

Susan B. Sinnott Guest Editor for this issue of MRS Bulletin Department of Materials Science and

Engineering, University of Florida, Gainesville, FL 32611, USA; tel. 352-846-3778; and email ssinn@mse.ufl.edu.

Sinnott is a professor of materials science and engineering and a University of Florida Research Foundation Professor. She received her BS degree in chemistry from the University of Texas, Austin, and her PhD degree in physical chemistry from Iowa State University. She was a postdoctoral associate at the Naval Research

Laboratory and was on the faculty at the University of Kentucky prior to joining the University of Florida. Her research interests include developing reactive empirical potentials and examining the properties and processing of materials using empirical and first-principles methods. Areas of interest include the chemical modification of polymer surfaces by ions, radicals and clusters, the stability of defects in oxides, the properties of heterogeneous interfaces, the stability of nanostructures, and investigating the origins of friction and wear. Sinnott is a Fellow of the Materials Research Society, American Vacuum Society, American Association for the Advancement of Science, and the American Ceramic Society.



Donald W. Brenner Guest Editor for this issue of MRS Bulletin

Department of Materials Science and Engineering, North Carolina State University, Raleigh, NC 27695-7907, USA; tel. 919-515-1338; and email brenner@ncsu.edu.

Brenner is a Kobe Steel Distinguished Professor in the Materials Science and Engineering Department at North Carolina State University (NCSU). He received his BS degree from the State University of New York in 1982 and his PhD degree from The Pennsylvania State University in 1987. He joined the Theoretical Chem-

istry Section at the US Naval Research Laboratory as a staff scientist in 1987, and joined the NCSU faculty in 1994. His research focuses on using atomic and mesoscale simulation and theory to understand technologically important processes and materials. Brenner's awards include the Reynolds Award for excellence in research, teaching, and outreach (2009) and the Feynman Award for Research in Nanotechnology (2002).



Michael Baskes

Department of Mechanical and Aerospace Engineering, University of California, San Diego (UCSD); email mbaskes@ucsd.edu. Baskes is an adjunct professor in the Depart-

ment of Mechanical and Aerospace Engineering at the University of California, San Diego (UCSD) and a laboratory associate-fellow at Los Alamos National Laboratory (LANL). He obtained his BS degree in engineering in 1965 and his PhD degree in materials science in 1970, both from the California Institute of Technology. He was then employed at Sandia National

Laboratories, LANL, and UCSD. Baskes's interests encompass the use of computational methods to investigate material properties. His major scientific accomplishments have been the development of the embedded atom method; the development of models to predict the behavior of helium in metals; and the development of a model to explain hydrogen isotope recombination. He is a member of The Minerals, Metals and Materials Society (TMS), Sigma Xi, the Materials Research Society, and a fellow of LANL, TMS, and the Institute of Physics. Baskes has authored or co-authored more than 190 technical publications that have had more than 5900 citations. Of these publications, three have more than 1000 citations, and 18 have more than 100 citations each. He has received two Department of Energy (DOE) awards for outstanding research and is in the DOE/BES Hall of Fame.

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#### Michael W. Finnis

Department of Materials and Department of Physics, Imperial College London, Exhibition Road, London SW7 2AZ, UK; tel. +44 207 594-6812; and email m.finnis@imperial.ac.uk. Finnis holds the chair in theory and simulation of materials at Imperial College, London, and is currently deputy director of the Thomas Young Centre—The London Centre for Theory and Simulation of Materials. Following his MA and PhD degrees at the Cavendish Laboratory in Cambridge, he was a staff scientist at AERE Harwell and subsequently worked at the Fritz-

Haber-Institut in Berlin and at the Max-Planck-Institut für Metallforschung in Stuttgart, Germany. His research interests include the derivation and application of interatomic force models and the link between thermodynamic potentials and underlying atomic scale quantities, especially in the theory of defects and interfaces. In 2005, Finnis was the recipient of the Born Medal and Prize of the Institute of Physics and the German Physical Society.



# **Stephen Foiles**

Computational Materials Science and Engineering Department, Sandia National Laboratories, Albuquerque, NM; tel. 505-844-7064; and email foiles@sandia.gov.

Foiles is a Distinguished Member of the Technical Staff in the Computational Materials Science and Engineering Department at Sandia National Laboratories. He received his BS degree in physics from Stanford University in 1978 and his PhD degree in theoretical physics from Cornell University in 1983. Foiles's research at Sandia has involved the application of atomic-

scale simulations to study a variety of materials science issues, with an emphasis on understanding more about internal interfaces.



### **Peter Gumbsch**

Fraunhofer Institute for Mechanics of Materials IWM, Freiburg and Institute for Applied Materials IAM, Karlsruhe Institute of Technology, Germany; tel. +49 721 608-44363; and email peter.gumbsch@kit.edu. Gumbsch is head of the Fraunhofer Institute for Mechanics of Materials IWM and chair for Mechanics of Materials at Karlsruhe Institute of Technology (KIT). His research interests are centered on the mechanical properties of materials, including microstructural and confinement aspects. His current focus is on tribology and atomistic aspects

of friction and wear. He is a member of the senate of the German National Academy of Sciences Leopoldina and has been multiply honored for his scientific work, most notably with the Gottfried-Wilhelm-Leibniz-Prize of the German Research Foundation DFG.



# Tao Liang

Department of Materials Science and Engineering, University of Florida, Gainesville, FL 32611, USA; tel. 352-392-6609; and email liang75@ufl.edu.

Liang is a research scientist in materials science and engineering at the University of Florida (UF). He received his BA degree from Jilin University, China, in 1997 and his PhD degree from The Ohio State University in 2005, both in materials science and engineering. He joined the Department of Materials Science and Engineering at UF as a postdoctoral researcher in 2006 and became a research scien-

tist in 2009. Liang's research focuses on developing advanced empirical potentials for multifunctional multicomponent systems and using atomistic, electronic-structure, and quantum chemical simulation methods to address the properties and processing of materials, including nanotribology, surface chemistry of target materials through polyatomic ion-beam deposition, physical, chemical, and electrical properties of organic materials, metals, oxides, semiconductors, and their interfaces.



#### Michael Moseler

Fraunhofer Institute for Mechanics of Materials IWM and Physics Department of the University of Freiburg, Germany; tel. +49 761 5142-332; and email michael.moseler@iwm.fraunhofer.de.

Moseler is a professor in the Physics Department of the University of Freiburg and is head of the work group "Multiscale Modeling and Tribosimulations" at the Fraunhofer Institute for Mechanics of Materials IWM. His work covers classical molecular dynamics simulations of friction, lubrication, and wear processes, phase

transformations in tribosystems, and nanoparticles, as well as multiscale models for thin-film growth. Further research activities are density functional calculations of finite size effects in free and supported clusters and their catalytic properties.



#### **Matous Mrovec**

Fraunhofer Institute for Mechanics of Materials IWM, Freiburg and Karlsruhe Institute of Technology, Germany; tel. +49 761 5142-375; and email matous.mrovec@kit.edu.

Mrovec is a staff scientist at the Fraunhofer Institute for Mechanics of Materials IWM in Freiburg with partial involvement at the Karlsruhe Institute of Technology (KIT) in Germany. He received his PhD degree in materials science and engineering from the University of Pennsylvania in 2002 under the supervision of Vasek Vitek. Between 2002 and 2004, Mrovec worked

as a postdoctoral fellow at the Max-Planck Institute for Metal Research in Stuttgart and at KIT. His main activities focus on atomistic modeling of materials, in particular with relation to their mechanical behavior.



Mark Noordhoek

Department of Materials Science and Engineering, University of Florida, Gainesville, FL 32611, USA; email minoord@gmail.com. Noordhoek is a graduate student in materials science and engineering at the University of Florida. He earned his BSE degree in materials science and engineering from the University of Michigan in 2009. His research uses atomic simulation methods to study corrosion in nuclear



Lars Pastewka

fuel claddings.

Department of Physics and Astronomy Johns Hopkins University, Baltimore, MD and Fraunhofer Institute for Applied Materials IWM, Freiburg, Germany; email lars.pastewka@iwm.fraunhofer.de.

Pastewka is currently at Johns Hopkins University holding a Marie-Curie postdoctoral fellowship. He holds graduate degrees in physics and microsystems engineering from North Carolina State University and the University of Freiburg, respectively. He received his doctorate degree in theoretical condensed matter physics from

the University of Freiburg in 2010, while a graduate research assistant at Fraunhofer IWM. Pastewka also has been a Fulbright fellow. His interests and current research topics include contact mechanics, tribology, and electrochemistry.



Simon R. Phillpot

Department of Materials Science and Engineering, University of Florida, Gainesville, FL 32611, USA; tel. 352-846-3782; and email sphil@mse.ufl.edu.

Phillpot is a professor of materials science and engineering at the University of Florida (UF) and a UF Research Foundation professor. He received his BA degree from Oxford University in 1980 and his PhD degree from UF in 1985, both in physics. He spent 16 years at Argonne National Laboratory in Chicago prior to joining UF in 2003. Phillpot's research focuses on using

atomistic and electronic-structure simulation methods to address issues in phonon-mediated heat transfer, ferroelectric and dielectric behavior, defect properties in oxides, mechanical behavior of metals, and tribology. He also works on developing advanced potentials for multifunctional systems. He is a fellow of the American Physical Society, the American Association for the Advancement of Science, the Institute of Physics (UK), and the Institute of Materials, Minerals and Mining (UK).



Steve Plimpton

Sandia National Laboratories, Albuquerque, NM; email sjplimp@sandia.gov.

Plimpton has been a member of the technical staff at Sandia National Laboratories since 1989. He earned his PhD degree in applied and engineering physics from Cornell University. Plimpton develops algorithms and software for materials modeling at various scales, including the LAMMPS molecular dynamic package discussed in his article in this issue of MRS Bulletin. He also works on more coarse-grained methods, including kinetic Monte Carlo techniques.



Tzu-Ray Shan

Sandia National Laboratories, Albuquerque, NM 87185-1322, USA; tel. 505-844-7009; and e-mail tnshan@sandia.gov.

Shan is a postdoctoral appointee at Sandia National Laboratories in Albuquerque, New Mexico. He was a graduate student in materials science and engineering at the University of Florida (UF), working with professors Susan Sinnott and Simon Phillpot. Shan received his BA and MS degrees in materials science and engineering from National Cheng Kung University in Taiwan in 2001 and 2003, respectively,

and his PhD degree from UF in 2011. He joined Sandia in September 2011. His research focuses on developing advanced interatomic potentials for multifunctional, heterogeneous systems. He also works on using atomistic and electronic-structure methods in modeling hypersonic shock propagation in molecular crystals.



Yun Kyung Shin

Department of Mechanical and Nuclear Engineering, Pennsylvania State University; email yks2@psu.edu.

Shin is a postdoctoral fellow working with Adri van Duin in the Department of Mechanical and Nuclear Engineering at The Pennsylvania State University. She received her PhD degree in 2011 in chemistry from The Ohio State University. Her current research focuses on development and applications of the ReaxFF force field to the study of oxidation reaction on complex nanoalloys and material properties.



Aidan Thompson

Scalable Algorithms Department, Sandia National Laboratories, Albuquerque, NM 87185-1316; tel. 505-844-9702; and email athomps@sandia.gov.

Thompson has been a member of the technical staff at Sandia National Laboratories for 14 years. He earned his PhD degree in chemical engineering from the University of Pennsylvania. Thompson develops and implements new algorithms, features, and interatomic potentials in LAMMPS. He also collaborates with other scientists, applying atomistic simulation meth-

ods to understand the effect of atomic-scale mechanisms on the behavior of condensed matter.



#### Adri van Duin

Pennsylvania State University, University Park, PA 16802; tel. 814-863-6277; and email acv13@psu.edu.

van Duin is an associate professor in the Department of Mechanical and Nuclear Engineering at The Pennsylvania State University (PSU). He earned his PhD degree from the Delft University of Technology in 1997. From 1997 to 2002, he worked at the University of Newcastle in Tyne, UK, as a postdoctoral scientist on computational chemical simulations applied to organic geochemistry. In 2002, van Duin joined the

California Institute of Technology. He moved to PSU in the fall of 2008. Since 2000, he has worked on the development and application of the ReaxFF reactive force field, which enables large scale (>>1000 atoms) and long-time (>1 ns) atomistic-scale, dynamical simulations of chemical reactions. He has applied this technique to a wide range of materials and research topics, including catalysis, combustion chemistry, and material failure.



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