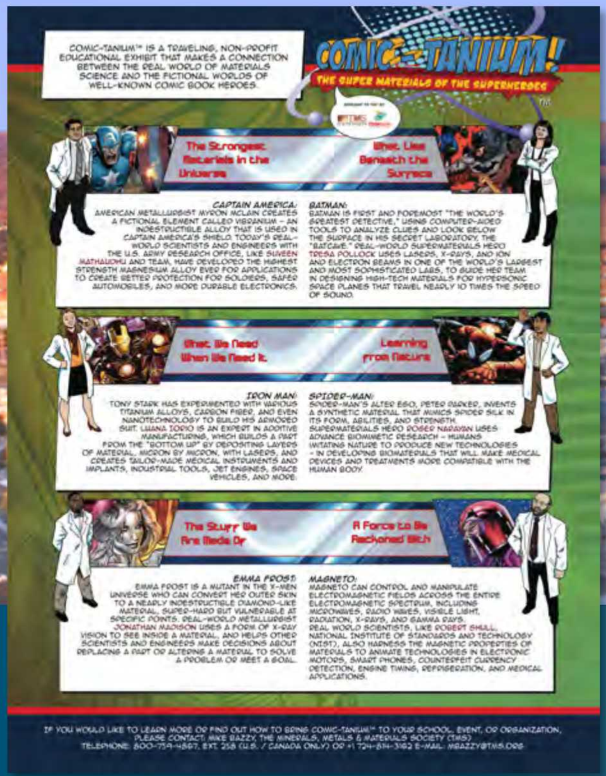
SAND2020-7773C



Science, Service, Collaboration & Diversity

Naval Research Laboratory,

HBCU/MI Summer Internship Seminar, Washington D.C.

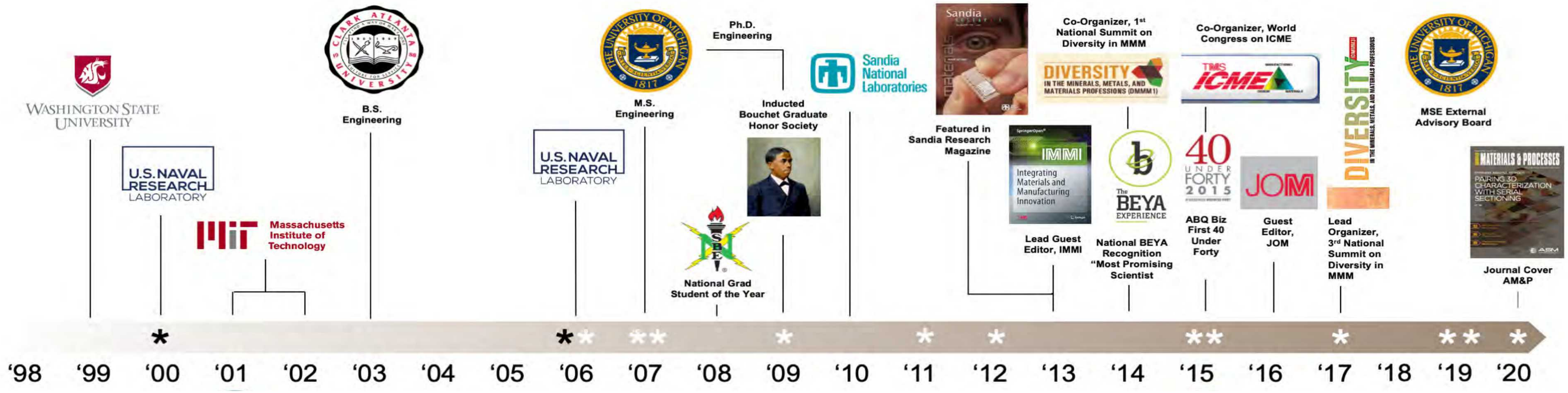
Wednesday, July 29th, 2020

Jonathan D. Madison, Ph.D.

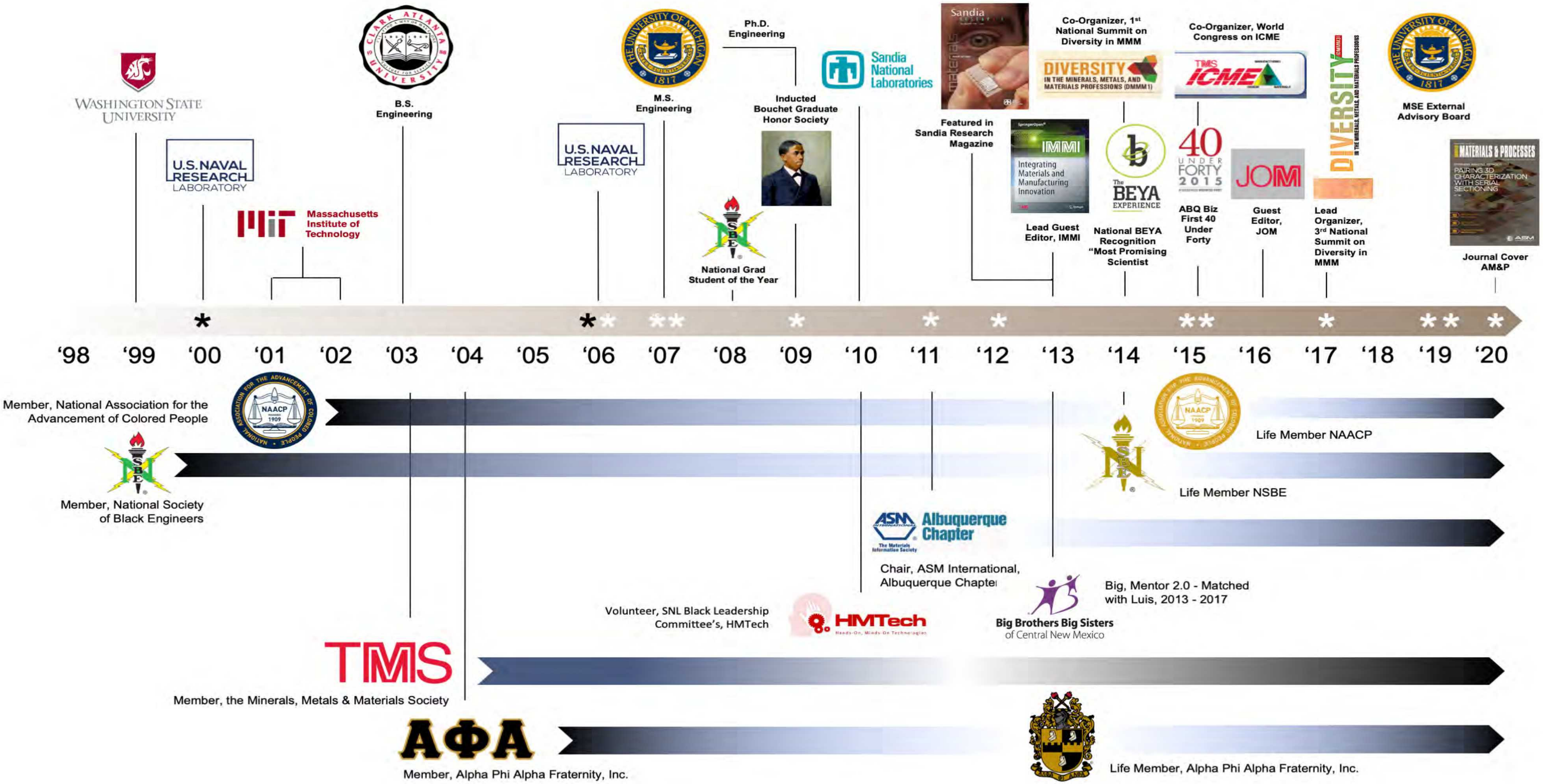
Sandia National Laboratories, Albuquerque, NM

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia LLC, a wholly owned subsidiary of Honeywell International Inc. for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

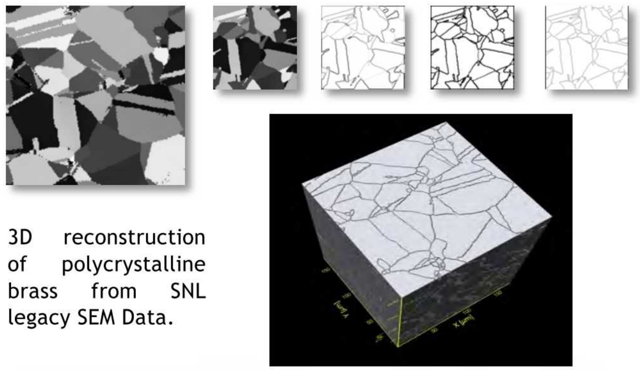
Professional Timeline



Service Involvement

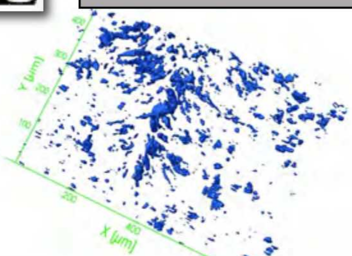


3D Reconstruction & Characterization

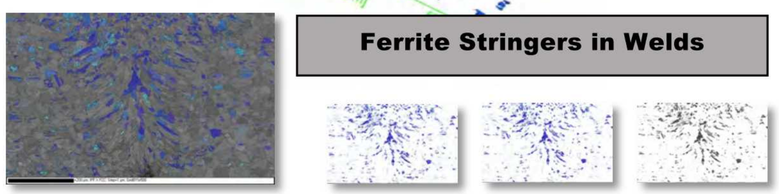


3D reconstruction of polycrystalline brass from SNL legacy SEM Data.

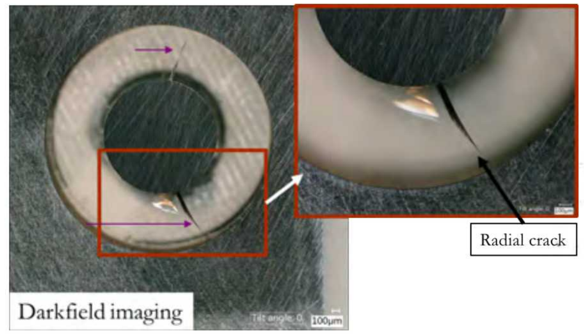
Polycrystalline Brass



3D reconstruction of ferrite stringers in a PW laser weld of 304L stainless steel from EBSD images.



Ferrite Stringers in Welds

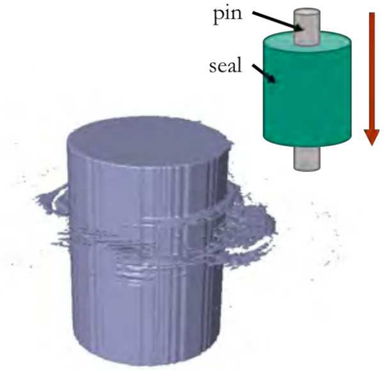


Cracks in Glass-to-Metal Seals

Determination of crack size, severity and depth in glass-to-metal seals for connectors

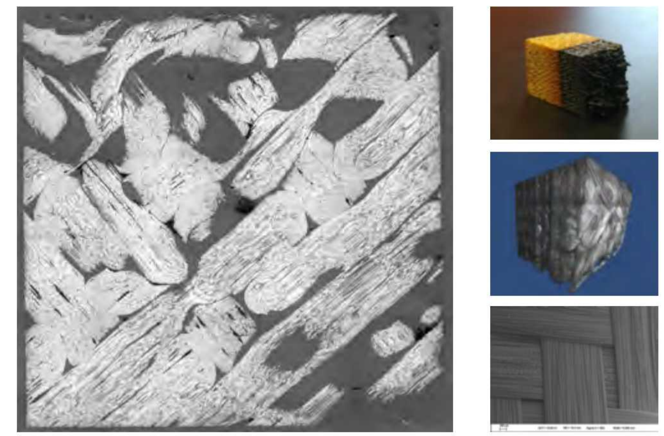
Weld Porosity

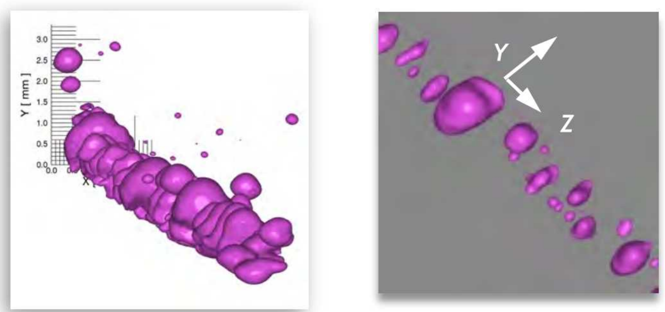
Below, 3D reconstruction and quantitative characterization of porosity in a CW laser weld of 304L stainless steel.

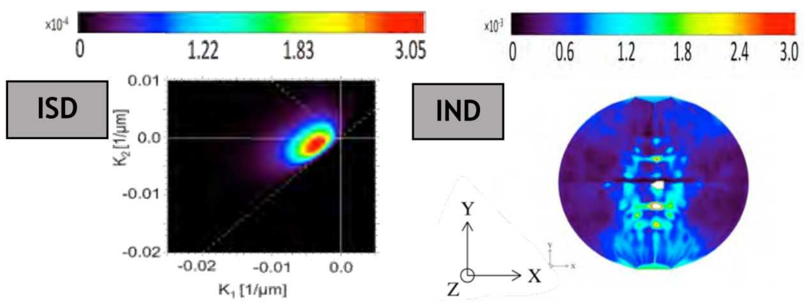


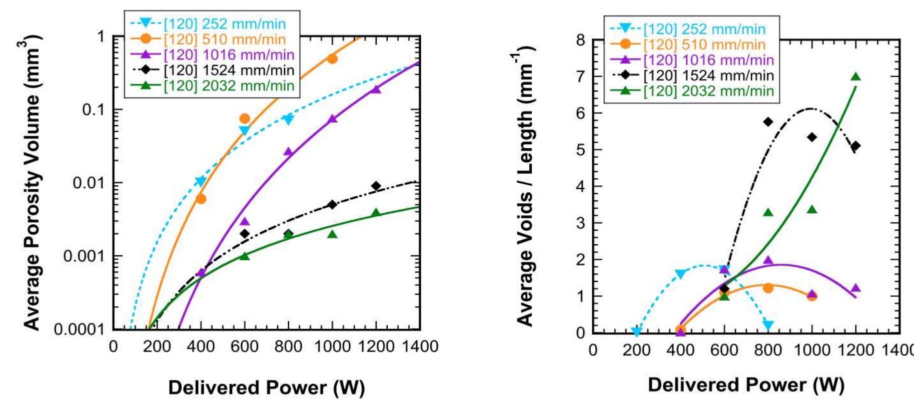
Carbon Fiber Composites for Thermal Protection Systems

Weave pattern consistency, voiding and resistance to charring in fiber-reinforced-composites*









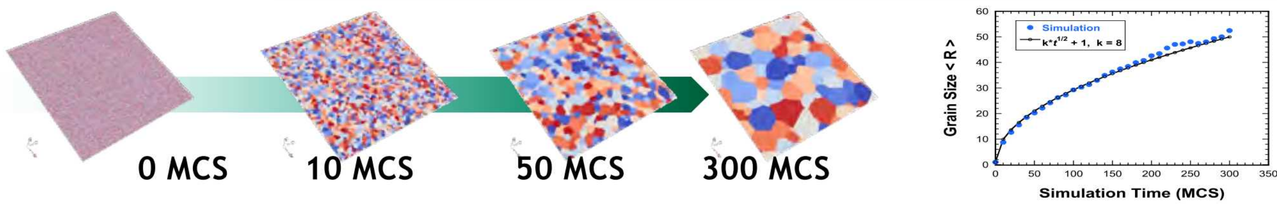
J. Madison, L. K. Aagesen, **Scripta Mat**, vol. 67, issue 9, (2012) pp. 783-786

J. Madison, et al. **IMMI**, vol. 3, issue 11 (2014

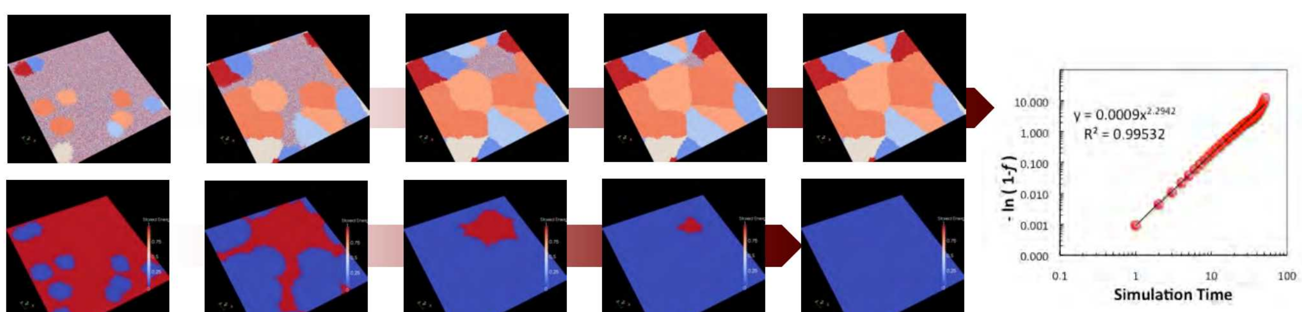
Microstructure Evolution Modeling

SPPARKS - Stochastic Parallel PARticle Kinetic Simulator

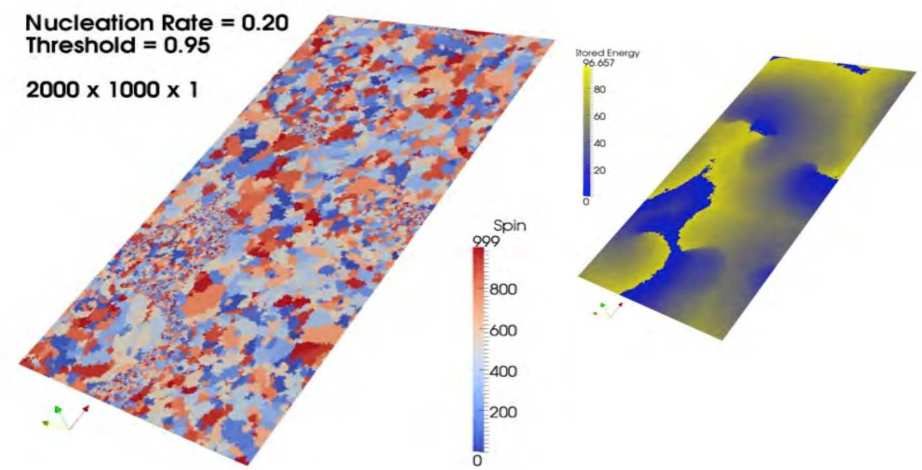
Grain Growth



Static Recrystallization

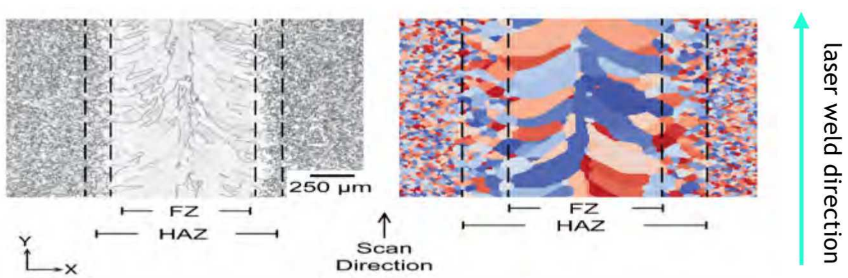


Dynamic Recrystallization



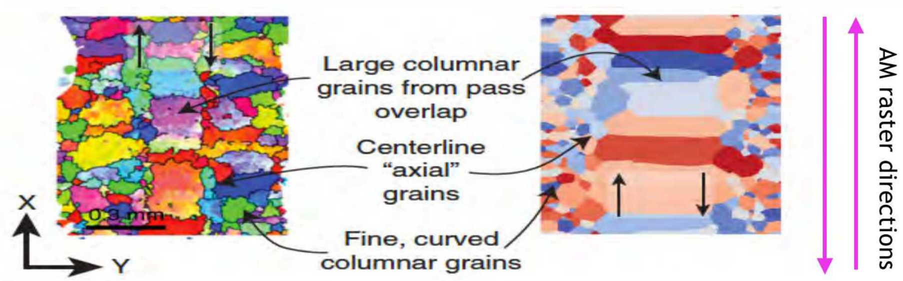
J. Madison, V. Tikare, E. Holm, **J. Nuc. Mater.**, vol. 425, (2012) pp. 173-180

Grain Structure In Vicinity of a Moving Heat Source



Experiment | **Simulation**

T. Rodgers, J. Madison, V. Tikare, **JOM**, vol. 68, no. 5, (2016) pp. 1419 – 1426



Experiment | **Simulation**

T. Rodgers, J. Madison, V. Tikare, **Comp. Mat. Sci.**, vol. 135, (2017) pp. 78 - 89

Using kMC methods we can generate a variety of synthetic microstructures by simple grain growth, static recrystallization, dynamic recrystallization as well as anisotropic grain structures resulting from interaction with a moving heat source. The dynamic recrystallization model exists as a hybrid in conjunction with cellular automata. All microstructural evolution models are performed in designed and created SNL open-source code entitled SPPARKS.

The **Advanced Simulation and Computing (ASC)** program develops, delivers and supports an HPC-based **modeling and simulation capability** in support of the NW mission, **including design, qualification and surveillance**.

Since its inception, ASC has created tremendous capabilities to **simulate the responses of NW components and structures to mechanical, thermal and other loadings.** However, **authoritative knowledge of material properties** for use in the models, and **capabilities to predict variabilities** in the material properties, **are still a challenge**. Inaccurate material properties result in inaccurate predictions. Lack of knowledge of material variabilities prevents prediction of uncertainty in performance.

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Advanced Simulation & Computing (ASC)

National Nuclear Security Administration

U.S. DEPARTMENT OF ENERGY

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The **Materials Margins Assurance program** will build capabilities and expertise that provide **physics-based material performance and variability margins** to support NW component design, analysis and qualification. Since material properties, in most instances, originate from phenomena at the microstructural level a multi-scale approach with **fundamental emphasis on microstructure** will remain a central focus

Advanced Simulation & Computing (ASC)

National Nuclear Security Administration

U.S. DEPARTMENT OF ENERGY

Materials Margins Assurance

How do we meaningfully and reasonably incorporate material variability in our simulation tools and code?

Materials Margins Assurance

How do we meaningfully and reasonably incorporate material variability in our simulation tools and code?

Staff	(x 12)
Post Docs	(x 2)
Students	(x 2)
Sites	(x 2)
Exemplars	(x 4)
Emphasis Areas	(x 5)

SNL NM & SNL CA

5 year activity ~ $1.3M / year

Materials Margins Assurance

Materials Margins Assurance

How do we meaningfully and reasonably incorporate material variability in our simulation tools and code?

EMPHASIS I	EMPHASIS II	EMPHASIS III	EMPHASIS IV	EMPHASIS UnPr
SYNTHETIC MICROSTRUCTURE PREDICTION	FINE-GRAIN ENSEMBLE DEFORMATION	CONTINUUM LEVEL DUCTILE DAMAGE AND FAILURE	CONSTITUTIVE MATERIAL MODEL DEVELOPMENT	UNCERTAINTY PROPAGATION
ADDITIVE MANUFACTURING	INCONEL X750 MICROSPRINGS	304L STAINLESS STEEL LASER WELDS	FE-CO-2V HIPERCO	

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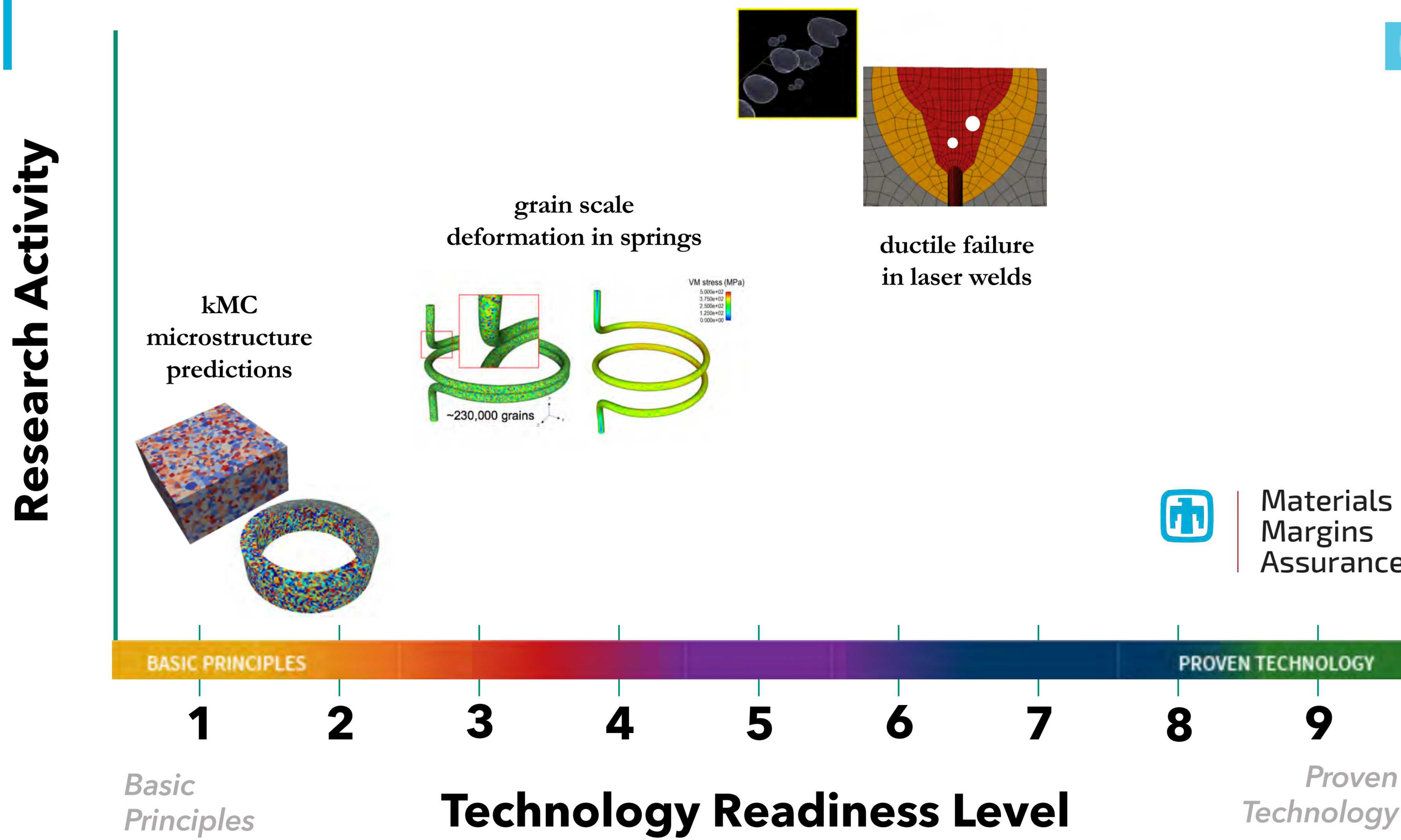
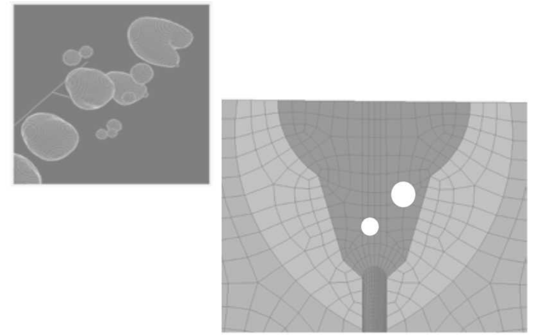


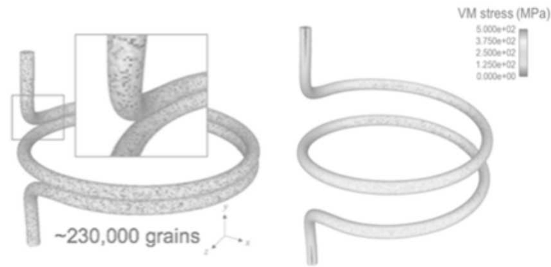
Materials Margins Assurance

Research Activity

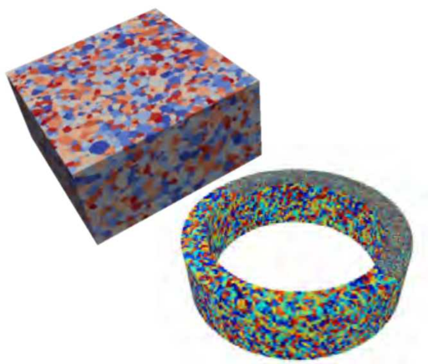
ductile failure
in laser welds



grain scale
deformation in springs



kMC
microstructure
predictions



Materials
Margins
Assurance

BASIC PRINCIPLES — PROVEN TECHNOLOGY

1 2 3 4 5 6 7 8 9

Basic Principles

Technology Readiness Level

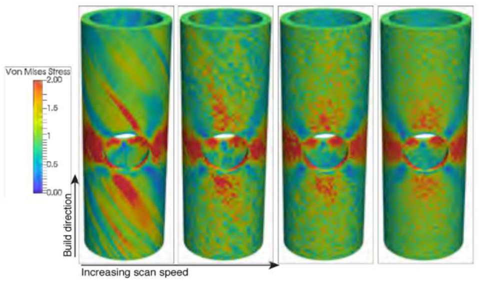
Proven Technology

Sandia's kMC Suite

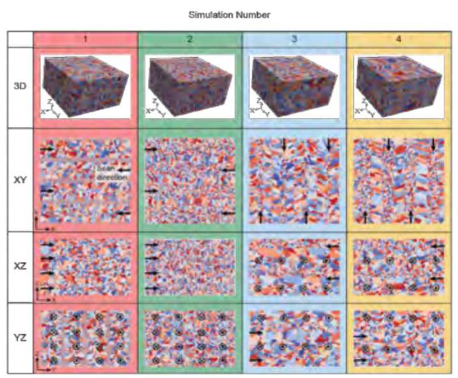
SPPARKS

Stochastic Parallel PARticle Kinetic Simulator

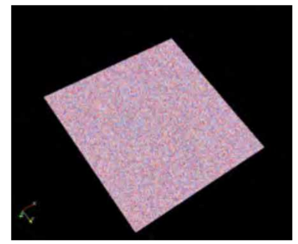
http://spparks.sandia.gov



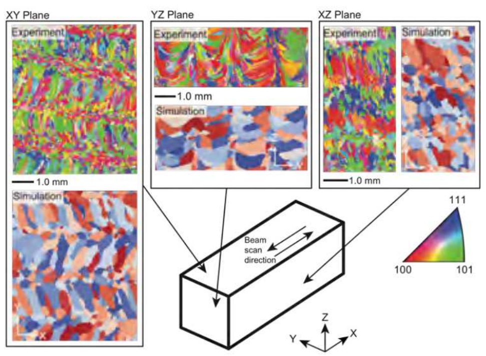
Rodgers et al., **MSMSE** (2018) vol. 26, pp. 055010 1-23



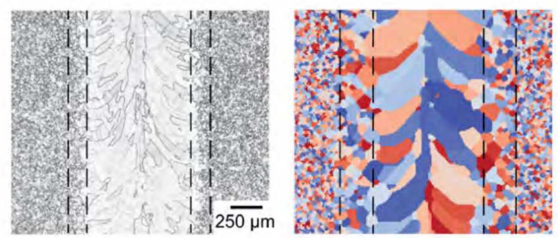
Popova et al. **IMMI** (2017) vol. 6, pp. 54-68



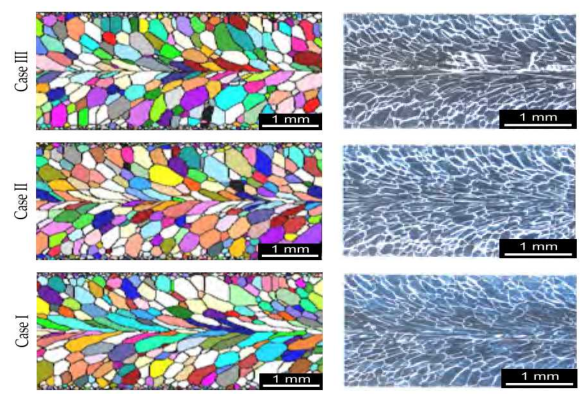
Holm & Battaile, ***JOM*** (2001) vol. 53, pp. 20-23



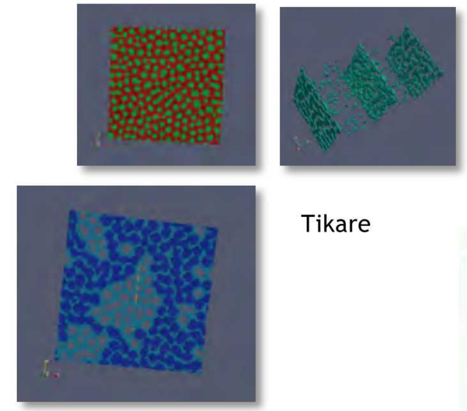
Rodgers et al., **Comp Mater Sci** (2017) vol. 135, pp. 78-89



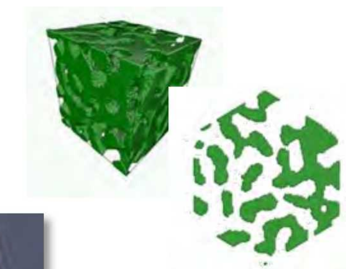
Rodgers, Madison, Tikare & Maguire, ***JOM*** (2016) vol. 68, pp. 1419-1426



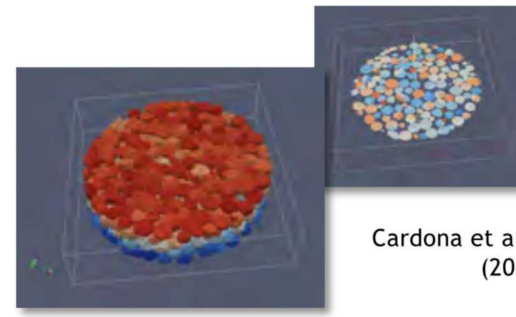
Rodgers et al., **MSMSE** (2017) vol. 25, pp. 064006



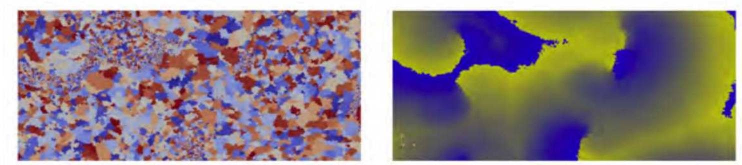
Tikare



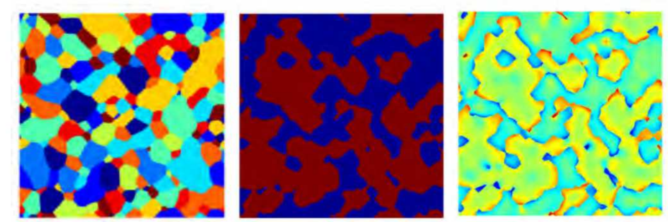
Wagner



Cardona et al. ***J. Am. Ceram. Soc.*** (2012) pp. 1-12



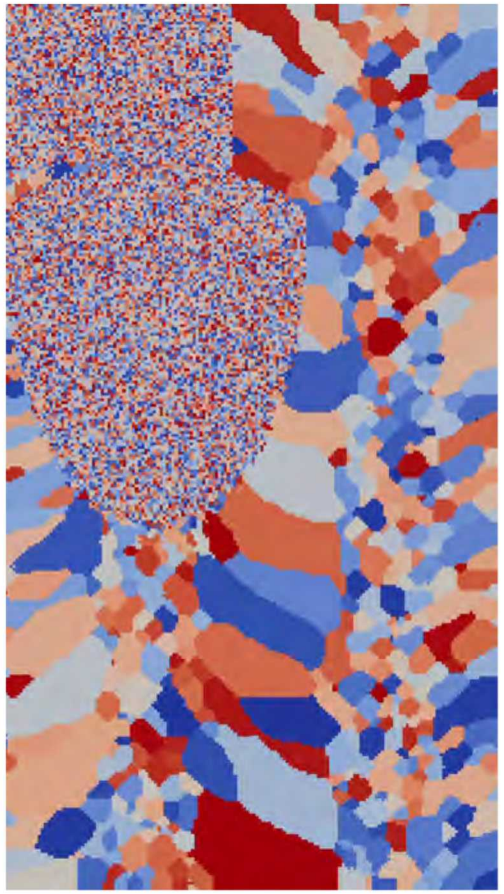
Madison, Tikare & Holm, ***J. Nuc. Mat.*** (2012) vol. 425 pp. 173-180



Homer, Tikare & Holm, ***Comp. Mat. Sci.*** (2013) vol. 69 pp. 414-423

- Open source kinetic Monte Carlo platform with user-editable "apps" for specific applications
- Used to study several mesoscale phenomena including sintering, recrystallization, vacancy diffusion, grain growth and welding
- Problems are easily parallelized and a range of Monte Carlo solvers are available

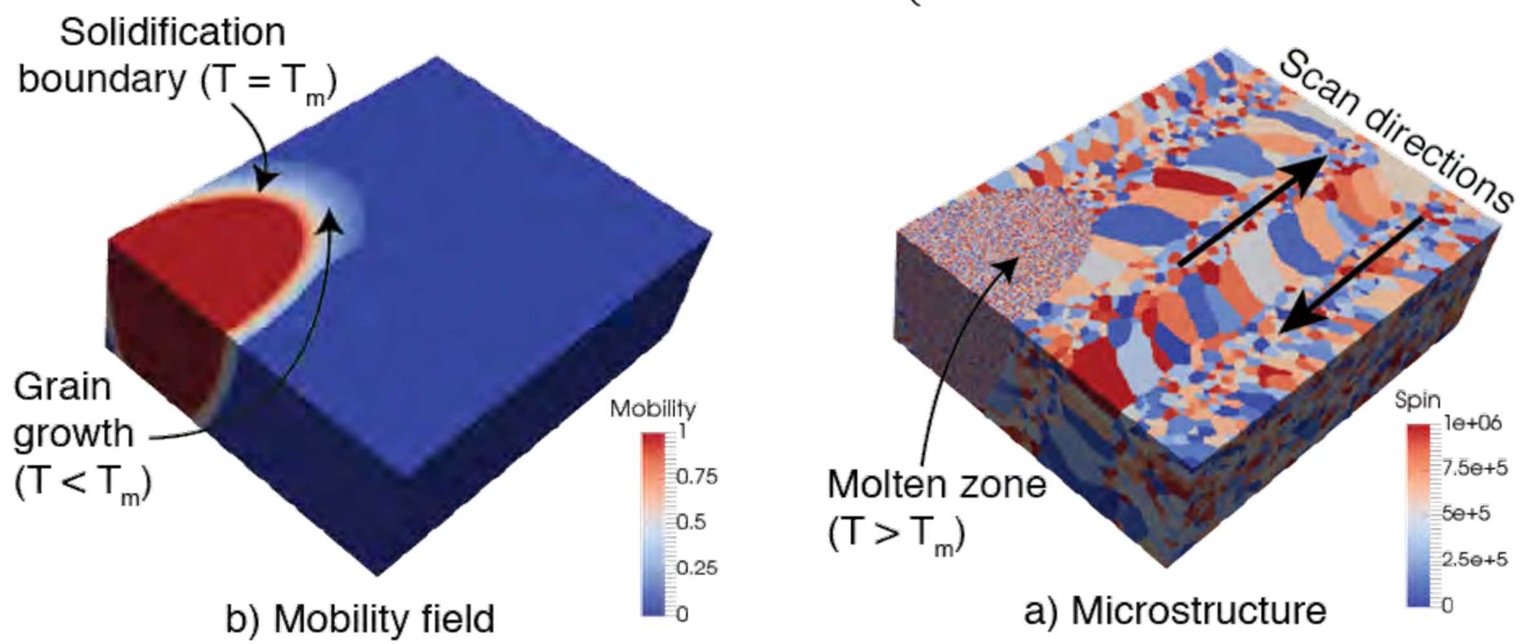
Approximating Solidification



kMC & Solidification Structure

$$M(T) = M_o \exp\left(\frac{-Q}{RT}\right)$$

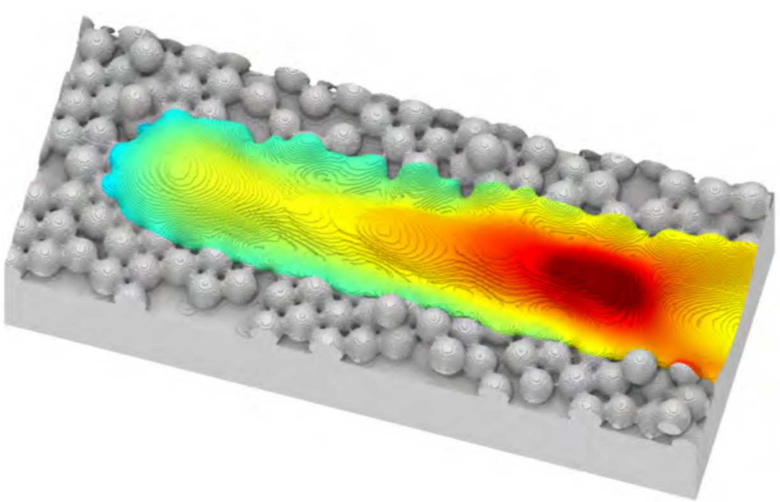
$$P = \begin{cases} M(T)\exp\left(\frac{-\Delta E}{k_B T_s}\right), & if\ \Delta E > 0 \\ M(T), & if\ \Delta E \leq 0 \end{cases}$$

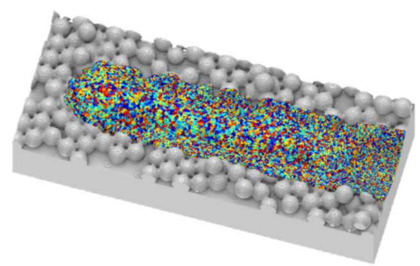


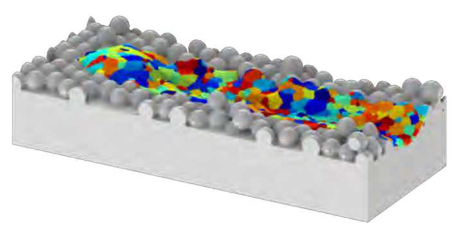
- The molten zone randomizes grain identities when it enters a region.
- Along the trailing surface, voxels either join existing columnar grains or form new grains.
- The temperature gradient creates a corresponding gradient of grain boundary mobilities via an Arrhenius relationship.

Model Improvements

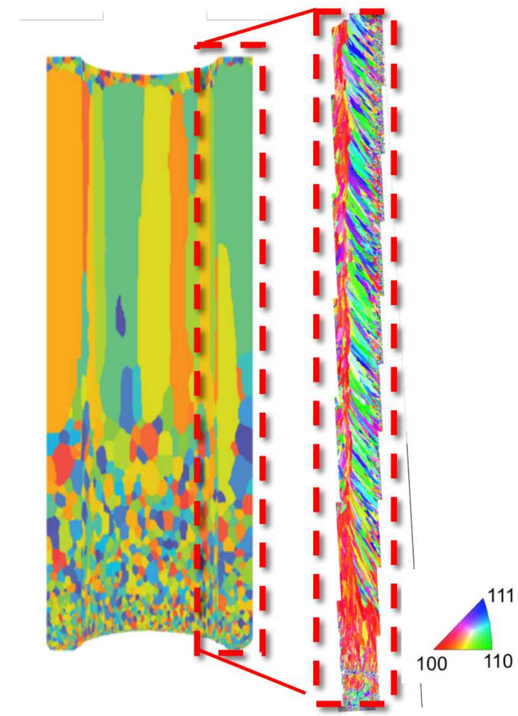
- Incorporate more **rigorous simulation of the molten zone** and solidification event
- Include **material specific parameters**
- Enable **non-powder bed** AM simulations



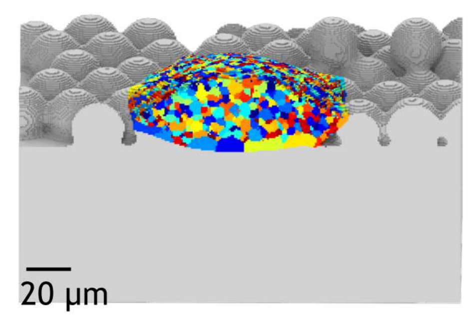


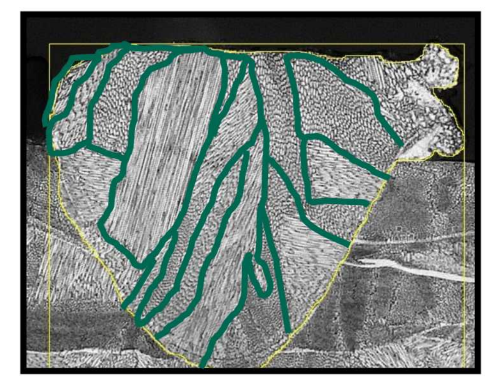


Large elements >> Under predict of nucleation



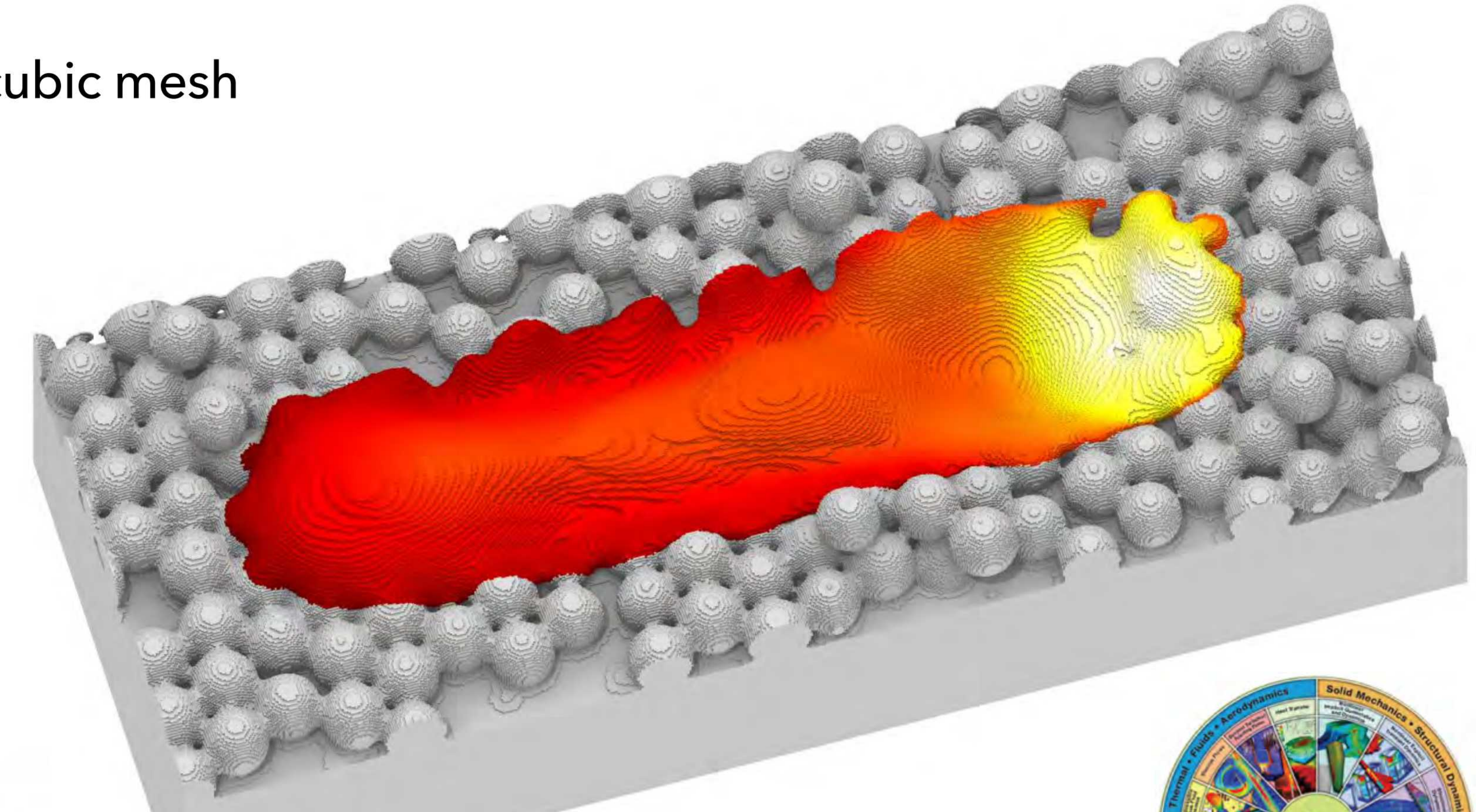
Small elements >> Over predict nucleation





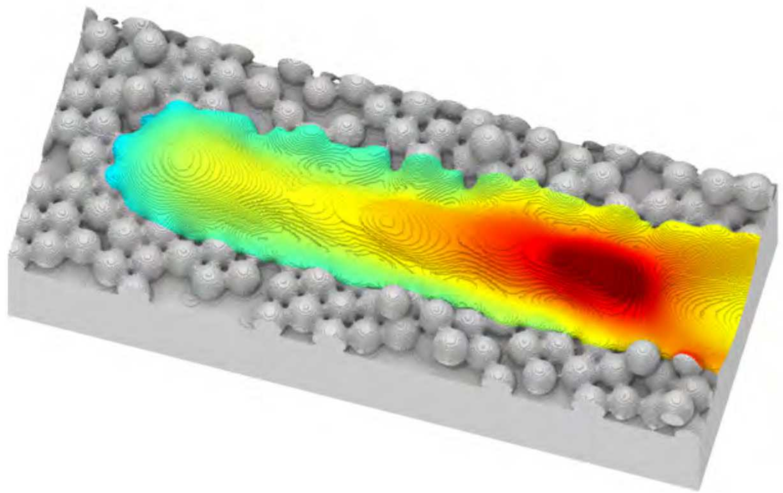
Thermofluid Powder Bed Simulations

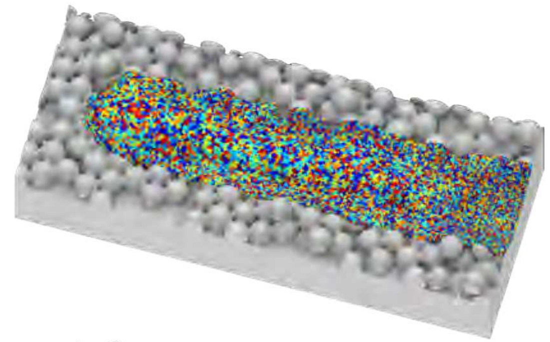
- Highly detailed level-set simulation with extensive physics
- CD-FEM mesh, mapped to a cubic mesh
- Molten metal & gas flow
- Vapor recoil pressure
- Very expensive to run
- 0.75 μm mesh size



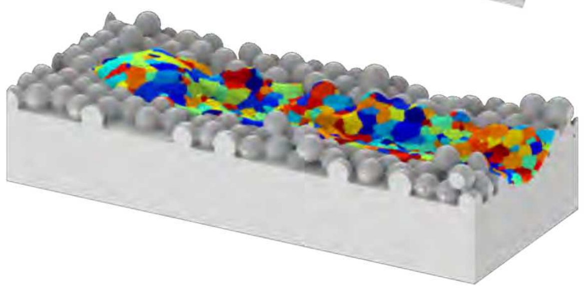
M. Martinez, D. Moser, T. Rodgers

Nucleation Rate

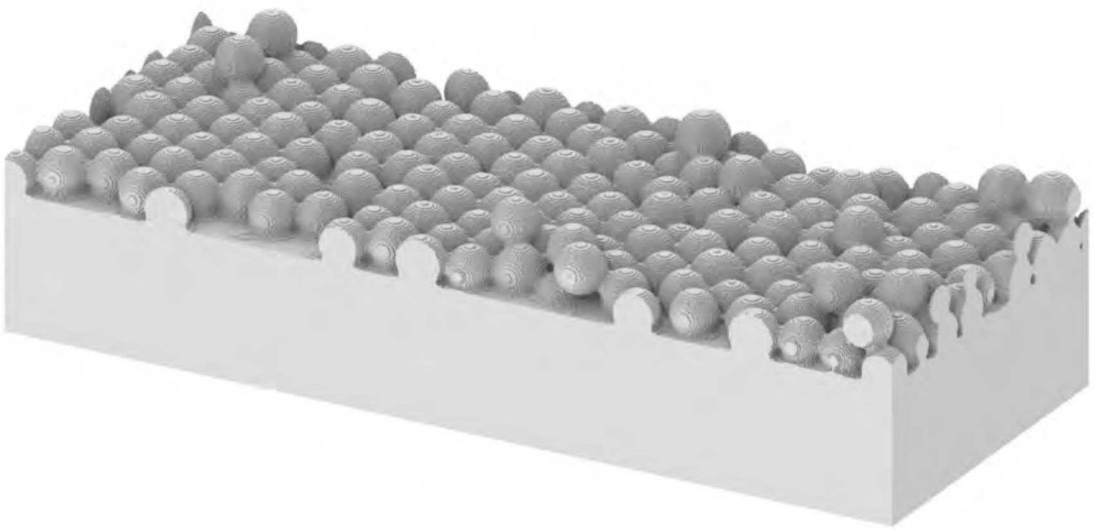




Unconstrained nucleation rate



Prescribed nucleation rate
$N_o = 10^{15}$



<u>Effect of nucleation site density:</u>

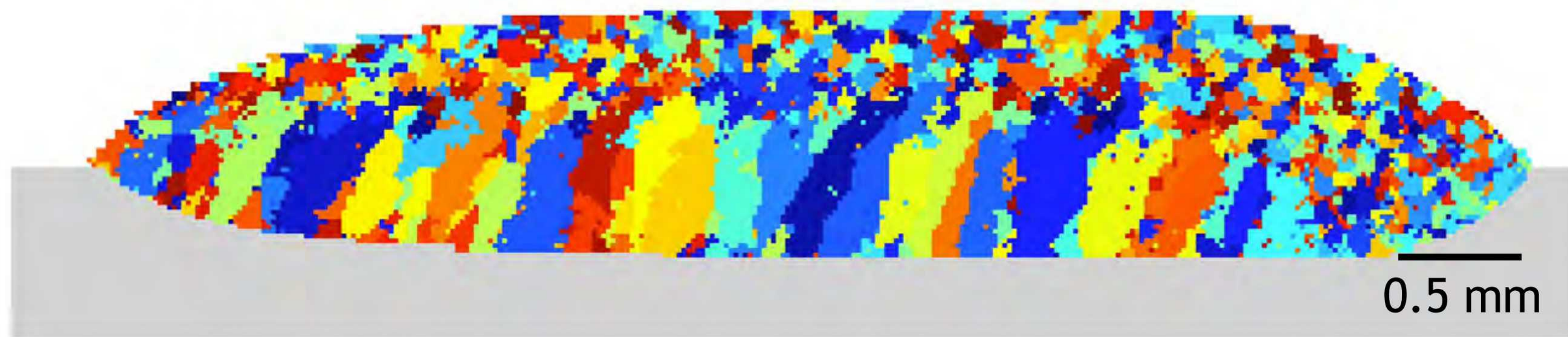
Particle-scale powder bed simulations used a much smaller lattice size than previous work (0.75 μm vs ~20 μm). With the old nucleation approach, these led to a large overprediction of nucleating grains, which resulted in a fine equiaxed structure (top).

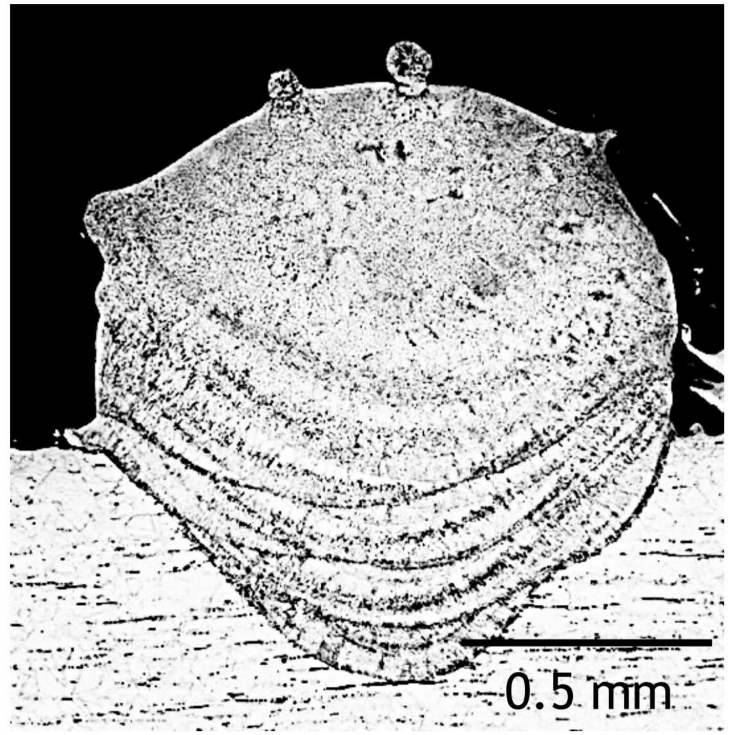
Introducing a N_o-dependent nucleation rule allowed only 1 nucleation site per 2,500 lattice sites and resulted in larger grains that grew from the substrate structure.

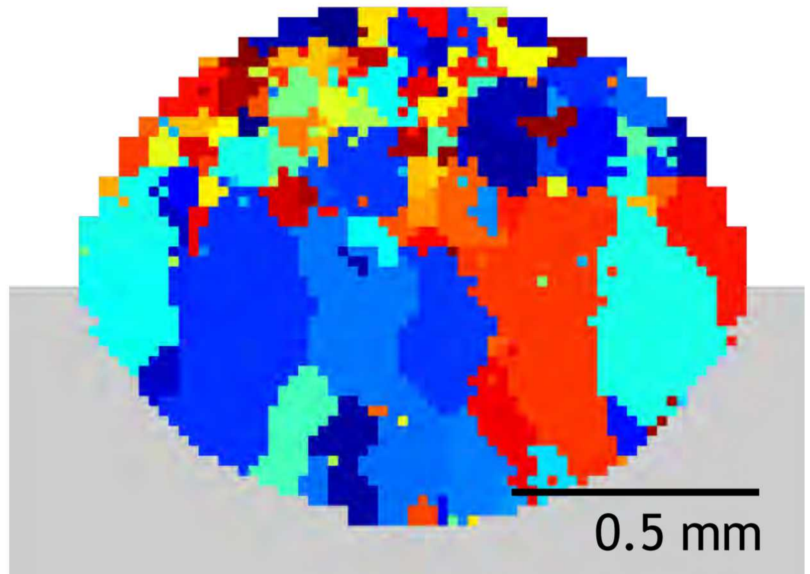
M. Martinez, D. Moser, T. Rodgers

Application to LENS

- Large (~1 mm) molten pool leads to mixed microstructures.
- Highly detailed level-set simulations with extensive physics.
- Molten metal & gas flow
- Incident powder jet momentum
- SPPARKS re-uses mesh created for in-process plasticity simulations.
- ~20 μm mesh size



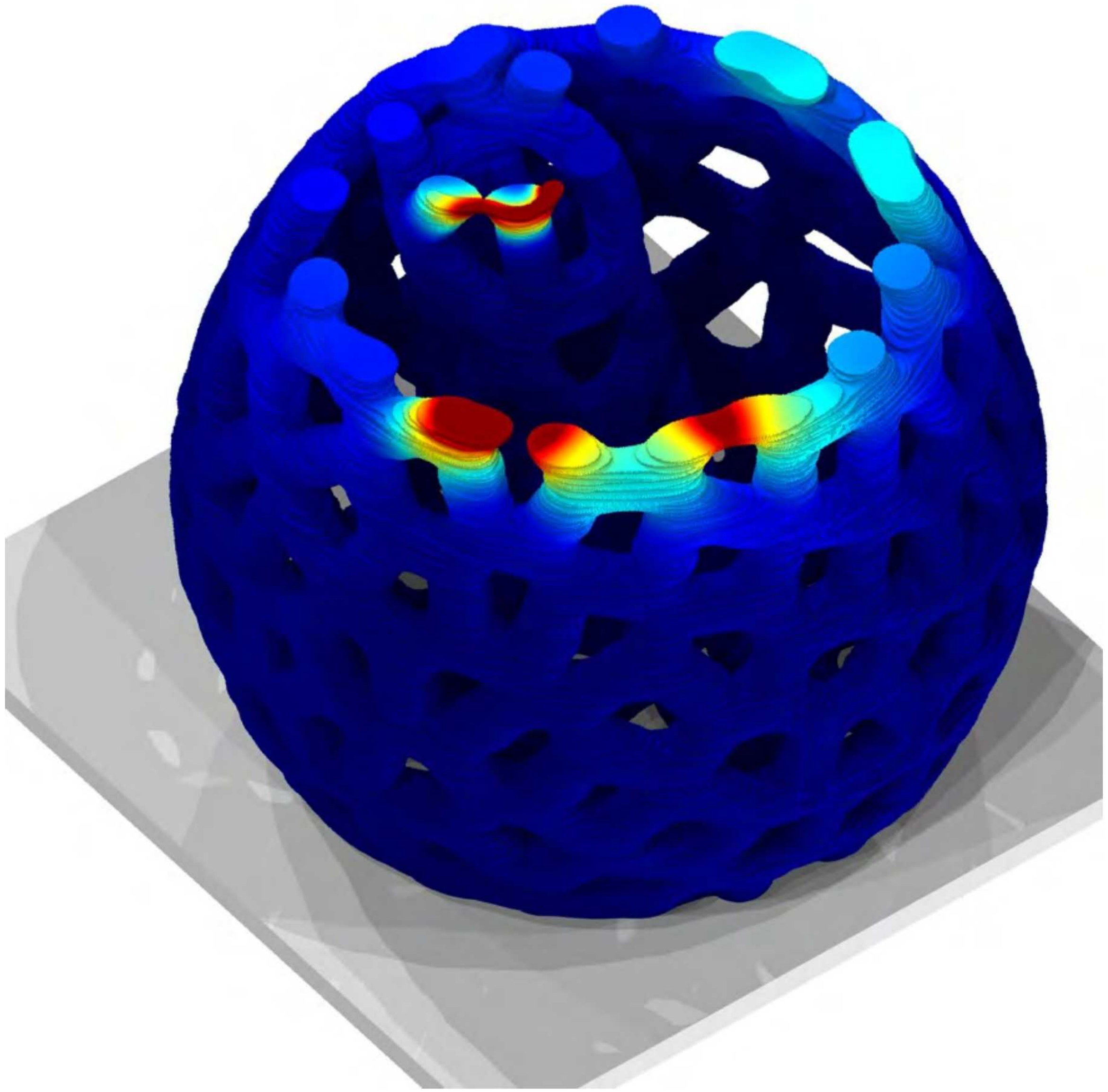


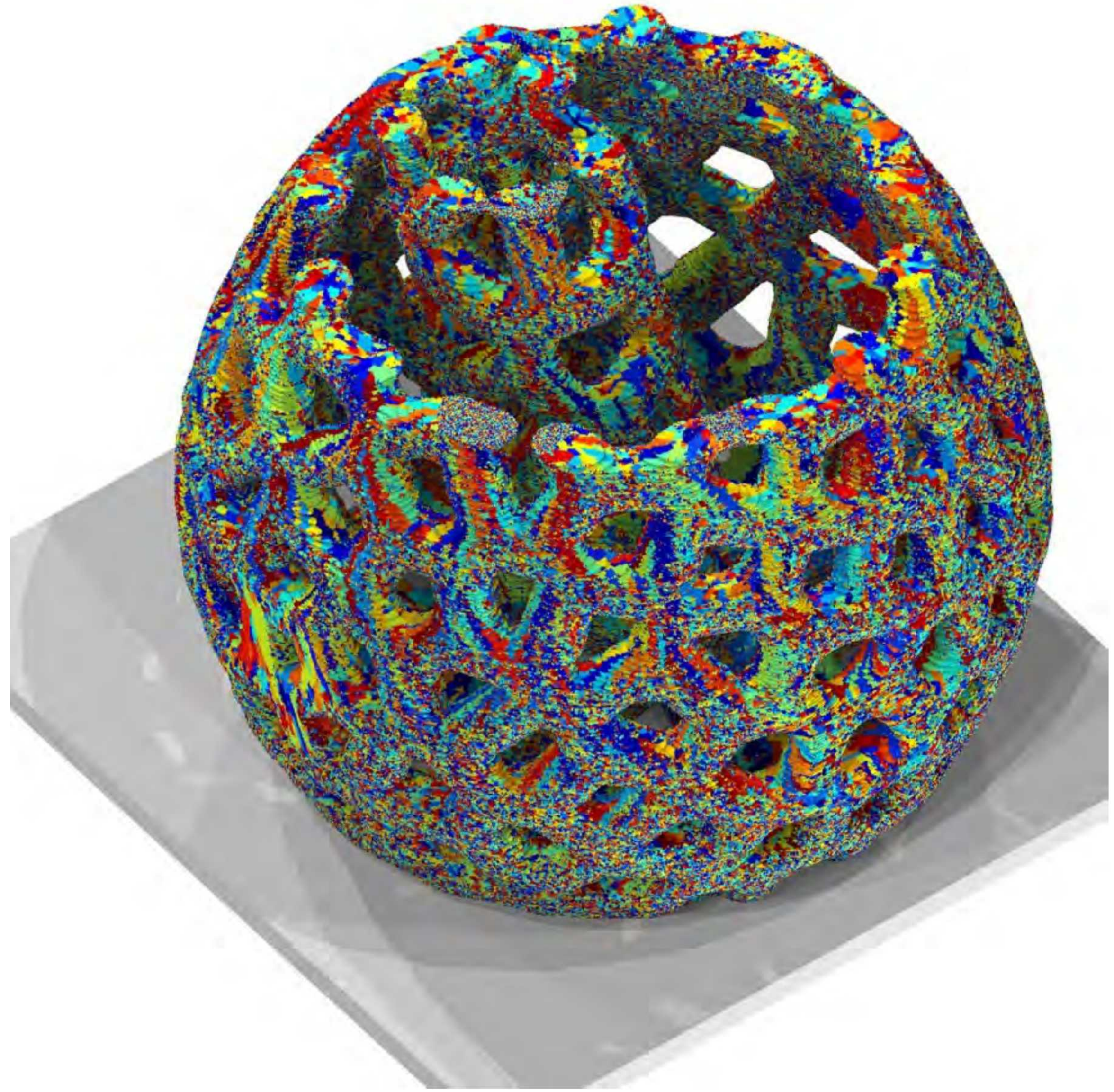


B. Trembecki, K. Ford, L. Beghini, M. Stender, T. Rodgers

Finite Difference Method on Complex Parts

Lattice Klein Bottle – 7.5 x 8 x 11.6 mm domain





Collaborators

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Mary Arnhart
Material Mechanics & Tribology

Greg Poulter
Computational Materials & Data Science

Andrew Polonsky
Material Mechanics & Tribology

Veena Tikare
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Thomas Ivanoff, Ph.D.
Experimental Environments

Alex Hickman
Metallurgy & Materials Joining

Olivia Underwood
Product Realization

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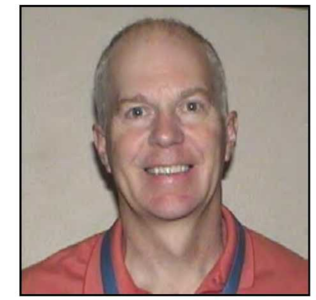
Kyle N. Karlson, M.S.
Multiscale Science

Kyle. Johnson, Ph.D.
Solid Mechanics



Joe Bishop, Ph.D.
Component Science & Mechanics

Sharlotte Kramer
Experimental Environments

Brad Boyce, Ph.D.
Nanostructure Physics

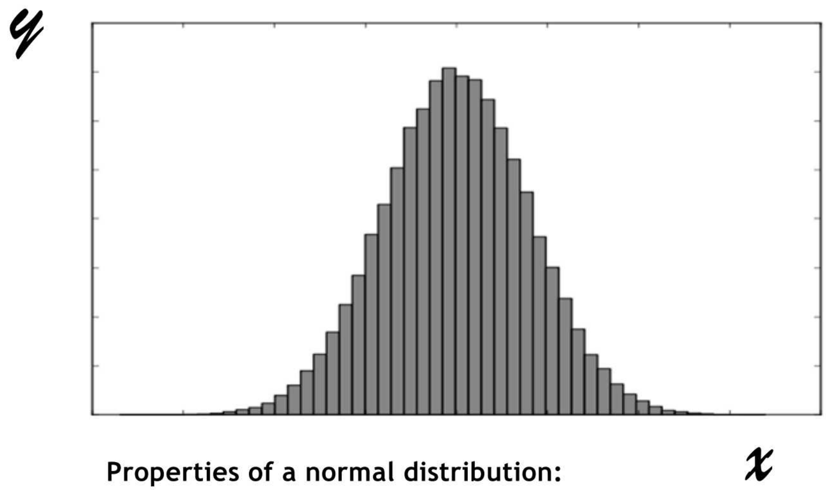
Laura Swiler
Optimization & UQ

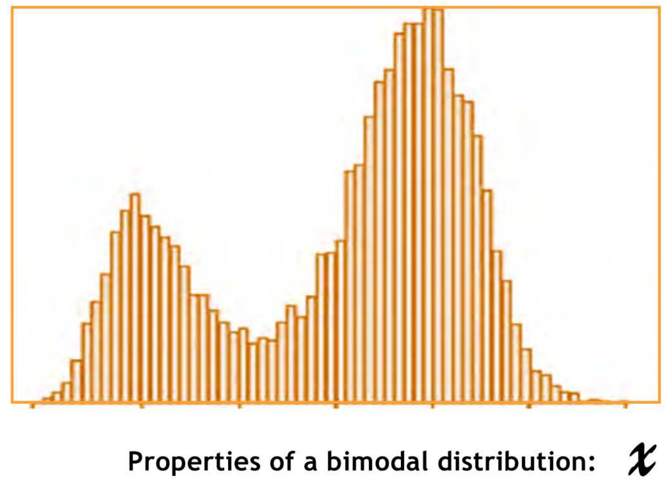
Bradley Jared, Ph.D.
Coatings and Additive Manufacturing

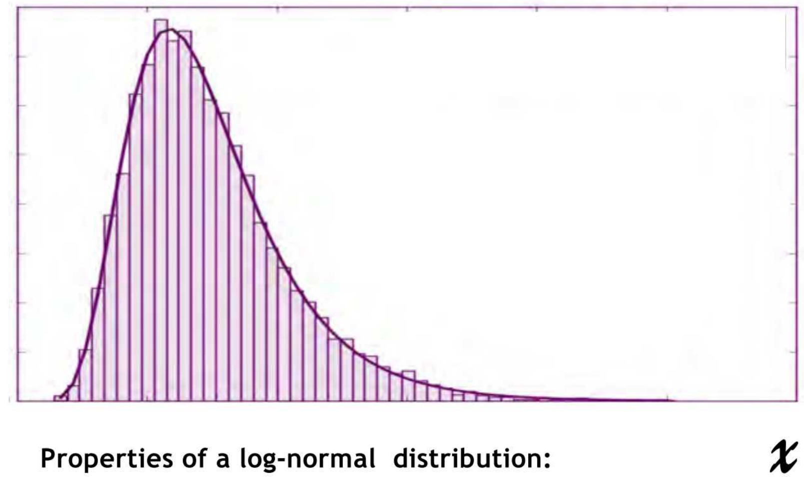
John Mitchell, Ph.D.
Multiscale Science

A few collaborators, colleagues & co-authors from the past five year

A Word on Distributions







Properties of a normal distribution:

- the mean, median and mode are all equal
- bell-shaped and symmetric about the mean
- total area under the curve is equal to one

Properties of a bimodal distribution:

- Has two distinct and identifiable modes
- Individual peaks do not have to exhibit an equivalent magnitude or population

Properties of a log-normal distribution:

- the mean and median are by definition different and both typically differ from the mode
- the lognormal distribution is asymmetric about the mean

Contents lists available at SciVerse ScienceDirect
International Journal of Fatigue
journal homepage: www.elsevier.com/locate/ijfatigue
ELSEVIER

Demonstration of an *in situ* microscale fatigue testing technique on a titanium alloy

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PERGAMON
Scripta Materialia 45 (2001) 1335–1340
Scripta MATERIALIA
www.elsevier.com/locate/scriptamat

Determining phase volume fraction in steels by electron backscattered diffraction

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Received 25 May 2001; received in revised form 2 July 2001; accepted 31 July 2001

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How Grain Growth Stops: A Mechanism for Grain-Growth Stagnation in Pure Materials

Elizabeth A. Holm* and Stephen M. Foiles

Metallogr. Microstruct. Anal.
DOI 10.1007/s13632-016-0290-0
CrossMark
TECHNICAL ARTICLE

An Examination of Abnormal Grain Growth in Low Strain Nickel-200

O. Underwood[1] · J. Madison[1] · R. M. Martens[2] · G. B. Thompson[3] · S. Welsh[4] · J. Evans[4]

ADVANCED ENGINEERING MATERIALS
FULL PAPER
DOI: 10.1002/adem.201700102

Extreme-Value Statistics Reveal Rare Failure-Critical Defects in Additive Manufacturing**

By Brad L. Boyce,* Bradley C. Salzbrenner, Jeffrey M. Rodelas, Laura P. Swiler, Jonathan D. Madison, Bradley H. Jared and Yu-Lin Shen

Means & modes of distributions are useful, but the really interesting things occur at the tails …

Current STEM Diversity Distributions

84% Percentage of working professionals in science and engineering jobs in the U.S. that are white OR Asian males

73% Over 70% of scientists and engineers are white

10% Only 1 in every 10 persons working in STEM are minority women

12% African-Americans, American-Indians and Hispanics between the ages of 18 and 24 account for 34% of the U.S. population but earn only 12% of all undergraduate degrees in engineering

50% vs. 30% Half of all Asian workers with STEM degrees have STEM jobs, compared to 30% of Hispanics, African Americans and American Indians

Sources:

U.S. News & World Report
Economics & Statistics Administration, U.S. Department of Commerce
U.S. Department of Education, National Assessment of Educational Progress in Math & Science, 2003 - 2013
Women, Minorities, and Persons with Disabilities in Science and Engineering: 2013, National Center for Science & Engineering, National Science Foundation
"5 Numbers that Explain Why STEM Diversity Matters to All of Us", WIRED,

The Power of the Diversity Distribution

"There is a pure and simple business case for diversity: Companies that are more diverse are more successful."

- Mindy Grossman –

#22 on Fortune's Top People in Business (2014)

"We have no hope of solving our problems without harnessing the diversity, the energy, and the creativity of all our people."

– Roger Wilkins –

15th U.S. Assistant Attorney General & Civil Rights Leader

"In most cases, you can't realize the full power of a distribution apart from the contribution of the tails"

– Jonathan Madison, Ph.D. –

Research Scientist

Questions ? ? ?