Integrated Computational Materials Science and Engineering in the ONR Portfolio

20 June 2011

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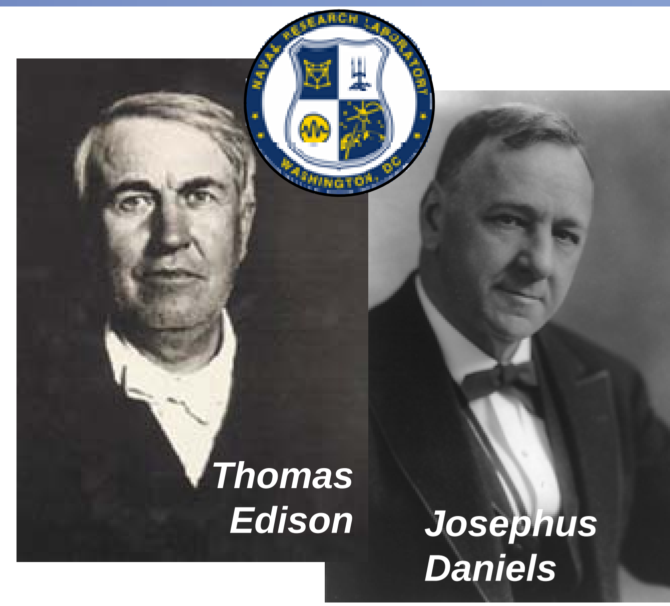
Sea Warfare & Weapons Department

Revolutionary Research . . . Relevant Results

Naval Research: Statutory Mission

Naval Research Laboratory *(Appropriations Act, 1916)*

"[Conduct] exploratory and research work . . . necessary . . . for the benefit of Government service, including the construction, equipment, and operation of a laboratory . . ."



Office of Naval Research *(Public Law 588, 1946)*

". . . plan, foster, and encourage scientific research in recognition of its paramount importance as related to the maintenance of future naval power, and the preservation of national security . . ."

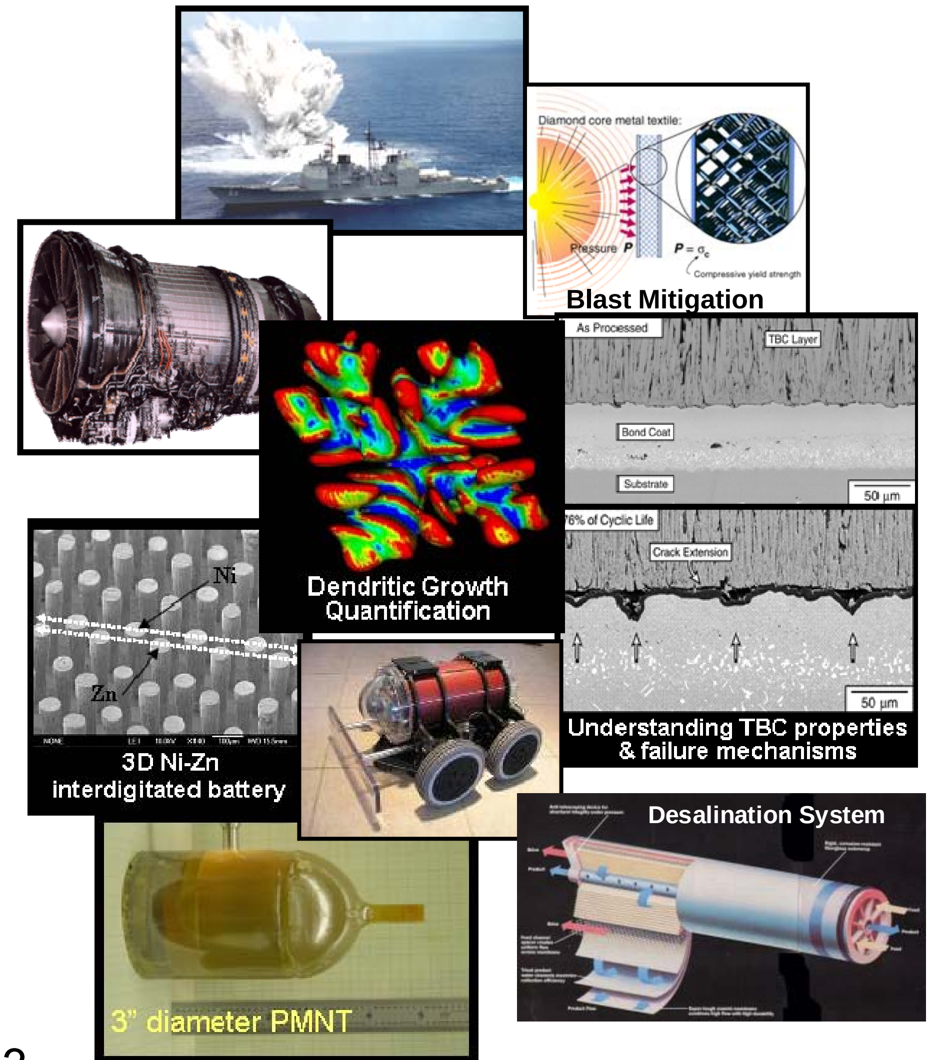
Transitioning S&T

(Defense Authorization Act, 2001)

". . . manage the Navy's basic, applied, and advanced research to foster transition from science and technology to higher levels of research, development, test, and evaluation."

Advanced Naval Materials

Integrated theoretical, computational and experimental programs to understand and develop the physics, chemistry, materials and processing that confidently meet critical naval needs



High Performance Functional Materials

- Power Generation & Energy Storage Materials
  - ✓ Electrochemical Materials
  - ✓ Polymeric and Organic Materials
- Piezoelectric Materials

High Performance Structural Materials

- Structural Metallic, Structural Cellular and Composite Materials
- High Temperature Turbine and Ultra-high Temperature Materials
- Welding and Joining
- Optical Ceramics

Environmental Quality

- Anti-fouling Release Coatings
- Solid and Liquid Waste Treatment

Optimization from Design thru System Life

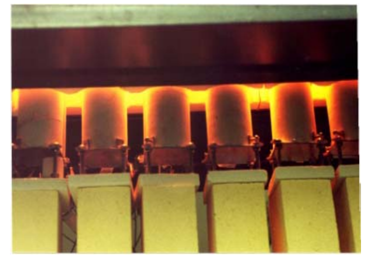
- Computer Aided Materials Design
- Solid Mechanics and Fatigue
- Non-Destructive Evaluation and Prognostics
- Integrated Computational Materials Science &Engineering

Acoustic Transduction Materials

Improve & Exploit Electromechanical Transduction Properties of Materials

Materials Synthesis, Evaluation and Analysis

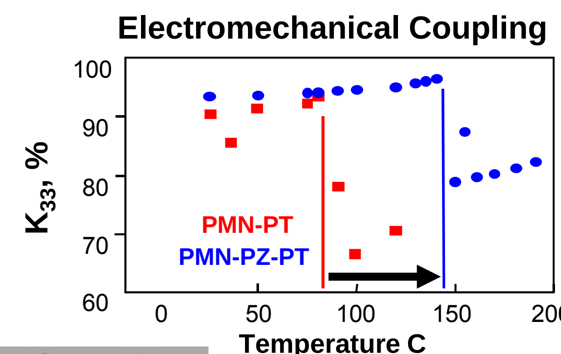
- Auto-feed melt crystal growth method
- Solid-state crystal growth method
- Micro domain engineering of PZT crystals
- Processes to increase mechanical robustness

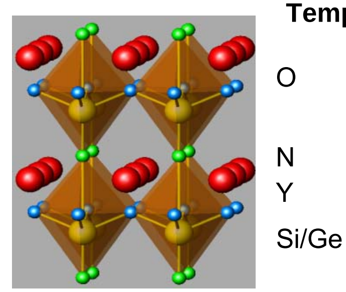


Scale-Up: Six Crucible Furnace

First-Principle Methods & Design

- Density functional theory, finite temperature and finite electric field based optimization
- Identification and optimization of morphotropic phase boundaries, layered superlattices, pressure induced phase transitions and dielectric tunability Enlarge temperature, field and stress operating domain





D&I Investments for System Performance

- Efficient, powerful and sensitive electromechanical transduction materials
- Order-of-magnitude improvements in system volume or performance

ONR POC: Dr. Wallace Smith; wallace.smith1@navy.mil

Propulsion Materials

Controlling Complex Interactions to Increase Operational Temperatures

Advanced High Temperature Materials (>1500˚C)

- Integration of computational thermodynamics and reaction kinetics to guide new alloy development
- Optimization of hot corrosion and oxidation resistance

Thermal and Environmental Barrier Coatings

- Multidisciplinary research to understand failure mechanisms
- Physics-based models for life prediction
- Validated coatings and affordable processes technologies

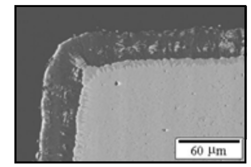
Advanced Materials Processing

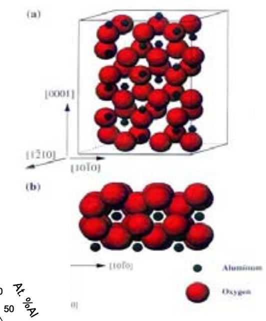
- Analytical process modeling and simulations
- Reduced costs through simplified processing schemes

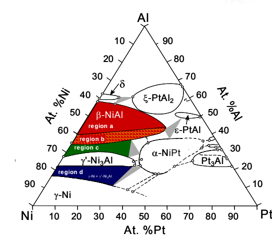
D&I and FNC Investments directly supporting VAATE and the NAE

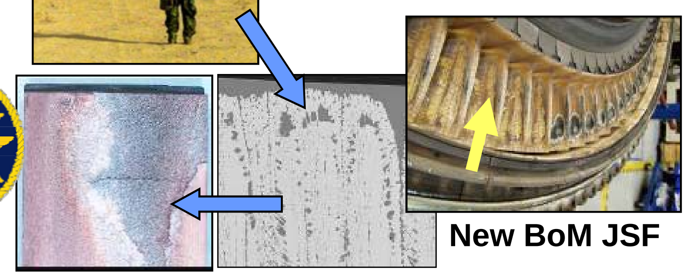
- Improved performance, fuel efficiency, reliability and time-on-wing, and reduced maintenance costs of naval aircraft (legacy, JSF and F-18E/F)
- Life prediction models for engine materials and coatings

DVTI spun from 6.1 Univ Virginia efforts; licensed to P&W for JSF doublet









New BoM JSF

ONR POC: Dr. David Shifler; david.shifler@navy.mil

Structural Metals

Understanding Material Response to Loading Events for Performance Optimization

Processing and Joining Technologies

- Friction stir welding of Naval steels to minimize distortion and rework in Naval structures
- Friction stir processing for surface properties, formability and repair
- Processing and welding technologies for marine titanium alloys

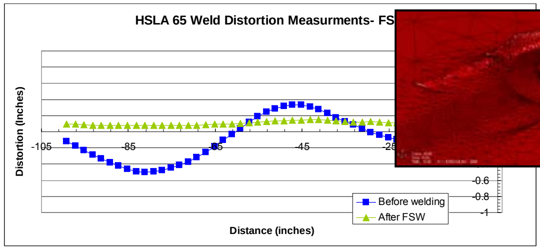
Steels, Titanium and Alloys of Interest

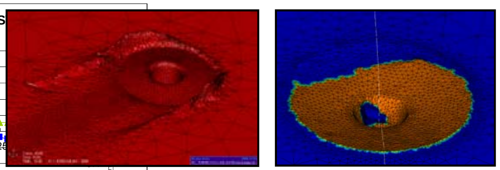
- Quantified descriptions of microstructural features, their evolution and properties
- Mechanisms affecting mechanical response and deformation under dynamic loading
- Design and prediction tools for structurally efficient materials in Naval environments and their rapid implementation

D&I for Performance and Affordability

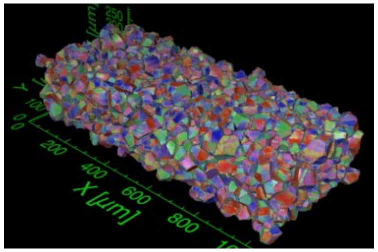
- Reduced weight and survivability Naval structures
- Confident prediction of alloy and weldment properties
- Accelerated certification of materials and processes

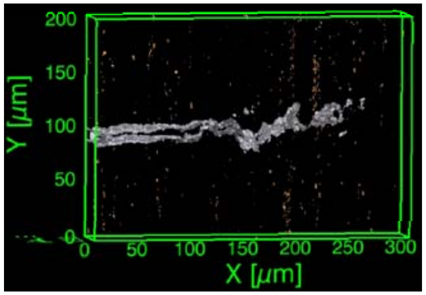
Cross section of Ti-5111 friction stir weld





Process development and material flow predictions





High resolution tomographic reconstruction of crack tip process zone

Tomography based micromechanical multiscale fracture simulation

ONR POC: Dr. William Mullins; william.m.mullins@navy.mil

Dynamic 3-D Digital Structure

Applying the ICME Methodology to Materials Research

Objectives:

Develop and demonstrate the fundamental research approaches and tools necessary to provide a computational basis for materials processing and behavior

- Proofs of concept for critical enablers
- Focused on Naval material needs

Key Technical Thrusts:

- *Digital representation of microstructure* across the nano-, micro- and meso-scales to effectively and quantitatively describe structures and features of interest
- *Simulation and prediction of microstructure evolution* in response to processing and/or use environment
  - Thermomechanical processing, environmental degradation, dynamic and/or fatigue loading, etc.
  - Microstructure-property relationships
  - Linking computational models to performance in a system
- *Tools for integration of computation and experiment*
  - Management of experimental and computational data

Dynamic 3-D Digital Structure: Motivation

Moving material science from ANALOG TO DIGITAL - from qualitative assessments of microstructure/property relationships to quantitative calculations

Influence of Microstructure on Properties of α/β Ti Alloys

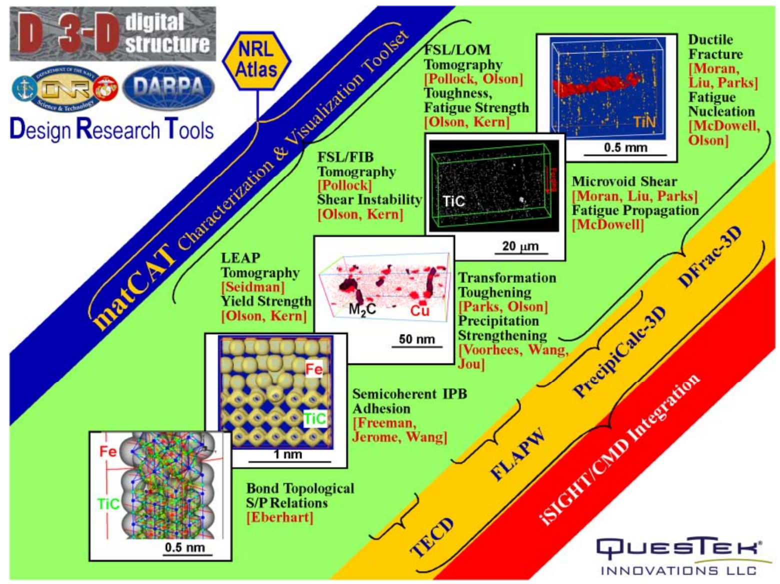
α+β Titanium Alloys	σ_y	ε_F	HCF	Micro-cracks da/dN	Macrocracks			Creep Strength 0.2%
					ΔK_{th} R=0.7	K_{IC}	ΔK_{th} R=0.1	
Aging (α_2) Oxygen	+	-	+	-	-	-	+	+
Bi-modal Structure	+	+	- / +	+	-	-	-	- / 0
GB α-Layers	0	-	-	-	0	-	0	0
Small α-Colonies α-Lamellae	+	+	+	+	-	-	-	-

G. Lütjering "Property Optimization Through Microstructure Control in Titanium and Aluminum Alloys." Technical University Hamburg-Harburg

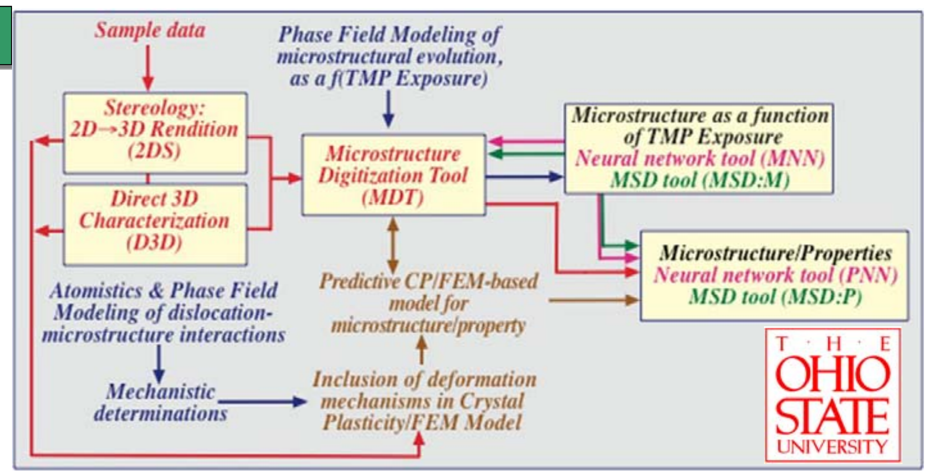
2003

3 Teams


D 3-D digital structure


D 3-D digital structure
NRL Atlas
DARPA
Design Research Tools
matCAT Characterization & Visualization Toolset
FSL/LOM Tomography [Pollock, Olson]
Toughness, Fatigue Strength [Olson, Kern]
Ductile Fracture [Moran, Liu, Parks]
Fatigue Nucleation [McDowell, Olson]
0.5 mm
TiN
FSL/FIB Tomography [Pollock]
Shear Instability [Olson, Kern]
TiC
20 µm
Microvoid Shear [Moran, Liu, Parks]
Fatigue Propagation [McDowell]
LEAP Tomography [Seidman]
Yield Strength [Olson, Kern]
Cu
50 nm
Transformation Toughening [Parks, Olson]
Precipitation Strengthening [Voorhees, Wang, Jou]
Fe
TiC
1 nm
Semicoherent IPB Adhesion [Freeman, Jerome, Wang]
Bond Topological S/P Relations [Eberhart]
0.5 nm
DFrac-3D
PrecipiCalc-3D
FLAPW
TECD
iSIGHT/CMD Integration
QuesTek Innovations LLC
Georgia Tech


Database and Data Analysis
.: Cornell :. Dawson
Statistical Analysis, "Digital Microstructure"
.: Iowa State :. Rajan
Data Mining
.: NRL :. Spanos
Serial Sectioning, EBSD
Dual-Beam FIB
.: Risø :. Lauridsen
4D XRD, Thermal and Stress Evolution, Small Scales
.: Cornell :. Miller
3DXRD, Mechanical Loading, Large Strains, Large Scales
3D Materials Atlas
.: NRL :. Geltmacher
Stress, Strain, Yield, Damage and Percolation Modeling
.: Cornell :. Dawson
Texture Evolution, Thermomechanical Response
.: Northwestern :. Voorhees
Phase Field Modeling
"Evolver" Modeling & Simulation
.: RPI :. Pearlman
Platform Development, Code Integration
Experimental Input
Software Development

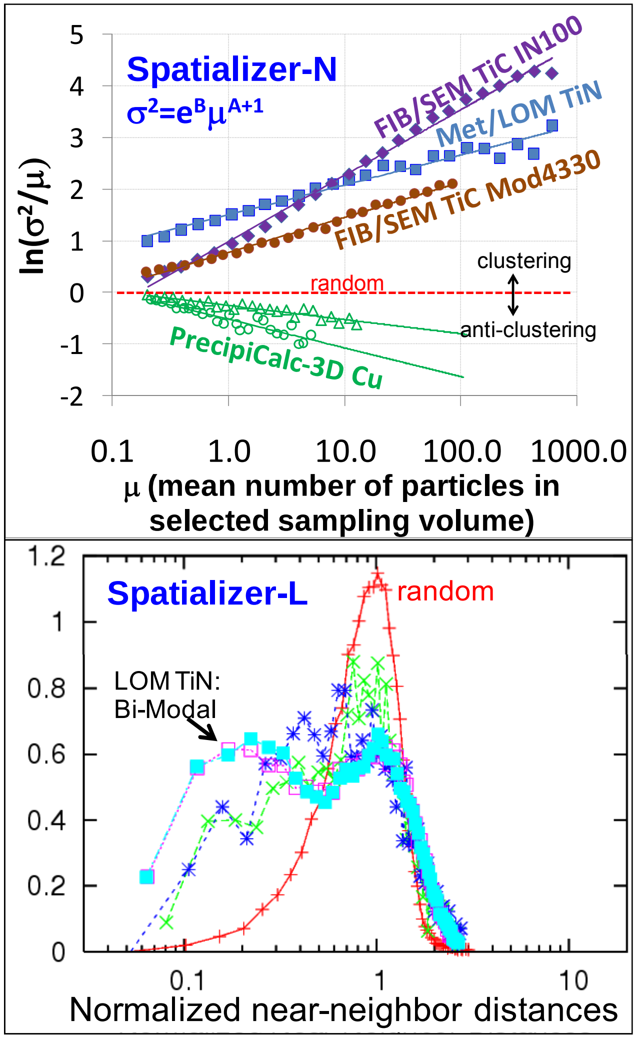

Sample data
Phase Field Modeling of microstructural evolution, as a f(TMP Exposure)
Stereology: 2D→3D Rendition (2DS)
Direct 3D Characterization (D3D)
Microstructure Digitization Tool (MDT)
Microstructure as a function of TMP Exposure
Neural network tool (MNN)
MSD tool (MSD:M)
Microstructure/Properties
Neural network tool (PNN)
MSD tool (MSD:P)
Atomistics & Phase Field Modeling of dislocation-microstructure interactions
Predictive CP/FEM-based model for microstructure/property
Mechanistic determinations
Inclusion of deformation mechanisms in Crystal Plasticity/FEM Model
THE OHIO STATE UNIVERSITY

Precipitation Spatial Quantification

Quantification and parameterization of spatial non-randomness of precipitate dispersion allows the next generation structure-property models to capture 3-D dispersion microstructure features.

High degrees of freedom inherent in real microstructures prevents comprehensive and complete parameterization.

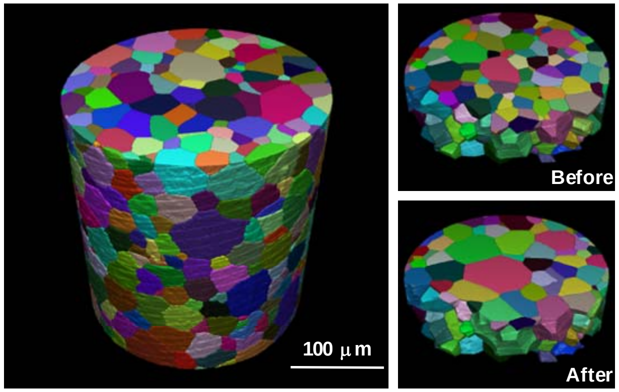
Quantification and parameterization relevant to the property models of interest, particularly precipitation strengthening and ductile fracture modeling are spatially non-random, but can be described quantitatively.



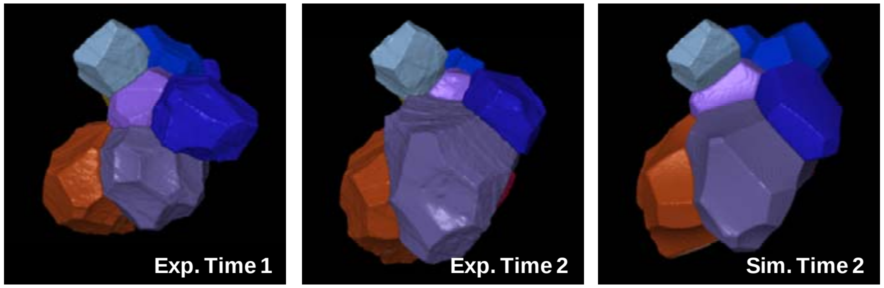
Grain Growth Kinetics in Ti

High fidelity 3-D synchrotron imaging techniques and robust phase field modeling allow capture of anisotropy effects

- Development of advanced non-destructive 3-D imaging tools based on phase-contrast X-ray tomography and diffraction contrast X-ray tomography.
- Acquisition of large (1000+ grains) data sets providing direct insight to the grain evolution in Ti-β-21S during grain growth.
- Developed a 3-D anisotropic phase field model for cubic materials.
- Simulated grain evolution in a Ti-β-21S sample with over 1200 grains.
- By comparing the morphologies of individual grains predicted by simulation with those measured experimentally we find that:
  a) The morphological evolution of a grain depends only on its local ensemble of grains.
  b) The mobilities of a grain's boundaries can vary by orders of magnitude and depend strongly on the grain boundary normal.
  c) Even without accounting for anisotropy in the grain boundary energy the model is capable of predicting surprisingly accurate morphologies and topologies in the isotropic regions of the experimental dataset.



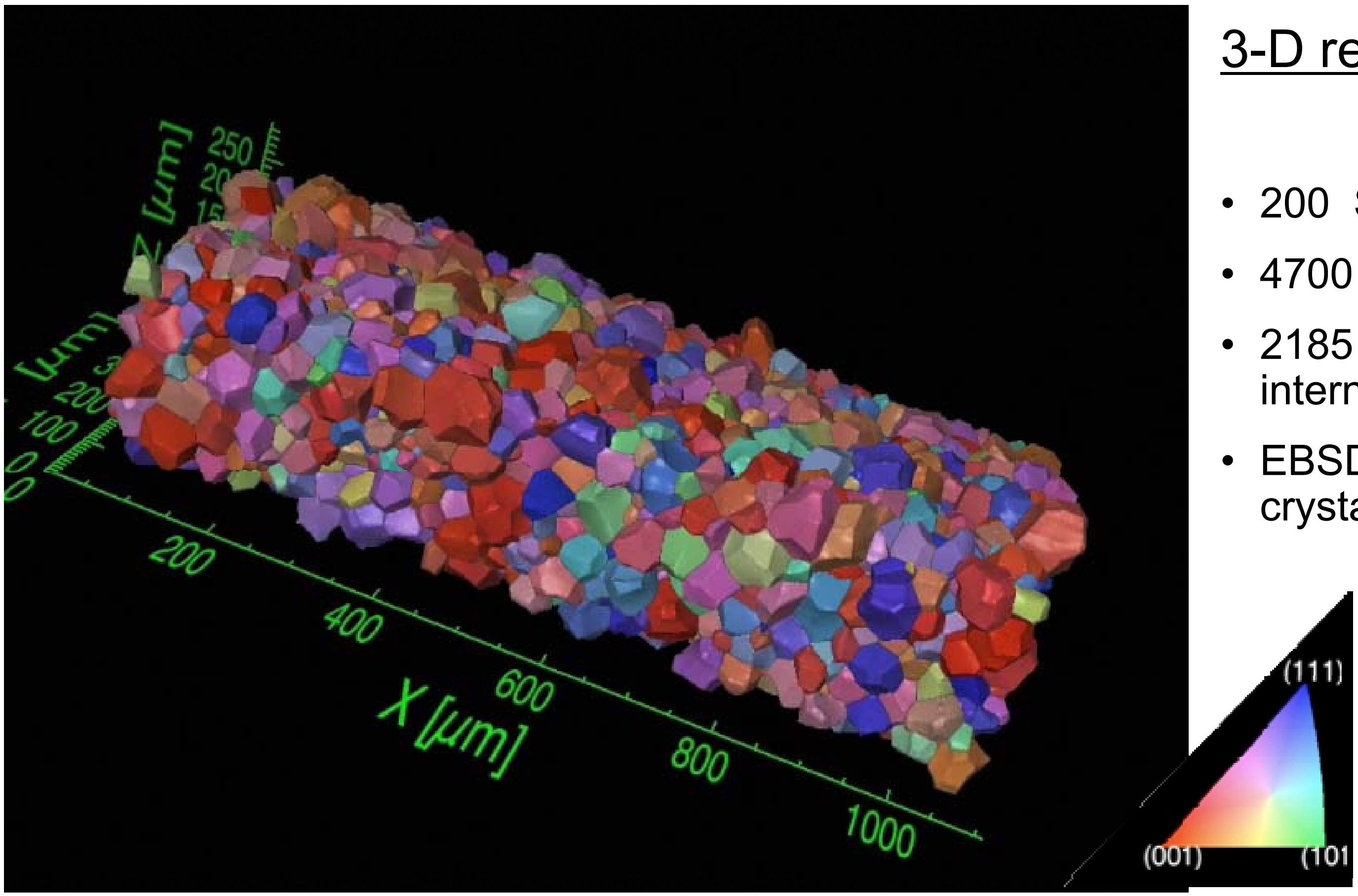
3-D experimental data of Ti-β-21S.
Left: Initial structure used in the phase field simulation comprising more than 1200 grains.
Right: Subset showing the grain structure before and after grain growth, respectively.



Comparison of an ensemble of grains in simulation with experiment

Erik Lauridsen, Risø-DTU; Peter Vorhees, Northwestern University

Reconstruction of β Grains in Ti-21S



<u>3-D reconstruction of β-Ti</u>

- 200 Sections
- 4700 grains reconstruction
- 2185 grains in unbiased internal volume
- EBSD data integrated for crystallography

Phase Field Models of Microstructure Evolution

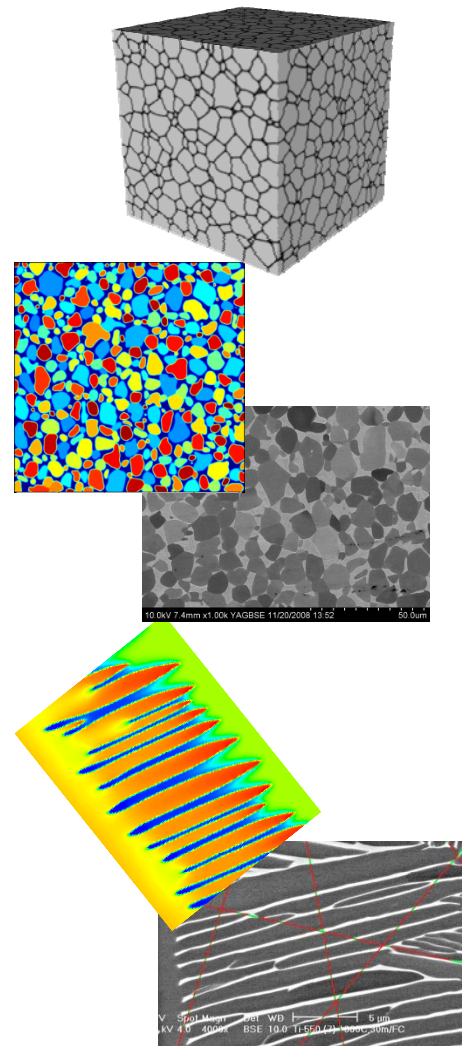
Phase field method captures influence of high volume fraction of precipitates and strong anisotropy, crystallography, and dislocation structures in evolution of α–β Ti structures.

Various complicated polycrystalline and two-phase (α+β) microstructures are accurately predicted, comparing well with experimental observations.

Parametric studies were carried out to explore the effect of anisotropy in interfacial energy and mobility on microstructural evolution.

The models have been applied directly to assist in 3-D microstructure reconstruction and to generate 3-D microstructure data to assist in developing D 3-D microstructure representation tools.

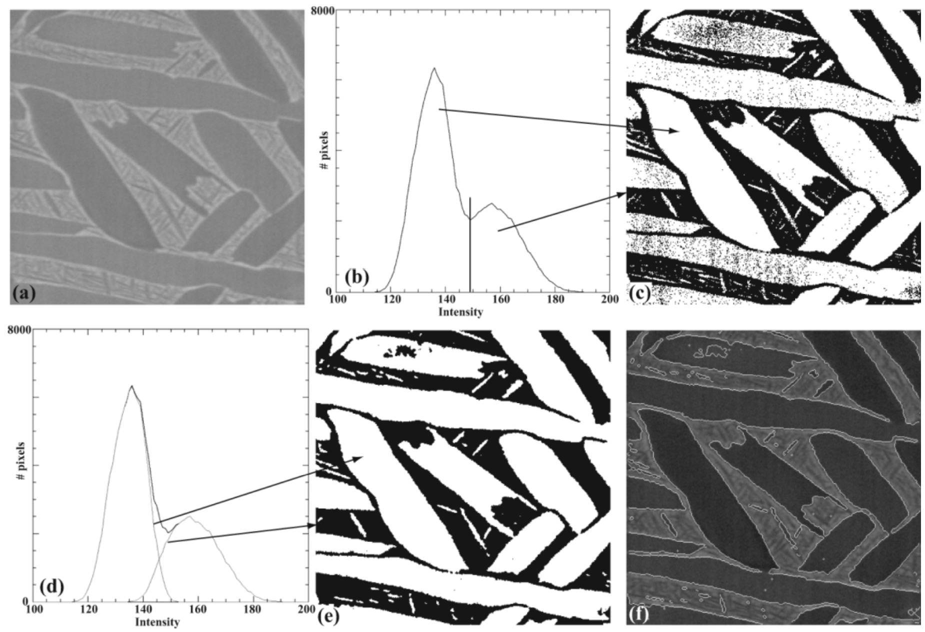
Combination of phase field models developed at different length scales provides a useful means in utilizing *ab initio* calculations, atomic potentials and experimental characterization to capture fundamental insights into phase transformation and deformation mechanisms and to establish physics-based models for engineering applications.



Automated Multimodal 3-D Image Segmentation

3-D data acquired by modern materials characterization instruments typically contain 10^7-10^9 voxels.

EMMPM:
(Expectation Maximization/Maximization of Posterior Marginals) is a stochastic segmentation technique to the automated segmentation of 2-D and 3-D microstructure data sets that minimizes the number of incorrectly classified voxels by means of a Bayesian approach.



In classical segmentation, an image (a), such as the two-phase Ti-6242 alloy microstructure above, is segmented by thresholding its intensity histogram (b); the resulting segmentation (c) is noisy and inaccurate.

We have combined EMMPM with a simulated annealing approach which accounts for each pixel's local neighborhood and allows for local smoothings.

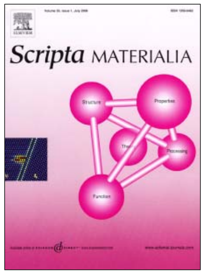
This allows for the deconvolution of the intensity histogram (d) into disjoint sets, in this case the two individual alloy phases (e).

In (f), the microstructure image (a) is shown along with the superimposed gradient of the segmentation, outlining the edges of the darker laths.

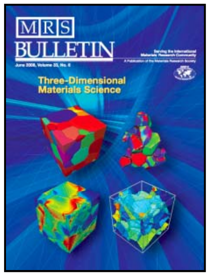
Impact

Over 270+ papers in print or preparation
Four Special Issues on 3-D Materials Science
15 Books and Book-Chapters written

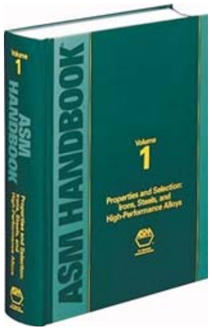
- Special *Scripta Materialia* Viewpoint Issue July, 2006: “3-D Analysis of Materials” (G. Spanos, guest editor)



- Special *Journal of Metals* issue December, 2006: “3-D Materials Science” (M. Uchic, guest editor)



- Special *MRS Bulletin* - June 2008: “3-D Materials Science: An Intersection of 3-D Reconstructions & Simulations” (H. Poulsen & K. Thornton, eds.)

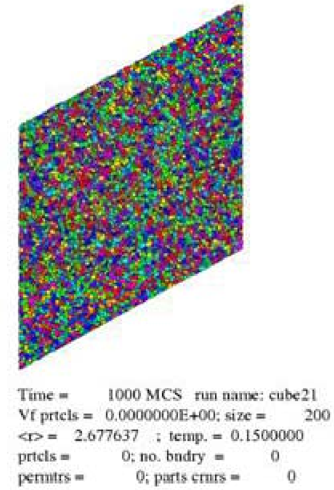


- ASM Handbook, Vol. 22 - 2009: “Modeling & Simulation” Sections on “3-D Microstructure Representation” & “Crystal Scale Simulations Using Finite Element Formulations”

Integration of Advanced Analysis with Materials Research

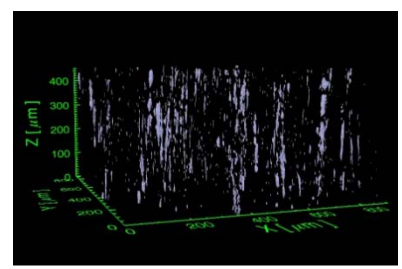
Objective: Materials design toolset

- Define a coherent framework for prediction & optimization of material properties
- Explore new approaches for modeling
- Computational efficiencies: less data but more information
- New approaches to performing calculations
- Exploit tight collaboration of experiment, characterization, modeling, and computation
- Rapid identification of new physical phenomena



Approach: Draw advanced analysis into each stage

- Explore reduced-order descriptions of microstructure
- Capture stochastic micromechanics of microstructure evolution
- Constitutive modeling that includes inherent randomness and emergent behavior
- Process modeling
- Investigate mappings of microstructure evolution models into reduced-order random-field descriptions
- Performance optimization



3D reconstruction of $LaSO_4$ inclusions in C-61 steel, created from 240 serial sections.

ONR POC: Dr. Bill Mullins; william.m.mullins@navy.mil

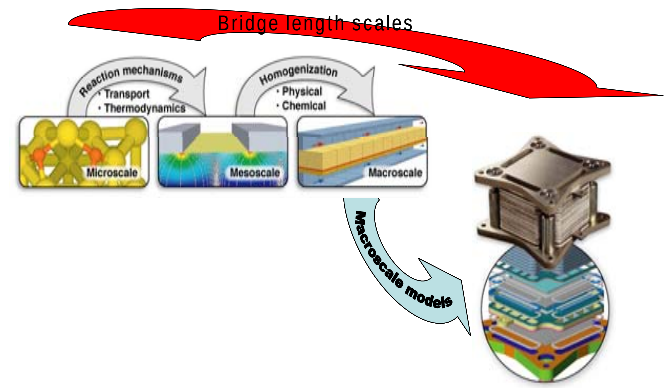
Integrated Efforts in Electrochemistry

Revolutionary Research . . . Relevant Results

Quantifying Surface/Interface Reactions for Advanced Battery and Fuel Cell Design

Objective: New high-performance electrochemical energy storage and power conversion systems

- Develop effective design tools, integrate validated physical models into robust CFD codes
- Collaborate with designers to develop and improve high-performance power systems
- Incorporate physical knowledge into real-time process control



Approach: Focus on science, tools, and systems

- Develop new approaches for modeling charge-transfer incorporating fundamental physics, chemistry, and electrochemistry
- Develop fully resolved models to represent effective properties of composite electrodes
- Develop model-predictive process-control algorithms for tubular SOFC stacks
- Develop model-predictive process-control algorithms for rechargeable battery design
- Initially develop and validate for solid oxide fuel cell (SOFC)
    - Apply to design a class of all-ceramic microchannel heat-exchangers and fuel-processing reactors
- Extend SOFC modeling tools to Li-ion batteries

Simulated transport in a reconstructed Li-ion cathode

All ceramic microchannel heat exchanger and reactor

COLORADO SCHOOL OF MINES 1874

ANSYS

Al-Alloy Accelerated Insertion of Materials

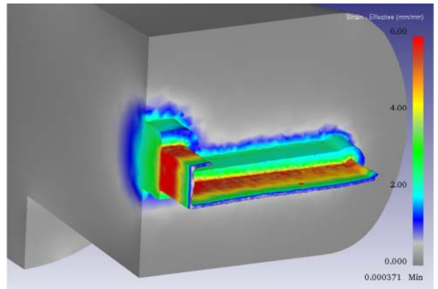
Using ICME to Rapidly Certify New Alloys & Known Alloys for New Applications

Objective:
Reduce certification testing requirements by 75%

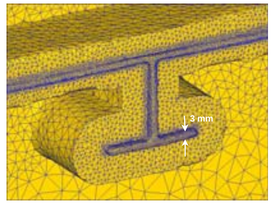
- Establish flexible architecture for integrating models and relevant data to assess and predict properties for a variety of materials systems
- Demonstrate utility of approach and establish “best practice”

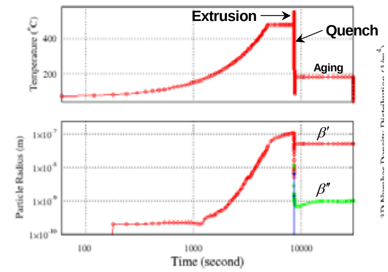
Approach: Focus on current need and build on established capabilities

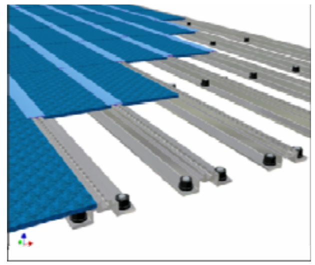
- Start with architecture demonstrated in the DARPA -AIM project *(Dan Backman as consultant)*
- Select application: AA6082 extrusion for LCS-2
- Purchase software and dedicated hardware, install, train users
- Thermo-Calc, PrecipiCalc, DEFORM, iSight-FD, material databases
- Develop thermodynamic, kinetic, deformation, and microstructure models and data sets
- Integrate applications with iSight
- Calculate microstructures, validate system
- Follow-on → develop similar 7XA models for Flexible Infrastructure



Simulated extrusion of AA6082 for an LCS-2 sidewall panel







7XA (Al-Sc) for Flexible Infrastructure application

ONR POC: Dr. William Mullins; william.m.mullins@navy.mil

COMPUTER-AIDED MATERIALS DESIGN (CAMD)

Developing Fundamental Understanding and the Tools for Discovery

De Nuevo Calculations and Exploration

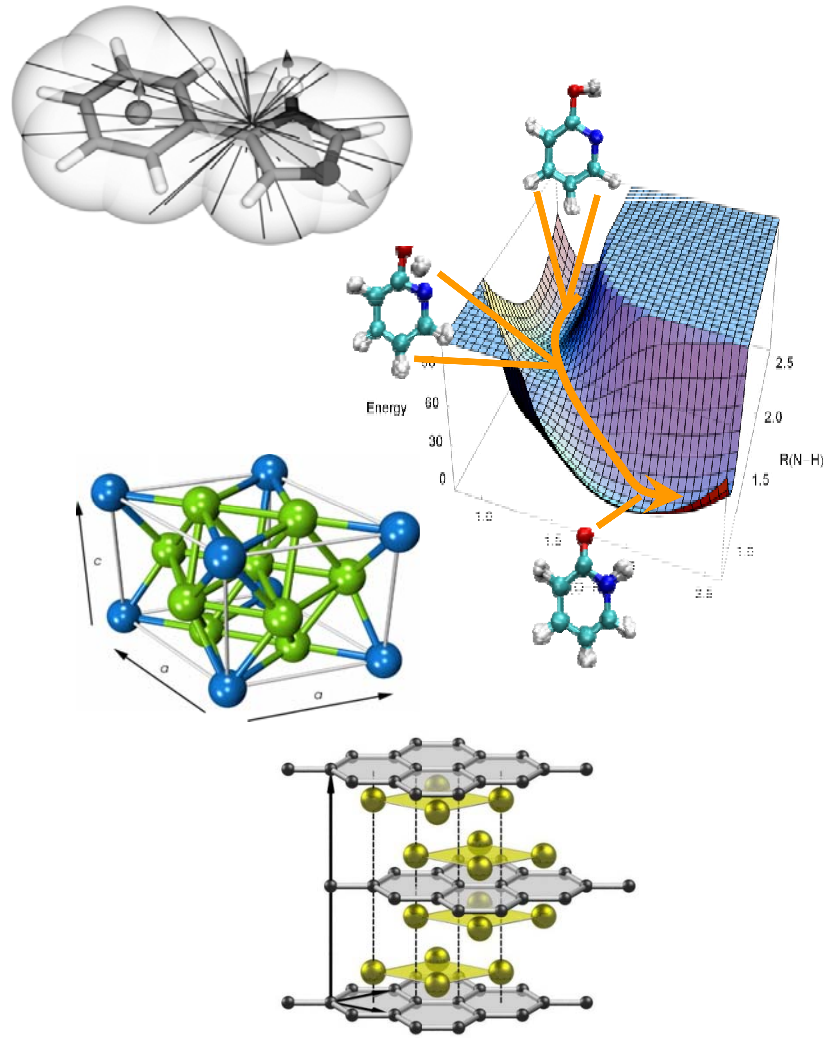
- Design strategies for new material creation
- Expand DoD materials portfolio

Introduce New Approaches/ Develop New Tools

- Develop heuristic-based modeling methodologies, akin to what is done in the pharmaceutical industry for “drug design,” to create new materials from new “lead” materials
- Develop design principles from the atomistic level through processing of bulk material (physics-based, multi-scale modeling methods)
- Develop data mining methods capable of exploring well established chemical databases for alternative materials

D&I Investments to Advance Materials Science and Application

- Theoretical tools are being developed to explore potential energy surfaces so that dynamical processes of molecules can be predicted.
- A new Hf/Sc alloy predicted by high-throughput quantum theory; now a candidate for synthesis and testing.
- A CAMD superconducting material; higher Tc materials are now being considered.



ONR POC: Dr. Kenneth Lipkowitz; kenny.lipkowitz@navy.mil