

# Solid–Liquid Interfaces: Molecular Structure, Thermodynamics, and Crystallization

Mark Asta, Frans Spaepen, and  
J. Friso van der Veen, Guest Editors

## Abstract

Materials phenomena ranging from the melting or freezing of ice to biomineralization in living organisms, to lubrication and the commercial casting of superalloys, are known to be critically influenced by molecular-scale structure and processes occurring at the interfaces between the crystalline solid and liquid phases. The properties of solid–liquid interfaces have long been a topic of intense interest in materials science, primarily because of their role in governing nucleation, growth, and morphological evolution in crystal growth from the melt or solutions. This issue of the *MRS Bulletin* provides an overview, highlighting new developments in experiment, theory, and modeling techniques that have led to substantial recent progress in the characterization of the molecular-level structural and thermodynamic properties of solid–liquid interfaces and their consequences for a variety of crystallization phenomena.

**Keywords:** crystallization, molecular structure, solid–liquid interfaces, thermodynamics.

Over the past two decades, intense practical interest in vapor-phase crystal growth has motivated the development of an advanced understanding of the molecular-level structure, thermodynamics, and kinetic properties of solid–vapor surfaces. Detailed investigations of crystal surfaces have been made possible by the development and application of powerful scanning probe and electron microscopies, surface-sensitive x-ray characterization techniques, and advanced atomistic, mesoscopic, and continuum-level theoretical tools.

In contrast to the situation for solid–vapor surfaces, a molecular-level understanding of solid–liquid interfacial properties has remained substantially less developed. This situation can be attributed in part to the inherent difficulties associated with experimental characterizations of “buried” interfaces between two condensed phases. In

addition, theoretical and simulation studies of solid–liquid interfaces require as a prerequisite the ability to accurately model the structural properties of both crystalline and fluid phases; system-specific theoretical studies have remained few in number, with the most detailed work being devoted to model systems with relatively simple interatomic interactions.

Despite the inherent challenges associated with molecular-level studies of solid–liquid interfaces, over the past decade a number of developments in experimental and simulation methods have been realized that are leading to rapid progress. It is the intent of this issue of *MRS Bulletin* to present some highlights of recent work in this area, focusing in particular on issues germane to the understanding of phenomena related to crystallization from the melt or solutions across a broad class of materials systems.

Traditionally, solid–liquid interfaces are characterized by the degree of structural order that they exhibit. “Smooth,” or faceted, interfaces are characterized by an atomically abrupt change in the degree of crystalline order across the solid–liquid boundary. Such interfaces have structures that can be described by analogy to the familiar picture of low-temperature solid–vacuum surfaces, where well-defined “terraces” are separated by abrupt atomic-scale steps. Molecularly “rough” solid–liquid interfaces, by contrast, are more suitably described as being structurally diffuse, with a degree of crystalline order that varies continuously over the scale of a few atomic planes across the solid–liquid boundary. Such interfaces are characteristically highly dynamic on an atomic scale, with interface atoms rapidly fluctuating between solid- and liquid-like environments. While “smooth” solid–liquid interfaces usually possess highly anisotropic properties, giving rise to faceted growth morphologies, molecularly rough interfaces are typically weakly anisotropic and lead to the formation of intricate dendritic solidification morphologies. The articles in this issue cover phenomena associated with both smooth and rough classes of solid–liquid interfaces in a broad range of materials systems and contrast the mechanisms involved in crystallization in both cases.

In the first article, Chernov et al. provide an overview of recent developments in the theoretical understanding of step and kink dynamics for faceted solid–liquid interfaces, in the context of the crystallization of inorganic and protein crystals from solution. Interest in solution growth originates from a variety of practical applications in materials, biological, and environmental sciences. Such general interest has motivated in-depth experimental studies over the past decade that have employed *in situ* atomic force microscopy and related techniques to characterize the structure and dynamics of steps during crystal growth from solution. These detailed experimental investigations have raised a number of new fundamental questions, which have been the focus of recent theoretical work aimed at advancing the state of understanding of step dynamics on faceted solid–liquid interfaces in solution growth. These theoretical developments and an overview of the key experimental observations that have motivated them form the focus of the review by Chernov et al.

While faceted solid–liquid interfaces are typically observed in crystal growth from solutions, molecularly rough interfaces are common in the solidification of materials such as metals and colloids from their melts. Until recently, much of the most de-

tailed information related to the structural and thermodynamic properties of molecularly rough solid–liquid interfaces has been provided by atomic-scale computer simulations, as represented by the pioneering work of Broughton and Gilmer<sup>1</sup> for model Lennard–Jones systems (i.e., systems interacting with repulsive  $1/r^{12}$  and attractive  $1/r^6$  interactions, where  $r$  is the interatomic separation).

The second article in this issue, by Hoyt et al., provides an overview of the state of understanding of the thermodynamic and kinetic properties of molecularly rough crystal–melt interfaces as they have been derived from recent atomistic simulations for a variety of model systems as well as several specific metals. These studies have provided new insights into variations in interfacial free energy with crystal structure, an issue germane to the nucleation of metastable phases in deeply undercooled melts. A particular emphasis in the article is given to the degree of anisotropy in interfacial free energies and mobilities exhibited in metallic crystal–melt interfaces. While such anisotropies are generally weak for rough solid–liquid interfaces, they nevertheless have important consequences for the morphologies observed in dendritic solidification. The predictions of numerical simulations for interfacial free energy anisotropies are shown to compare favorably with recent equilibrium crystal shape measurements in metal alloy systems, which are also described. The authors discuss how these predictions have led to new insights into unusual dendritic growth morphologies observed in commercial Al-based alloy systems.

In seminal work by Turnbull<sup>2</sup> more than 50 years ago, the first measurements of solid–liquid interfacial free energies in metals were derived from nucleation studies in undercooled melts (see Figure 1). Since that time, experimental studies of nucleation have continued to provide one of the most common frameworks for investigating thermodynamic properties of solid–liquid interfaces. The article by Kelton et al. provides an overview of the current state of the art in such studies. The authors describe recent experimental work employing novel “containerless processing” (e.g., electrostatic or electromagnetic levitation) methods, which enable one to deeply undercool alloy melts. Experiments employing this technique have provided new evidence for the development of icosahedral order in undercooled melts, and the significance of this finding for the nucleation of solids is discussed. Specifically, experimental observations and theoretical analyses indicate that the solid–liquid interfacial free energy is a decreasing function of the

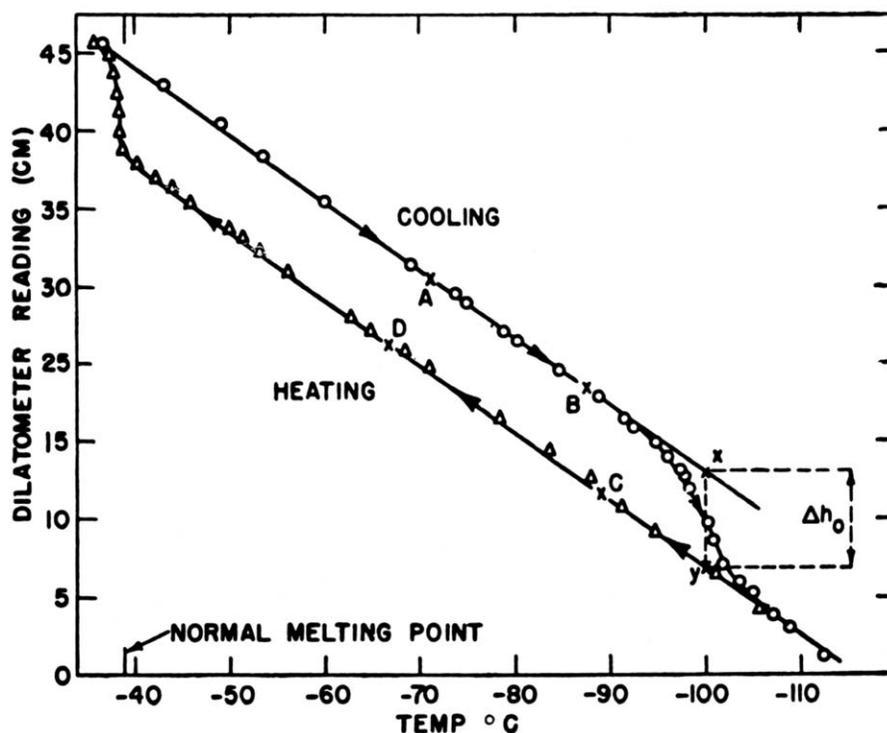


Figure 1. Turnbull's demonstration (1952) of large undercooling of liquid mercury.<sup>2</sup> Emulsification of the liquid into micron-sized droplets isolated the heterogeneous nucleants (“motes”) into a small number of droplets, so that most of the liquid crystallized by homogeneous nucleation. The crystallization was observed by the change in volume, measured as a dilatometer height,  $\Delta h_0$ . These experiments established that the structure of the liquid is fundamentally different from that of the crystal and inspired Frank's hypothesis of icosahedral (polytetrahedral) short-range order in simple liquids.<sup>3</sup> Turnbull's analysis of the data with classical nucleation theory showed that the solid–liquid interfacial energy is large (equivalent to melting 61% of a monolayer) and increases with temperature.

degree of local tetrahedral and icosahedral order in the crystalline solid phase. The specific emphasis in the article is on the effects that ordering in the liquid and at solid–liquid interfaces have upon both heterogeneous and homogeneous nucleation processes in alloy melts. Thus, the article also describes experimental investigations of magnetic ordering in deeply undercooled melts of ferromagnetic alloys and the influence of substrate structure of “catalysts” on heterogeneous crystal nucleation.

The article by Wu et al. is a more detailed look at the problem of extracting a value for the solid–liquid interfacial energy from crystal nucleation experiments. Gibbs first calculated the work to form a spherical crystal nucleus in an undercooled melt by separating it into a bulk term proportional to the number of atoms in the cluster, and a surface term proportional to its surface area. Even though the approach has been remarkably successful, especially for condensation from the vapor, a number of fundamental questions remain, some of

them related to the fundamentals of nucleation and others to the specifics of the solid–liquid phase transformation. This article reviews the thermodynamics necessary for a rigorous calculation of the reversible work, as well as the assumptions commonly used to calculate a nucleation rate from this work. Aspects of the problem that complicate the Gibbsian picture include the nonspherical shape of the nucleus (which can be highly irregular for small interfacial energies, as in the crystallization of colloidal suspensions), the temperature coefficient of the interfacial energy (generally thought to be positive due to the entropy loss in the liquid near the interface), and the possible dependence of the interfacial energy on the size of the nucleus. The article shows how theory (thermodynamic, density functional), computer simulation (molecular dynamics, phase field), and experimental simulation (confocal microscopy on colloidal suspensions) can shed light on the problem.

The final two articles highlight the current state of the art in the application of

electron microscopy and x-ray scattering techniques to investigations of the structural, kinetic, and thermodynamic properties of solid–liquid interfaces.

The article by Howe and Saka describes how *in situ* transmission electron microscopy (TEM) studies allow determination of the structure, chemistry, and kinetic behavior of solid–liquid interfaces with sub-nanometer spatial resolution. Examples are given illustrating the applications of TEM to measurements of equilibrium ordering and compositional profiles across solid–liquid interfaces. It is also demonstrated how, through the use of calibrated heating holders, it is possible to study the dynamics of interface motion with growth velocities as low as  $\sim 2$  nm/s. Such investigations open the way for the first direct analyses of the kinetics and mechanisms governing interface migration. The measurement of size-dependent melting temperatures in small particles provides a strategy for probing interfacial thermodynamic properties, through the well-known Gibbs–Thomson relations. Howe and Saka include as a final example the application of TEM to studies of the equilibrium melting

temperatures of small particles embedded in a crystalline matrix. They demonstrate that the melting point of such particles can be either elevated or depressed depending on the relative magnitudes of the solid–matrix, liquid–matrix, and solid–liquid interfacial free energies.

The final article, by van der Veen and Reichert, highlights recent applications of state-of-the-art synchrotron x-ray scattering measurements to the study of structural ordering at solid–liquid interfaces. The article includes a brief overview of the techniques used to probe solid–liquid interface structure with x-rays and discusses a range of applications illustrating the detailed information that can be derived from such techniques. Specifically, the article includes examples taken from recent work by the authors to water–solid interfaces, liquid–metal/solid–semiconductor interfaces and colloids in confinement between solids. In general, the solid surface is found to induce ordering within the liquid both in the perpendicular and in-plane directions. For liquid Pb on Si(100), a fivefold local symmetry was observed adjacent to the

silicon wall, evidencing the icosahedral ordering discussed in the article by Kelton et al. for metallic bulk melts. The authors also treat the effect of two opposing interfaces, which may differ substantially from that of a single interface. The most interesting example in nature is that of water sandwiched by two solids. Studies of the melting of ice in contact with silica revealed interfacial melting as a precursor of bulk melting, where the watery layer was found to have an anomalously high density.

How freezing and melting phenomena are influenced by the presence of interfaces may be predicted by consideration of interfacial free energies and classical nucleation, but these depend strongly on local atomic-scale ordering effects, about which we have only recently begun to gain more knowledge.

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**Mark Asta**, Guest Editor for this issue of *MRS Bulletin*, is an associate professor in the Department of Materials Science and Engineering at Northwestern University in Evanston, Ill. His group works in the area of computational materials science, focusing on the development and application of atomistic and first-principles methods for simulating thermodynamic and kinetic properties in bulk alloys and at surfaces and interfaces. These methods are currently being applied in the modeling of surface phase diagrams, microstructural evolution in crystal growth from the melt and vapor, and as an integral component in computer-aided materials design projects.

From 1988 to 1993, Asta did his PhD work at the University of California at Berkeley with D. de Fontaine on the topic of *ab initio* calculations of alloy phase diagrams.

He subsequently joined Sandia National Laboratories at Livermore, Calif., as a postdoctoral researcher and then as a member of technical staff. He joined the faculty at Northwestern in 2000.

In 2002, Asta was awarded ASM International's Materials Research Silver Medal Award. He is currently on the editorial board for the journal CALPHAD and is a key reader for *Metallurgical and Materials Transactions*.

Asta can be reached at the Department of Materials Science and Engineering, Northwestern University, 2225 N. Campus Dr., Evanston, IL 60208 USA; tel. 847-491-5940 and e-mail m-asta@northwestern.edu.

**Frans Spaepen**, Guest Editor for this issue of *MRS Bulletin*, is the John C. and Helen F. Franklin Professor of Applied Physics at Harvard University. His research in-



Mark Asta

terests span a wide range of experimental and theoretical topics in materials science, such as amorphous metals and semiconductors (viscosity, diffusion, mechanical properties), the structure and thermodynamics of interfaces (crystal/melt, amorphous/crystalline semiconductors, grain boundaries), mechanical properties of thin films, the perfection of silicon crystals for metrological applications, and colloidal systems as models for the study of dynamics and defects in crystals and glasses.



Frans Spaepen

Spaepen earned his undergraduate degree in metallurgical engineering at the K.U. Leuven in 1971, and his PhD degree in applied physics from Harvard in 1975. He joined the faculty of the Division of Applied Sciences at Harvard in 1977 as assistant professor, was appointed associate professor in 1981, and full professor in 1983. In 1984, he was a visiting professor in Leuven, and in 2000 and 2002 he was a Humboldt visitor at DLR-Köln and FZ-Jülich. From 1990 to



J. Friso van der Veen

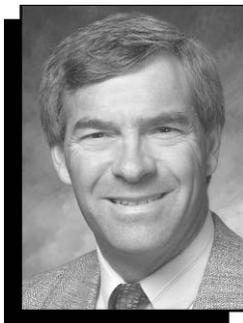
1998, Spaepen was Director of the Harvard Materials Research Laboratory/Materials Research Science and Engineering Center. He has been the director of the Rowland Institute at Harvard since 2001. He is co-editor of *Solid State Physics*.

Spaepen can be reached by e-mail at spaepen@deas.harvard.edu.

**J. Friso van der Veen**, Guest Editor for this issue of *MRS Bulletin*, has been a professor of experimental physics at the ETH Zurich since



Alexander A. Chernov



James J. De Yoreo



László Gránásy



A. Lindsay Greer



Tomorr Haxhimali



Dieter M. Herlach

2000. He heads the Research Department for Synchrotron Radiation and Nanotechnology at the Paul Scherrer Institute, in Villigen, Switzerland. This department is home of the Swiss Light Source (SLS). His current research interests lie in the application of synchrotron x-ray scattering techniques for studies of the structural properties of solid–liquid interfaces and of confined fluid films. His earlier work includes the use of medium-energy ion scattering and synchrotron radiation-based XUV electron spectroscopy and x-ray diffraction for studies of the geometric and electronic structure of single-crystal surfaces. He studied physics at the University of Utrecht and earned his doctorate in 1978 with a thesis on a surface science topic. In 1980, after spending a year as postdoctoral researcher at IBM Yorktown Heights, van der Veen joined the staff at the FOM–Institute for

Atomic and Molecular Physics in Amsterdam. In 1987, he became head of the surface physics department, and in 1997, he was appointed professor of experimental physics at the Van der Waals–Zeeman Institute of the University of Amsterdam.

He has authored or co-authored more than 200 research papers. In 1998, van der Veen was awarded the IUVSTA Prize by the International Union for Vacuum Science, Techniques, and Applications for his research, in particular, for his studies of surface melting.

Van der Veen can be reached by e-mail at [friso.vanderveen@psi.ch](mailto:friso.vanderveen@psi.ch).

**Alexander A. Chernov** is a chief scientist at the NASA Marshall Space Flight Center, and employed by BAE Systems Analytical Solutions. He graduated with a degree in physics from Moscow State University, then

joined the Institute of Crystallography of the USSR (later Russian) Academy of Sciences.

Chernov's major scientific interests are in all branches of crystallization, surface science, inorganic, and biological materials sciences. His work includes layer crystal growth theory and stability, impurities and the formation of other defects, the first computer simulation of crystal growth, kinetic phase transitions, surface melting, CVD, epitaxy, protein crystallization, and deformation.

Chernov has authored approximately 300 publications, including two books. In 1987, he was elected to the Russian Academy of Sciences (RAS). Chernov has been awarded the Russian Federation Government Prize for science and technology, the inaugural F.C. Frank Prize from the International Organization for Crystal Growth, and the E.S. Fyodor Prize from the RAS.

Chernov can be reached by e-mail at [alex.chernov@msfc.nasa.gov](mailto:alex.chernov@msfc.nasa.gov).

**James J. De Yoreo** is director of the Bio-Security and Nanosciences Laboratory and is a physicist in the Chemistry and Materials Science Directorate at Lawrence Livermore National Laboratory (LLNL). His research has spanned a wide range of materials-related disciplines including solid-state physics, geophysics and geochemistry, crystal growth, and biomolecular materials. His current focus is the physics of materials organization at solid–liquid interfaces in biomolecular and biomineral systems.

De Yoreo received his BA degree in physics from Colby College in 1978 and his MA and PhD degrees in experimental physics from Cornell University in 1985. Following post-doctoral work at the University of Maine and Princeton University, he became a member of the LLNL technical staff in 1989. He was the recipient of an R&D 100 award in 1994 and the 2001 LLNL Science and Technology Award. He is a member of the executive committee of the American Association for Crystal Growth (AACG) and is vice president of AACG–West.

De Yoreo can be reached by e-mail at [deyoreo1@llnl.gov](mailto:deyoreo1@llnl.gov).

**László Gránásy** is the leader of the Phase Field Group at the Research Institute for Solid-State Physics and Optics of the Hungarian Academy of Sciences. He has been working for more than 10 years on nucleation problems using various discrete and continuum approaches including

cluster dynamics, density functional, and phase field techniques. His current research is concentrated on field theoretic modeling of polycrystalline solidification.

Gránásy has been a guest scientist at Tohoku University (Sendai, Japan), Max-Planck-Institut für Eisenforschung (Düsseldorf), the German Aerospace Center (Cologne, Alexander von Humboldt scholarship), the University of Sheffield (British Council fellowship), the University of Chicago, the University of Bergen (Norway), and the National Institute of Standards and Technology. He has a PhD degree in physics from the Roland Eötvös University, Budapest (1982), and received the Candidate of Science degree of the Hungarian Academy of Sciences in 1989.

In 2000, Gránásy was awarded a Széchenyi Professorship at the Technical University of Budapest. He has received various awards, including the Research Award of the Hungarian Academy of Sciences (2000). He has authored or co-authored more than 120 scientific publications and has over 870 independent citations to his work. He is a member of various Topical Teams of the European Space Agency.

Gránásy can be reached by e-mail at [grana@szfki.hu](mailto:grana@szfki.hu).

**A. Lindsay Greer** is deputy head of the Department of Materials Science and Metallurgy at the University of Cambridge. After earning a PhD degree at Cambridge, he undertook postdoctoral work and was an assistant professor of applied physics at

Harvard University before returning to a faculty position in Cambridge. Greer's research interests are in microstructural kinetics, specifically on glass formation and crystal nucleation. His work on nucleation has concentrated on the grain refinement of aluminum alloys. Other interests are bulk metallic glasses, chalcogenide thin films for phase-change data storage, and electromigration in thin-film conductors. Greer is editor of *Philosophical Magazine* and has been chair of the *MRS Bulletin* Editorial Board.

Greer can be reached by e-mail at [alg13@cam.ac.uk](mailto:alg13@cam.ac.uk).

**Tomorr Haxhimali** is currently completing his PhD thesis in the Physics Department at Northeastern University in Boston under the supervision of Alain Karma. His thesis focuses on phase-field computations of dendritic evolution.

Haxhimali can be reached by e-mail at [haxhimali.t@neu.edu](mailto:haxhimali.t@neu.edu).

**Dieter M. Herlach** is a professor of physics at the Ruhr-Universität Bochum and a senior scientist at the German Aerospace Center (Cologne), where he is group leader of the Institute of Space Simulation. He studied physics at the Technical University Aachen and earned his PhD degree at the same university in 1981, for his research on low-temperature physics. After his education in Aachen, he was employed at the University Duisburg as a university assistant, where he focused on the science of magnetism. In 1983,



**Dirk Holland-Moritz**

Herlach moved to the German Aerospace Center and established a new research area on nonequilibrium solidification of undercooled melts. In 1991, he received the degree of a university lecturer at Ruhr-Universität Bochum, and he was nominated as professor in experimental physics in 1998. He has spent sabbaticals at the University of Cambridge (1988) and at Harvard University (1997). He was appointed full professor at the Ruhr-Universität Bochum in 2001.

Herlach can be reached by e-mail at [Dieter.Herlach@dlr.de](mailto:Dieter.Herlach@dlr.de) and via URL [www.dlr.de/rs/forschung/zeus/UK/mitarbeiter/Herlach](http://www.dlr.de/rs/forschung/zeus/UK/mitarbeiter/Herlach).

**Dirk Holland-Moritz** is a research scientist at the Institute of Space Simulation within the German Aerospace Center (Cologne). He studied physics at the University of Cologne, earning the diploma degree in 1990. In 1994, he earned his PhD degree in physics from the Technical University Aachen. From 1999 to 2000, he was a guest scientist in the Division of Engineering and Applied Sciences at Harvard University. In 2004, he qualified as a private lecturer at the Ruhr-Universität Bochum. Holland-



**James M. Howe**



**Leonid N. Rashkovich**

Moritz's main research fields are the physics of undercooled metallic melts, solidification behavior in undercooled metallic liquids, and quasicrystalline solids.

Holland-Moritz can be reached by e-mail at [dirk.holland-moritz@dlr.de](mailto:dirk.holland-moritz@dlr.de).

**James M. Howe** is a professor in the Department of Materials Science and Engineering at the University of Virginia. His current research emphasizes the application of high-resolution and analytical transmission electron microscope techniques to study the mechanisms and kinetics of phase transformations in nanoparticles and the behavior of interphase boundaries at the atomic level. He received his PhD degree in materials science from the University of California at Berkeley in 1985 and joined the Department of Metallurgical Engi-



**Jeffrey J. Hoyt**



**Harald Reichert**

neering and Materials Science at Carnegie Mellon University as Alcoa Assistant Professor of Physical Metallurgy. While at Carnegie Mellon, Howe became an associate professor and served as technical director for the Alcoa Center for Engineered Materials. In 1991, Howe joined the Materials Science and Engineering faculty at the University of Virginia. He has served as director of the Electron Microscope Facility since then and was promoted to full professor in 1999.

Howe has received several awards for his research, including a Presidential Young Investigator Award from the National Science Foundation in 1985, a Humboldt Senior Research Award from the Alexander von Humboldt Foundation in Germany in 1999, and the Materials Science Research Silver Medal



**Alain Karma**



**Hiroyasu Saka**

from ASM International in 2000. He was elected a fellow of ASM International in 1997.

Howe has published more than 190 technical papers, two book chapters, and two symposium proceedings on transformation interfaces and electron microscopy. He is the author of the textbook *Interfaces in Materials* (1997) and co-author with B. Fultz of the textbook *Transmission Electron Microscopy and Diffractometry of Materials*, published in 2001.

Howe can be reached by e-mail at [jh9s@virginia.edu](mailto:jh9s@virginia.edu).

**Jeffrey J. Hoyt** is a Principal Member of Technical Staff at Sandia National Laboratories in the Materials and Process Modeling and Simulation Department. His research involves molecular dynamics and Monte Carlo simulations of solidification processes in alloys as



**Kenneth F. Kelton**



**Brian B. Laird**



**James R. Morris**



**Ralph E. Napolitano**

interfaces, liquids, and amorphous materials and the development of advanced algorithms for molecular dynamics simulation. He is also the team leader of the molecular modeling group for the Center for Environmentally Beneficial Catalysis, a multi-university Engineering Research Center sponsored by the National Science Foundation and headquartered at the University of Kansas.

Laird received his PhD degree in theoretical chemistry (theory and simulation of the freezing transition) in 1987 from the University of California at Berkeley.

Laird can be reached by e-mail at [blaird@ku.edu](mailto:blaird@ku.edu), and via URL <http://www.chem.ku.edu/blaird/>.

**James R. Morris** is a member of Senior Research and Development Staff in the Alloy Behavior and Design Group of the Metals and Ceramics Division at Oak Ridge National Laboratory. He received a BS degree in physics from Colorado State University in 1987 and a PhD degree from Cornell University in 1992. From 1992 to 2003, Morris was a researcher in the Metals and Engineering Physics Program at Ames Laboratory and Iowa State University. His research interests include structure of liquid metals and alloys; nucleation and solidification from the melt; phase stability, defects, and mechanical properties in metals and alloys; and martensitic phase transformations.

Morris can be reached by e-mail at [morrisj@ornl.gov](mailto:morrisj@ornl.gov).

**Ralph E. Napolitano** has been assistant pro-

St. John's College. Kelton's primary research interests are nucleation in condensed phases and the formation and structures of liquid, amorphous, quasicrystal, and complex crystal phases. His work on nucleation has focused on time-dependent nucleation, coupled kinetic processes, and the relations between the structures of the initial and final phases and the nucleation barrier. His research activities have also focused on the structure of Ti/Zr-based quasicrystals and their possible use in hydrogen storage applications. Kelton is the U.S. regional editor for the *Journal of Non-Crystalline Solids*.

Kelton can be reached by e-mail at [kfk@wuphys.wustl.edu](mailto:kfk@wuphys.wustl.edu), and via URL <http://wuphys.wustl.edu/~kfk/>.

**Brian B. Laird** is a professor in the Chemistry Department at the University of Kansas, where he also serves as associate chair for graduate programs. His research interests involve the application of statistical mechanics and computer simulation to the determination of chemically relevant materials properties. Specific areas of research include fundamental investigations into the structure, dynamics, and thermodynamics of crystal–melt



**Rohit Trivedi**



**Peter G. Vekilov**



**David T. Wu**

well as irradiation effects in materials. Prior to joining Sandia, Hoyt was on the faculty of the Department of Mechanical and Materials Engineering at Washington State University. Hoyt holds a PhD degree from the University of California, Berkeley, and is the author of more than 50 scientific publications in the area of thermodynamics and phase transformations.

Hoyt can be reached by e-mail at [jjhoyt@sandia.gov](mailto:jjhoyt@sandia.gov).

**Alain Karma** is a College of Arts and Sciences Distinguished Professor in the Physics Department at Northeastern University in Boston. He received his PhD degree in physics from the University of California at Santa Barbara in 1985 and subsequently spent three years, from 1985 to 1988, at the California Institute of Technology as a Weingart Fellow in

Theoretical Physics before joining Northeastern in 1988.

His group works on developing theoretical models and computational tools to probe fundamental aspects of nonequilibrium interfacial patterns in condensed matter, including microstructural pattern formation in alloy solidification, surface growth, crack propagation, and corrosion. A main focus over the last decade has been the development of quantitative phase field approaches to these problems, with the most recent efforts concentrating on combining atomistic- and continuum-scale methods.

Karma is currently co-leading, with A.D. Rollet (Carnegie Mellon University), a 30-member Cooperative Research Team that is part of the DOE-funded CMSN (Computational Materials Science Network). This

team regroups computational materials scientists from U.S. universities and DOE labs with expertise in atomistic- and continuum-scale modeling of both solid–liquid and solid–solid interfaces and focuses on modeling microstructural evolution based on fundamental thermodynamic and kinetic properties of these interfaces.

Karma can be reached by e-mail at [a.karma@neu.edu](mailto:a.karma@neu.edu).

**Kenneth F. Kelton** is a professor of physics at Washington University in St. Louis, Mo. After earning a PhD degree at Harvard University in 1983, he continued in a postdoctoral position at Harvard and became an assistant professor in the Physics Department at Washington University in 1985. He has spent extended periods at Cambridge University, most recently as an Overseas Visiting Scholar in

essor in the Department of Materials Science and Engineering at Iowa State University since 2000. He received a BS degree in materials science and engineering from the University of Florida in 1989. From there, he worked as a research engineer for the Research and Development Division at Babcock & Wilcox until 1992, when he enrolled at the Georgia Institute of Technology, earning an MS degree in metallurgical engineering in 1994 and a PhD degree in materials science and engineering in 1996. From 1996 to 1998, he was an NRC Postdoctoral Fellow at the National Institute of Standards and Technology. Since 1998, he has been an assistant scientist and coordinator of the Solidification Science Area at Ames Laboratory.

Napolitano has received numerous awards, including the Excellence in Research Award from Iowa State University's Department of Materials Science and Engineering (2004), the Council of Outstanding Young Engineering Alumni from the Georgia Institute of Technology (2000), and the Grodsky Outstanding Senior Scholarship from the University of Florida's Department of Materials Science and Engineering in 1989.

Napolitano can be reached by e-mail at [ralphn@iastate.edu](mailto:ralphn@iastate.edu).

**Leonid N. Rashkovich** graduated from the D.I. Mendeleev Institute of Chemical Technology. After graduation, he joined the Institute of Building Materials; since 1964, he has been a faculty member and professor in the Physics Department at Moscow

State University and chair of Polymer and Crystal Physics. His major scientific interests are in the mechanisms and kinetics of crystallization in inorganic materials, proteins, and polymers. Rashkovich pioneered fast crystal growth technology from solution, which earned him the 1994 R&D 100 Award (for KDP crystal growth) and *in situ* high-precision laser interferometry to study processes on crystal surfaces growing from solution. He is the author of approximately 150 professional publications, including two books.

Rashkovich can be reached by e-mail at [rashk@polly.phys.msu.ru](mailto:rashk@polly.phys.msu.ru).

**Harald Reichert** is a group leader at the Max Planck Institute for Metal Research in Stuttgart, Germany. His research interests include the investigation of surface phase transformations, alloy physics, and the structure of solid–liquid interfaces, for which he is developing instrumentation at synchrotron radiation sources. In 2002, he received the Walter Schottky Award for Solid State Physics from the German Physical Society. He received his PhD degree in physics from Ludwigs-Maximilians-Universität in Munich and worked at the University of Houston as a postdoctoral researcher.

Reichert can be reached by e-mail at [reichert@mf.mpg.de](mailto:reichert@mf.mpg.de).

**Hiroyasu Saka** has been a professor in the Department of Quantum Engineering at Nagoya University in Japan since 1994. He received his bachelor's (1964), master's (1966), and

doctorate (1972) degrees in engineering from Nagoya University. In the intervening years, he has been a research associate for the Department of Metallurgy at Nagoya University (1970–1979), a British Council Scholar for the Department of Science of Materials at the University of Oxford (1977–1979), an associate professor in the Department of Metallurgy at Nagoya University (1979–1987), and a professor in the Department of Materials Science and Engineering at Nagoya University (1988–1994). His research interests include electron microscopy (conventional and *in situ*) of defects in crystalline materials and phase transformations (solid/solid, solid/liquid), specimen preparation techniques using a focused ion beam, and toughening of brittle materials by means of dislocations. Saka has authored or co-authored more than 300 publications in various scientific journals and proceedings.

Saka can be reached by e-mail at [saka@numse.nagoya-u.ac.jp](mailto:saka@numse.nagoya-u.ac.jp).

**Rohit Trivedi** is the Anson Marston Distinguished Professor in Engineering (since 1991), a professor of materials science and engineering, and a senior scientist and group leader at Ames Laboratory (since 1975) at Iowa State University. Previously, he was a research assistant (1962–1963), project engineer (1964–1965), assistant professor (1966–1970), and an associate professor (1970–1975) at Carnegie Mellon University. He has received numerous honors including the Iowa Distinguished

Faculty in Engineering Lecturer from the University of Iowa (2000), the Bruce Chalmers Award from the Metals, Minerals, and Materials Society (1995), the Senior Fulbright Award (1977–1978), and the Senior Alexander von Humboldt Award (1977–1978, 1984). He has been an invited or guest professor at numerous institutions and has published more than 170 papers and presented over 180 invited talks.

Trivedi can be reached by e-mail at [trivedi@ameslab.gov](mailto:trivedi@ameslab.gov).

**Peter G. Vekilov** is currently associate professor of chemical engineering at the University of Houston (UH) and a faculty member within the Institute for Molecular Design at UH and at the Keck Center for Computational Biology at Rice University. He earned his MS degree in chemistry from M.V. Lomonosov Moscow State University and his PhD degree in chemistry from the Russian Academy of Sciences. After postdoctoral appointments at the Bulgarian Academy of Sciences, the Institute for Bioscience and Human Technology in Tsukuba, Japan, and the University of Alabama in Huntsville (UAH), he became an assistant professor of chemistry at UAH. He is a recipient of the Dupont Research Award, the UAH Foundation Research Award, the International Union of Crystallography Young Scientist Award, and various other international and national awards. He serves as a member of the U.S. National Committee for Crystallography and the

Executive Council of the International Organization for Biological Crystallization, and he is a topic editor for *Crystal Growth and Design*. The main thrusts of Vekilov's research group are the physico-chemical fundamentals of phase transitions in protein solutions related to protein condensation diseases (sickle-cell anemia, cataracts, Alzheimer's disease, etc.), processes in healthy organisms, and other technological processes. His group has published approximately 100 papers.

Vekilov can be reached by e-mail at [vekilov@uh.edu](mailto:vekilov@uh.edu).

**David T. Wu** is an associate professor in the Department of Mechanical Engineering at Yale University. He received an AB degree in physics and SM and PhD degrees in applied physics from Harvard University. He has worked in teaching positions at Yale and Harvard in addition to being a systems engineer for Rockwell International's Electro-Optics Division. He was also a staff member and U.S. Department of Energy Distinguished Postdoctoral Fellow at Los Alamos National Laboratory and a visiting scientist at Universität des Saarlandes in Germany. Over the years, he has been honored with the Junior Faculty Fellowship in the Natural Sciences, the Hellman Family Fellowship for Junior Faculty, and the Moore Memorial Fund for Improving Undergraduate Curriculum, all from Yale.

Wu can be reached by e-mail at [d.wu@yale.edu](mailto:d.wu@yale.edu). □