Nanofabrication with Single Atomic Plane Precision: Atomic-Level Sculpting Of Crystalline Oxides

Stephen Jesse, Qian He, Andrew Lupini, Donovan Leonard, Mark Oxley, Oleg Ovchinnikov, Raymond Unocic, Alexander Tselev, Miguel Fuentes-Cabrera, Bobby Sumpter, Stephen Pennycook, Sergei Kalinin, and Albina Borisevich

Researchers developed a unique method to create epitaxial nanostructure of a complex oxide with single atomic plane precision and arbitrary pre-defined shapes. This achievement not only provides another technique for manipulation and control of matter at the nanometer scale, which may advance the fundamental understandings of e-beam matter interaction and epitaxial growth mechanisms of complex oxides, but also suggests a way of larger scale atomic-level fabrication using existing e-beam lithography systems, providing a bottom-up, atomic-level complement to 3D printing.

This work was coordinated through ORNL’s Institute for Functional Imaging of Materials (IFIM), as collaboration between a MSED-funded project, a strategic LDRD, and CNMS staff research.


The e-beam of an electron microscope is used to crystallize amorphous SrTiO3 with atomic plane precision. The word “small” is epitaxially patterned onto a 160 x 80 nm area. The background is a zoomed-in, atomic resolution view of the letter “s”.

The research was sponsored by the by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.
### In-situ Environment Shines Light and Neutrons on Structure–Function Evolution of Polymers

J. Zhu, Y. Han, R. Kumar, Y. He, K. Hong, P. V. Bonnesen, B. G. Sumpter, S. C. Smith, G. S. Smith, I. N. Ivanov, and C. Do

Researchers developed a sample environment where neutron and optical probes worked in concert to track molecular dynamics in solution and in thin films. They used their new capability—in situ multimodal interrogation of structures and functions—to make discoveries likely to improve photovoltaic materials, including assembling a polymer into functional structures in aqueous solution using a detergent-like molecule as a template and improving a solid’s performance via an additive.

Once placed in the test chamber, a sample can be transported to different instruments for measurements. The chamber has a transparent face to allow entry of laser beams to probe materials. Probing modes include neutrons, X-rays, photons, electrical charge, magnetic spin, and calculations aided by high-performance computing; they can operate simultaneously to characterize matter under a broad range of conditions. The chamber can track molecules under changing temperature, pressure, humidity, light, solvent composition, etc. It extends the probing of materials from typical environments under resting conditions to operating environments that allow scientists to assess how working materials change over time and explore ways to improve their performance.

Work was performed at the Center for Nanophase Materials Sciences and the Spallation Neutron Source, both at ORNL, and the Advanced Photon Source at Argonne National Laboratory.

### Assessment of quasi-laminar flaws in Belgian nuclear reactor pressure vessels

Richard Bass, Terry Dickson, Sarma Gorti, Hilda Klasky, Randy Nanstad, Mikhail Sokolov, Paul Williams, and William Server

ORNL performed a detailed technical review of the 2015 Electrabel (EBL) Safety Cases prepared for the Belgium reactor pressure vessels (RPVs) at Doel 3 and Tihange 2 (D3/T2), and based on an independent quantitative assessment, confirmed the structural integrity of D3/T2 under all design transients with ample margin in the presence of the quasi-laminar flaws found in each RPV. The Federal Agency for Nuclear Control (FANC) in Belgium commissioned ORNL to provide an independent assessment of the existing safety margins against cracking of the RPVs at D3/T2 due to the presence of quasi-laminar flaws found in each RPV. Based partly on the conclusions of the ORNL assessment and reviews by other independent experts, FANC authorized the restart of D3/T2 in November 2015.

Work was sponsored by the Belgian Federal Agency for Nuclear Control. Development of the FAVOR code was sponsored by the U.S. Nuclear Regulatory Commission.

### ORNL's in-situ multimodal test chamber tracks molecular dynamics in solutions as well as solids.

This work was supported by the Laboratory Directed Research and Development program at Oak Ridge National Laboratory


### Section of T2 RPV (left) and mesh used (right) for analysis of flaw #1660 using ABAQUS XFEM

TOTAL + ADIOS for Seismic simulations

S. Klasky and N. Podhorszki - ORNL
Pierre-Yves Aquilanti and Jyothi Bhaskar - TOTAL E&P

Using ADIOS, simulations on ORNL's Titan (1024 Processes) achieve a 6X I/O speedup from using Parallel HDF5.

TOTAL (a global, integrated energy producer and provider, the world's fourth-largest international oil and gas company and second-largest solar operator) has evaluated the Adaptable IO System (ADIOS) software for the I/O needs of their seismic imaging efforts. TOTAL found that ADIOS provides the best alternative for their applications. These applications take terabytes of data as inputs, and output petabytes of result data along with intermediate data. For TOTAL, it was especially important to achieve good performance for structured grid data. For the evaluation, TOTAL used one of the applications (Reverse Time Migration - RTM) and their SGI system and OLCF’s Titan and compared the performance of the MPI-IO, HDF5, ADIOS and SIONLib I/O implementations. During the tests, the ADIOS team provided guidance for optimizing ADIOS for their use cases. As a result of these positive first evaluations, TOTAL has decided to put more effort into integrating ADIOS into their codes where they will further evaluate its performance.

Supported by TOTAL and the Oak Ridge Leadership Computing Facility

Supporting the Development of Soft-Error Resilient Message Passing Applications using Simulation

Christian Engelmann and Thomas Naughton

Researchers developed the very first simulation-based Message Passing Interface performance tool that supports both, the injection of process failures and bit flip faults. This work enables the development of soft-error resilient high-performance computing (HPC) applications by permitting the investigation of their correctness and performance under various fault conditions using simulated HPC systems.

This work was performed at Oak Ridge National Laboratory and was sponsored by the US Department of Energy's Office of Advanced Scientific Computing Research.

News

HPC Leading Institutes Announce Formation of the UCX Consortium to Expand Collaboration within HPC Community

Group Aims to Expedite Advances in High Performance Computing Worldwide; Takes the Next Step toward Achieving Exascale Performance

The OpenUCX community today, under the leadership of Oak Ridge National Laboratory, announced its intention to form the UCX Consortium, an industry group focused on the proliferation and continued evolution of the UCX High-Performance Computing Communication Framework. The Consortium will be formed to increase collaboration between government laboratories, universities and commercial businesses within the HPC community, expanding the possibilities for discovery and advancement. Members of the Consortium will benefit from shared knowledge and resources, a fast and flexible access to a wide range of worldwide utilities and communication directives. Furthermore, they will profit from a production-grade low-level flexible communication software environment, which can be used as a vehicle for revolutionary research, a key to foster innovation.


Process variation threatens to slow down and even pause chip miniaturization

For past several decades, the processor industry has enjoyed the benefits of chip miniaturization and the exponential increase in the number of on-chip transistors as predicted by Moore's law. However, as process technology scales to small feature sizes, precise control of fabrication processes has become increasingly difficult. As a result, 'process variation' (PV), which refers to the deviation in parameters from their nominal specifications, has greatly worsened.

In his paper "A Survey Of Architectural Techniques for Managing Process Variation" Sparsh Mittal investigates the impact of PV along with strategies for mitigating it in a wide range of system architectures, e.g. in CPUs, GPUs, in processor components (cache, main memory, processor core), in memory technologies (SRAM, DRAM, eDRAM, non-volatile memories e.g. PCM, resistive RAM) and in both 2D and 3D processors.


New ORNL Paper: Survey on Asymmetric Multicore Processors

ORNL researcher Sparsh Mittal has authored a new paper entitled “A Survey Of Techniques for Architecting and Managing Asymmetric Multicore Processors.” Now accepted for ACM Computing Surveys 2015, the document reviews nearly 125 papers.

Modern computing systems have become highly diverse in terms of their workloads, usage pattern, scale and optimization objective. Hence, even a highly-optimized “monolithic core” cannot simultaneously meet such diverse and often conflicting requirements. To address this challenge, asymmetric multicore processors have been proposed which feature cores of different types (e.g. big and LITTLE) in the same processor. Qualcomm Snapdragon 810, Samsung Exynos 5 Octa and Nvidia Tegra X1 are some examples of asymmetric multicore.

Download the paper here - [https://www.academia.edu/18301534/A_Survey_Of_Techniques_for_Architecting_and_Managing_Asymmetric_Multicore_Processors](https://www.academia.edu/18301534/A_Survey_Of_Techniques_for_Architecting_and_Managing_Asymmetric_Multicore_Processors)

Oak Ridge National Laboratory to Co-Lead DOE’s New HPC for Manufacturing Program

Oak Ridge National Laboratory (ORNL) is collaborating with Lawrence Livermore and Lawrence Berkeley National Laboratories (LLNL and LBNL) to lead a new US Department of Energy (DOE) program designed to fund and foster public-private R&D projects that enhance US competitiveness in clean energy manufacturing.

“The Manufacturing Demonstration Facility (MDF) has worked with numerous industry partners to overcome challenges in areas of advanced manufacturing, and ORNL is excited by the prospect of extending and accelerating this success through modeling and simulation,” said John Turner, Group Leader for Computational Engineering and Energy Sciences and ORNL lead for HPC4Mfg. He added, “We look forward to collaborating with colleagues at LLNL and LBNL, and with industry partners, to apply our computational expertise to challenging clean energy manufacturing problems.”


Awards and Recognition

Maier Named Fellow of the American Physical Society

Thomas Maier, a senior research staff member in ORNL's Computer Science and Mathematics Division and in the Center for Nanophase Materials Sciences, focuses on many-body theory of correlated electron systems including unconventional superconductors, multilayers and nanostructures. He was cited by APS's Division of Condensed Matter Physics for "numerical and phenomenological calculations that have provided insight into cuprate and iron-pnictide superconductors."

Thomas was selected for the honor by the APS Council of Representatives and will be formally recognized at the APS's March meeting.

CSMD’s Sen receives Drell Academic Award

Satya Sen of the Computer Science and Mathematics Division has been awarded the 2016 Sidney D. Drell Academic Award by Intelligence and National Security Alliance, an organization of public, private and academic sectors within the national security and intelligence communities. Satya came to ORNL as a Wigner Fellow and is currently a member of CSMD’s Complex Systems group. His award is based on his contributions to the Department of Homeland Security Domestic Nuclear Detection Office’s Intelligent Radiation Sensing System projects. The award is named for Sidney Drell, a Fermi Award-winning theoretical physicist and arms control expert and professor emeritus at Stanford Linear Accelerator Center.

CORE-Direct Wins R&D100 Award

Manjunath Gorentla Venkata and Pavel Shamis receive the R&D100 Award at the awards ceremony in Las Vegas

CORE-Direct (Collectives Offload Resource Engine), developed with Mellanox Technologies with Pavel Shamis as ORNL team leader.

Oak Ridge National Laboratory’s CORE-Direct is an application acceleration and scaling technology available with the InfiniBand HCA ecosystem for HPC, big data and data center applications. CORE-Direct’s software and hardware is available by Mellanox. CORE-Direct technology accelerates the main determinant of performance and scalability in parallel applications, the group data exchange operations. To achieve this, it adds software and hardware capabilities to offload and execute the data exchange operations on the network, abstract the memory hierarchies on the node and provide a powerful abstraction to be used by applications, offering a novel and comprehensive solution. The testament to this is the wide and successful adoption of the technology-more than 28% of supercomputers on the Top 500 list of world’s fastest supercomputers use CORE-Direct technology.

Widely recognized as the “Oscars of Invention,” the R&D 100 Awards identify and celebrate the top technology products of the year. Past winners have included sophisticated testing equipment, innovative new materials, chemistry breakthroughs, biomedical products, consumer items, and high-energy physics. The R&D 100 Awards spans industry, academia, and government-sponsored research.

This research was done in the context of the Department of Energy Office of Science’s FastOS program. This program is focused on exploratory work in operating systems and runtimes for petascale and beyond supercomputers.

Agarwal awarded patent by USPTO

Pratul Agarwal was awarded patent number 9,195,795 by the USPTO. The patent, titled "Identification and modification of dynamical regions in proteins for alteration of enzyme catalytic effect" describes a method to provide an inexpensive and efficient solution by utilizing computer simulations, in combination with available experimental data, to build suitable models and investigate the enzyme activity.

Community Service

• David E. Bernholdt, program committee, Hawaii International Conference on System Sciences (HICSS-49)
• David E. Bernholdt, program committee, Second International Workshop on Hardware-Software Co-Design for High Performance Computing (Co-HPC 2015)
• David E. Bernholdt, program committee, Second Annual Workshop on HPC User Support Tools (HUST15)
• David E. Bernholdt, program committee, Third International Workshop on Software Engineering for High Performance Computing in Computational Science and Engineering (SEHPCCE15)
• David E. Bernholdt, program committee, Second Workshop on Accelerator Programming with Directives (WACCPD 2015)
• Michael Brim, participant, 9th Scalable Tools Workshop in Lake Tahoe, California
• Michael Brim, program committee, 2015 International Workshop on Data Intensive Scalable Computing Systems (DISCS-2015)
• Wael Elwasif, reviewer, Computer Physics Communications.
• Christian Engelmann, reviewer, Journal of Computational Science (JCONS)
• Christian Engelmann, reviewer, Journal of Parallel and Distributed Computing (JPDC)
• Christian Engelmann, program committee, International Conference on Algorithms and Architectures for Parallel Processing (ICA3PP) 2015
• Christian Engelmann, Technical Papers Member, System Software, SuperComputing2015
• Christian Engelmann, BOF Resilience Chair, System Software, SuperComputing2015
• Manjunath Gorentla Venkata, co-chair, OpenSHMEM 2015: Second workshop on OpenSHMEM and Related Technologies
• Manjunath Gorentla Venkata, program committee, 21st IEEE International Conference on Parallel and Distributed Systems (ICPADS 2015)
• Liz Hebert, Assistant to the Technical Program Chair, SuperComputing2015
• Forrest Hoffman, co-convened, AGU session - Earth and Space Science Informatics Session (IN43A)
• Forrest Hoffman, co-convened, AGU session - Biogeosciences Session (B21E)
• Forrest Hoffman, co-convened, AGU session - Town Hall (TH15C)
• Forrest Hoffman, co-convened, AGU session - International Workshop on Spatial and Spatiotemporal Data Mining (SSTDM-15)
• Forrest Hoffman, co-convened, AGU session - IEEE International Conference on Data Mining (ICDM 2015)
• Chung-Hsing Hsu, program committee, Second Workshop on OpenSHMEM and Related Technologies
• Chung-Hsing Hsu, co-chair, The First Workshop on HPC Power Management
• Christos Kartsaklis, program committee, ICT-DMi2015: International Conference on Information and Communication Technologies for Disaster Management
• Christos Kartsaklis, program committee, International Workshop on Sustainable Higher Performance Computing (SHPC 2015)
• Christos Kartsaklis, program committee, Workshop on Extreme-Scale Programming Tools (ESPT2015)
• Christos Kartsaklis, program committee, Workshop on Extreme Data Parallel Processing, Exascale Systems Engineering and Energy Efficiency (HPC-E5)
• Christos Kartsaklis, program committee, 2nd International Workshop on Hardware-Software Co-Design for High Performance Computing (Co-HPC 2015)
• Christos Kartsaklis, program committee, 2nd Workshop on Accelerator Programming Using Directives (WACCPD 2015)
• Christos Kartsaklis, program committee, CANDAR 2015: The Third International Symposium on Computing and Networking
• Christos Kartsaklis, Program Committee Member, Co-HPC 2015, SuperComputing2015
• Christos Kartsaklis, Program Committee Member, WACCPD, SuperComputing2015
• Christos Kartsaklis, Program Committee Member, Fourth Workshop on Extreme-Scale Programming Tools, SuperComputing2015
• Scott Klasky, Posters Committee Member, SuperComputing2015
• Seyong Lee, program committee for ICPADS 2015, WACCPD 2015, and WRAp 2015
• Seyong Lee, reviewer of DOE SBIR proposal
• Seyong Lee, reviewer of International Journal of High Performance Computing
Community Service (Continued)

- Seyong Lee, reviewer of International Journal of Computing Science and Applications (CyS)
- Qing Gary Liu, Technical Papers Member, Data Analytics, Visualization and Storage, SuperComputing2015
- Tiffany M. Mintz, program committee, International Conference on Contemporary Computing (IC3) 2016
- Tiffany M. Mintz, poster committee co-chair, Smoky Mountains Computational Sciences and Engineering Conference 2015
- Sparsh Mittal, reviewer for ACM TACO, IEEE JETCAS, IEEE CAL, IEEE Transactions on Computers and ACM Computing Surveys
- Sarah Powers, hostess, Dr. Blair Sullivan for a Women in Computing seminar titled "Searching for Structure in Network Science."
- David Pugmire, Scientific Visualization and Data Analytics Showcase Committee Member, SuperComputing2015
- Philip C. Roth, Security Chair, SuperComputing2015
- Phil Roth, General Chair, 2015 Data Intensive Scalable Computing Systems Workshop (DISCS-2015), co-located with SC15
- Pavel Shamis, co-chair, OpenSHMEM 2015: Second workshop on OpenSHMEM and Related Technologies
- Jeffrey Vetter, technical program chair, SuperComputing2015
- Jeffrey Vetter, participated in the IEEE Rebooting Computing Summit in December to review emerging technologies.
- Jeffrey Vetter, ACM Gordon Bell Prize Committee Member, SuperComputing2015
- Jeffrey Vetter, Steering Committee Member, SuperComputing2015

Events

UPCOMING

First International Workshop on Performance Portable Programming Models for Accelerators (P^3MA) - June 23, 2016

Graham Lopez

This workshop will be held on June 23, 2016, collocated with the ISC High Performance Conference in Frankfurt, Germany (http://www.isc-hpc.com).

The workshop will provide a forum for bringing together researchers, vendors, users and developers to brainstorm aspects of heterogeneous computing and its various tools and techniques.


Looking Beyond CMOS Technology for Future HPC - April 5-6, 2016

Jeff Nichols, Neena Imam, Barney Maccabe

The goal of this workshop will be to explore common areas of interest among various stake holders to enable the supercomputers of the future. As such, this workshop will focus on novel approaches that overcome the limitations of CMOS technology with the potential to enable paradigm shifts in the HPC realm. The workshop will have four sessions based on the following focus areas: nanomaterials, quantum computing, superconducting computing, and emerging processor and memory architectures. Experts from federal agencies, national laboratories, industry, and academia will be invited to give talks in these areas. Common to the four focus areas will be the consideration of technological gaps and challenges to developing supporting ecosystem and infrastructure for "beyond CMOS" technologies.

Workshop site here - http://beyondcmos.ornl.gov/

SOS20 - March 22-25, 2016

John Turner

SOS is an invitation-only series of highly interactive workshops on Distributed Supercomputing organized by Sandia National Laboratories, Oak Ridge National Laboratories and the Swiss National Supercomputing Centre.

Participants in the SOS Workshops have been key players in remarkable changes in High Performance Computing over the past two decades, and this 20th anniversary meeting will provide an opportunity to both look back over those changes and look ahead to Exascale and beyond. In addition to a retrospective panel featuring some of the founding and long-time figures in SOS, participants will discuss the following topics:

- Are we entering a new age of software development for HPC?
- Application software longevity - a blessing or a curse?
- What evolving applications and workflows are driving HPC today?
- Is co-design having an impact on system design?
- How have HPC operating systems and runtime environments evolved?

Workshop site here - http://www.csm.ornl.gov/SOS20/
2nd International Workshop on the Lustre Ecosystem: Enhancing Lustre Support for Diverse Workloads
Neena Imam, Michael Brim, Sarp Oral

The Lustre Ecosystem workshop series is intended to help explore improvements in the performance and flexibility of Lustre for supporting diverse application workloads. The 2015 workshop was the inaugural edition, and the goal was to initiate a discussion on the open challenges associated with enhancing Lustre for diverse applications, the technological advances necessary, and the associated impacts to the Lustre ecosystem. The workshop program featured a day of tutorials and a day of technical paper presentations.

In this workshop, we seek contributions that explore improvements in the performance and flexibility of the Lustre file system for supporting diverse workloads. Specific topics of interest include, but are not limited to:

- Using Lustre as a Shared Resource
- Adaptability and Scalability of Lustre for Diverse Workloads
- Resilience and Serviceability of Lustre
- Knowledge Provenance in Lustre
- Application-driven Lustre Benchmarking
- Integrating Big Data Technologies with Lustre
- Performance Monitoring Tools for Lustre

Workshop site here - http://lustre.ornl.gov/ecosystem

PAST
Language, Network and System Software (LENS) Workshop
Manjunath Gorentla Venkata

Manjunath Gorentla Venkata was invited to talk about OpenSHMEM programming model at Language, Network and System Software (LENS) workshop in Tokyo, Japan (http://wallaby.aics.riken.jp/lens/) on October 30th, 2015. The workshop was organized by CREST program (http://www.jst.go.jp/kisoken/crest/en/index.html). The goal of the workshop was to create a dialogue among the PGAS communities in the US, Europe, and Asia, and to discuss the relevance of PGAS for the exascale era.

The CREST program aims to develop technologies, hardware, and software for post-peta scale computing. It is a flagship program of Japan Science and Technology Agency.

The OpenSHMEM is a predominant PGAS library interface specification. It is a community effort to standardize the SHMEM programming models, driven by Oak Ridge National Laboratory (ORNL), Department of Defense (DoD), and University of Houston (UH). The community has released three versions of the OpenSHMEM specification, and it will the latest version version 1.3 at SC15. In this talk, first, I will introduce OpenSHMEM, present its history, and discuss the upcoming features. Then, I will discuss the efforts preparing OpenSHMEM for the exascale era, and provide an overview of the OpenSHMEM activities, which includes specification development, reference implementation, and research. Lastly, I will provide an overview of OpenSHMEM reference implementation and its network layer, UCX.

This work was performed for the DoD.

CSMD Seminars
- Madhu Hari: Using Software Engineering Methodologies to Port a Scientific Code to GPUs
- Kathleen Hamilton: Percolation bounds for decoding thresholds with correlated erasures in quantum codes
- Christoph Beckermann: Modeling of Microstructure Evolution in Solidification Processes
- Ferrol Aderholdt: Virtual Machine Introspection-based Checkpoint/Restart for Survivable Clouds
- Mike Leuze: DNA2Face: Predicting Faces from a DNA Sample
- Alvin R. Lebeck: Molecular-Scale Nanophotonics for Network-on-Chip and Probabilistic Computing Functional Units
- Jian Huang: Interactive Selection of Multivariate Features in Large Spatiotemporal Data
- Tonglin Li: Distributed NoSQL Storage for Extreme-Scale System Services in Clouds and Supercomputers
- Todd Gamblin: Build and Test Automation at Livermore Computing
- Ian Foster: Accelerating Discovery Via Science Services
- Edmond Chow: Very Fine-Grained Parallelization of Sparse Linear Algebra Computations
- Vivek Seshadri: Can DRAM do more than just store data?
- Alexander M. Feldt: Thinking About Vulnerability: Climate Change, Human Rights, and Moral Thresholds

CAM Seminars
- Rick Archibald: Sparse Sampling Methods for Image Processing and Data Analysis
- Frank Pinski: Rare Events, the Thermodynamic Action and the Continuous-Time Limit
- Edriss Titi: Finite Number of Determining Parameters for the Navier-Stokes Equations with Applications into Feedback Control and Data Assimilation
Events (Continued)

- Balasubramaniam Radhakrishnan: Modeling Nucleation in Solid State Phase Transformations
- Fei Han: Coupling Peridynamics with Damage Mechanics to Achieve Objective Simulation of Material Failure
- Srikanth Allu: Multi-Scale Modeling for Performance and Safety of Lithium Ion Batteries
- Heng Xiao: Quantifying and Reducing Model-Form Uncertainties in Reynolds-Averaged Navier-Stokes Simulations: An Open-Box, Physics-Based Approach
- Ben Thompson: Boundary Element Analysis of Active Tectonics and Earthquakes in the Longmen Shan and Himalaya: Insights and Computational Methodology
- Peter Jantsch: Analysis and Approximation of Parametric Hyperbolic PDE
- Nicholas Dexter: Explicit Cost Bounds of Stochastic Galerkin Approximations for Parameterized PDEs with Random Coefficients
- Guowei Wei: Geometry and Topology of the Biomolecular World

CAEBAT III Kick-off
Srikanth Allu, Sergiy Kalnaus, Abhishek Kumar, Damien Lebrun-Grandie, Srdjan Simunovic, John Turner, Wael Elwasif, and Hsin Wang

On Nov. 3, 2015, a joint kickoff for the third phase of the Computer Aided Engineering for Batteries (CAEBAT) program was held in Washington, DC.

The kickoff for the third phase of CAEBAT also marks the start of the ORNL-led Consortium for Advanced Battery Simulation (CABS), a collaboration between ORNL, Lawrence Berkeley National Laboratory (LBNL) and Sandia National Laboratories (SNL). CABS is a three-year, $1.525M/yr. effort.

Two major barriers for increasing battery energy density and power, increasing safety and reducing cost are: (1) insufficient understanding of the underlying physical phenomena that limit battery performance and safety, particularly the role of microstructure, and (2) lack of validated predictive simulation tools. CABS will address (1) by developing new experiments for properties with largest uncertainties and developing new validated models that allow researchers to explore battery response under both normal and abusive conditions, and will address (2) by deploying increasingly capable and computationally efficient releases of the Open Architecture Software (OAS) and components of the Virtual Integrated Battery Environment (VIBE), developed as part of CAEBAT 1.

CABS will operate as an integrated partnership. LBNL will provide data for properties and validation of microstructure models. SNL will perform high-resolution microstructure simulations. ORNL will develop and perform new mechanics experiments, develop homogenized, layer-resolved, and microstructure models, and will deploy software components through VIBE/OAS while enhancing its extensibility and improving computational performance through implementation of new hybrid / adaptive methods and other numerical improvements. ORNL will also serve as the lead institution, performing overall management.

Publications of Note

Multiscale modeling and characterization for performance and safety of lithium-ion batteries

ABSTRACT: Lithium-ion batteries are highly complex electrochemical systems whose performance and safety are governed by coupled nonlinear electrochemical-electrical-thermal-mechanical processes over a range of spatiotemporal scales. Gaining an understanding of the role of these processes as well as development of predictive capabilities for design of better performing batteries requires synergy between theory, modeling, and simulation, and fundamental experimental work to support the models. This paper presents the overview of the work performed by the authors aligned with both experimental and computational efforts. In this paper, we describe a new, open source computational environment for battery simulations with an initial focus on lithium-ion systems but designed to support a variety of model types and formulations. This system has been used to create a three-dimensional cell and battery pack models that explicitly simulate all the battery components (current collectors, electrodes, and separator). The models are used to predict battery performance under normal operations and to study thermal and mechanical safety aspects under adverse conditions. This paper also provides an overview of the experimental techniques to obtain crucial validation data to benchmark the simulations at various scales for performance as well as abuse. We detail some initial validation using characterization experiments such as infrared and neutron imaging and micro-Raman mapping. In addition, we identify opportunities for future integration of theory, modeling, and experiments.
Modeling the evolution of lithium-ion particle contact distributions using a fabric tensor approach
A.J. Stershic, S. Simunovic, J. Nanda

ABSTRACT: Electrode microstructure and processing can strongly influence lithium-ion battery performance such as capacity retention, power, and rate. Battery electrodes are multi-phase composite structures wherein conductive diluents and binder bond active material to a current collector. The structure and response of this composite network during repeated electrochemical cycling directly affects battery performance characteristics. We propose the fabric tensor formalism for describing the structure and evolution of the electrode microstructure. Fabric tensors are directional measures of particulate assemblies based on inter-particle connectivity, relating to the structural and transport properties of the electrode. Fabric tensor analysis is applied to experimental data-sets for positive electrode made of lithium nickel manganese cobalt oxide, captured by X-ray tomography for several compositions and consolidation pressures. We show that fabric tensors capture the evolution of inter-particle contact distribution and are therefore good measures for the internal state of and electronic transport within the electrode. The fabric tensor analysis is also applied to Discrete Element Method (DEM) simulations of electrode microstructures using spherical particles with size distributions from the tomography. These results do not follow the experimental trends, which indicates that the particle size distribution alone is not a sufficient measure for the electrode microstructures in DEM simulations.

Internal configuration of prismatic lithium-ion cells at the onset of mechanically induced short circuit
Hsin Wang, Srdjan Simunovic, Hossien Maleki, Jason N. Howard, Jerald A. Hallmark

ABSTRACT: The response of Li-ion cells to mechanically induced internal electrical shorts is an important safety performance metric design. We assume that the battery internal configuration at the onset of electrical short influences the subsequent response and can be used to gauge the safety risk. We subjected a series of prismatic Li-ion cells to lateral pinching using 0.25”, 0.5”, 1”, 2” and 3” diameter steel balls until the onset of internal short. The external aluminum enclosure froze the internal cell configuration at the onset of short and enabled us to cross-section the cells, and take the cross-section images. The images indicate that an internal electric short is preceded by extensive strain partitioning in the cells, fracturing and tearing of the current collectors, and cracking and slipping of the electrode layers with multiple fault lines across multiple layers. These observations are at odds with a common notion of homogeneous deformation across the layers and strain hardening of electrodes that eventually punch through the separator and short the cell. The faults are akin to tectonic movements of multiple layers that are characteristic of granular materials and bonded aggregates. The short circuits occur after extensive internal faulting, which implies significant stretching and tearing of separators.

Atomic-Level Sculpting of Crystalline Oxides: Toward Bulk Nanofabrication with Single Atomic Plane Precision

ABSTRACT: The atomic-level sculpting of 3D crystalline oxide nanostructures from metastable amorphous films in a scanning transmission electron microscope (STEM) is demonstrated. Strontium titanate nanostructures grow epitaxially from the crystalline substrate following the beam path. This method can be used for fabricating crystalline structures as small as 1–2 nm and the process can be observed in situ with atomic resolution. The fabrication of arbitrary shape structures via control of the position and scan speed of the electron beam is further demonstrated. Combined with broad availability of the atomic resolved electron microscopy platforms, these observations suggest the feasibility of large scale implementation of bulk atomic-level fabrication as a new enabling tool of nanoscience and technology, providing a bottom-up, atomic-level complement to 3D printing.

Patterning: Atomic-Level Sculpting of Crystalline Oxides: Toward Bulk Nanofabrication with Single Atomic Plane Precision
Stephen Jesse, Qian He, Andrew R. Lupini, Donovan N. Leonard, Mark P. Oxley, Oleg Ovchinnikov, Raymond R. Unocic, Alexander Tselev, Miguel Fuentes-Cabrera, Bobby G. Sumpter, Stephen J. Pennycook, Sergei V. Kalinin and Albina Y. Borisevich

ABSTRACT: Q. He, A. Y. Borisevich, and co-workers describe how an aberration-corrected e-beam in a scanning transmission electron microscope can be used to crystallize amorphous complex oxides with atomic plane precision. Using this control system, epitaxial growth of SrTiO3 is achieved to pattern text onto a 90 × 25 nm area, as shown in the image. Each feature shown is about 20 unit cells (about 8 nm) wide.
Controlling Molecular-Ordering in Solution-State Conjugated Polymers
Jiahua Zhu, Youngkyu Han, Rajeev Kumar, Youjun He, Kunlun Hong, Peter Bonnesen, Bobby G. Sumpter, Changwoo Do, Sean Smith, Ilia Ivanov, Changwoo Do

ABSTRACT: Rationally encoding molecular interactions that can control the assembly structure and functional expression in a solution of conjugated polymers hold great potential for enabling optimal organic optoelectronic and sensory materials. In this work, we show that thermally-controlled and surfactant-guided assembly of water-soluble conjugated polymers in aqueous solution is a simple and effective strategy to generate optoelectronic materials with the desired molecular ordering. We have studied a conjugated polymer consisting of a hydrophobic thiophene backbone and hydrophilic, thermo-responsive ethylene oxide side groups, which shows a step-wise, multi-dimensional assembly in water. By incorporating the polymer into phase-segregated domains of an amphiphilic surfactant in solution, we demonstrate that both chain conformation and degree of molecular ordering of the conjugated polymer can be tuned in hexagonal, micellar and lamellar phases of the surfactant solution. The controlled molecular ordering in conjugated polymer assembly is demonstrated as a key factor determining the electronic interaction and optical function.

Two-Dimensional, Ordered, Double Transition Metals Carbides (MXenes)
Babak Anasori, Yu Xie, Majid Beidaghi, Jun Lu, Brian C. Hosler, Lars Hultman, Paul R. C. Kent, Yury Gogotsi, and Michel W. Barsoum

ABSTRACT: The higher the chemical diversity and structural complexity of two-dimensional (2D) materials, the higher the likelihood they possess unique and useful properties. Herein, density functional theory (DFT) is used to predict the existence of two new families of 2D ordered, carbides (MXenes), M′2M″C2 and M′2M″2C3, where M′ and M″ are two different early transition metals. In these solids, M′ layers sandwich M″ carbide layers. By synthesizing Mo2TiC2Tx, Mo2Ti2C3Tx, and Cr2TiC2Tx (where T is a surface termination), we validated the DFT predictions. Since the Mo and Cr atoms are on the outside, they control the 2D flakes’ chemical and electrochemical properties. The latter was proven by showing quite different electrochemical behavior of Mo2TiC2Tx and Ti3C2Tx. This work further expands the family of 2D materials, offering additional choices of structures, chemistries, and ultimately useful properties.
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Contact Information

CONTACTS

CSMD Director - Barney Maccabe - maccabeab@ornl.gov
Division Secretary - Lora Wolfe - wolfelm@ornl.gov
Division Finance Officer - Ursula Henderson - hendersonuf@ornl.gov
Technical Communications - Daniel Pack - packdl@ornl.gov

LINKS

Computer Science and Mathematics Division - www.csm.ornl.gov
Computing and Computational Sciences Directorate - computing.ornl.gov
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