and Assembly of Microscale Discrete Electronic Components.”*

Platinum microelectrodes were fabricated on a sapphire substrate by lithographic patterning and used to manipulate 1.58  $\mu\text{m}$  silica particles in the plane of the substrate. A digital video system captured the motion of particles far from the electrodes and their deposition onto the working electrode during application of a DC potential. The role of electrode reversibility was investigated by comparing as-deposited electrodes with electrodes modified by electrolytic plating of platinum. Particles were also observed adhering to the substrate before reaching the electrode. The  $\zeta$ -potential of the particles and substrate was measured. The differing surface chemistry of the two systems and a local reduction in pH due to the production of hydrogen ion at the anode can explain the adhesion phenomena. Force distance curves were recorded using a colloid probe atomic force microscopy technique to directly measure the interaction of the silica particles with the sapphire substrate. These data validated the observed adhesion at the electrode and provided further support for the temporal and spatial reduction in pH. The role of Faradaic processes and the diffusion of potential determining ions in electrophoretic deposition were also considered.

Farrell, Martin V., and **Nancy Ma**, “Macrosegregation during alloyed semiconductor crystal growth in strong axial and transverse magnetic fields,” *International Journal of Heat and Mass Transfer*, 47, 3047-3055, 2004.

*The authors are at North Carolina State University where Professor Ma is the Principal Investigator on the ground-based project “Models of Mass Transport during Microgravity Crystal Growth of Alloyed Semiconductors in a Magnetic Field.”*

This paper presents a model for the unsteady species transport during bulk growth of alloyed semiconductor crystals with both axial and transverse magnetic fields. During growth of alloyed semiconductors such as germanium–silicon (GeSi) and mercury–cadmium–telluride (HgCdTe), the solute's concentration is not small so that density differences in the melt are very large. These compositional variations drive compositionally-driven buoyant convection, or solutal convection, in addition to thermally-driven buoyant convection. These buoyant convections drive convective transport which produce non-uniformities in the concentration in both the melt and the crystal. This transient model predicts the distribution of species in the entire crystal grown in a magnetic field. The present study investigates the effects of magnetic field orientation and strength on the segregation in alloyed semiconductor crystals, and presents results of concentration in the crystal and in the melt at several different times during crystal growth.

L<sup>3</sup>Espérance D. , C. F. M. Coimbra, **J. D. Trolinger** and R. H. Rangel, “Experimental verification of fractional history effects on the viscous

dynamics of small spherical particles,” *Experiments in Fluids*, 38, on-line, 2004.

*L’Esperance and Trolinger are with MetroLaser Incorporated, where Dr. Trolinger is the Principal Investigator on the flight experiment “Spaceflight Holography Investigation in a Virtual Apparatus.” Professor Coimbra is at University of Hawaii-Manoa, and Professor Rangel is at University of California, Irvine.*

We investigate the low Reynolds, high-frequency particle response of non-neutrally buoyant particles suspended in a fluid. Gravity effects are suppressed by means of a very thin tether, whose effect on the horizontal movement of the particle is negligible due to the small amplitude, high-frequency nature of the forcing. The measured stationary responses of particles of different densities closely match the theoretical predictions for the full solution, including Basset history effects for both the amplitude ratio and the phase, and clearly differ from the solution where the history force is neglected.

Narayanan, Velamur Asokan Badri, and **Nicholas Zabaras**, “Stochastic inverse heat conduction using a spectral approach,” *International Journal for Numerical Methods in Engineering*, 60, 1569-1593, 2004.

*The authors are with Cornell University where Professor Zabaras is PI on the ground-based project “On the control of the effects of gravity on the solidification microstructures using optimally designed thermal boundary fluxes and electromagnetic fields.”*

An adjoint-based functional optimization technique in conjunction with the spectral stochastic finite element method is proposed for the solution of an inverse heat conduction problem in the presence of uncertainties in material data, process conditions and measurement noise. The ill-posed stochastic inverse problem is restated as a conditionally well-posed  $L_2$  optimization problem. The gradient of the objective function is obtained in a distributional sense by defining an appropriate stochastic adjoint field. The  $L_2$  optimization problem is solved using a conjugate-gradient approach. Accuracy and effectiveness of the proposed approach is appraised with the solution of several stochastic inverse heat conduction problems.

Kershner, R., J. W. Bullard, and **M. J. Cima**, "Zeta Potential Orientation Dependence of Sapphire Substrates" *Langmuir*, 20, 4101-4108, 2004.

*The authors are from the Massachusetts Institute of Technology, where Professor Cima is the Principal Investigator of the ground-based project “Forces during Manufacture and Assembly of Microscale Discrete Electronic Components.”*

The zeta potential of planar sapphire substrates for three different crystallographic orientations was measured by a streaming potential technique in the presence of KCl and  $(\text{CH}_3)_4\text{NCl}$  electrolytes. The streaming potential was measured for large single

crystalline C-plane (0001), A-plane (11-20), and R-plane (1-102) wafers over a full pH range at three or more ionic strengths ranging from 1 to 100 mM. The roughness of the epi-polished wafers was verified using atomic force microscopy to be on the order of atomic scale, and X-ray photoelectron spectroscopy (XPS) was used to ensure that the samples were free of silica and other contaminants. The results reveal a shift in the isoelectronic point (iep) of the three samples by as much as two pH units, with the R-plane surface exhibiting the most acidic behavior and the C-plane samples having the highest iep. The iep at all ionic strengths was tightly centered around a single pH for each wafer. These values of iep are substantially different from the range of pH 8-10 consistently reported in the literature for  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> particles. Particle zeta potential measurements were performed on a model powder using phase analysis light scattering, and the iep was confirmed to occur at pH 8. Modified Auger parameters (MAP) were calculated from XPS spectra of a monolayer of iridium metal deposited on the sapphire by electron beam deposition. A shift in MAP consistent with the observed differences in iep of the surfaces confirms the effect of surface structure on the transfer of charge between the Ir and sapphire, hence accounting for the changes in acidity as a function of crystallographic orientation.

Kim, Jung-Whan, Hojin Kim, Myoungbae Lee, and **Jules J. Magda**, "Interfacial Tensions of a Nematic Liquid Crystal/Water Interface with Homeotropic Surface Alignment," *Langmuir*, 20, 8110-8113, 2004.

*The authors are from the University of Utah, where Professor Magda is the Principal Investigator on the project, "Novel Microstructures for Polymer-Liquid Crystal Composite Materials."*

Pendant drop experimental results are presented for the temperature dependence of the interfacial tension between water and the immiscible nematic liquid crystal 4'-pentyl-4-biphenylcarbonitrile (5CB) in the presence of the absorbed surfactant cetyltrimethylammonium bromide (CTAB). Absorption of the surfactant lowers the interfacial tension value and is also known from earlier work to induce a transition in liquid crystal surface alignment from planar to homeotropic [Brake et al. *Langmuir* **2003**, 19, 6436.]. Discrepancies exist in the literature regarding the density of 5CB, and the density difference between 5CB and water in any case is very small. However, from the ability to form pendant 5CB drops, one may infer that the density of 5CB exceeds that of water over the entire temperature range studied (28-41°C), in disagreement with the predictions of one earlier report on 5CB. The interfacial tension is shown to exhibit a relative maximum near the bulk 5CB nematic-isotropic transition temperature  $T_{NI}$ , regardless of which published data set of 5CB density values is used to analyze the measurements, with a possible discontinuity in tension occurring at  $T_{NI}$ . The anomalous shape of the interfacial tension curve, depending on the choice of the 5CB density data set, may be quite similar to that recently reported for the interfacial tension between 5CB and a hydrophobic, isotropic molten polymer (Rai et al. *Langmuir* **2003**, 19, 7370).

Bossuyt, Sven, Jan Schroers, Won-Kyu Rhim, and **William L. Johnson**, "Minimizing convection effects in liquid droplets during high-temperature electrostatic levitation," *Review of Scientific Instruments*, 76, 033909 (9 pages), 2005.

*Dr. Bossuyt is at Vrije Universiteit, Brussel. The other authors are at California Institute of Technology, where Professor Johnson is the Principal Investigator on the ground-based project "Thermodynamic and Transport Properties of Glass Forming Alloy Liquids Using the Caltech High Vacuum Electrostatic levitator Platform."*

We present an approach to reduce the convective flow in an electrostatically levitated liquid droplet to such an extent that diffusion is the dominant mechanism for mass transport, thus enabling direct measurements of atomic diffusion in reactive liquids at elevated temperatures. Convection is minimized by containerless processing, and reducing temperature variations in the sample. The diffusion tracer is deposited in situ in the electrostatic levitation device used for containerless processing. Uniform noncontact heating of the sample is achieved by laser heating with multiple beams arranged symmetrically, e.g., in a tetrahedral geometry. The expected temperature variations and the resulting convection flows are estimated for a Zr-based glass-forming alloy. The analysis suggests that diffusion experiments are possible throughout the entire undercooled liquid temperature range of this alloy and, in microgravity, up to 50 K above the liquidus temperature.

Boettinger, W. J., G. B. McFadden, S.R. Coriell, **R.F. Sekerka** and J.A. Warren, "Lateral deformation of diffusion couples," *Acta Materialia*, 53, 1996-2008, 2005.

*Professor Sekerka is at Carnegie Mellon University and is Principal Investigator on the ground-based project "Lattice Boltzmann Computations of Binary Diffusion under Stochastic Microgravity." The other authors are at National Institute of Standards and Technology.*

A model is used to describe the shape change of a binary diffusion couple when the diffusivities of the two species differ. The classical uniaxial Kirkendall shift is obtained only if the displacement is constrained to be in the diffusion direction. For traction-free conditions at the external surfaces of a diffusion couple, a more general displacement field is obtained that accounts for the lateral shape change data of Voigt and Ruth [Journal of Physics-Condensed Matter 7 (1995) 2655-2666]. The model employs an isotropic stress-free strain rate and equal and constant partial molar volumes. In this case the displacement field is shown to be independent of the various elastic/plastic moduli. Depending on the lateral dimension of the diffusion couple, the displacement in the diffusion direction can be reduced by up to a factor of three compared to the case of a pure uniaxial displacement.

Hyers, Robert W., "Fluid flow effects in levitated drops," *Measurement Science and Technology*, 16, 394-401, 2005.

*Dr. Hyers is at University of Massachusetts. The work was done under the auspices of Professor Kelton, the PI on the flight project "Studies of Nucleation and Growth, Specific Heat and Viscosity of Undercooled Melts of Quasicrystals and Polytetrahedral-Phase-Forming Alloys," at Washington University, St. Louis*

Levitation techniques have been applied to a staggering range of materials, from liquid helium to aqueous solutions of proteins, to metals, ceramics, glasses and semiconductors. These experiments have encompassed temperatures from cryogenic to greater than 2500 °C, and samples from micrograms to tens of kilograms. It should come as no surprise that a wide variety of levitation principles have been employed for processing these samples, including electromagnetic (EML), electrostatic (ESL), aerodynamic and gas film, acoustic and dia- or paramagnetic levitation, as well as combinations of these and others. All of these containerless techniques share one key feature: internal flow in liquid samples. The flow may be driven directly by the positioning force, as in EML and aerodynamic levitation, or by temperature gradients through Marangoni convection and/or natural buoyancy, as in ESL. It is possible to reduce the positioning-driven and buoyancy flows by performing the experiments in microgravity; however, often even the reduced levels are important. For some experiments, such as viscosity measurements, only whether the flow is laminar or turbulent must be established. For other experiments, however, quantitative assessments of velocity, shear stress or shear strain rate are required. In most cases, it is difficult or impossible to measure the internal flow in levitated droplets directly. The samples are usually small, and often opaque, reactive, high-temperature, metastable, or all of the above. Furthermore, recirculating flow limits the utility of tracking surface particles, since they tend to collect in stagnation points rather than following the flow. Most research groups have chosen mathematical modelling to assess the internal flow in levitated droplets. Several different classes of experiments are examined in terms of the effect of fluid flow and the impact of flow modelling. This paper focuses on EML and ESL, although the techniques and many of the results are applicable to other levitation methods.

Mukherjee, S., Z. Zhou, J. Schroers, W. L. Johnson, and W. K. Rhim, “Overheating threshold and its effect on time–temperature–transformation diagrams of zirconium based bulk metallic glasses,” *Applied Physics Letters*, 84, 5010-5012, 2004.

*The authors are at California Institute of Technology, where Professor Johnson is the Principal Investigator on the ground-based project “Thermodynamic and Transport Properties of Glass Forming Alloy Liquids Using the Caltech High Vacuum Electrostatic levitator Platform.”*

A pronounced effect of overheating is observed on the crystallization behavior for the three zirconium-based bulk metallic glasses:  $Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$ ,  $Zr_{57}Cu_{15.4}Ni_{12.6}Al_{10}Nb_5$ , and  $Zr_{52.5}Cu_{17.9}Ni_{14.6}Al_{10}Ti_5$ . A threshold overheating temperature is found for each of the three alloys, above which there is a drastic increase in the undercooling level and the crystallization times. Time–temperature–transformation (TTT) diagrams were measured for the three alloys by overheating above their respective threshold temperatures. The TTT curves for  $Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$  and  $Zr_{57}Cu_{15.4}Ni_{12.6}Al_{10}Nb_5$  are very similar in shape and scale with their respective glass transition temperatures, suggesting that system-specific properties do not play a crucial role in defining crystallization kinetics in these alloys. The critical cooling rates to vitrify the alloys as determined from the TTT curves are about 2 K/s for  $Zr_{41.2}Ti_{13.8}Cu_{12.5}Ni_{10}Be_{22.5}$  and 10 K/s for  $Zr_{57}Cu_{15.4}Ni_{12.6}Al_{10}Nb_5$ . The measurements were conducted in a high-vacuum electrostatic levitator.

Sonda, Paul, Andrew Yeckel, Prodromos, and **Jeffrey J. Derby**, “Hopf bifurcation and solution multiplicity in a model for destabilized Bridgman crystal growth,” *Chemical Engineering Science*, 60, 1323-1336, 2005.



*The authors are University of Minnesota, where Professor Derby is the PI on the ground based project “Theoretical Analysis of 3D, Transient Convection and Segregation in Microgravity Bridgman Crystal Growth.”*

Flow instabilities are analyzed within a destabilized vertical Bridgman crystal growth system, first studied experimentally by Kim et al. (J. Electrochem. Soc. 119(1972) 1218), using a distributed-parameter model consisting of balance equations for energy and momentum transport. Numerical solution of the governing equations via a Galerkin finite element method reveals multiple operating states and dynamic phenomena. Bifurcation analysis shows that the onset of time-periodic flows occurs in the model system via a supercritical Hopf bifurcation, consistent with prior experimental observations on the dynamics of flow in similar systems.

Echebarria, Blas, Roger Folch, **Alain Karma**, and Mathis Plapp, “Quantitative phase-field model of alloy solidification,” *Physical Review E*, 70, 61604 (22 pages), 2005.

*Dr. Echebarria and Professor Karma, the Principal Investigator on the ground-based project “Phase-field simulations of Dendritic Growth at Low Undercooling: Confronting Theory and Experiment,” are from Northeastern University. Dr. Folch is from Universiteit Leiden, The Netherlands, while Dr. Plapp is from CNRS/Ecole Polytechnique, France.*

We present a detailed derivation and thin interface analysis of a phase-field model that can accurately simulate microstructural pattern formation for low-speed directional solidification of a dilute binary alloy. This advance with respect to previous phase-field models is achieved by the addition of a phenomenological “antitrapping” solute current in the mass conservation relation [A. Karma, Phys. Rev. Lett. **87**, 115701 (2001)]. This antitrapping current counterbalances the physical, albeit artificially large, solute trapping effect generated when a mesoscopic interface thickness is used to simulate the interface evolution on experimental length and time scales. Furthermore, it provides additional freedom in the model to suppress other spurious effects that scale with this thickness when the diffusivity is unequal in solid and liquid [R. F. Almgren, SIAM J. Appl. Math. **59**, 2086 (1999)], which include surface diffusion and a curvature correction to the Stefan condition. This freedom can also be exploited to make the kinetic undercooling of the interface arbitrarily small even for mesoscopic values of both the interface thickness and the phase-field relaxation time, as for the solidification of pure melts [A. Karma and W.-J. Rappel, Phys. Rev. E **53**, R3017 (1996)]. The performance of the model is demonstrated by calculating accurately within a phase-field approach the Mullins-Sekerka stability spectrum of a planar interface and nonlinear cellular shapes for realistic alloy parameters and growth conditions.

Steinbach, I., H.-J. Diepers, and **C. Beckermann**, “Transient growth and interaction of equiaxed dendrites,” *Journal of Crystal Growth*, 275, 624-638, 2005.

*Professor Beckermann, the Principal Investigator for the NRA project “Equiaxed Dendritic Growth Experiment,” is at The University of Iowa. Drs Steinbach and Diepers are at ACCESS, Aachen Germany. This project, originally selected for flight and having passed the Science Concept Review was subsequently transitioned to ground.*

An improved version of a previously developed mesoscopic model is used to simulate transients and thermal interactions during growth of equiaxed dendrites of a pure substance. The model is validated through comparisons with exact, analytical solutions and direct, fully resolved phase-field simulations. The issue of constancy in the selection parameter,  $\sigma^*$ , during transients is addressed in some detail. The model is first applied to realistically simulate previously performed microgravity experiments involving the growth of succinonitrile dendrites from a stinger inside a growth chamber. It is shown how the thermal interactions between the seed and the dendrite and between the growth chamber wall and the dendrite cause temporal variations in the dendrite tip velocities. Excellent agreement with microgravity measurements is obtained. A scaling relation is derived that provides the duration of the seed size effect during the initial transient. The model is also used to investigate the transients arising during the growth of two equiaxed dendrites towards each other. A scaling relation for the duration of the transient decay of the tip velocities is derived. Additional study is needed to fully understand cases where equiaxed grains interact early before a fully dendritic structure is established.

Tucker, Dennis S., **Edwin C. Ethridge**, Guy A. Smith, and Gary Workman, "Effects of Gravity on ZBLAN Glass Crystallization," *Annals of the New York Academy of Science*, 1027, 129-137, 2004.

*Drs Tucker and Ethridge are at Marshall Space Flight Center, while Drs Smith and Workman are at University of Alabama in Huntsville. Dr. Ethridge is the Principal Investigator on the NRA project "Mechanisms for the Crystallization of ZBLAN."*

The effects of gravity on the crystallization of  $ZrF_4$ - $BaF_2$ - $LaF_3$ - $AlF_3$ - $NaF$  glasses have been studied using the NASA KC-135 and a sounding rocket. Fibers and cylinders of ZBLAN glass were heated to the crystallization temperature in unit and reduced gravity. When processed in unit gravity the glass crystallized, but when processed in reduced gravity, crystallization was suppressed. A possible explanation involving shear thinning is presented to explain these results.

Matson, Douglas M., David J. Fair, Robert W. Hyers, and Jan R. Rogers, "Contrasting Electrostatic and Electromagnetic Levitation Experimental Results for Transformation Kinetics of Steel Alloys," *Annals of the New York Academy of Science*, 1027, 435-446, 2004.

*Dr. Matson and Mr. Fair are at Tufts University, Dr. Hyers is at University of Massachusetts, while Dr. Rogers is at Marshall Space Flight Center. Dr. Matson is the Co-Investigator on the project of **Professor Flemings** of Massachusetts Institute of Technology. This NRA project, "The role of convection and growth competition in phase selection in microgravity," has passed its Science Concept Review and has just been transitioned from flight to ground status.*

The delay between conversion of metastable ferrite to stable austenite during ternary Fe-Cr-Ni alloy double recalescence is seen to differ by over an order of magnitude for tests conducted using electrostatic and electromagnetic levitation. Several possible

reasons for this deviation are proposed. Thermodynamic calculations on evaporation rates indicate that potential composition shifts during testing are minimized by limiting test time and thermal history. Simulation indicates that deviation would be limited to a factor of 1.5 under worst-case conditions. Possible effects due to differences in sample size are also eliminated since the metastable array, where stable phase nucleation must occur, is significantly smaller than the sample. Differences in internal convection are seen to be the most probable reason for the observed deviation.

**Sadhal, S. S.**, A. Rednikov, and K. Ohsaka, "Shape Relaxation of Liquid Drops in a Microgravity Environment," *Annals of the New York Academy of Science*, 1027, 447-463, 2004.

*The authors are at University of Southern California, where Professor Sadhal is the Principal Investigator on the NRA project "Non-intrusive Measurement of Thermophysical Properties of Liquids by Electrostatic-Acoustic Hybrid Levitation."*

We investigated shape relaxation of liquid drops in a microgravity environment that was created by letting the drops fall freely. The drops were initially levitated in air by an acoustic/electrostatic hybrid levitator. The levitated drops were deformed due to the force balance among the levitating force, surface tension, and gravity. During the free fall, the deformed drops underwent shape relaxation driven by the surface tension to restore a spherical shape. The progress of the shape relaxation was characterized by measuring the aspect ratio as a function of time, and was compared to a simple linear relaxation model (in which only the fundamental mode was considered) for perfectly conductive drops. The results show that the model quite adequately describes the shape relaxation of uncharged/charged drops released from an acoustically levitated state. However, the model is less successful in describing the relaxation of drops that were levitated electrostatically before the free fall. This may be due to finite electrical conductivities of liquids, which somehow affects the initial stage of the shape relaxation process.

Hyers, Robert W., Douglas M. Matson, **Kenneth R. Kelton**, and Jan R. Rogers, "Convection in Containerless Processing," *Annals of the New York Academy of Science*, 1027, 474-494, 2004.

*Dr. Hyers is at University of Massachusetts, Dr. Matson is at Tufts University, Professor Kelton is at Washington University, St. Louis while Dr. Rogers is at Marshall Space Flight Center. Professor Kelton is the Principal Investigator on the NRA project "Studies of Nucleation and Growth, Specific Heat and Viscosity of Undercooled Melts of Quasicrystals and Polytetrahedral-Phase-Forming Alloys." This project, which has passed its Science Concept Review has recently been transitioned from flight to ground status, having passed its Science Concept Review.*

Different containerless processing techniques have different strengths and weaknesses. Applying more than one technique allows various parts of a problem to be solved separately. For two research projects, one on phase selection in steels and the other on nucleation and growth of quasicrystals, a combination of experiments using electrostatic levitation (ESL) and electromagnetic levitation (EML) is appropriate. In both experiments, convection is an important variable. The convective conditions achievable

with each method are compared for two very different materials: a low-viscosity, high-temperature stainless steel, and a high-viscosity, low-temperature quasicrystal-forming alloy. It is clear that the techniques are complementary when convection is a parameter to be explored in the experiments. For a number of reasons, including the sample size, temperature, and reactivity, direct measurement of the convective velocity is not feasible. Therefore, we must rely on computation techniques to estimate convection in these experiments. These models are an essential part of almost any microgravity investigation. The methods employed and results obtained for the projects levitation observation of dendrite evolution in steel ternary alloy rapid solidification (LODESTARS) and quasicrystalline undercooled alloys for space investigation (QUASI) are explained.

Kang, Namhyun, **Jogender Singh**, and Anil K. Kulkarni, "Gravitational Effects on the Weld Pool Shape and Microstructural Evolution During Gas Tungsten Arc and Laser Beam Welding of 304 Stainless Steel and Al-4 wt% Cu Alloy," *Annals of the New York Academy of Science*, 1027, 529-549, 2004.

*The authors are at Pennsylvania State University where Professor Singh is the Principal Investigator on the NRA project "Gravitational Effect on the Development of Laser Weld-Pool and Solidification Microstructure."*

Effects of gravitational acceleration were investigated on the weld pool shape and microstructural evolution for 304 stainless steel and Al-4wt% Cu alloy. Effects of welding heat source were investigated by using laser beam welding (LBW) and gas tungsten arc welding (GTAW). As the gravitational level was increased from low gravity (LG  $\sim 1.2 g$ ) to high gravity (HG  $\sim 1.8 g$ ) using a NASA KC-135 aircraft, the weld pool shape for 304 stainless steel was influenced considerably during GTAW. However, insignificant change in the microstructure and solute distribution was observed at gravitational levels between LG and HG. The GTAW on Al-4 wt% Cu alloy was used to investigate the effect of gravitational orientation on the weld solidification behavior. Gravitational orientation was manipulated by varying the welding direction with respect to gravity vector; that is, by welding upward opposing gravity ( $\uparrow$ -U) and downward with gravity ( $\downarrow$ -D) on a vertical weld piece and welding perpendicular to gravity ( $\perp$ ) on a horizontal weld piece. Under the same welding conditions, a larger primary dendrite spacing in the  $\uparrow$ -U weld was observed near the weld pool surface and the fusion boundary than in the case of  $\perp$  or  $\downarrow$ -D welds. The  $\downarrow$ -D weld exhibited different solidification morphology and abnormal S shape of solidification rate curve during its growth. For 304 stainless steel GTAW, significant effects of gravitational orientation were observed on the weld pool shape that was associated with weld surface morphology and convection flow. However, the weld pool shape for LBW was mostly constant with respect to the gravitational orientation.

**Trolinger, James D.**, Drew L'Esperance, Roger H. Rangel, Carlos F. M. Coimbra, and William K. Witherow, "Design and Preparation of a Particle Dynamics Space Flight Experiment, SHIVA," *Annals of the New York Academy of Science*, 1027, 550-566, 2004.

*This work pertains to the NRA project "Spaceflight Holography Investigation in a Virtual Apparatus (SHIVA)," which has passed its Science Concept Review and has just been transitioned from flight to ground status. Dr. Trolinger, the Principal Investigator is at*

*MetroLaser Incorporated, as is Dr. L'Esperance. Dr. Rangel is at University of California at Irvine, Dr. Coimbra at University of Hawaii, while Mr. Witherow is at Marshall Space Flight Center.*

This paper describes the flight experiment, supporting ground science, and the design rationale for a project on spaceflight holography investigation in a virtual apparatus (SHIVA). SHIVA is a fundamental study of particle dynamics in fluids in microgravity. Gravitation effects and steady Stokes drag often dominate the equations of motion of a particle in a fluid and consequently microgravity provides an ideal environment in which to study the other forces, such as the pressure and viscous drag and especially the Basset history force. We have developed diagnostic recording methods using holography to save all of the particle field optical characteristics, essentially allowing the experiment to be transferred from space back to Earth in what we call the "virtual apparatus" for microgravity experiments on Earth. We can quantify precisely the three-dimensional motion of sets of particles, allowing us to test and apply new analytic solutions developed by members of the team. In addition to employing microgravity to augment the fundamental study of these forces, the resulting data will allow us to quantify and understand the ISS environment with great accuracy. This paper shows how we used both experiment and theory to identify and resolve critical issues and to produce an optimal experimental design that exploits microgravity for the study. We examined the response of particles of specific gravity from 0.1 to 20, with radii from 0.2 to 2 mm, to fluid oscillation at frequencies up to 80 Hz with amplitudes up to 200 microns. To observe some of the interesting effects predicted by the new solutions requires the precise location of the position of a particle in three dimensions. To this end we have developed digital holography algorithms that enable particle position location to a small fraction of a pixel in a CCD array. The spaceflight system will record holograms both on film and electronically. The electronic holograms can be downlinked providing real-time data, essentially acting like a remote window into the ISS experimental chamber. Ground experiments have provided input to a flight system design that can meet the requirements for a successful experiment on ISS. Moreover the ground experiments have provided a definitive, quantitative observation of the Basset history force over a wide range of conditions. Results of the ground experiments, the flight experiment design, preliminary flight hardware design, and data analysis procedures are reported.

**Weber, Richard**, "Control of Liquid Properties and Structure *via* Melt Chemistry," *Ceramic Transactions*, 170, 21-30, 2005.

*Dr. Weber, the Principal Investigator on the ground-based project, "Microgravity Studies of Liquid-Liquid Phase Transitions in Undercooled Alumina-Yttria Melt," is with Containerless Research, Inc.*

The properties and structures of molten oxides can be strongly influenced by small changes in both cation and anion chemistry. The application of containerless techniques allows precise control of ambient oxygen pressure in equilibrium with a high temperature melt and avoids secondary contamination by crucible materials. Elimination of container-driven nucleation of crystals can access deeply undercooled, metastable liquids to provide a glimpse of the region between the ordered crystal and disordered liquid states. It is in the metastable region that there are opportunities to synthesize and study new materials. This paper briefly reviews results of studies of the effect of ambient oxygen pressure and melt composition on the properties and structure of liquid oxides and oxide glasses. The theme of controlling liquid structure through melt chemistry to obtain new glasses, influence liquid phase transitions, and to develop optical materials is illustrated with examples.

**Kelton, K. F.**, “Coupled Processes in Nucleation,” *Ceramic Transactions*, 170, 147-162, 2005.

*Professor Kelton, is from is at Washington University, St. Louis. He is the PI on the project “Studies of Nucleation and Growth, Specific Heat and Viscosity of Undercooled Melts of Quasicrystals and Polytetrahedral-Phase-Forming Alloys, ”which has recently been transitioned from flight to ground status, having passed its Science Concept Review.*

Coupled phase transitions are common, with amorphous phase separation preceding crystallization, for example. The coupling can be more complicated than this, however, such as when long-range diffusion becomes competitive with the interfacial attachment processes underlying nucleation in the classical theory, or when fluctuations in one order parameter catalyze the fluctuations underlying nucleation during glass crystallization. Three case studies are used for illustration, (i) phase separation or nano-scale precipitation followed by glass devitrification, (ii) time-dependent nucleation when the initial and final phases have a different composition, and (iii) structural fluctuations that catalyze the nucleation of particular phases. While these examples are drawn from crystallization processes in metallic glasses or liquids, as well as silicate glasses, they demonstrate general nucleation features that are relevant to all nucleation-based first order phase transitions.

Fuss, Tihana, **Delbert E. Day**, Charles E. Lesher, and Chandra S. Ray, “Crystallization of a  $\text{Li}_2\text{O}\cdot 2\text{SiO}_2$  Glass under High Hydrostatic Pressures,” *Ceramic Transactions*, 170, 312-224, 2005.

*Dr. Fuss and Professor Day are University of Missouri-Rolla, Dr. Lesher is at University of California-Davis, while Dr. Ray is with Marshall Space Flight Center. Professor Day is the Principal Investigator on the project, “Kinetics of Nucleation and Crystal Growth in Glass Forming Melts in Microgravity,” which has just been transitioned for flight to ground status, having passed its Science Concept Review.*

The crystallization behavior of a  $\text{Li}_2\text{O}\cdot 2\text{SiO}_2$  (LS2) glass subjected to a uniform hydrostatic pressure of 4.5 or 6 GPa was investigated between 543 and 750°C using XRD, IR, Raman, TEM and DTA. The density of all the glasses (or glass-ceramics) subjected to high pressures was higher than that of the glass at ambient pressures (one atmosphere), and was  $2.43 \pm 0.01$  g/cm<sup>3</sup> for the 4.5 GPa glass and between  $2.52 \pm 0.01$  g/cm<sup>3</sup> and  $2.57 \pm 0.01$  g/cm<sup>3</sup>, depending upon processing temperature, for the 6 GPa glasses. The crystallization tendency for the glasses decreased (the crystal growth rate curve moved to higher temperatures) with increasing pressure. A decrease in the diffusion coefficient and/or developing additional stress at the glass-crystal interface at high pressures could be the likely reasons for suppressing the crystal growth rates. Like the glass at ambient pressure, the glass subjected to 4.5 GPa crystallized only LS2 (orthorombic, Ccc2) crystals. The density of both glasses, ambient and 4.5 GPa, was smaller than that of the crystal,  $2.46 \pm 0.01$  g/cm<sup>3</sup>. The structure of the crystals formed in the glasses that were subjected to 6 GPa pressure and whose density was higher than that of  $\text{Li}_2\text{O}\cdot \text{SiO}_2$  (LS) crystals, was complex and unknown. The structure of these crystals is believed to be a deformed LS-type, whose parameters yield a calculated crystal density of 2.61 g/cm<sup>3</sup> which is higher than the measured density of these glass-ceramics. It is believed that crystallization of these glasses follows a route which favors forming only those crystals that are accompanied by a positive, but lowest possible density change.

Chen, Su, Jianjun Sui, Li Chen, and **John A. Pojman**, “Polyurethane–Nanosilica Hybrid Nanocomposites Synthesized by Frontal Polymerization,” *Journal of Polymer Science Part A: Polymer Chemistry*, 43, 1670–1680, 2005.

*Professor Pojman is the Principal Investigator on the project, “Transient Interfacial Phenomena in Miscible Polymer Systems,” which has just been transitioned from flight to ground, having passed its Science Concept Review. He is at University of Southern Mississippi. The other authors are at Nanjing University of Technology, China*

Polyurethane–nanosilica hybrids were synthesized with frontal polymerization. Structurally well-dispersed and stable hybrids were obtained via a two-step functionalization process: First, the silica was encapsulated with 3-aminopropyltriethoxysilane (APTS). Second, poly(propylene oxide) glycol, toluene 2,4-diisocyanate, 1,4-butanediol, and a catalyst (stannous caprylate) were dissolved in dimethylbenzene and mixed together at room temperature along with the modified nanosilica. A constant-velocity propagating front was initiated via the heating of the end of the tubular reactor. For the complete encapsulation of the silica with APTS, different weight ratios of APTS to silica were investigated. The polyurethane hybrids were characterized with Fourier transform infrared, differential scanning calorimetry, and transmission electron microscopy. The polyurethane hybrids produced by frontal polymerization had the same properties as those produced by batch polymerization with stirring, but the frontal polymerization method required significantly less time and lower energy input than the batch polymerization method.

Kim, Jung-Whan, Hojin Kim, Myoungbae Lee, and **Jules J. Magda**, “Interfacial Tension of a Nematic Liquid Crystal/Water Interface with Homeotropic Surface Alignment,” *Langmuir*, 20, 8110 – 8113, 2004.

*The authors are at University of Utah where Professor Magda is the Principal Investigator on the ground-based project “Novel Structures for Polymer-Liquid Crystal Composite Materials.”*

Pendant drop experimental results are presented for the temperature dependence of the interfacial tension between water and the immiscible nematic liquid crystal 4'-pentyl-4-biphenylcarbonitrile (5CB) in the presence of the adsorbed surfactant cetyltrimethylammonium bromide (CTAB). Adsorption of the surfactant lowers the interfacial tension value, and is also known from earlier work to induce a transition in liquid crystal surface alignment from planar to homeotropic [Brake *et al. Langmuir* **2003**, *19*, 6436.]. Discrepancies exist in the literature regarding the density of 5CB, and the density difference between 5CB and water in any case is very small. However, from the ability to form pendant 5CB drops, one may infer that the density of 5CB exceeds that of water over the entire temperature range studied (28 – 41 °C), in disagreement with the predictions of one earlier report on 5CB. The interfacial tension is shown to exhibit a relative maximum near the bulk 5CB nematic-isotropic transition temperature  $T_{NI}$ , regardless of which published data set of 5CB density values is used to

analyze the measurements, with a possible discontinuity in tension occurring at  $T_{NI}$ . The anomalous shape of the interfacial tension curve, depending on the choice of the 5CB density data set, may be quite similar to that recently reported for the interface between 5CB and a hydrophobic, isotropic molten polymer (Rai *et al.*, *Langmuir* **2003**, *19*, 7370).

Huo, Y., and **B. Q. Li**, "A Mathematical Model for Marangoni Flow and Mass Transfer in Electrostatically Positioned Droplets," *Metallurgical and Materials Transactions B*, 36B, 271-281, 2005.

*Mr. Huo and Professor Li are at Washington State University, where Li is the Principal Investigator on the ground-based project "Modeling Study of Instability and Internal Flows in Levitated Droplets Under Microgravity."*

A mathematical model is developed for the free surface deformation, full three-dimensional (3-D) Marangoni convection and solute transport phenomena in electrostatically levitated droplets under microgravity. The electric field is calculated by the boundary element method and the shape deformation by the weighted residuals method. The numerical model for the transport phenomena is developed based on the Galerkin finite-element solution of the Navier-Stokes equations, the energy balance equation, and the mass transport equation. Numerical simulations are carried out for droplet deformation by electrostatic forces and 3-D Marangoni convection in droplets heated by three different heating source arrangements. Results show that the electric forces deform a droplet into an oval shape under microgravity by pulling the droplet apart at the two poles. A two-beam heating arrangement results in an axisymmetric flow and temperature distribution in the droplet. Complex 3-d Marangoni flow structure occurs when a tetrahedral or octahedral heating arrangement is applied. The thermal transport in the droplet is conduction dominant for the cases studied. In general, the convection is stronger with higher melting point melts. The internal convection has a strong effect on the concentration distribution in the droplet. For melts with high viscosities, a significant reduction in velocity can be achieved with an appropriate laser beam arrangement, thereby permitting a diffusion-controlled condition to be developed.

Mukherjee S., **W. L. Johnson**, and W. K. Rhim, "Noncontact measurement of high-temperature surface tension and viscosity of bulk metallic glass-forming alloys using the drop oscillation technique," *Applied Physics Letters*, 86, 014104 (3 pages), 2005.

*The authors are at California Institute of Technology, where Professor Johnson is the Principal Investigator on the ground-based project "Thermodynamic and Transport Properties of Glass Forming Alloy Liquids Using the Caltech High Vacuum Electrostatic levitator Platform"*

High-temperature surface tension and viscosities for five bulk metallic glass-forming alloys with widely different glass-forming abilities are measured. The measurements are carried out in a high-vacuum electrostatic levitator using the drop oscillation technique.



The surface tension follows proportional mathematical addition of pure components' surface tension except when some of the constituent elements have much lower surface tension. In such cases, there is surface segregation of the low surface tension elements. These alloys are found to have orders of magnitude higher viscosity at their melting points compared to the constituent metals. Among the bulk glass-forming alloys, the better glass former has a higher melting-temperature viscosity, which demonstrates that high-temperature viscosity has a pronounced influence on glass-forming ability. Correlations between surface tension and viscosity are also investigated.

Sano, T., C.-S. Kim, and **G. S. Rohrer**, "Shape Evolution of SrTiO<sub>3</sub> Crystals During Coarsening in a Titania-Rich Liquid," *Journal of the American Ceramic Society*, 88, 993-996, 2005.

*The authors are at Carnegie Mellon University where Professor Rohrer is the PI on the ground-based project "Shape evolution kinetics of small ceramic particles."*

To identify factors that might affect capillary driving forces and interface structure-dependent mechanisms for coarsening, we have used a stereological analysis to determine the changes in the morphology of SrTiO<sub>3</sub> crystals in contact with a titania-rich liquid at 1500°C. A combination of flat and curved surfaces is observed in contact with the liquid. The (100) surface is the most common, followed by (110). A range of surfaces in the <100> zone are also found, but with a lower frequency. The areas of the {100} and {110} surfaces are approximately equal at the initial stage, but after 24 h of growth, the {100} surface area is more than twice as great as the {110} surface area. At this point, {100} surfaces make up more than 25% of the surface area in contact with the liquid. The results suggest that morphological changes during growth continuously reduce the average surface energy and interface mobility. This provides a plausible explanation for coarsening rates that decrease faster than predicted by the classical theory.

**Rohrer, Gregory S.**, "Influence of Interface Anisotropy on Grain Growth and Coarsening," *Annual Review of Materials Research*, 35, 2005.

*Professor Rohrer, the PI on the ground-based project "Shape evolution kinetics of small ceramic particles," is from Carnegie Mellon University.*

It has recently become possible to measure the anisotropic distribution of interfaces in polycrystals and composites. Because classical theories for grain growth and coarsening assume isotropic interface properties, they are incapable of explaining how these distributions arise. The purpose of this paper is to review the results of recent experiments, simulations, and theories that document the effects of anisotropy on the capillarity-driven evolution of granular systems. The results suggest that meaningful predictions of evolving microstructural characteristics can be made using models that incorporate the anisotropy of the interfacial energy and mobility.

**Rohrer, Gregory S.**, and Chang-Soo Kim, "The influence of singular and morphological changes on coarsening," *Zeitschrift fur Metallkunde*, 96, 191-196, 2005.

*The authors are at Carnegie Mellon University where Professor Rohrer is the PI on the ground-based project "Shape evolution kinetics of small ceramic particles."*

When the interface energy between coarsening crystals and an intervening phase is anisotropic, mechanisms that do not affect isotropic systems become important. If there are singular surfaces, then growth and dissolution must occur by the lateral motion of steps, formed at a defect center, or by two-dimensional nucleation. Here, it is shown that two-dimensional nucleation is not plausible under typical experimental conditions and that persistent step-creating defects are required for a singular surface to advance or retract during coarsening. The simultaneous presence of crystals with and without defects leads to two populations that grow at very different rates, and this provides an explanation for abnormal coarsening. The influence of extrinsic morphological changes is also considered. It is assumed that when relatively high-energy, non-equilibrium shapes in the starting materials evolve during coarsening to shapes increasingly bound by lower-energy surfaces, the mean surface energy is reduced. Simulations show that under these conditions, non-classical coarsening kinetics arise in which the rate constant decreases linearly with the mean surface energy.

Palosz, W., M. P. Volz, S. Cobb, S. Motakef, and **F. R. Szofran**, “Detached growth of germanium by directional solidification,” *Journal of Crystal Growth*, 277, 124-132, 2005.

*Drs. Palosz, Volz, Cobb and Szofran are at Marshall Space Flight Center. Dr. Szofran is the Principal Investigator on the project “Influence of Containment on Defects in GeSi Crystals: Comparison of Detached Bridgman and Floating-Zone Growth” which has passed Science Concept Review and has been transitioned from flight to ground status. Dr. Motafek is with Cape Simulations Inc.*

The conditions of detached solidification under controlled pressure differential across the meniscus were investigated. Uncoated and graphite- or BN-coated silica and pBN crucibles were used. Detached and partly detached growth was achieved in pBN and BN-coated crucibles, respectively. The results of the experiments are discussed based on the theory of Duffar et al.

Jackson, J. B., and **N. J. Halas**, “Surface-enhanced Raman scattering on tunable plasmonic nanoparticle substrates,” *Proceedings of the National Academy of Sciences of the United States of America*, 101, 17930-17935, 2004.

*The authors are from Rice University where Professor Halas is the Principal Investigator on the ground-based project “Metal Nanoshell Functionalization and Materials Assembly: Effects of Microgravity Conditions.”*

Au and Ag nanoshells are investigated as substrates for surface-enhanced Raman scattering (SERS). We find that SERS enhancements on nanoshell films are dramatically different from those observed on colloidal aggregates, specifically that the Raman enhancement follows the plasmon resonance of the individual nanoparticles. Comparative finite difference time domain calculations of fields at the surface of smooth and roughened nanoshells reveal that surface roughness contributes only slightly to the total enhancement. SERS enhancements as large as  $2.5 \times 10^{10}$  on Ag nanoshell films for the nonresonant molecule *p*-mercaptoline are measured.

Anilkumar, A.V., **R. N. Grugel**, J. Bhowmick, and T. G. Wang, "Suppression of thermocapillary oscillations in sodium nitrate half-zones by high-frequency end-wall vibrations, *Journal of Crystal Growth*, 276, 194-203, 2005.

Experiments to suppress thermocapillary oscillations by using high-frequency end-wall vibrations were carried out in sodium nitrate floating half-zones. Such a half-zone is formed by melting one end of a vertically held sodium nitrate crystal rod with a hot surface at the top. Thermocapillary convection occurs in the melt due to the imposed temperature gradient at the free surface. When this temperature gradient is large enough, steady thermocapillary convection becomes unstable, and thermocapillary oscillations occur. In such a context, the bottom end of the crystal rod was vibrated at a high frequency to generate a streaming flow in a direction opposite to that of thermocapillary convection. It is observed that by generating a sufficiently strong streaming flow, the thermocapillary oscillations can be quenched everywhere in the melt zone.

*Dr Grugel is at Marshall Space Flight Center and is the Principal Investigator on the ground based project "Utilizing Controlled Vibrations in a Microgravity Environment to Understand and Promote Microstructural Homogeneity during Floating-Zone Crystal Growth." The other authors are at Vanderbilt University.*

**Koss, M. B.**, J.C. LaCombe, A. Chait, V. Pines, M. Zlatkowsky, M.E. Glicksman and P. Kar, "Pressure-mediated effects on thermal dendrites," *Journal of Crystal Growth*, 279, 179-185, 2005.

*Professor Koss is at College of the Holy Cross, and is the Principal Investigator on the transition experiment "Transient Dendritic Solidification Experiment (TDSE)," which passed its Science Concept Review in July 2000. Dr. LaCombe and Dr. Kar are at University of Nevada, Drs Chait, Pines and Zlatkowsky are at NASA Glenn Research Center, and Professor Glicksman is at Rensselaer Polytechnic Institute.*

We subjected succinonitrile dendrites growing under steady-state conditions to a rapid change in thermal driving force through a step-change in pressure. This change in pressure caused a corresponding change in the equilibrium melting temperature due to the Clapeyron effect, and a shift in the temperature field due to an adiabatic temperature change in both the solid and its melt. The new thermal conditions caused the dendrites to transition from well-characterized initial steady states to states appropriate for the new operating conditions. The initial and final states are clearly discernable, but the onset of the change in tip radius lags behind the change in tip velocity even though the total transition times appear to be similar. During the transition, a fast growing, small dendrite emerges out of the tip of a slow growing, large dendrite. Lastly, the pressure changes appear to destabilize the interface, which leads to the initiation of a dominant side branch. This work constitutes evidence that pressure changes quantifiably change growth behavior and can be used as a perturbation to influence interfacial morphology in a well-characterized free dendritic growth system. This hints at how such a mechanism may be used to control growth microstructures.

Michna, Sarah, Willie Wu, and **Jennifer Lewis**, "Concentrated hydroxyapatite inks for direct-write assembly of 3-D periodic scaffolds," *Biomaterials*, 26, 5632-5639, 2005.

*The authors are from University of Illinois, Urbana, where Professor Lewis is the Principal Investigator on the ground-based project "Directed Colloidal Assembly of Mesoporous Hydroxyapatite Tissue Engineering Scaffolds with Microporous Domains."*

Hydroxyapatite (HA) scaffolds with a 3-D periodic architecture and multiscale porosity have been fabricated by direct-write assembly. Concentrated HA inks with tailored viscoelastic properties were developed to enable the construction of complex 3-D architectures comprised of self-supporting cylindrical rods in a layer-by-layer patterning sequence. By controlling their lattice constant and sintering conditions, 3-D periodic HA scaffolds were produced with a bimodal pore size distribution. Mercury intrusion porosimetry (MIP) was used to determine the characteristic pore size and volume associated with the interconnected pore channels between HA rods and the finer pores within the partially sintered HA rods.

Wang, Jingbo, and **Nicholas Zabaras**, "Hierarchical models for inverse problems in heat conduction," *Inverse Problems*, 21, 183-206, 2005.

*The authors are with Cornell University where Professor Zabaras is the Principal Investigator on the ground-based project "On the control of the effects of gravity on the solidification microstructures using optimally designed thermal boundary fluxes and electromagnetic fields."*

Stochastic inverse problems in heat conduction with consideration of uncertainties in the measured temperature data, temperature sensor locations and thermophysical properties are addressed using a Bayesian statistical inference method. Both parameter estimation and thermal history reconstruction problems, including boundary heat flux and heat source reconstruction, are studied. Probabilistic specification of the unknown variables is deduced from temperature measurements. Hierarchical Bayesian models are adopted to relax the prior assumptions on the unknowns. The use of a hierarchical Bayesian method for automatic selection of the regularization parameter in the function estimation inverse problem is discussed. In addition, the method explores the length scales in the estimation of thermal variables varying in space and time. Markov chain Monte Carlo (MCMC) simulation is conducted to explore the high dimensional posterior state space. The methodologies presented are general and applicable to a number of data-driven engineering inverse problems.

Bessonov, N., **J. A. Pojman**, and V. Volpert, "Modelling of miscible liquids and microgravity experiments," *Matapli, (Journal of Société de Mathématiques Appliquées & Industrielles)*, 75, 51-66, 2004.

*Professor Pojman is the Principal Investigator on the project, "Transient Interfacial Phenomena in Miscible Polymer Systems," which has just been transitioned from flight to ground status, having passed its Science Concept Review. He is at University of Southern Mississippi. Dr. Bessonov is at Institute of Problems of Mechanical Engineering, Saint*

*Petersburg, Russia, while Dr. Volpert is at Laboratoire des Mathématiques Appliquées, Université Lyon*

Temperature and concentration gradients can create volume forces which result, in the case of immiscible liquids, in various capillary phenomena. However, even for miscible liquids, where a thermodynamically stable interface between them does not exist, we can expect transient interfacial phenomena before the liquid becomes homogeneous due to diffusion. This hypothesis was first suggested in 1901 by Korteweg, who also derived a mathematical model to describe this effect. A century after that, the questions about its experimental confirmation and about agreement between the theory and experiments remain basically open. Recent theoretical studies, essentially motivated by microgravity experiments, but also terrestrial experiments, give hope for obtaining a definitive confirmation of existence of transient interfacial tension in miscible liquids.

Antrim, Daniel, Patrick Bunton, Lydia Lee Lewis, Brian D. Zoltowski, and **John A. Pojman**, "Measuring the Mutual Diffusion Coefficient for Dodecyl Acrylate in Low Molecular Weight Poly(Dodecyl Acrylate) Using Laser Line Deflection (Wiener's Method) and the Fluorescence of Pyrene," *Journal of Physical Chemistry Part B* 109, 11842-11849, 2005.

*Professor Pojman is the Principal Investigator on the project, "Transient Interfacial Phenomena in Miscible Polymer Systems," which has just been transitioned from flight to ground status, having passed its Science Concept Review. He, Antrim and Zoltowski are at University of Southern Mississippi while Patrick Bunton is at William Jewell College and Lydia Lewis is at Millsaps College.*

Diffusion of small molecules into glassy polymers is quite complicated and almost non-Fickian. Little work has been done with the diffusion of low molecular weight polymer that are liquids at room temperature (such as poly(dodecyl acrylate)) into their miscible monomers. We have studied three molecular weights under 20 000 to determine if poly(dodecyl acrylate) diffusion into dodecyl acrylate could be treated with Fick's law and if so to determine the values of the diffusion coefficients. We compare two methods for measuring the diffusion of dodecyl acrylate into poly(dodecyl acrylate): We used laser line deflection (Wiener's method) and improved upon the method from published reports. We also used the dependence of pyrene's fluorescence on the viscosity to measure the concentration distribution, and thus to extract the diffusion coefficient. After an initial relaxation period, diffusion in all cases followed Fick's law with a single concentration-independent diffusion coefficient obtained by both methods yielded the same order of magnitude for the diffusion coefficients ( $10^{-7}$  cm<sup>2</sup>/s) and showed the same trend in the dependence on the average molecular weight of the polymer (a decrease in the diffusion coefficient with an increase in the molecular weight).

Wang, K. G., Z. Guo, W. Sha, **M. E. Glicksman**, and K. Rajan, "Property predictions using microstructural modeling," *Acta Materialia*, 53, 3395-3402, 2005.

*Professor Glicksman, Principal Investigator for the Flight Project "Isothermal Dendritic Growth Experiment," is at Rensselaer Polytechnic Institute, as are Messrs Kang and*

*Rajan. Dr. Guo is at Sente Software Ltd, England, while Dr. Sha is at The Queen's University of Belfast, Northern Ireland.*

Precipitation hardening in an Fe–12Ni–6Mn maraging steel during overaging is quantified. First, applying our recent kinetic model of coarsening [Phys. Rev. E, 69 (2004) 061507], and incorporating the Ashby–Orowan relationship, we link quantifiable aspects of the microstructures of these steels to their mechanical properties, including especially the hardness. Specifically, hardness measurements allow calculation of the precipitate size as a function of time and temperature through the Ashby–Orowan relationship. Second, calculated precipitate sizes and thermodynamic data determined with Thermo-Calc<sup>®</sup> are used with our recent kinetic coarsening model to extract diffusion coefficients during overaging from hardness measurements. Finally, employing more accurate diffusion parameters, we determined the hardness of these alloys independently from theory, and found agreement with experimental hardness data. Diffusion coefficients determined during overaging of these steels are notably higher than those found during the aging – an observation suggesting that precipitate growth during aging and precipitate coarsening during overaging are not controlled by the same diffusion mechanism.

Lu, Y., **C. Beckermann**, and J.C. Ramirez, “Three-dimensional phase-field simulations of the effect of convection on free dendritic growth,” *Journal of Crystal Growth*, 280, 320-334, 2005.

*The authors are at The University of Iowa, where Professor Beckermann is the Principal Investigator on the ground-based project “Microstructure Evolution in Free Dendritic Growth.”*

Three-dimensional free dendritic growth of a pure material into an undercooled melt in the presence of fluid flow is investigated numerically using the phase-field method. Such computations are made possible by solving the Navier–Stokes equations for the flow and the energy equation for the heat transport on a grid that is twice as coarse as the grid for the phase-field equation. The effect of the flow on the upstream growing dendrite tip velocity and radius of curvature is investigated as a function of the imposed flow velocity, undercooling, crystalline anisotropy, and Prandtl number. The results are compared to available theories of dendritic growth with and without convection. The predicted growth Péclet numbers as a function of the flow Péclet number are in reasonable agreement with the theoretical predictions. The dendrite tip selection parameter is essentially independent of the flow velocity within the range studied, which is also in accordance with theory. The three-dimensional dendrite tip shape is found to be well fitted by the same universal scaling relation as without flow.

Johnson, John L., Justin J. Brezovsky, and **Randall M. German**, "Effect of Liquid Content on Distortion and Rearrangement Densification of

Liquid Phase Sintered W-Cu," *Metallurgical and Materials Transactions*. 36A, 1557-1565, 2005.

*Messrs. Johnson and Brezovsky are with The Pennsylvania State University where Professor German is the Principal Investigator on the Project "Gravitational Effects on Distortion in Sintering." This project has passed its Science Concept Review and is being transitioned from flight to ground status.*

Tungsten and copper exhibit negligible solubility for each other, so densification during liquid phase sintering of W-Cu is limited to rearrangement of the W particles and solid-state sintering of the W skeleton. Experiments are conducted to evaluate the effects of Cu volume fraction on liquid phase sintering of W-Cu. Sintered microstructures are quantitatively analyzed and are used to define critical microstructural parameters that prevent distortion and rearrangement densification. Slumping is prevented first by capillary forces, then by formation of a rigid W skeleton at critical values of contiguity and connectivity which depend on the dihedral angle. A refined expression for the dependence of contiguity on volume fraction that includes the effect of dihedral angle is developed. An analysis of gravitational, capillary, and bonding forces acting on W particles in liquid Cu explains the ability to achieve high sintered densities through rearrangement despite a lack of distortion with up to 80 vol pct liquid. Capillary forces are sufficient to break weak solid-solid bonds that form during heating, enabling rearrangement to occur even without dissolution of these bonds. At higher solid volume fractions, sufficient particle contacts form to prevent rearrangement by these capillary forces, thus limiting sintered densities.

Li, C., R. N. Scripa, H. Ban, B. Lin, **C.-H. Su**, and S. L. Lehoczky, "Thermophysical properties of  $\text{Hg}_{0.8}\text{Cd}_{0.2}\text{Te}$  melt: Density, electrical conductivity and viscosity," *Journal of Non-Crystalline Solids*, 351, 1179-1184, 2005.

*Drs Li, Su and Lehoczky are at MSFC, where Dr. Su is the Principal Investigator on the ground based project "Cadmium Zinc Telluride ( $\text{CdZnTe}$ ) High-Energy Radiation Sensors and Structural Transformation of Group I-III-VI Melts." Drs Scripa, Ban, and Lin are with University of Alabama at Birmingham.*

Thermophysical properties, namely, density, viscosity, and electrical conductivity of  $\text{Hg}_{0.8}\text{Cd}_{0.2}\text{Te}$  melt were measured as a function of temperature. A pycnometric method was used to measure the melt density in the temperature range of 1072–1122 K. The viscosity and electrical conductivity were simultaneously determined using a transient torque method from 1068 to 1132 K. The density result from this study is within 0.3% of the published data. However, the current viscosity result is approximately 30% lower than the existing data. The electrical conductivity of  $\text{Hg}_{0.8}\text{Cd}_{0.2}\text{Te}$  melt as a function of temperature, which is not available in the literature, is also determined. The analysis of the temperature dependent electrical conductivity and the relationship between the kinematic viscosity and density indicated that the structure of the melt appeared to be homogeneous when the temperature was above 1090 K. A structural transition occurred in the  $\text{Hg}_{0.8}\text{Cd}_{0.2}\text{Te}$  melt as the temperature was decreased from 1090 K to the liquidus temperature.

**Kassemi, M.,** S. Barsi, J. I. D. Alexander, and M. Banish, “Contamination of microgravity liquid diffusivity measurements by void-generated thermocapillary convection,” *Journal of Crystal Growth*, 276, 621-634, 2005.

*Dr. Barsi and Dr. Alexander are at Case Western Reserve University. Dr. Kassemi, the Principal Investigator for the ground-based project “Effect of Marangoni Convection Generated by Voids on Segregation during Low-g and 1-g Solidification,” is at Glenn Research Center. Dr. Banish is at the University of Alabama in Huntsville.*

This paper examines the effects of thermocapillary convection generated by a void or bubble on the self-diffusion measurement of molten indium in microgravity. The study is based on the thermophysical and geometrical configurations of the self-diffusion in liquid elements (SDLE) microgravity experiment. A transient finite element model of the diffusion capillary is presented. Numerical simulations of the transport processes in the diffusion capillary indicate that the concentration stratification in the enclosure is greatly modified by void-generated convection when small temperature non-uniformities are present in the system. The extent to which this modification can contaminate the diffusion data obtained by the Harned-Codastefano methodology is determined. In order to generalize the findings, results are summarized by relating the extent of the convective contamination of the diffusion data to the thermocapillary Reynolds number of the bubble and the Schmidt number of the system.

Lupulescu, A., **M. E. Glicksman,** and M. B. Koss, “Conduction-limited crystallite melting,” *Journal of Crystal Growth*, 276, 549-565, 2005.

*Professor Glicksman, Principal Investigator for the Flight Project “Isothermal Dendritic Growth Experiment,” is at Rensselaer Polytechnic Institute, as is Dr. Lupulescu. Dr. Koss is at the College of the Holy Cross.*

High-purity pivalic acid (PVA) dendrites were observed growing under convection-free conditions during the isothermal dendritic growth experiment (IDGE) flown on NASA's space shuttle *Columbia* on STS-87. The IDGE was part of the complement of primary scientific experiments designated as the United States Microgravity Payload Mission (USMP4) launched late in 1997. The IDGE video data show that PVA dendrites may be melted without exhibiting any detectable relative motion with respect to the surrounding quiescent melt phase. Thus, melting occurs by heat conduction alone. When a small fixed superheating is imposed on pre-existing dendritic fragments, they melt steadily toward extinction. Individual fragments steadily decrease in size according to a square-root of time dependence predicted using quasi-static conduction-limited theory. Agreement between analytic melting theory and microgravity experiments was found originally if the melting process occurs under the restriction of shape-preserving conditions, where needle-like crystal fragments may be approximated as ellipsoids with a constant axial ratio. Among the new results reported here is the influence of capillarity effects on melting in needle-like crystallites, observed as a dramatic change in their axial ratio, when the size scale of a crystallite decreases below a critical value. In microgravity melting experiments, the axial ratio of individual crystallites does not remain constant, because of interactions with neighboring fragments within the mushy zone. The kinetic data were then “sectorized” to divide the total melting process into a series of short intervals. Each melting sector for a crystallite could then be approximated by a constant average value of the axial ratio. Sectorization also allows accurate prediction of melting kinetics by applying quasi-static heat conduction theory,



despite the suspected presence of capillarity and the occurrence of fragmentation. These additional processes that accompany the melting of slender crystallites currently lie outside conventional melting theory. The data presented show that melting kinetics of small crystallites remains dominated by heat conduction from the surrounding melt, which is modified by the appearance of additional heat fluxes. These additional heat fluxes flow within the crystallites. They arise from capillary effects induced by steep interfacial curvature gradients that accompany the small crystallite size scales prior to their extinction.

Shu, Y., **B. Q. Li**, and H. C. de Groh, III, "Convection and Solidification in Constant and Oscillating Thermal Gradients: Measurements and Simulations," *Journal of Thermophysics and Heat Transfer*, 19, 199-208, 2005.

*Messrs Shu and Li are at Washington State University where Professor Li is the PI on the ground-based project "Study of magnetic field effects on convection and solidification in normal and microgravity." Dr. de Groh is at Glenn Research Center.*

An experimental and numerical study of natural convection and solidification in a two-dimensional cavity driven by constant and oscillating temperature gradients is presented. Finite element models are developed to predict the flowfield, the temperature distribution, and the solid-liquid interphase shapes during solidification. Both the fixed-grid and moving-grid methods are applied in the numerical simulations, using the former to illustrate the oscillating thermal gradient conditions and using the latter to illustrate the constant temperature gradient conditions. An experimental system is set up where succinonitrile is used as a working fluid. The flow pattern, the velocity field, and the solidification interface shape are measured using the laser-based particle-image-velocimetry system. Numerical simulations and experiments are conducted for various configuration and different thermal gradients. In most cases, convection is dominated by one recirculating loop. With an inverted temperature gradient, however, multiple convection loops are observed. Both the convective flow pattern and the velocity strongly affect the solid-liquid interface shapes during solidification. In a majority of the cases studied, the model predictions are in good agreement with the experimental measurements.

Ganapathysubramanian, Baskar, and **Nicholas Zabaras**, "Control of solidification of non-conducting materials using tailored magnetic fields," *Journal of Crystal Growth*, 276, 299-316, 2005.

*The authors are with Cornell University where Professor Zabaras is PI on the ground-based project "On the control of the effects of gravity on the solidification microstructures using optimally designed thermal boundary fluxes and electromagnetic fields."*

The structure of fluid flow in a solidifying melt plays a critical role in the quality/properties of the solid. It follows that by controlling the flow behavior, the final solidified material can be suitably affected. Most of the magnetic control approaches used depend on the variation of the Lorentz force for suppression of flow and are limited to conducting materials alone. The application of a magnetic gradient gives rise to an additional force that can be used to affect the melt flow of any material. In this work, a

computational method for the design of solidification of a non-conducting material is addressed such that diffusion-dominated growth is achieved by the suppression of convection. The control parameter in the design problem is the time history of the imposed magnetic field. The design problem is posed as an unconstrained optimization problem. The adjoint method for the inverse design of continuum processes is adopted. Examples of designing the time history of the imposed magnetic field for the directional growth of various non-conducting materials are presented to demonstrate the developed formulation.

Zawilski, Kevin T., M. Claudia C. Custodio, Robert C. DeMattei, and **Robert S. Feigelson**, "Control of growth interface shape using vibroconvective stirring applied to vertical Bridgman growth," *Journal of Crystal Growth*, 282, 236-250, 2005.

*The authors are at Stanford University where Professor Feigelson is the Principal Investigator on the ground based project "Investigation of the Crystal Growth of Dielectric Materials by the Bridgman Technique Using Vibrational Control."*

The ability of vibroconvective stirring to control the growth interface shape during vertical Bridgman growth was demonstrated using the coupled vibrational stirring (CVS) technique. CVS involves the application of low-frequency vibrations to the outside of the growth ampoule and produces strong flows emanating from the fluid surface. Previous studies showed that the growth rate and interface shape fluctuations occurred under growth with a constant vibrational frequency. In order to eliminate these fluctuations, this paper examines methods to lower the vibrational frequency as growth progressed to maintain a constant fluid flow rate in the vicinity of the growth interface. These flow control methods were tested on two growth systems: NaNO<sub>3</sub> and lead magnesium niobate–lead titanate (PMNT). The previously observed fluctuations were greatly reduced when flows were appropriately controlled. Using this control method, CVS flows were then applied to reduce the concavity of the growth interface in the NaNO<sub>3</sub> system at fast growth rates (>10 mm/h).

Wang, K. G., **M. E. Glicksman**, and K. Rajan, "Length scales in phase coarsening: Theory, simulation, and experiment," *Computational Materials Science*, 34, 235-253, 2005.

*The authors are at Rensselaer Polytechnic Institute where Professor Glicksman is the Principal Investigator on the flight project "Evolution of Local Microstructures: Spatial Instabilities of Coarsening Clusters."*

The collective interactions occurring within a population of spherical precipitates dispersed throughout a contiguous matrix may be described on the basis of a diffusion screening length. This critical length scale is derived from the quasi-static theory of diffusion-limited phase coarsening of spherical precipitates. This theory predicts as functions of the dispersoid volume fraction the changes in diffusion screening length, the maximum particle size, the population's coarsening rate, and, finally, the affine particle-size distribution. Furthermore, by considering fluctuations observed in the growth rates of individual particles, we formulate a stochastic theory of phase

coarsening. Results obtained from simulating phase coarsening using multiparticle diffusion approaches and phase field model are then compared to the kinetic theories. Finally, particle-size distributions and the maximum radii predicted from theory and simulations are shown to agree well with experimental results obtained from measurements performed on  $\delta$  ( $\text{Al}_3\text{Li}$ ) precipitates in binary Al–Li alloys.

Minke, M. V., and **K.A. Jackson**, “Diffusion of germanium in silica glass,” *Journal of Non-Crystalline Solids*, 351, 2310-2316, 2005.

*The authors are at the University of Arizona, where Professor Jackson is the Principal Investigator on the ground-based project and “Non-Equilibrium Phase Transformations.”*

The first measurements of the diffusion coefficient of substitutional germanium in silica glass are reported. Samples were prepared by implanting germanium ions into high purity silica. The concentration of germanium at the surface remained essentially zero, indicating that germanium evaporated readily from the surface of the sample. It was found that, during an initial anneal, the peak concentration of germanium shifted toward the surface. We attribute this to a drift motion of ions in the field created by the implant. The motion of the ions during an anneal could be changed by applying a DC electric field. A preliminary annealing procedure was established which eliminated the drift motion, so that the subsequent motion of germanium could be described as simple diffusion. EXAS measurements indicated that germanium was clustered together in the as-implanted samples, but that after this pre-anneal, germanium was incorporated into the matrix. The diffusion coefficient of the substitutional germanium in silica was found to be  $7250 \exp(-6.6 \times 10^4/T) \text{ cm}^2/\text{s}$ , which corresponds to an activation energy,  $Q = 131 \text{ kcal/mol}$ .

Zawilski, Kevin T., M. Claudia C. Custodio, Robert C. DeMattei, and **Robert S. Feigelson**, “Control of growth interface shape using vibroconvective stirring applied to vertical Bridgman growth,” *Journal of Crystal Growth*, 282, 236-250, 2005.

*The authors are at Stanford University where Professor Feigelson is the Principal Investigator on the ground based project “Investigation of the Crystal Growth of Dielectric Materials by the Bridgman Technique Using Vibrational Control.”*

The ability of vibroconvective stirring to control the growth interface shape during vertical Bridgman growth was demonstrated using the coupled vibrational stirring (CVS) technique. CVS involves the application of low-frequency vibrations to the outside of the growth ampoule and produces strong flows emanating from the fluid surface. Previous studies showed that the growth rate and interface shape fluctuations occurred under growth with a constant vibrational frequency. In order to eliminate these fluctuations, this paper examines methods to lower the vibrational frequency as growth progressed to maintain a constant fluid flow rate in the vicinity of the growth interface. These flow control methods were tested on two growth systems:  $\text{NaNO}_3$  and lead magnesium niobate–lead titanate (PMNT). The previously observed fluctuations were greatly reduced when flows were appropriately controlled. Using this control method, CVS flows were

then applied to reduce the concavity of the growth interface in the NaNO<sub>3</sub> system at fast growth rates (>10 mm/h).

Minke, M. V., and **K.A. Jackson**, "Diffusion of germanium in silica glass," *Journal of Non-Crystalline Solids*, 351, 2310-2316, 2005.

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Xu, B., and **B. Q. Li**, "Hot-film measurement of temperature gradient induced natural convection in liquid gallium," *Experimental Thermal and Fluid Science*, 29, 697-704, 2005.

*The authors are at Washington State University where Professor Li is the PI on the ground-based project "Study of magnetic field effects on convection and solidification in normal and microgravity."*

An experimental study on temperature gradient induced natural convection in molten gallium is presented in this paper. The induced temperature and velocity fields are mapped simultaneously. A standard hot-film anemometer working under constant temperature mode is used to measure the velocity profile, and the temperature profile is measured using a standard T type thermocouple. The obtained velocity and temperature distributions are compared with previous numerical simulations and reasonably good agreements have been achieved.

Volz, M. P., J. S. Walker, M. Schweizer, S. D. Cobb, and **F. R. Szofran**, "Bridgman growth of germanium crystals in a rotating magnetic field," *Journal of Crystal Growth*, 282, 305-312, 2005.

Professor Walker is at the University of Illinois, Urbana. The other authors are at Marshall Space Flight Center where Dr. Szofran is the Principal Investigator on the transition experiment "Reduction of Defects in Germanium Silicon."

A series of (1 0 0)-oriented gallium-doped germanium crystals has been grown by the vertical Bridgman method and under the influence of a rotating magnetic field (RMF). Time-dependent flow instabilities occur when the critical magnetic Taylor number ( $T_m^*$ ) is exceeded, and this can be observed by noting the appearance of striations in the grown crystals.  $T_m^*$  decreases as the aspect ratio of the melt increases, and approaches the theoretical limit expected for an infinite cylinder. Intentional interface demarcations are introduced by pulsing the RMF on and off. The RMF has a marked effect on the interface shape, changing it from concave to nearly flat as the RMF strength is increased.

Mendoza, R., J. Alkemper, and **P. W. Voorhees**, "Three-dimensional morphological characterization of coarsened microstructures," *Zeitschrift für Metallkunde*, 96, 155-160, 2005.

*Drs. Mendoza and Voorhees are at Northwestern University, where Professor Voorhees is the Principal Investigator on the ground-based project "The Evolution of Dendrite Morphology during Isothermal Coarsening." Dr. Alkemper is at the General Electric Corporate Research and Development Center, Schenectady.*

The three-dimensional morphological evolution of a directionally solidified Al-15 wt.% Cu alloy during isothermal coarsening was examined. The microstructure was analyzed using the Interfacial Shape Distribution (ISD), which gives the probability of locating an interfacial patch with a given pair of principle curvatures. By scaling the ISDs by a characteristic length, the inverse of the surface area per unit volume, it was possible to determine if the system reached a time-invariant state. During coarsening, cylindrical interfaces appear in the second coarsened sample and remained for later coarsening times. The appearance of the corresponding peak in the ISD indicated that the microstructure was not evolving in a self-similar manner, despite the linear relationship between the inverse surface area per unit volume and the cube root of coarsening time. Stereographic projections of the interfacial normals indicated that the microstructure of the earliest coarsened sample had a four-fold symmetry that disappeared during coarsening and that the majority of interfacial area for all coarsened samples is parallel to the direction in which the pre-coarsened samples were solidified.

Li, C., **C.-H. Su**, S. L. Lehoczky, R. N. Scripa, B. Lin, and H. Ban, "Thermophysical properties of liquid Te: density, electrical conductivity and viscosity," *Journal of Applied Physics*, 97, 83513-1-7, 2005.

*Drs Li, Su and Lehoczky are at MSFC, where Dr. Su is the Principal Investigator on the ground based project "Cadmium Zinc Telluride (CdZnTe) High-Energy Radiation Sensors and Structural Transformation of Group I-III-VI Melts." Drs Scripa, Ban, and Lin are with University of Alabama at Birmingham.*

The thermophysical properties of liquid Te, namely, density, electrical conductivity, and viscosity, were determined using the pycnometric and transient torque methods from

the melting point of Te (723 K) to approximately 1150 K. A maximum was observed in the density of liquid Te as the temperature was increased. The electrical conductivity of liquid Te increased to a constant value of  $2.9 \times 10^5 \text{ } \Omega^{-1} \text{ m}^{-1}$  as the temperature was raised above 1000 K. The viscosity decreased rapidly upon heating the liquid to elevated temperatures. The anomalous behaviors of the measured properties are explained as caused by the structural transitions in the liquid and discussed in terms of Eyring's [A. I. Gubanov, *Quantum Electron Theory of Amorphous Conductors* (Consultants Bureau, New York, 1965)] and Bachinskii's [Zh. Fiz.-Khim. O-va. **33**, 192 (1901)] predicted behaviors for homogeneous liquids. The properties were also measured as a function of time after the liquid was cooled from approximately 1173 or 1123 to 823 K. No relaxation phenomena were observed in the properties after the temperature of liquid Te was decreased to 823 K, in contrast to the relaxation behavior observed for some of the Te compounds.

Goldenfeld, Nigel, Badrinarayan P. Athreya, and **Jonathan A. Dantzig**, "Renormalization group approach to multiscale simulation of polycrystalline materials using the phase field crystal model," *Physical Review E*, 72, 020601-1-4, 2005.

*The authors are at University of Illinois at Urbana-Champaign, where Professor Dantzig is the Principal Investigator on the ground based project "Phase Field Modeling of Microstructure Development in Microgravity."*

We propose a computationally efficient approach to multiscale simulation of polycrystalline materials, based on the phase field crystal model. The order parameter describing the density profile at the nanoscale is reconstructed from its slowly varying amplitude and phase, which satisfy rotationally covariant equations derivable from the renormalization group. We validate the approach using the example of two-dimensional grain nucleation and growth.

Zhao, Q., M. Buongiorno Nardelli, W. Lu, and **J. Bernholc**, "Carbon Nanotube-Metal Cluster Composites: A New Road to Chemical Sensors?," *Nano Letters*, 5, 847-851, 2005.

*The authors are from North Carolina State University where Professor Bernholc is the Principal Investigator on the ground-based project "Growth and Properties of Carbon Nanotubes."*

Novel carbon nanotube-metal cluster structures are proposed as prototype systems for molecular recognition at the nanoscale. Ab initio calculations show that already the bare nanotube cluster system displays some specificity because the adsorption of ammonia on a carbon nanotube-Al cluster system is easily detected electrically, while diborane adsorption does not provide an electrical signature. Since there are well-established procedures for attaching molecular receptors to metal clusters, these results provide a "proof-of-principle" for the development of novel, high-specificity molecular sensors.

Wang, Hui, Glenn P. Goodrich, Felicia Tam, Chris Oubre, Peter Nordlander, and **Naomi J. Halas**, “Controlled Texturing Modifies the Surface Topography and Plasmonic Properties of Au Nanoshells,” *Journal of Physical Chemistry B*, 11083-11087, 109, 2005.

*The authors are from Rice University where Professor Halas is the Principal Investigator on the ground-based project “Metal Nanoshell Functionalization and Materials Assembly: Effects of Microgravity Conditions.”*

We report a facile and controllable method for the postfabrication texturing of the surface topography of Au nanoshells based on site-selective chemical etching of the polycrystalline Au nanoshell surface by a bifunctional alkanethiol molecule, cysteamine. This nanoscale surface texturing process systematically introduces dramatic changes to the plasmonic properties of the Au nanoshells. The modification of the plasmon resonant properties of nanoshells as a function of increased surface roughness was examined experimentally and modeled theoretically using three-dimensional finite difference time domain (FDTD) simulations.

Rowenhorst, D. J., and **P. W. Voorhees**, “Measurements of the Grain Boundary Energy and Anisotropy in Tin,” *Metallurgical and Materials Transactions A*, 36A, 2127-2135, 2005.

*The authors are at Northwestern University, where Professor Voorhees is the Principal Investigator on the ground-based project “The Evolution of Dendrite Morphology during Isothermal Coarsening.”*

The three-dimensional (3-D) geometry of the triple junction formed between two solid Sn-rich particles and a Pb-rich liquid matrix is used to measure the interfacial energy and its anisotropy for individual grain boundaries. The anisotropy is determined using a Cahn-Hoffman capillary vector analysis of the energy balance at a triple junction. The absolute solid-solid grain boundary energy for each individual boundary is then determined by using the known value for the solid-liquid energy. A total of 136 boundaries are analyzed, with 46 of them forming grain boundaries. The remaining boundaries are found to be wetted boundaries with thin-liquid films formed between the two particles. A correlation between the low interfacial energy and the probability of occurrence for that disorientation is also observed. We also show that the anisotropy, as quantified by the magnitude of the torque term, is a significant portion of the total interfacial energy, especially for low energy boundaries. The degree of twist *vs* tilt of the boundaries is also analyzed. As expected, there are more tilt boundaries within the system than twist boundaries and most of the low energy boundaries have a mixed tilt-twist character.

Sofonea, Victor, and **Robert F. Sekerka**, “Boundary conditions for the upwind finite difference Lattice Boltzmann model: Evidence of slip velocity in micro-channel flow,” *Journal of Computational Physics*, 207, 639-659, 2005.

*Dr. Sofonea is at the Center for Fundamental and Advanced Technical Research, Romanian Academy, Romania. Professor Sekerka, the Principal Investigator for the ground-based project "Lattice Boltzmann Computations of Binary Diffusion under Stochastic Microgravity" is at Carnegie Mellon University.*

We conduct a systematic study of the effect of various boundary conditions (bounce back and three versions of diffuse reflection) for the two-dimensional first-order upwind finite difference Lattice Boltzmann model. Simulation of Couette flow in a micro-channel using the diffuse reflection boundary condition reveals the existence of a slip velocity that depends on the Knudsen number  $\varepsilon = \lambda/L$ , where  $\lambda$  is the mean free path and  $L$  is the channel width. For walls moving in opposite directions with speeds  $\pm u_w$ , the slip velocity satisfies  $u_{\text{slip}} = 2\varepsilon u_{\text{wall}}/(1 + 2\varepsilon)$ . In the case of Poiseuille flow in a micro-channel, the slip velocity is found to depend on the lattice spacing  $\delta s$  and Knudsen number  $\varepsilon$  to both first and second order. The best results are obtained for diffuse reflection boundary conditions that allow thermal mixing at a wall located at half lattice spacing outside the boundary nodes.

Mukherjee, S., J. Schroers, **W. L. Johnson**, and W.-K. Rhim, "Influence of Kinetic and Thermodynamic Factors on the Glass-Forming Ability of Zirconium-Based Bulk Amorphous Alloys," *Physical Review Letters*, 94, 245501 (4 pages), 2005.

*The authors are at California Institute of Technology, where Professor Johnson is the Principal Investigator on the ground-based project "Thermodynamic and Transport Properties of Glass Forming Alloy Liquids Using the Caltech High Vacuum Electrostatic Levitator Platform."*

The time-temperature-transformation curves for three zirconium-based bulk amorphous alloys are measured to identify the primary factors influencing their glass-forming ability. The melt viscosity is found to have the most profound influence on the glass-forming ability compared to other thermodynamic factors. Surprisingly, it is found that the better glass former has a lower crystal-melt interfacial tension. This contradictory finding is explained by the icosahedral short-range order of the undercooled liquid, which on one hand reduces the interfacial tension, while on the other hand increases its viscosity.

Ganapathysubramanian, Baskar, and **Nicholas Zabaras**, "On the control of solidification of conducting materials using magnetic fields and magnetic field gradients," *International Journal of Heat and Mass Transfer*, 48, 4174-4189, 2005.

*The authors are with Cornell University where Professor Zabaras is PI on the ground-based project "On the control of the effects of gravity on the solidification microstructures using optimally designed thermal boundary fluxes and electromagnetic fields."*



Solidification from the melt to near net shape is a commonly used manufacturing technique. The fluid flow patterns in the melt affect the quality of the final product. By controlling the flow behavior, the final solidified material can be suitably affected. Most of the magnetic field approaches to melt flow control rely on the application of a constant magnetic field. A constant magnetic field results in the Lorentz force which is used to damp and control the flow. However, simultaneous application of a magnetic gradient results in the Kelvin force along with the Lorentz force. This can be used for better control of the melt flow resulting in higher crystal quality. In the present work, a computational method for the design of solidification of a conducting material is addressed. The control parameter in the design problem is the time history of the imposed magnetic field. A steady, constant magnetic gradient is also maintained during the process. The design problem is posed as an unconstrained optimization problem. The adjoint method for the inverse design of continuum processes is adopted. Examples of designing the time history of the imposed magnetic field for the directional growth of various materials are presented to demonstrate the developed formulation.

Sofonea, Victor, and **Robert F. Sekerka**, “Diffuse-reflection boundary conditions for a thermal lattice Boltzmann model in two dimensions: Evidence of temperature jump and slip velocity in microchannels,” *Physical Review E*, 71, 066709-1-10, 2005.

*Dr. Sofonea is at the Center for Fundamental and Advanced Technical Research, Romanian Academy, Romania. Professor Sekerka, the Principal Investigator for the ground-based project “Lattice Boltzmann Computations of Binary Diffusion under Stochastic Microgravity” is at Carnegie Mellon University.*

We discuss the implementation of diffuse reflection boundary conditions in a thermal lattice Boltzmann model for which the upwind finite difference scheme is used to solve the set of evolution equations recovered after discretization of the velocity space. Simulation of heat transport between two parallel walls at rest shows evidence of temperature jumps at the walls that increase with Knudsen number. When the walls move in opposite directions with speeds  $\pm u_w$ , fluid velocity slip is observed at the walls, together with temperature jumps.

**Su, Ching-Hua**, “Composition – Temperature – Partial Pressures Data for  $\text{Cd}_{0.8}\text{Zn}_{0.2}\text{Te}$  by Optical Absorption Measurements,” *Journal of Crystal Growth*, 281, 577-586, 2005.

*Dr. Su is at Marshall Space Flight Center, and is the Principal Investigator on the ground-based project “Cadmium Zinc Telluride ( $\text{CdZnTe}$ ) High-Energy Radiation Sensors and Structural Transformation of Group I-III-VI Melts.”*

Known weights of Cd, Zn and Te were reacted in silica optical cells of known volume, and the partial pressures of  $\text{Te}_2$  and Zn between 485 and 1160°C were determined by measuring the optical density of the vapor in the ultra-violet to visible range. The composition of the condensed phase or phases was calculated from the original weights and the amount of material in the vapor phase. The corresponding composition – temperature – partial pressures,  $x_{\text{Te}}-T-P_{\text{Te}_2}$ , data, including five Te-rich solidus points,

were established. The solubility range for the Te-rich  $\text{Cd}_{0.8}\text{Zn}_{0.2}\text{Te(s)}$  is similar to that of  $\text{CdTe(s)}$  with  $x_{\text{Te}} = 0.50005$  at  $809^\circ\text{C}$  and an estimated maximum solubility of  $x_{\text{Te}} = 0.50012$  at about  $1000^\circ\text{C}$ . The partial pressures of Cd and  $\text{Te}_2$  measured over the  $\text{Cd}_{0.8}\text{Zn}_{0.2}\text{Te}$  melt at  $1140^\circ\text{C}$  were about 1.55 and 0.02atm, respectively, and the corresponding Zn partial pressure was estimated to be 0.05atm. It was recommended that a Cd reservoir maintained at 800 to  $820^\circ\text{C}$  should be used during directional solidification of  $\text{Cd}_{0.8}\text{Zn}_{0.2}\text{Te}$  to prevent the preferential loss of Cd to the vapor phase.

Lin, John J., Frank S. Bates, **Daniel A. Hammer**, and James A. Silas, "Adhesion of Polymer Vesicles," *Physical Review Letters*, 95, 026101-1-4, 2005.

*Messrs Lin, Hammer and Silas are at University of Pennsylvania, where Professor Hammer is the Principal Investigator on the ground based project "Polymosomes: Tough, Giant Vesicles from Block Copolymers." Professor Bates is at University of Minnesota.*

The adhesion and bending modulus of polybutadiene-poly(ethylene oxide) block copolymer vesicles made from a bidisperse mixture of polymers is measured using micropipette aspiration. The adhesion energy between biotinylated vesicles and avidin beads is modeled by incorporating the extension of the adhesive ligands above the surface brush of the vesicle according to the blob model of bidisperse polymer mixtures of Komura and Safran assuming the polymer brush at the surface of the vesicle is compact. The same model accurately reproduces the scaling of the bending modulus with polymer composition.

Woods, Vincent, Jayantha Senawirante, and **Nikolaus Dietz**, "Nucleation and Growth of InN by high-pressure chemical vapor deposition: Optical monitoring," *Journal of Vacuum Science and Technology*, B23, 1790-1794, 2005.

*The authors are at Georgia State University where Dr. Dietz is the Principal Investigator on the ground-based project "Optical characterization of gas phase, gas phase chemistry, and surface chemistry during high pressure vapor phase deposition processes under laminar and turbulent flow conditions."*

The growth of high quality, stoichiometric InN presents a challenge because of the volatility of atomic nitrogen. To overcome the associated difficulties, a high-pressure chemical vapor deposition (HPCVD) system has been developed, which has opened the avenue for achieving stoichiometric single-phase surface compositions for materials such as InN for which thermal decomposition pressures are large at optimum processing temperatures. We report results obtained during InN growth in the pressure range of 2-15 bar to achieve the earlier objectives and to obtain insights into the InN nucleation and growth process. Using real-time optical ultraviolet absorption spectroscopy, we characterized the chemistry of the gas-phase precursors as functions of flow, pressure, and temperature. Highly surface sensitive probing on InN nucleation and steady state growth is achieved by principal-angle-reflectance spectroscopy, allowing the characterization of surface chemistry at a submonolayer level. The InN layers grown at lower temperatures exhibit an absorption edge at 1.85 eV, which is

shifted towards lower energies as the growth temperatures increase. Absorption edges as low as 0.7 eV are observed, values reported for molecular beam epitaxy-grown InN material. The real-time optical monitoring techniques employed demonstrated their superiority in optimizing and controlling the growth process, as well as in gaining insight in gas phase and surface chemistry processes during HPCVD.

**Dietz, Nikolaus**, Martin Straßburg, and Vincent Woods, “Real-time optical monitoring of ammonia flow and decomposition kinetics under high-pressure chemical vapor deposition conditions,” *Journal of Vacuum Science and Technology*, A23, 1221-1227, 2005.

*The authors are at Georgia State University where Dr. Dietz is the Principal Investigator on the ground-based project “Optical characterization of gas phase, gas phase chemistry, and surface chemistry during high pressure vapor phase deposition processes under laminar and turbulent flow conditions.”*

Understanding the gas phase decomposition kinetics of the chemical precursors involved in the nucleation and thin-film growth processes is crucial for controlling the surface kinetics and the growth process. The growth of emerging materials such as InN and related alloys requires deposition methods operating at elevated vapor densities due to the high thermal decomposition pressure of these materials. High nitrogen overpressure has been demonstrated to suppress the thermal decomposition of InN, but has so far not been explored in chemical vapor deposition experiments. In this contribution we present research results on the decomposition kinetics of ammonia in the laminar flow regime of a high-pressure flow channel reactor. Ultraviolet absorption spectroscopy is applied to analyze absorption features of ammonia with respect to the ammonia flow rate during continuous flow and pulsed ammonia injection. Pulsed ammonia injection has been used to analyze the average gas flow velocity in the high-pressure chemical vapor deposition system as a function of the total gas flow rate and the reactor pressure. The onset of the kinetics related to the decomposition of ammonia was found to start above 900 K and showed a marked decrease for higher reactor pressures, thus decreasing the discrepancy of trimethylindium and ammonia decomposition temperatures.

**N. Dietz**, M. Alevi, V. Woods, M. Strassburg, H. Kang, and I. T. Ferguson, “The characterization of InN growth under high-pressure CVD conditions,” *physica status solidi (b)*, 242, 2985-2994, 2005.

*Messrs Dietz, Alevi, Woods, and Strassburg are at Georgia State University where Dr. Dietz is the Principal Investigator on the ground-based project “Optical characterization of gas phase, gas phase chemistry, and surface chemistry during high pressure vapor phase deposition processes under laminar and turbulent flow conditions.” Messrs Kang and Ferguson are at Georgia Institute of Technology.*

Gaining insight into the gas phase and surface chemistry processes that govern the growth of InN and indium-rich group III-nitrides alloys is of crucial importance for understanding and controlling their materials properties. *High pressure chemical vapor deposition (HPCVD)* has been shown to be a valuable method for achieving this goal. First results show that InN layers can be grown under HPCVD conditions at 850-900 °C in the laminar flow regime of the HPCVD reactor at pressures around 15 bar and

ammonia to TMI precursor flow ratio below 200. This is a major step towards the growth of indium rich group III-nitride heterostructures due to the close processing windows. The *ex situ* InN layers analysis shows that the absorption edge in the InN depends strongly on the precursor flow ratio, indicating that the debated InN properties are strongly influenced by the indium-to-nitrogen stoichiometry. By controlling the InN point defect chemistry we showed that the absorption edge shifts from 1.8 eV down to 0.7 eV. The results show a close relation between absorption edge shift in InN and In-N stoichiometry. In order to study the growth under high-pressure CVD conditions, real-time optical characterization techniques have been developed and applied to analyze gas phase constituents as well as the film nucleation and steady state growth at elevated pressures. Principal angle reflection and laser light scattering are employed to study surface chemistry processes at a sub-monolayer level, showing their superiority in optimizing and controlling the growth process.

**Trivedi, R.**, and J. H. Shin, “Modelling of microstructure evolution in peritectic systems,” *Materials Science and Engineering*, A413-414, 288-295, 2005.

*The authors are from Iowa State University. Professor Trivedi is Principal Investigator for the flight experiment “Interface Pattern Selection in Directional Solidification,” which has been transitioned to ground-based having passed its Science Concept Review.*

Theoretical models for directional solidification microstructures are largely developed for steady-state growth conditions. In the two-phase region of peritectic system, a rich variety of two-phase microstructures form in which the two phases often form under non-steady-state conditions and the microstructure evolution depends on the nucleation characteristics of the two phases as well as on the competitive growth of the two phases under dynamical growth conditions. Theoretical models, based on nucleation and diffusive growth, are presented to establish the mechanisms that lead to different microstructure formation in peritectic systems. The critical role played by nucleation in the selection of oscillatory microstructures is discussed, and experimental studies to select different nucleation sites are described. Experimental studies in the Sn-Cd system are carried out in thin capillary samples to minimize fluid flow effects that are dominant in most experiments. Critical conditions for the observation of composite microstructures are evaluated. These results will be presented to support the predictions of the models.

**Perepezko, J. H.**, “Nucleation controlled phase selection during solidification,” *Materials Science and Engineering*, A413-414, 389-397, 2005.

*Professor Perepezko is at the University of Wisconsin-Madison, where he is the Principal Investigator on the ground-based project “The Dynamics of Heterogeneous Solidification Microstructure Genesis in Undercooled Composite Systems.”*

An important and long-standing goal in the analysis and modeling of solidification processing is the identification and prediction of microstructural evolution in order to

provide a control over solidification structure. The advances towards achieving the goal are significant especially with regard to the role of growth kinetics competition in microstructure selection. At the same time there have been advances in the analysis of the initial phase selection during nucleation that plays a central role in the overall evolution of solidification microstructure. During product phase transitions that develop with changing undercooling level or alloy composition, competitive nucleation can yield mixed phase microstructures of both stable and metastable phases as shown for rapid solidification of eutectic, peritectic and glass forming alloys. At low undercooling the key role of interface catalysis is evident as well as an inhibited growth to allow for the optimization of the nucleation density during grain refining processes. At high undercooling, during crystallization of bulk melts or devitrification of metallic glass, the nucleation onset and the initial phase selection are usually determined by a heterogeneous nucleation on catalytic sites that are developed through either ex situ or in situ processes. The complete analysis of solidification microstructure evolution requires the consideration of the dynamic kinetic competition that is the basis of phase selection transitions.

Ko, Eunjung, M. M. G. Alemany, **Jeffrey J. Derby**, and James R. Chelikowsky, “*Ab initio* simulations of nonstoichiometric  $\text{Cd}_x\text{Te}_{1-x}$  liquids,” *Journal of Chemical Physics*, 123, 1-8, 2005.

*Dr. Alemany is at Universidad de Santiago de Compostela, Spain. The other authors are at University of Minnesota where Professor Derby is the Principal Investigator on the ground-based project “First Principles Calculations of Molten II-VI Compounds and their Solidification Behavior.”*

We present *ab initio* molecular-dynamics simulations for  $\text{Cd}_x\text{Te}_{1-x}$  liquids where the composition is nonstoichiometric. The simulations are performed following Born-Oppenheimer molecular dynamics. The required forces are obtained from a solution of the Kohn-Sham equation using *ab initio* pseudopotentials. We consider stoichiometries of the form:  $\text{Cd}_x\text{Te}_{1-x}$ , where  $x=0.2, 0.4, 0.6$ , and  $0.8$ . For each composition of the melt, we consider a range of temperatures near the experimentally determined liquid temperatures. We examine the microstructural properties of the melt, the viscosity, and self-diffusion properties of the liquid as a function of the stoichiometry and temperature. We also perform an analysis of the distribution of the electronic density of states in these liquids. We find that structural changes in the local order, experimentally predicted to occur when the concentration of Cd is increased, are closely related to changes in the electronic properties of the melt.

Ko, Eunjung, M. M. G. Alemany, and James R. Chelikowsky, “Viscosities of liquid CdTe near melting point from *ab initio* molecular-dynamics calculations,” *Journal of Chemical Physics*, 121, 942–945, 2004.

*The work was supported by NASA. The authors are at the University of Minnesota, Minneapolis, where **Professor Derby** is the Principal Investigator on the ground-based project “First Principles Calculations of Molten II-VI Compounds and their Solidification Behavior.”*

Recent experimental results for the viscosity of liquid CdTe exhibit disparate behavior as a function of temperature. While some measurements show the expected Arrhenius-type behavior, other measurements show an anomalous temperature dependence indicating an increase in viscosity with increasing temperature. We present *ab initio* molecular-dynamics simulations of liquid cadmium telluride near its melting point and use the Stokes–Einstein relation to extract values of the viscosity constant. We find no anomalous behavior; the viscosity decreases monotonically with temperature and is consistent with an Arrhenius like behavior. Although calculated values are slightly smaller than those measured, the predicted activation energy agrees well with experiment.

Zhu, Dongmei , C. S. Ray, Wancheng Zhou and **D. E. Day**, “On glass formation for a  $\text{Na}_2\text{O}\cdot 4\text{TeO}_2$  melt: Effect of melting temperature, time, and raw material,” *Journal of Materials Science*, 39, 7351-7357, 2005.

*Dr. Zhou is at Northwestern Polytechnic University, Xi’an, Shaanxi. Dr. Ray is at MSFC, while the other authors are at University of Missouri-Rolla, where Professor Day is the Principal Investigator on the transition experiment “Kinetics of Nucleation and Crystal Growth in Glass Forming Melts in Microgravity,” which has passed its Science Concept Review.*

The effect of melting temperature, time, and the type of raw material,  $\text{NaNO}_3$  or  $\text{Na}_2\text{CO}_3$ , as a source for  $\text{Na}_2\text{O}$  on the glass formation for a  $\text{Na}_2\text{O}\cdot 4\text{TeO}_2(\text{NT}_4)$  melt was investigated. Melting with  $\text{NaNO}_3$  at  $750^\circ\text{C}$  for a short time (15 min) produced a glass that is slightly more chemically durable and more resistant to crystallization than glasses melted at a higher temperature ( $800^\circ\text{C}$ ), or for a longer time (60 min), or using  $\text{Na}_2\text{CO}_3$ . A thin surface layer (<1.5 nm) that contains some nitrogen and a higher concentration of bridging oxygen is suspected to be the reason for the higher chemical durability and higher resistance to crystallization for this glass. However, melting at  $800^\circ\text{C}$  for 60 min produced a glass, whose properties were independent of the type of raw material,  $\text{NaNO}_3$  or  $\text{Na}_2\text{CO}_3$ , used.

Heinen, O., D. Holland-Moritz, D.M. Herlach, and **K.F. Kelton**, “In situ diffraction studies of the phase selection in undercooled Ti–Fe–Si–O melts,” *Journal of Crystal Growth*, 286, 146-151, 2006.

*Professor Kelton, is from Washington University, St. Louis. He is the Principal Investigator on the project “Studies of Nucleation and Growth, Specific Heat and Viscosity of Undercooled Melts of Quasicrystals and Polytetrahedral-Phase-Forming Alloys,” a flight*

*project which has transitioned to ground, having passed the Science Concept Review. The other authors are at Insitut für Raumsimulation, DLR, Germany.*

A time-resolved in situ determination of the phase formation sequence in undercooled Ti-Fe-Si-O melts was performed using the combination of electromagnetic levitation and energy-dispersive X-ray diffraction of synchrotron radiation. Ti-Fe-Si-O alloys are known to form a large variety of stable and metastable phases, including quasicrystals and approximant phases. Different solidification pathways are found as a function of undercooling, with the primary nucleation of the 1/1 crystal approximant phase from the liquid occurring at the largest undercoolings. The results on phase selection are discussed with respect to the influence of the short-range order in the undercooled liquid on the nucleation behavior of solid phases.

Cui, X. and **B. Q. Li**, “Discontinuous finite element solution of 2-D radiative transfer with and without axisymmetry,” *Journal of Quantitative Spectroscopy and Radiative Transfer*, 96, 383-407, 2005.

*The authors are at Washington State University where Professor Li is the PI on the ground-based project “Study of magnetic field effects on convection and solidification in normal and microgravity.”*

A discontinuous Galerkin finite element methodology is presented for the computation of two-dimensional (2-D) radiative transfer in participating media with and without axisymmetry. The central idea of the discontinuous formulation is that the variables are allowed to be discontinuous across the inter-element boundaries. Consequently, the formulation should be particularly useful for radiative transfer calculations where the radiation intensity experiences a jump across the boundary. Being able to compute an axisymmetric problem over a 2-D mesh rather than using one three-dimensional (3-D) scenario results in reduced computing time and lower memory storage requirements. Mathematical formulations and numerical implementations using the discontinuous finite element (DFE) method for radiative transfer are given. The procedures for incorporating the mapping of the discontinuous formulation of radiative transfer develop a unified approach to both 2-D and 2-D axisymmetric problems are discussed in detail. The computed results are given, and they compare well with the solutions reported in the literature that were obtained using other methods. Examples include both non-scattering and scattering cases. The effects of the solid-angular and spatial discretization on the accuracy of results are discussed. Numerical simulations show that an even discretization of solid angle is important to ensure an adequate numerical accuracy.

Kim, T. H., G. W. Lee, B. Sieve, A. K. Gangopadhyay, R. W. Hyers, T. J. Rathz, J. R. Rogers, D. S. Robinson, **K. F. Kelton**, and A. I. Goldman, “*In situ* High-Energy X-Ray Diffraction Study of the Local Structure of

Supercooled Liquid Si,” *Physical Review Letters*, 95, 085501 (4 pages), 2005.

*Professor Kelton, the PI on the project “Studies of Nucleation and Growth, Specific Heat and Viscosity of Undercooled Melts of Quasicrystals and Polytetrahedral-Phase-Forming Alloys,” is at Washington University, St. Louis, as are Messrs. Kim, Gangopadhyay and Lee. This is a transition project which had passed its Science Concept Review. Dr. Rogers and Mr. Rathz are at MSFC, while Dr. Hyers is at University of Massachusetts. Drs Sieve and Robinson are at Iowa State University.*

Employing the technique of electrostatic levitation, coupled with high-energy x-ray diffraction and rapid data acquisition methods, we have obtained high quality structural data more deeply into the supercooled regime of liquid silicon than has been possible before. No change in coordination number is observed in this temperature range, calling into question previous experimental claims of structural evidence for the existence of a liquid-liquid phase transition.

Sofonea, V, and **R. F. Sekerka**, “Diffusivity of Two-component Isothermal Finite Difference Lattice Boltzmann Models,” *International Journal of Modern Physics C*, 16, 1075-1090, 2005.

*Dr. Sofonea is at the Center for Fundamental and Advanced Technical Research, Romanian Academy, Romania. Professor Sekerka, the Principal Investigator for the ground-based project “Lattice Boltzmann Computations of Binary Diffusion under Stochastic Microgravity” is at Carnegie Mellon University.*

Diffusion equations are derived for an isothermal lattice Boltzmann model with two components. The first-order upwind finite difference scheme is used to solve the evolution equations for the distribution functions. When using this scheme, the numerical diffusivity, which is a spurious diffusivity in addition to the physical diffusivity, is proportional to the lattice spacing and significantly exceeds the physical value of the diffusivity if the number of lattice nodes per unit length is too small. Flux limiter schemes are introduced to overcome this problem. Empirical analysis of the results of flux limiter schemes shows that the numerical diffusivity is very small and depends quadratically on the lattice spacing.

**Chernov, A. A.**, L. N. Rashkovich, and P. G. Velikov, “Steps in solution growth: dynamics of kinks, bunching and turbulence,” *Journal of Crystal Growth*, 275, 1-18, 2005.

*Dr. Chernov is with BAE Systems, and is the Principal Investigator on the ground based project “Morphological Stability of Stepped Interfaces Growing From Solution.” Dr. Rashkovich is at Moscow State University, while Dr. Vekilov is at University of Houston.*

New findings on calcium oxalate monohydrate, monoclinic lysozyme and potassium dihydrophosphate crystal growth are presented and discussed. Atomic force microscopy was applied to measure step rates on CaOx and monoclinic lysozyme faces to understand kink kinetics. High precision Michelson interferometry allowed to discover step splitting on the (1 0 1) KH<sub>2</sub>PO<sub>4</sub> face growing from turbulent solution. In all three cases, aqueous solutions at room temperature were used.



CaOx was grown from solution in which the ion concentration ratio  $\xi = [\text{Ox}]/[\text{Ca}] = 5 \times 10^{-2}$ ,  $10^{-1}$ , 1, 10, 20. The rate  $v$  of steps one lattice spacing high on the (1 0 0) face reach maximum at  $\xi = 1$ . Attachment and detachment statistics of two types of particles (Ca and Ox) to a kink on the step of a non-Kossel crystal predicted the reciprocal kink propagation rate to be  $1/v \sim \xi^{1/2} + \xi^{-1/2}$ , consistent with experiment.

Step morphology on the (1 0 1) face of monoclinic lysozyme suggests rhombic, about rectangular 2D critical nucleus. In such a nucleus, two mutually parallel, though crystallographically different steps making the opposite edges, are supposed to be equal. The segment lengths pinned at dislocation outcrop are found to be very different and experience huge scattering. These phenomena, treated as a result of different kink nucleation rates on parallel nearly kink-free steps "looking" to the opposite directions, are of kinetic rather than of thermodynamic origin.

Contrary to conventional observations, in a turbulent solution flow the average step bunch width and height were found to reach limits as bunches propagate along the face. These limits decrease when the flow rate increases from  $\sim 60$  to 200 cm/s. The phenomenon is explained by the turbulent nature of the solution flow. In this flow, due to penetration of turbulent eddies, diffusivity within the viscous solution boundary layer,  $D = D_0 + 0.5 u_t y$ , quickly increases with the distance  $y$  from the interface since the friction velocity,  $u_t$ , reaches several cm/s. Therefore, molecular diffusivity,  $D_0 \cong 10^{-5}$  cm<sup>2</sup>/s, is significant only within the  $\sim 20$ –40 nm thick solution layer over the interface. As the flow rate increases, the turbulent mixed solution approaches the growing stepped crystal face closer and shrinks the range within which steps interact with one another through their diffusion fields. This weak interaction results in step splitting.

Churilov, A., and **A. Ostrogorsky**, "Model of Te and Zn doped InSb Solidification in Space," *Journal of Thermophysics and Heat Transfer*, **19**, 542-547, 2005.

*The authors are at Rensselaer Polytechnic Institute where Professor Ostrogorsky is the Principal Investigator on the transition experiment "Space and Ground Based Crystal Growth Using a Magnetically Coupled Baffle," which has passed its Science Concept Review.*

Numerical simulations were performed to determine the effect of residual microaccelerations on the distribution of dopants (Te and Zn) during solidification of InSb in space. A moving geometry model was developed and used to account for the reduction in melt size during growth. The model demonstrates that diffusion controlled segregation in doped InSb can be obtained at  $10^{-5}g_0$  gravity for the considered growth parameters. The results for the moving geometry and semi-infinite melt domain models are compared to each other and to the analytical correlations for the case of diffusion controlled segregation.

Zhang, Haoyu, Yanghee Kim, and **Prabir K. Dutta**, “Controlled release of paraquat from surface-modified zeolite Y,” *Microporous and Mesoporous Materials*,” 88, 312-318, 2006.

*The authors are from The Ohio State University where Professor Dutta is the Principal Investigator on the ground-based project on “Reverse Micelle Based Synthesis of Microporous Materials in Microgravity.”*

The surface hydroxyl groups of zeolite Y were reacted with 1,1,3,3-tetramethyldisilazane,  $\text{HN}(\text{SiHMe}_2)_2$  under ambient conditions and the grafting of siloxy functionality on the zeolite was confirmed by infrared, NMR spectroscopy and elemental analysis. Paraquat (methyl viologen) was ion-exchanged into the zeolite, followed by treatment with the disilazane reagent. Surface modification of paraquat-loaded zeolites encapsulates the guest molecules in the zeolite cages and release of paraquat by ion-exchange with sodium ions was studied. The total amount of paraquat released was dependent on the concentration of  $\text{Na}^+$  in solution, and was similar for the derivatized and underivatized samples. In the absence of surface modification, equilibration occurred within 20 min, whereas with surface modification, the equilibration time was extended to 7 days. These kinetics are reflected in the effective diffusion coefficients ( $D$ ) of paraquat, with  $D = 1.2 \times 10^{-15} \text{ cm}^2 \text{ s}^{-1}$  for derivatized zeolite Y and  $D = 0.2\text{--}1.1 \times 10^{-7} \text{ cm}^2 \text{ s}^{-1}$  for the underivatized sample. Paraquat was chosen as the guest molecule, since it is widely used as an herbicide and its controlled release is of interest in agricultural applications.