Trevor Keller, Ph. D.

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Education

Rensselaer Polytechnic Institute Troy, NY

Ph.D., Materials Engineering Dr. Daniel Lewis, research advisor 2011 to 2015

Thesis: "Bias in Polycrystal Topology Caused by Grain Boundary Motion by Mean Curvature." Performed large-scale phase field simulations of normal isotropic grain growth on high performance computing clusters including AMOS, an IBM Blue Gene/Q supercomputer. Designed and implemented algorithms to reconstruct polyhedral grain topology (faces, edges, and vertices) from diffuse interfaces in 2D and 3D phase field datasets. Found the process of triangular face elimination responsible for biasing topology in populations of polyhedral grains in synthetic, simulated, and real metal microstructures. Open source code: http://github.com/tkphd/trijunctionThreshold.

M.S., Materials Engineering Dr. Daniel Gall, research advisor 2009 to 2011

Thesis: "Effects of Magnesium(II) on Zinc Oxide Nanorod Growth From Aqueous Solution." Designed experiments to deposit ZnO on glass substrates using a novel flow-through aqueous chemical reactor under various combinations of temperature, pH, reactant concentrations, and flow rate. Found minor effects of Mg^{2+} ions on ZnO film stress and lattice parameters.

B.S., Chemical Engineering 2002 to 2006

Experience

National Institute of Standards and Technology Gaithersburg, MD

NRC Postdoctoral Associate, 40 hours/week July 2015 to present

Implemented phase field model for solid-state transformation in alloy systems with three components and four phases, analogous to Inconel 625. Designed initial conditions based on electron micrographs of additively manufactured Inconel 625 to simulate microstructure evolution during heat treatment. Produced thermodynamic models through simplification of quantitative CALPHAD databases while retaining key phase diagram features, using computer algebra systems to accurately generate expressions and multivariable derivatives for import into phase field software. Open source code: http://github.com/usnistgov/phasefield-precipitate-aging.

Mesoscale Microstructure Simulation Project http://github.com/mesoscale

Software Developer January 2013 to present

MMSP implements a grid class in C++ with parallel domain decomposition for finite difference applications, especially phase field methods and Monte Carlo models. Invited to join project as co-developer based on voluntary contribution of patches to eliminate memory leaks and resolve race conditions in parallel computing environments. Eliminated corruption in parallel I/O on large-block filesystems, enabling clean execution of phase field and kinetic Monte Carlo research simulations on IBM Blue Gene/Q supercomputers with up to 4096 cores. Implemented testing of proposed source code changes through automatic online continuous integration.

Veeco Instruments Solar Process Development Center, Clifton Park, NY

Process Engineer, 20 hours/week July 2009 to August 2011

Researched non-toxic alternatives to CdS, reporting to senior management. Traveled to Helsinki, Finland to evaluate state-of-the-art atomic layer deposition reactor.

DayStar Technologies Materials Development Group, Clifton Park, NY

Process Engineer, 40 hours/week January 2009 to June 2009

Process Technician, 40 hours/week July 2006 to December 2008

Researched alternatives to chemical bath deposition of CdS thin films, including nontoxic materials and novel reactor geometries. Achieved 72× scaleup in CdS deposition area with only 6× increase in waste generation.

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Publications

- T. Keller, G. Lindwall, S. Ghosh, L. Ma, B. Lane, F. Zhang, U. Kattner, J. Heigel, E. Lass, Y. Idell, M. Williams, A. Allen, J. Guyer, and L. Levine. "Application of Finite Element, Phase-field, and CALPHAD-based Methods to Additive Manufacturing of Ni Alloys." Manuscript in preparation (2017).
- T. Keller, B. Cutler, E. Lazar, and D. Lewis. "Comparative Grain Topology." *Acta Materialia* **66** (2014) 414–423. DOI: 10.1016/j.actamat.2013.11.039
- T. Keller, B. Cutler, M. Glicksman, and D. Lewis. "Enumeration of Polyhedra for Grain Growth Analysis." In *Proceedings of the First International Conference on 3D Materials Science* (3DMS'12), Seven Springs, PA, July 8–12, 2012, pages 97–106.

Presentations

- *T. Keller*, G. Lindwall, U. Kattner, and J. Guyer. "Study on the Effects of Microsegregation, Temperature, and Stress on IN625 Microstructures by Phase Field Simulations." TMS Annual Meeting. San Diego, CA: February 28, 2017.
- *T. Keller*, G. Lindwall, U. Kattner, and J. Guyer. "Arresting deleterious particle growth in Inconel 625: Phase field model description." MS&T Annual Meeting. Salt Lake City, UT: October 27, 2016.
- *T. Keller*, B. Cutler, and D. Lewis. "Finite grain boundary networks from phase-field grain growth data." Invited talk to the NIST Material Science & Engineering Division. Gaithersburg, MD: December 8, 2014.
- T. Keller, B. Cutler, and *D. Lewis*. Invited talk: "Comparative analysis of polycrystals in simulated & experimental datasets." MS&T Annual Meeting. Pittsburgh, PA: October 15, 2014.
- T. Keller, D. Crist, *D. Lewis*, Y. Tan, K. Huang, and C. Li. "Realtime prediction of grain growth during materials processing." PICS3. Marseille, France: May 2014.
- *T. Keller* and D. Lewis. "Topological characterization of 3D microstructures with diffuse interfaces." TMS Annual Meeting. San Diego, CA: February 19, 2014.
- *T. Keller*, D. Lewis, B. Cutler, and E. Lazar. "Topological comparison of synthetic microstructures." MS&T Annual Meeting. Montreal, QC, Canada: October 28, 2013.
- T. Keller, *D. Lewis*, B. Cutler, B. Yener, S. Rock, G. Saunders, and M. Muench. "The topology of polycrystals." PICS3. Marseille, France: July 2013.
- T. Keller, B. Cutler, G. Yauney, and *D. Lewis*. "Topological analysis of collapsing grains." MS&T Annual Meeting. Pittsburgh, PA: October 10, 2012.
- T. Keller, B. Cutler, G. Yauney, and *D. Lewis*. "Polyhedral graphs & grain topology." International Conference on 3-Dimensional Materials Science (3DMS). Seven Springs, PA: July 11, 2012.

Posters

- *T. Keller* and D. Lewis. "Trijunction Drag Affects Grain Topology." NIST Chapter of Sigma Xi, Annual Postdoctoral Poster Session. Gaithersburg, MD: February 19, 2016.
- *T. Keller* and D. Lewis. "Grain topology from 3D phase-field simulations." Eastern New York Chapter of ASM International, Spring Symposium. Troy, NY: November 18, 2014.
- *T. Keller*, B. Cutler, G. Yauney, and D. Lewis. "Grain topologies in synthetic, simulated, and real microstructures." Rensselaer Moves into Petascale Computing: Celebration & Workshop. Troy, NY: October 3, 2013.
- *T. Keller*, B. Cutler, G. Yauney, and D. Lewis. "Topological distributions in synthetic microstructures and grains." 8th International Conference on Porous Metals and Metallic Foams (MetFoam). Raleigh, NC: June 23-26, 2013.
  - Won Second Place Poster Award.
- D. Lewis, G. Saunders, S. Rock, *T. Keller*, J. Mao, M. Muench, J. Symons, D. Hoffman, M. Oullette, and C. LaBarre. "Development of an automated serial sectioning system." CATS/CEG Advanced Manufacturing Conference. Troy, NY: April 22, 2013.
- *T. Keller*, G. Yauney, B. Cutler, and D. Lewis. "Grain populations in topological space." Eastern New York Chapter of ASM International, Spring Symposium. Troy, NY: December 5, 2012.

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Special Skills

Scientific Computing: Open source software portfolio available at http://github.com/tkphd. Experienced in parallel programming for high performance computing environments with C++ and MPI-2; using git version control software; typesetting technical documents using LaTeX2e; building and maintaining workstation computers based on Debian GNU/Linux with multiple users; managing software RAID 1/5/6; maintaining small computer clusters using Ansible.

Experimental Techniques: Experienced in sample preparation and analysis using the following techniques: metallographic polishing and etching of Fe-, Cr-, Cu-, Zn-, and Ni-based alloys for optical microscopy and EBSD; scanning electron microscopy of inorganic specimens; X-ray diffractometry, UV-visible light spectrophotometry, and profilometry of thin films.

Professional Development

- CHiMaD Phase-Field Workshop IV Northwestern University January 17–20, 2017
  Detailed discussion of the state of phase-field community codes following time-limited installation and execution of CHiMaD benchmark problems with unfamiliar software (PRISMS-PF).
- Women in STEM: STEM Role Model Training NIST November 29, 2016
  Panel discussion on engaging students, highlighting diversity, and making STEM relatable. Emphasis on constructive mindset and responsible fulfillment of mentor and role model duties.
- Women in STEM: Meal with a Mentor NIST June 28, 2016
  Lunchtime panel and break-out discussions with 24 summer undergraduate and graduate students on trajectories, opportunities, and obstacles in STEM research. Emphasis on answering questions and presenting a range of individual perspectives.
- CHiMaD Phase-Field Workshop III Northwestern University May 3–5, 2016
  Detailed discussion of the state of phase-field community codes through the lens of hackathon problems (anisotropic solidification and elasticity), solved using FiPy in collaboration with two developers.
- CHiMaD Phase-Field Workshop II Northwestern University October 13–16, 2015
  Detailed discussion of the state of phase-field community codes through the lens of hackathon problems (spinodal decomposition and Ostwald ripening), solved using MMSP.
- Software Carpentry Workshop NIST September 23–24, 2015
  Interactive lecture topics included Unix shell scripts, Python programming and visualization, git version control, and data management in SQL databases.
- IIMEC Summer School Texas A&M University June 2–11, 2014
  "Computational Materials Science Across Scales." Lecture topics included density functional theory, molecular dynamics, thermodynamics, phase-field models, and continuum mechanics. Equal coverage of theory and numerical exercises in collaborative workshops.
- Member of the Society for Industrial and Applied Mathematics (SIAM) since 2014
- Played intramural soccer in 15-team league RPI Team captain, Fall 2014