Atomistic Simulations of Mechanics of Nanostructures

Hanchen Huang and Helena Van Swygenhoven, Guest Editors

Abstract

Nanostructures can be in the form of nanoparticles or nanograins, nanowires or nanotubes, and nanoplates or multilayers. These nanostructures may be used individually or embedded in a bulk material. In both cases, they share two common features. First, the small dimensions minimize or even eliminate the presence of defects. Second, nanostructures entail large surface or interface areas. The absence of defects makes nanostructure materials stronger than their bulk counterparts, leading to the eventual realization of ideal strength. The presence of surfaces and interfaces may either reduce or increase the strength. Atomistic simulations can provide insight into the deformation mechanism at the atomic and electronic level, something that is very difficult to obtain from experiments. This article describes generic features of nanostructures and summarizes the five areas presented in the articles in this issue.

Introduction

A structure becomes nanoscale when at least one of its three dimensions is below 100 nm. Gleiter[1] classified nanostructures according to their dimensionality, as schematically shown in Figure 1a. In nanoparticles or nanograins, all three dimensions are nano, making them zero-dimensional (0D). Nanowires or nanotubes are large in only one dimension, making them one-dimensional (1D). Analogously, thin films, multilayers, or membranes exceed the nanometer regime in two of the three dimensions, making them two-dimensional (2D). Confinements of electron distribution in small dimensions can lead to both quantitative and qualitative changes of materials functionalities. In connection with mechanics, these three types of nanostructures share two common features. On one hand, the smaller the structure, the less chance it incorporates defects. On the other hand, the number of atoms situated in the surface or interface increases drastically. These two structural characteristics of nanostructures determine, to a great extent, their elastic and plastic responses in the presence of surfaces and interfaces. For example, the Young's modulus of a nanostructure can increase or decrease with dimension, as shown in Figure 1b. These aspects form the focus of this theme issue.

At an interface, the periodicity of atomic arrangement terminates. This termination means the loss of atomic neighbors at a free surface, and therefore the change of electron distribution. As an example, Figure 2 shows electron redistribution near a ZnO $(11\bar{2}0)$ surface.[2] Due to the loss of atomic neighbors, each of the surface bonds (S1, S2, and S3) is strengthened, as indicated by the overlap of electron distribution (as shown by the red contours in Figure 2). This tendency of electron redistribution moves the surface atoms and exerts strain on atoms under the surface. At a metallic surface, similar electron redistribution occurs, leading to surface stress and strain. The surface stress may lead to or facilitate surface reconstruction, change of elastic moduli, phase transformation, dislocation nucleation and motion, and self-organization of nanostructures.[3–5] When surface stress itself is insufficient, additional mechanical stress helps facilitate the phase transformation.[5,6,7]

Local electronic structure plays a key role in determining the nature of defects in crystals. For instance, the general planar fault energy curves, which represent the energy dependency of rigidly shearing a crystal, influence the nature of slip activity in nanocrystalline systems.[8] Figure 3a displays the valence electron density in face-centered-cubic (fcc) Al that is rigidly sheared at a {111} plane along the $\langle 1\bar{1}2\rangle$ slip direction. The inter {111}-plane bonding is substantially altered. This alteration results in the maximum energy configuration in the generalized stacking fault energy (GSFE) curve displayed in Figure

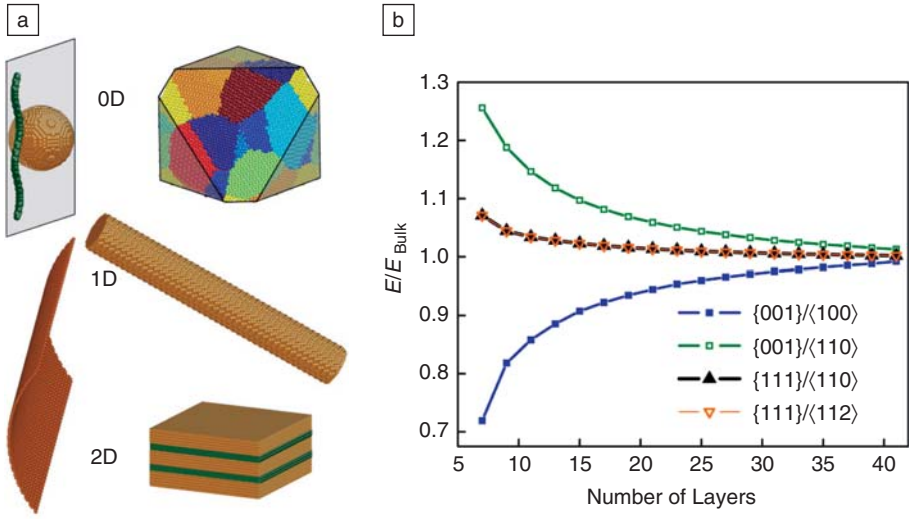

Figure 1. (a) Schematic of nanostructures—0D nanoparticles and nanograins, 1D nanowires, and 2D membranes and multilayers; (b) Variation of normalized Young's modulus (E) as a function of Cu nanoplate thickness. Reprinted with permission from Reference 3. © 2004, American Institute of Physics.

3b and is referred to as the unstable stacking fault energy.[9] Atomistic simulations have shown that when the unstable stacking fault energy is close in value to the stable stacking fault energy (such as in Al), the nucleation of full dislocations at the grain boundary becomes more likely within the simulation time.[8] A similar rationale applies to twin fault and twin migration activity within the nanocrystalline system.[10] Beyond the demonstrating examples in Figures 2 and 3, interfaces serve as sinks and sources of defects and conspire with dislocations in a variety of mechanical deformation processes.

Atomistic simulations have been instrumental to the understanding of the deformation mechanism responsible for the mechanical behavior of materials and are particularly prominent for nanostructures. Individual nanostructures are generally much smaller than 100 nm in dimension. This dimension is well within the reach of classical atomic simulations such as molecular dynamics and kinetic Monte Carlo simulations. For those of even smaller dimensions, electronic (full electronic or tight-binding) calculations are feasible, providing full details of atomic/electronic behavior. Such details are usually beyond the reach of direct experimental characterizations, and yet they dictate the mechanical deformation of nanostructures.

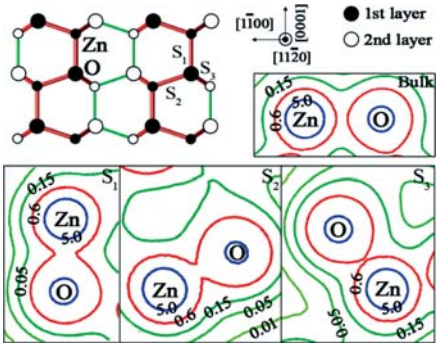

Figure 2. Top view of the atomic structure of the ZnO (11$\bar{2}$0) surface, the density contour of electrons at S_1, S_2, and S_3, and that in the bulk for comparison. Reprinted with permission from Reference 2. © 2006, American Institute of Physics.

In synergy with experiments, the atomistic simulations can provide useful guidance to experiments in suggesting deformation mechanisms, especially since the method provides direct access to many "hidden" parameters in experiments such as the interface structure at the atomic and electronic level, the stored excess energy, the free volume, and the internal stress distribution.[11] However, atomistic simulations, even at the full electronic level, involve approximations and idealizations such as the representation of many-body electronic effects. The short time steps required in molecular dynamics result in using strain rates that are incredibly high when compared with experimental values. Therefore, extrapolation toward experimental observations has to be done with extreme care, making it almost impossible to determine the true rate-limiting processes.

There are, however, several success stories of synergetic effects between simulations and experiments such as surface reconstruction and the dislocation mechanism in nanograins, both of which have been predicted by atomistic simulations and confirmed by experiments.

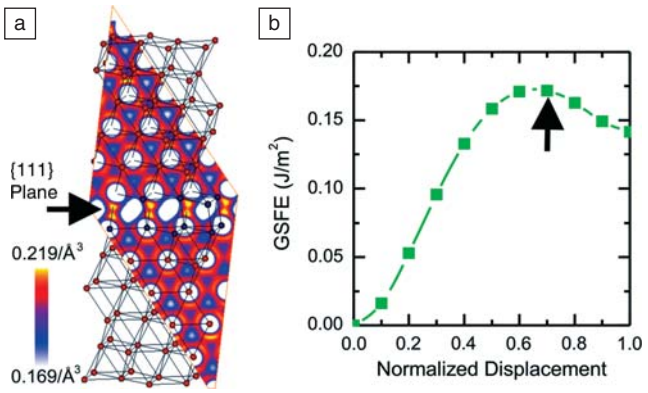

Figure 3. Al fcc (face-centered cubic) electronic charge density map of a {111} plane that intersects a rigidly sheared {111} plane along the ⟨$\bar{1}$ $\bar{1}$2⟩ slip direction. (b) The energy dependence as a function of normalized rigid displacement—the generalized stacking fault energy (GSFE) curve. In (a) the configuration is taken at the maximum energy of (b) (black arrow), the unstable stacking fault energy.

Coverage of This Issue

This issue focuses on crystalline nanostructures. Nanotubes are not the main focus because they have been covered in previous issues of the *MRS Bulletin*.[12] Two aspects of mechanics are addressed by simulations: mechanical deformation driven by stress or strain and mechanics-driven synthesis of nanostructures. The five overview articles cover the topics of ultra-strength of nanostructures, the strengthening role of nanoparticles, elastic and plastic responses of nanowires, plastic deformation of nanoscale multilayers and nanograins,[13,14] and advancements in mechanics-driven synthesis of nanostructures.

Looking at a generic feature, Zhu et al. review recent advancements in understanding the ultra-high strength of nanostructures. The strength is dictated by dislocation nucleation and motion at low temperatures. In the absence of mobile dislocations, plastic deformation will not proceed until new dislocations are nucleated, which can lead to a much higher strength, approaching the ideal strength. The ultra-high strength is reachable, for example, during nanoindentation of single crystalline solids. When dislocations, although available to facilitate plastic deformation, do not have sufficient time to respond to a stress, the strength can also increase; this is the case in high strain-rate deformation. In nanostructures, additional obstacles such as interfaces and nanoparticles also serve to increase the strength. Zhu et al. review the length- and time-scale effects on the deformation processes in nanostructures with ultra-high strength. They emphasize the critical role of activation volume in understanding the strength-controlling mechanisms.

One possible application of the extremely high strengths of nanoparticles is to exploit their role as reinforcement to improve the mechanical properties of bulk materials. Chrzan et al. consider the strengthening of alloys through the introduction of nanoscale precipitates, hindering the propagation of dislocations in the crystalline matrix. The precise mechanism by which nanoparticles strengthen a bulk material is size dependent: The very small particles can be cut by dislocations, whereas dislocations are forced to circumvent larger precipitates. The structure of the precipitates also can be altered through its interaction with dislocations. However, exceptional structural stability and strength can be obtained by introducing nanoscale particles; for example, small nanoparticles of 3–5 nm in diameter can be structurally stable at high temperatures and lead to a six orders-of-magnitude increase in creep resistance. The deforma-

tion mechanisms derived from atomistic simulations are critical input for elasticity-based dislocation dynamics, a simulation technique at a higher lengthscale.[15–17]

Focusing on 1D nanostructures, Park et al. review recent developments in nanowire mechanics. Near surfaces, atoms have fewer bonding neighbors, leading to a redistribution of electrons that results in the rearrangement of surface atoms for metallic solids or reconstructions for covalent solids. The rearrangement or reconstruction also leads to elastic stiffening or softening of the surfaces. At the same time, it also imposes a large strain on the nanowire interior, triggering nonlinear elastic stiffening or softening. When the cross-sectional dimension is small enough, surface rearrangement or reconstruction also can lead to phase transformations, such as fcc to body-centered-tetragonal (bct) in gold nanowires. Defects nucleated due to surface stresses can couple with those created due to externally applied forces. Under large deformation, the strength of nanowires depends on whether nucleation or glide requires larger stress. As a result, metallic nanowires can become either stronger or slightly weaker with the introduction of twin boundaries.

Focusing on 2D multilayers and nanocrystalline metals where each crystal is a nanograin, Derlet et al. review recent advancements in mechanics in confined volumes, particularly the interaction between dislocations and grain boundaries. The complex lifetime of a dislocation is reviewed, starting with its nucleation at the grain boundary, followed by its propagation and eventual absorption in the surrounding grain boundary network. Dislocation nucleation at grain boundaries is studied in systematic bicrystal simulations that consider coincident site lattice boundaries and in simulations using fully 3D crystalline networks in which general high angle boundaries with tilt and twist components can be studied. The latter also allows the study of the effect of triple and higher order junctions on the dislocation-interface interactions. The unique properties of fcc/bcc (body-centered cubic) nano-layered composite systems and the details of their interface properties are also reviewed. Their concluding discussion focuses on the limitations of finite temperature molecular dynamics. New transition path methods may be used to overcome the inherent high-strain rate/high-stress regime through the calculation of activation volumes that characterize the strain-rate sensitivity of the atomic scale plastic processes studied.

Turning to the applications of nanomechanics, Liu et al. review recent advancements in mechanics-driven synthesis of nanostructures. Strain generates long-range fields, such as Columbic fields, of charged particles. This long range nature enables the self-organization of structures so as to minimize the thermodynamic free energy. Quantum dot formation during hetero-epitaxy is one such example. Driven by the mismatch strain between epilayer and substrate, the quantum dots tend to be periodic and uniform to minimize the strain energy. Size uniformity in the synthesis of these quantum dots affects their functional behavior, such as monochromic light emission. Crystalline surfaces, already under intrinsic surface stress, are very responsive to additional stresses. Introduction of gas molecules onto a surface can generate sufficient stress to peel off the surface layer and drive it to form tubular structures. This mechanics-driven self-organization of tubular nanostructures offers the advantage of structure control. In contrast, vapor-based synthesis usually leads to nanostructures of mixed structures (e.g., nanotubes of mixed chirality).

Prospects

The overview articles in this volume show that atomistic simulations have had a large effect on the advancement of nanostructure mechanics, and there is still opportunity for further advances. Much effort has been invested in the basic science of nanostructure mechanics.[18] Looking forward, there are two areas that pose great challenges and offer potentials of reward.

The first area is the bridging of time scales in atomistic simulations. In contrast to the bridging of length scales, there has been less progress in bridging time scales. Both electronic structure and classical molecular dynamics simulations are limited to nanoseconds in time scale. Hyper-molecular dynamics and similar approaches enable simulations lasting microseconds for selective materials systems in which diffusion kinetics is simpler. Unfortunately, this condition is not satisfied most of the time. By associating atoms to lattice points, lattice kinetic Monte Carlo simulations extend the time scale to microseconds or seconds. However, the use of the lattice renders it impossible to directly represent mechanical deformation. Fortunately, strain and stress can be represented by strain energy. Incorporating strain energy into the lattice kinetic Monte Carlo simulations and coupling this method with other simulation methods (such as classical molecular dynamics and a continuum approach) may lead to atomistic methods over multiple time scales.

The second area concerns the hierarchy of nanostructures. So far, the majority of atomistic simulations have focused on a single type of nanostructure. Realistic applications will likely involve hierarchies of nanostructures. For example, a future integrated circuit may include doped nanowires or nanotubes as *p-n* junctions, nanofilms as insulators, and nanoparticle-reinforced composites as case materials. The hierarchies will likely include hetero-interfaces where charge transfer is critical. Coupling of electronic structure calculations and classical molecular dynamics simulations may enable rigorous simulations of charge transfer and also allow the efficient treatment of large dimensions.

Acknowledgments

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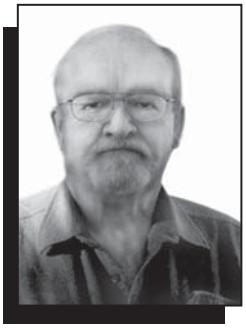

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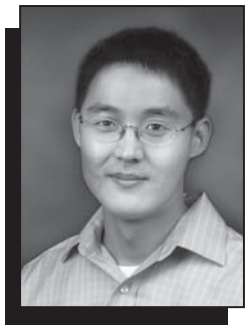

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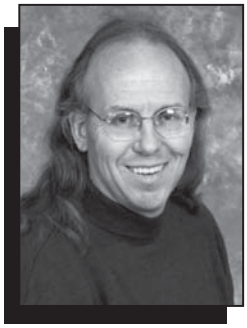

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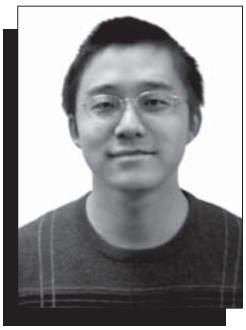


Ji Zang

Ting Zhu

Steven J. Zinkle

Wang is a postdoctoral research associate in the Materials Science and Technology Division at Los Alamos National Laboratory. He received his PhD degree in mechanical engineering from Rensselaer Polytechnic Institute in 2006. He has approximately 45 publications in books and journals. His work focuses on modeling deformation behavior of composites and growth mechanisms of nanostructures.

Sidney Yip can be reached at the Department of Nuclear Science and Engineering at the Massachusetts Institute of Technology, Cambridge, MA 02139, USA; e-mail syip@mit.edu.

Yip has been a professor of nuclear science and engineering since 1965 and a professor of materials science and engineering since 2000 at the Massachusetts Institute of Technology. After receiving undergraduate and graduate degrees from the University of Michigan, he spent a year as a postdoctoral fellow at the University of Michigan and two years as a research associate at Cornell University. His interest lies in multiscale materials modeling theory and simulation, particularly at the atomistic level. Most recently he edited the *Handbook of Materials Modeling* (Springer, 2005). He is a fellow of the American Physical Society and a member of the Materials Research Society.

Ji Zang can be reached at the School of Chemical and Biomolecular Engineering at the Georgia Institute of Technology, Atlanta, GA 30332, USA; tel. 404-894-7608, and e-mail ji.zang@chbe.gatech.edu.

Zang is a postdoctoral fellow at the Georgia Institute of Technology and works on the diffusion of water and gas molecules in carbon nanotubes and metal oxide nanotubes. He received his BS and MS degrees from the School of Materials Science and Engineering at Xi'an Jiaotong University, Xi'an, China, in 1999 and 2001, respectively. In 2007, Zang obtained his PhD degree in materials science and engineering at the University of Utah, where he focused on theoretical modeling and molecular dynamics simulation of mechanical properties of carbon nanotubes under hydrostatic pressure and bending behavior of Si/Ge nanofilms.

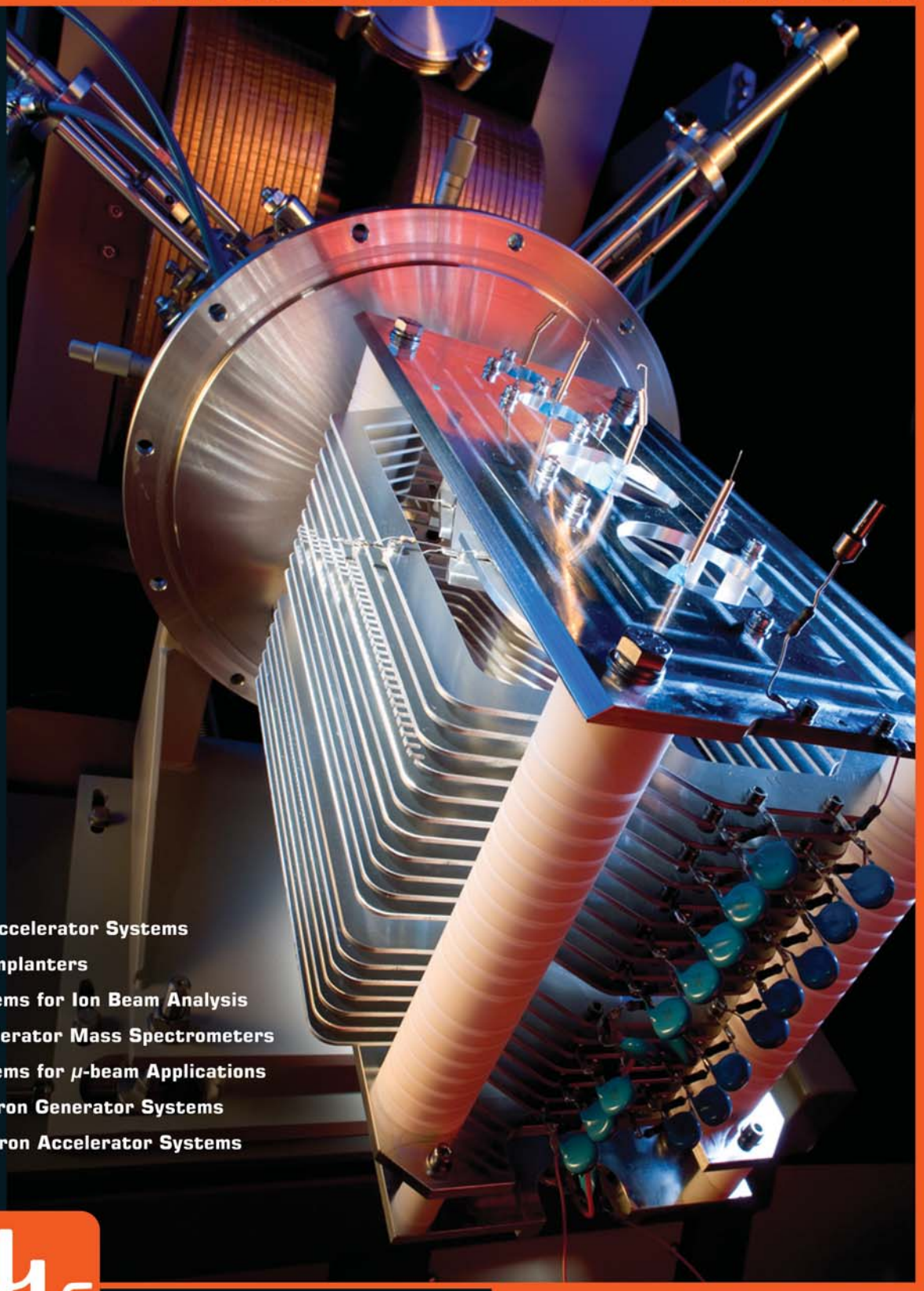
Ting Zhu can be reached at the Woodruff School of Mechanical Engineering at the Georgia Institute of Technology, Atlanta, GA 30332, USA; e-mail ting.zhu@me.gatech.edu.

Zhu is an assistant professor in the Woodruff School of Mechanical Engineering at the Georgia Institute of Technology. His research is focused on materials modeling and nanomechanics of materials (http://www.me.gatech.edu/zhugroup/). Zhu received his PhD degree from the Massachusetts Institute of Technology (2004) and was a postdoctoral research associate at Harvard University (2004–2005).

Steven J. Zinkle can be reached at the Materials Science and Technology Division, Oak Ridge National Laboratory (ORNL), P.O. Box 2008, Oak Ridge, TN 37831-6132, USA; tel. 865-574-4065, fax 865-574-4066, and e-mail zinklesj@ornl.gov.

Zinkle is a corporate fellow and director of the Materials Science and Technology Division at ORNL. He received a PhD in nuclear engineering and an MS in materials science from the University of Wisconsin—Madison in 1985 and subsequently joined ORNL as a Wigner Fellow. He has been a visiting scientist at Risø National Laboratory in Roskilde, Denmark and Forschungszentrum Jülich in Germany. His research interests include deformation and fracture mechanisms in structural materials and investigation of radiation effects in metals and ceramics for fusion and fission energy systems. He has written more than 220 peer-reviewed publications and is a fellow of the American Ceramic Society, ASM International, and the American Nuclear Society (ANS). He has received numerous awards, including the U.S. Department of Energy E.O. Lawrence Award, the IEEE Nuclear and Plasma Sciences Society Fusion Technology Award, and the ANS Mishima award for outstanding R&D on nuclear fuels and materials. □

PARTICLE ACCELERATOR SYSTEMS



- Ion Accelerator Systems
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- Systems for Ion Beam Analysis
- Accelerator Mass Spectrometers
- Systems for μ-beam Applications
- Neutron Generator Systems
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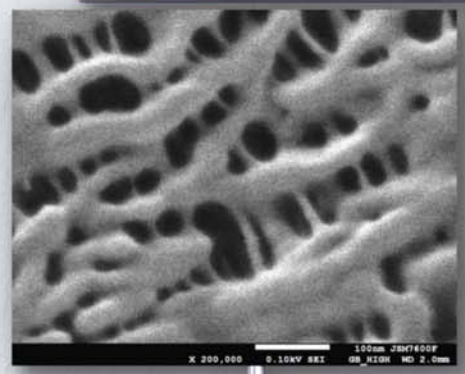
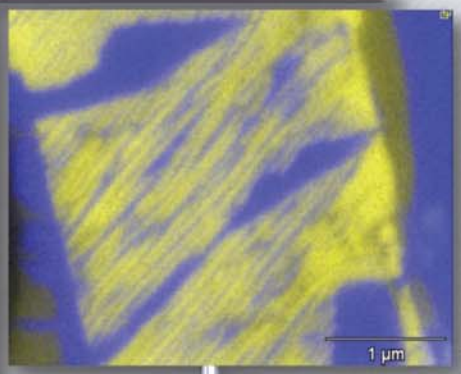
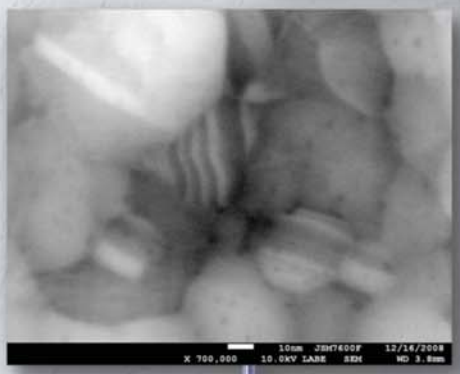
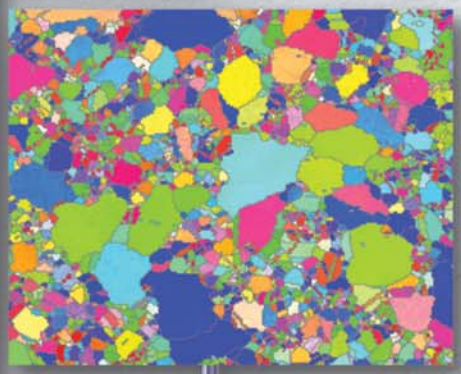




EDS/WDS
EDS map of TiO_2 in FeOx with <100nm spatial resolution 30,000x

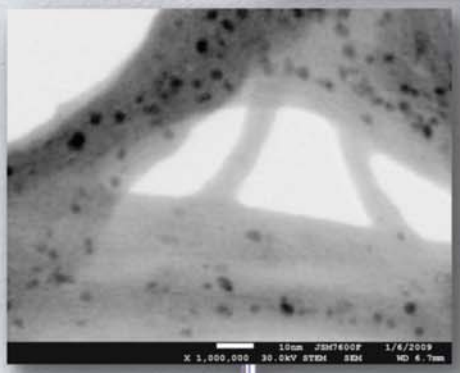
LABe
1-3 nm twinning in mineral BSE image

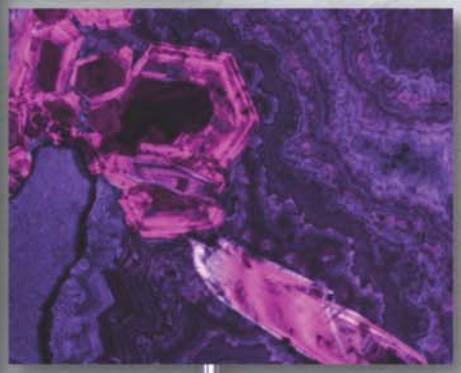




EBSD
Orientation map of Ni alloy

STEM
CNT with 1-3 nm Pt nanoparticles





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