ICME in Education: General Perspectives, and the Role of Government and Materials Societies

G. Spanos

TMS

Contributors:

W. Hunt, TMS

D. Rowenhorst, A. Lewis, A. Geltmacher, NRL

S. Chan and Greg Olson, Northwestern Univ.

Financial Support – TMS, ONR & DARPA (D 3-D program)

Talk Outline

- Background on ICME (from my perspective – NRL, TMS)

- Another aspect of <u>I</u>ntegrated in <u>I</u>CME:
  - ➢Integration of four types of organizations
  - ➢Critical issue to emphasize in ICME-related curriculum

- ICME tools development in NRL-led "D3-D" program
  - ➢Involvement of four organization types
  - ➢Importance of critical experiments (recurring theme)
  - ➢Importance of 3D (vs. 2D)
  - ❖All must be considered in any ICME-related curriculum

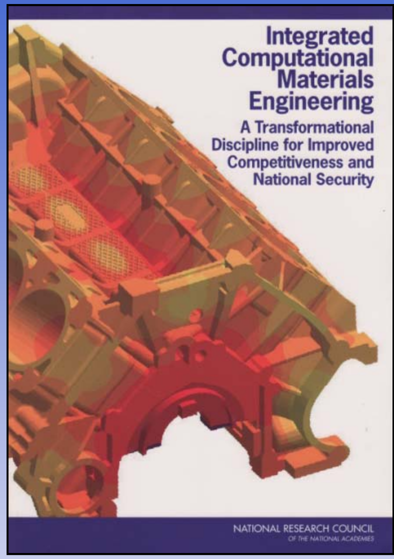
- Role of Government in ICME, implications in education

- Role of Materials Societies in ICME, implications

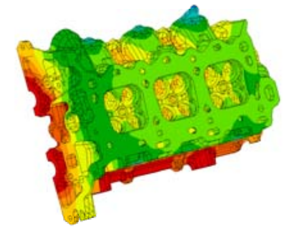
- Final Thoughts and Comments

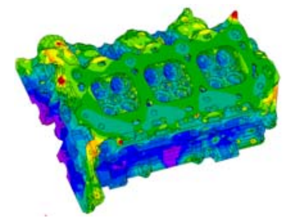
Integrated Computational Materials Engineering (ICME)

- National Academies report/study
  - Summary in beginning: recommends strong support from Industry, Government, Academia, and Materials Societies to establish a foundation for materials design and manufacturing
  - Will result in large savings of $ and time toward implementation of new optimized materials and manufacturing processes



- Case studies:
  - Ford virtual aluminum castings program: > 7:1 ROI for $15M investment
  - DARPA AIM program: Rotor Design Tool, etc.
  - Others……..
  - ❖ Must learn from (and include in education)

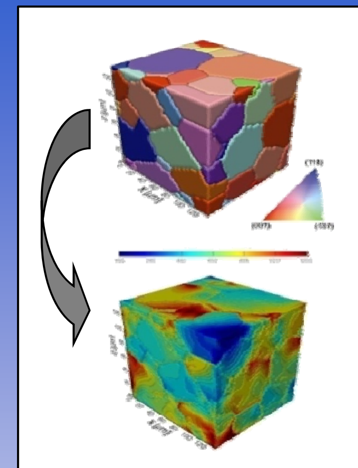

Thermal Analysis


Local Fatigue Strength

(courtesy J. Allison)

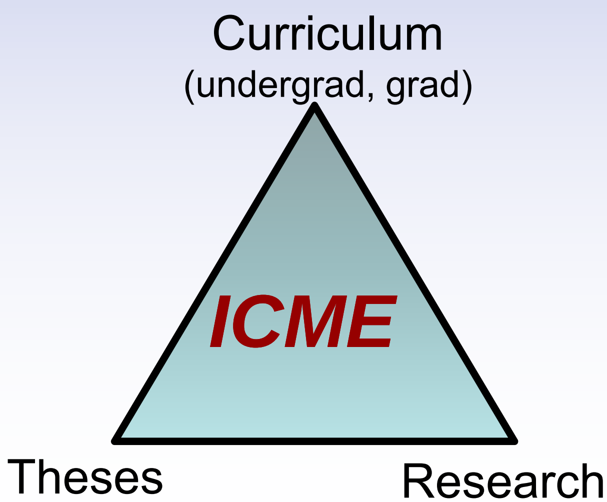
ICME in Education

- As a materials community, now in position to bring together our more fundamental experimental & computational efforts (particularly in 3D) with more applied manufacturing efforts



3D experimental reconstruction & FEM model in a titanium alloy

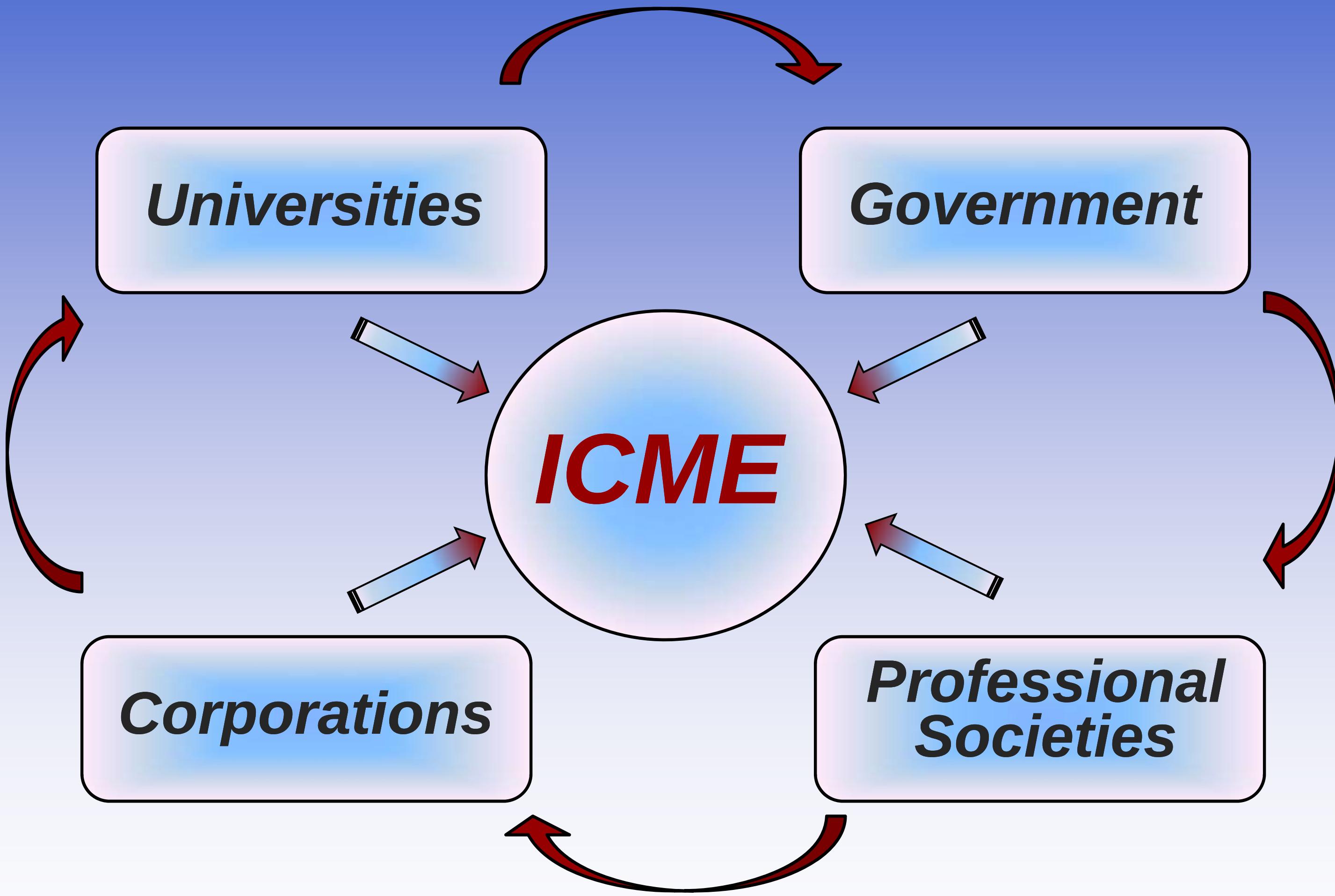
- What role will/should universities play and how will this be implemented in academia?



In addition to an R&D foundation for ICME, develop "human capital" for future ICME efforts (our professionals)

TMS

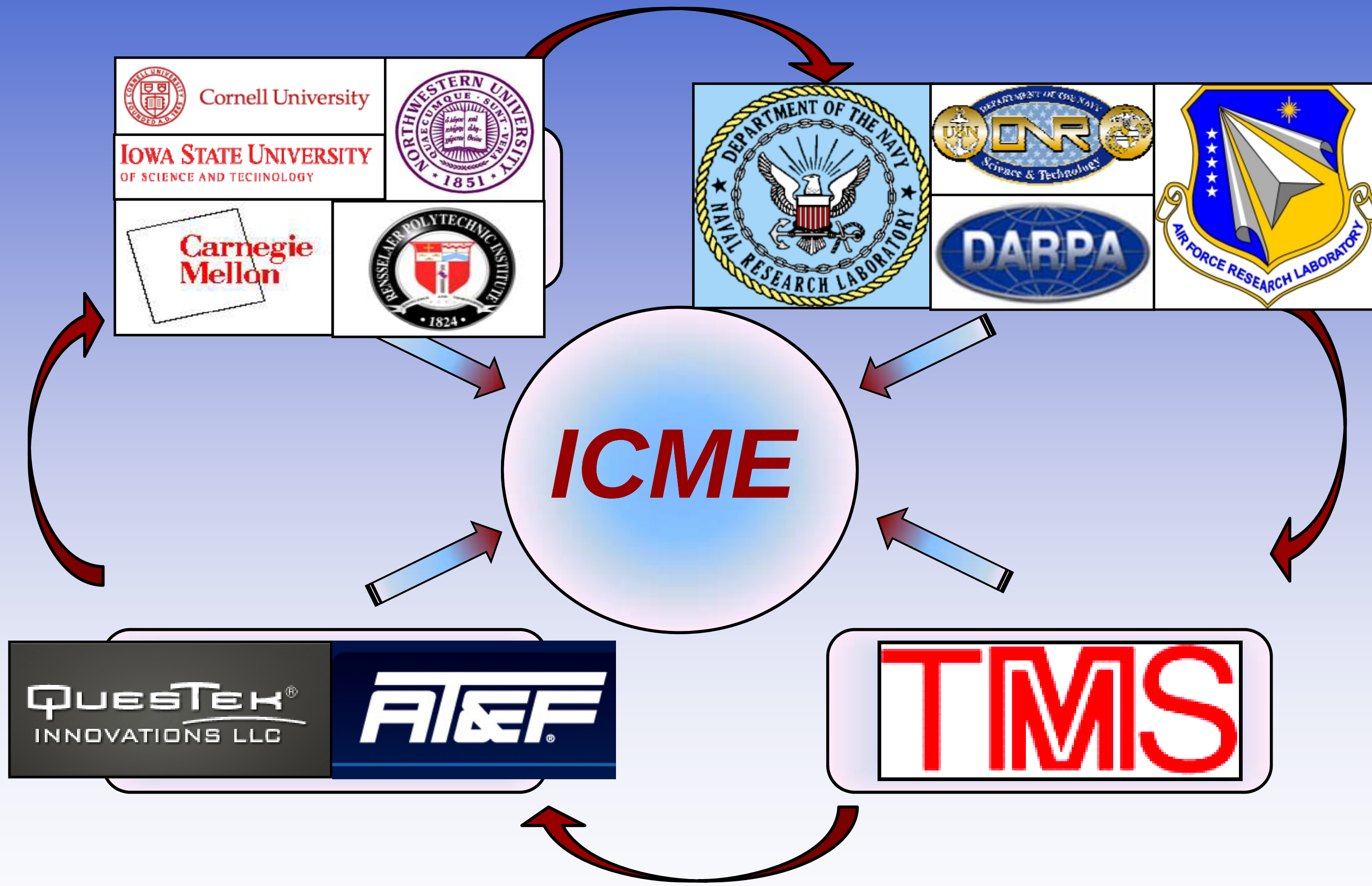
One Aspect of "Integrated" in ICME – Synergy Amongst Four Groups



- ***Must coordinate all four for optimal leveraging***
- ***This approach to ICME must be considered "upstream" in any curriculum development, or academic research***

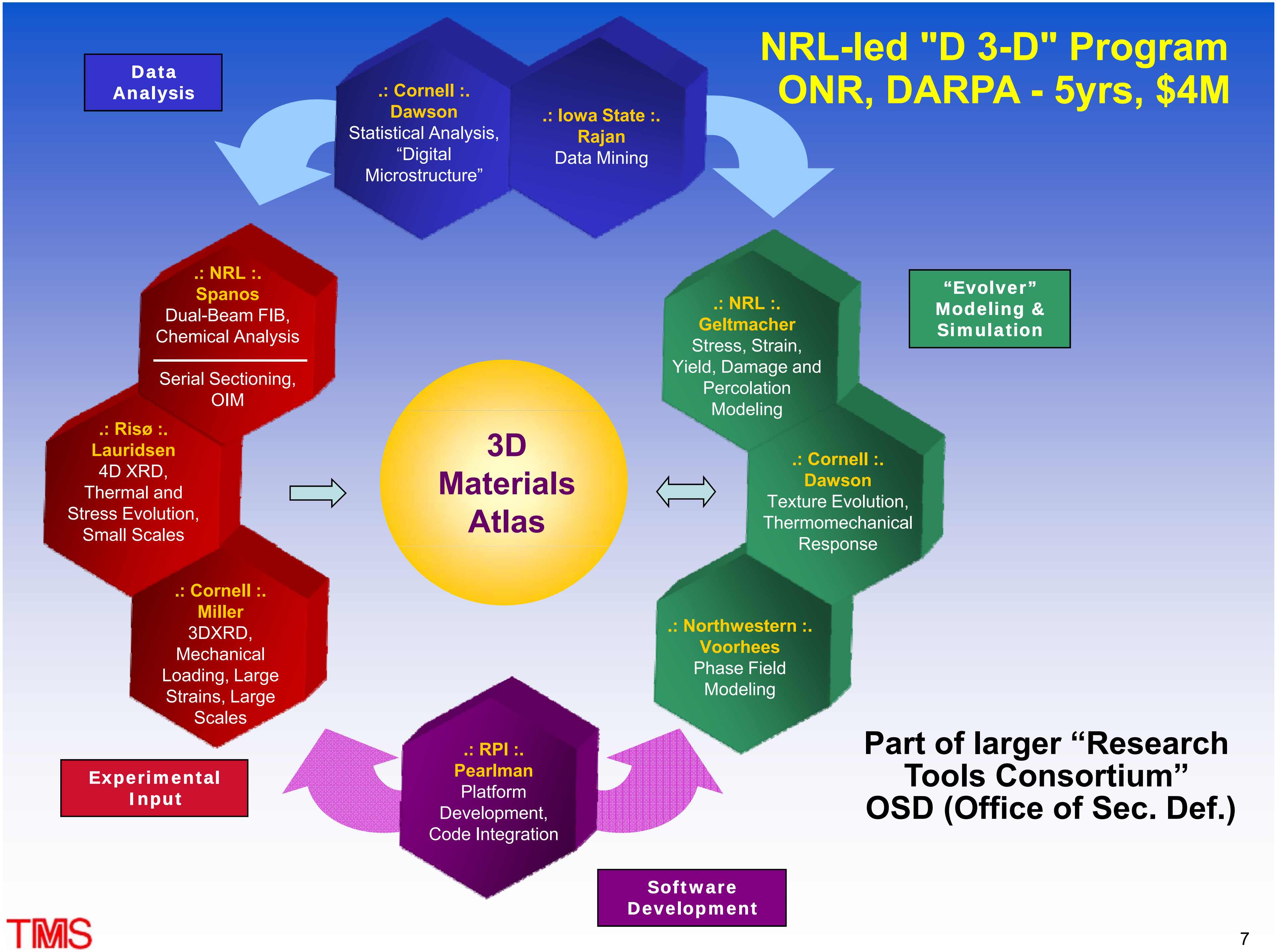
TMS

One Example of Integration Amongst Four Groups: NRL-led "D3D" and Steels Programs



- **Will discuss how four types of organizations interacted to develop ICME tools and methodology in NRL program**

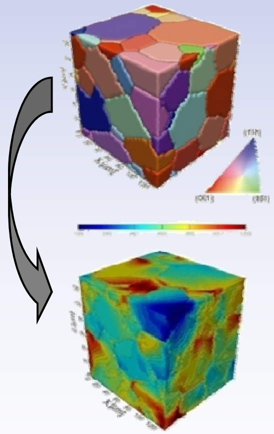
TMS


NRL-led "D 3-D" Program
ONR, DARPA - 5yrs, $4M
Data Analysis
.: Cornell :.
Dawson
Statistical Analysis, "Digital Microstructure"
.: Iowa State :.
Rajan
Data Mining
.: NRL :.
Spanos
Dual-Beam FIB, Chemical Analysis
Serial Sectioning, OIM
.: Risø :.
Lauridsen
4D XRD, Thermal and Stress Evolution, Small Scales
.: Cornell :.
Miller
3DXRD, Mechanical Loading, Large Strains, Large Scales
3D Materials Atlas
"Evolver" Modeling & Simulation
.: NRL :.
Geltmacher
Stress, Strain, Yield, Damage and Percolation Modeling
.: Cornell :.
Dawson
Texture Evolution, Thermomechanical Response
.: Northwestern :.
Voorhees
Phase Field Modeling
.: RPI :.
Pearlman
Platform Development, Code Integration
Experimental Input
Software Development
Part of larger "Research Tools Consortium"
OSD (Office of Sec. Def.)
TMS

Model Validation and 3D Microstructural Analyses are Critical to ICME

- **Validation/Calib.** of models critical
  - Many speakers at last GRC on ICME mentioned this (Lee, Gottstein, Pollock, Krajewshi), & importance of 3D
  - Powerful 3D models continuously upgrading functionality, but *validation lagging far behind*

- **Input** for models - realistic (not idealized)
  - "Image-based" or "microstructure-based" modeling
  - Provide for enhancement of models
  - 3D critical - examples where 2D is insufficient

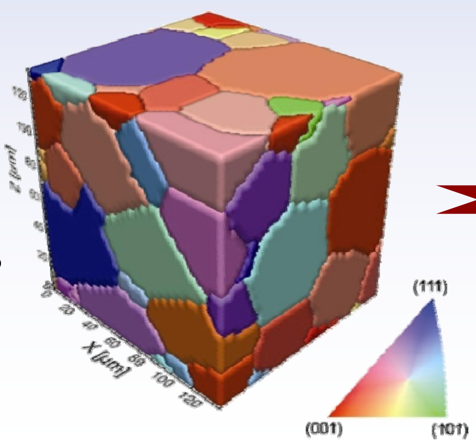


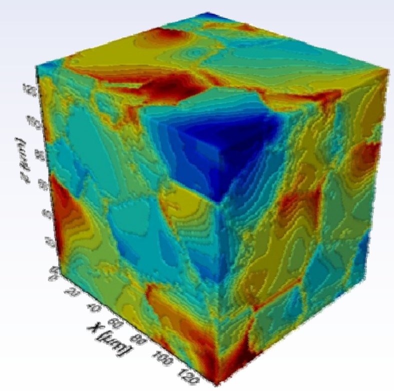
* Reminder: In Nat. Academies ICME report, and J. Allison past TMS talk: **~50%** of Ford ICME Virtual Al Castings effort was ***experimental***

Reasons for Studying Materials Microstructures in 3D

- 3D shapes, distributions, & crystallography of grains and defects:
  - Dictate mechanical/physical properties
  - Critical for accurate predicative models
    - microstructural evolution, materials response, materials & process design
- Typical microscopy techniques have in the past viewed 2D sections only - shown as inadequate for determining true 3D microstructure
- Groundbreaking 3D experimental capabilities and powerful computer hardware & software now available
- ***Recent 3D modeling approaches ("imaged-based") take as input real 3D experimental data - for accurate predictability and design in computational materials modeling***

Experimental Reconstructions





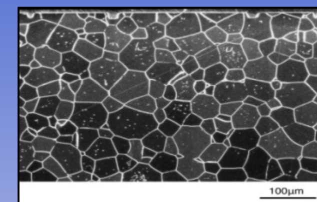
"Image-based" Simulations

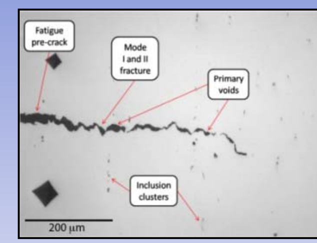
TMS

Two 3D Studies at NRL

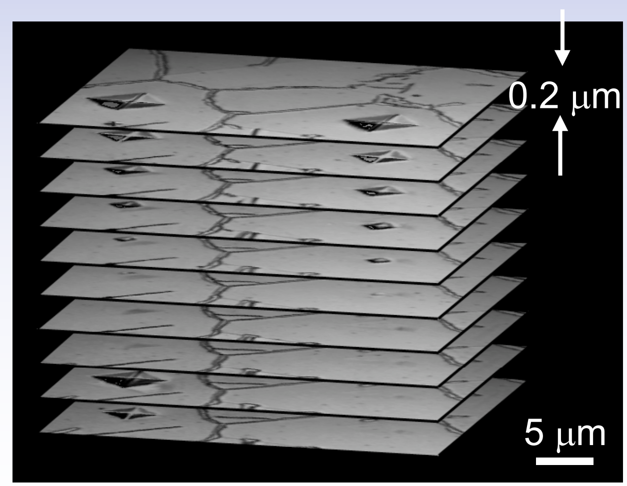
- Will highlight recurring themes for ICME tools/research
  (1) interaction of four organizational types, (2) synergy between computation and experiment, (3) need for 3D

- Systems/problems studied:
  - Beta grain structure in a Ti alloy (Ti-21S)
  - Cracks, voids, inclusions – 4330 steel (collaboration with Northwestern)



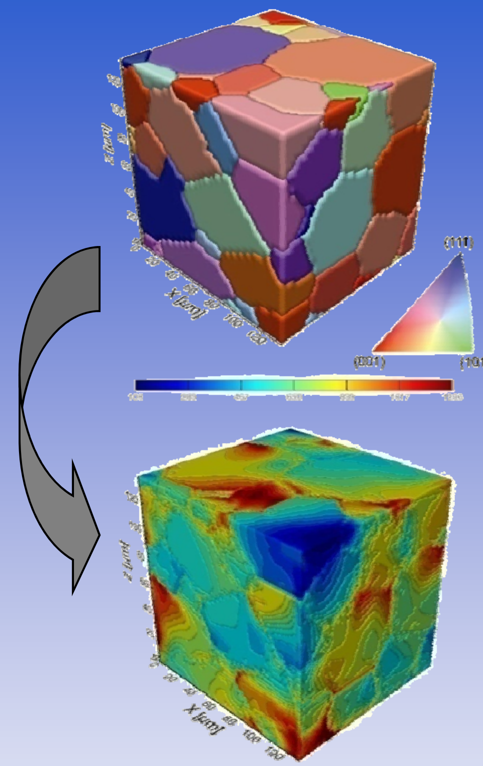


- Methodology:
  - ▼Define goals, system, problem
  - ▼Serial sectioning
  - ▼Imaging & segmentation
  - ▼3D reconstruction
  - ▼Quantitative 3D analysis
  - ▼“Image-based” computational modeling (for ICME approach)

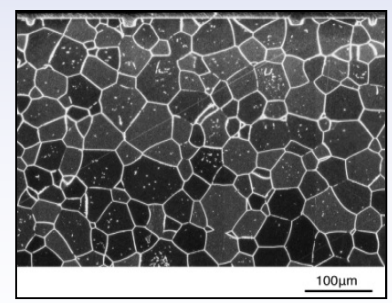


Goals and problem set-up: β Ti alloy

- Goal:
  - ➢Reconstruct a large (statistically significant) data set of space filling grains in 3D
    - – Start with simple system – single phase
  - ➢Needed for predictive modeling (ICME):
    - – Thermal processing (Phase Field)
    - – Mechanical response (FEM)
  - ➢**Navy/DARPA** interest: Ti & steel alloy and process development

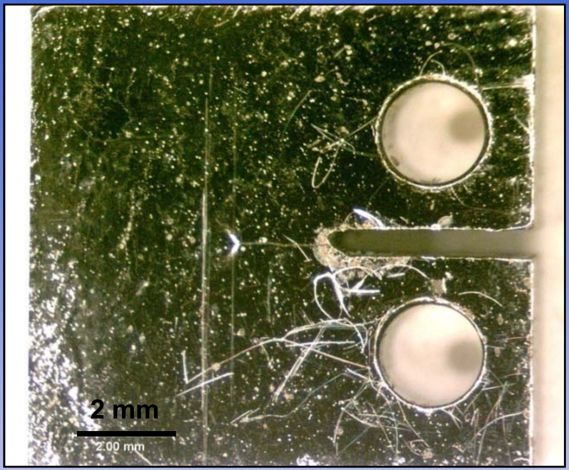


- Initial problem set up
  - ➢After much consultation (**J. Williams, OSU**), chose a beta stabilized Ti alloy – β 21S (Ti-15Mo-2.8Nb-2.0Al-0.2Si-0.2Fe-0.13O)
    - – Although other simpler alloys, this one slowed down kinetics enough to control grain size

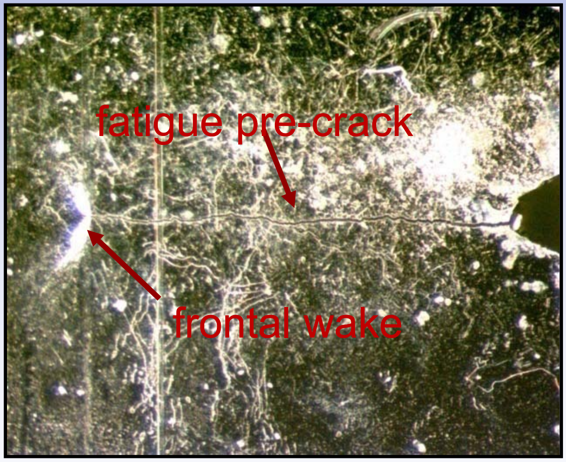


Goals and problem set-up: Steel

- Goal:
  - Reconstruct crack tip, voids, inclusions in frontal wake of cracked specimen
  - 3D data needed for multi-scale ductile fracture models
  - **Navy** interest: predictability and mitigation of failure in advanced steels

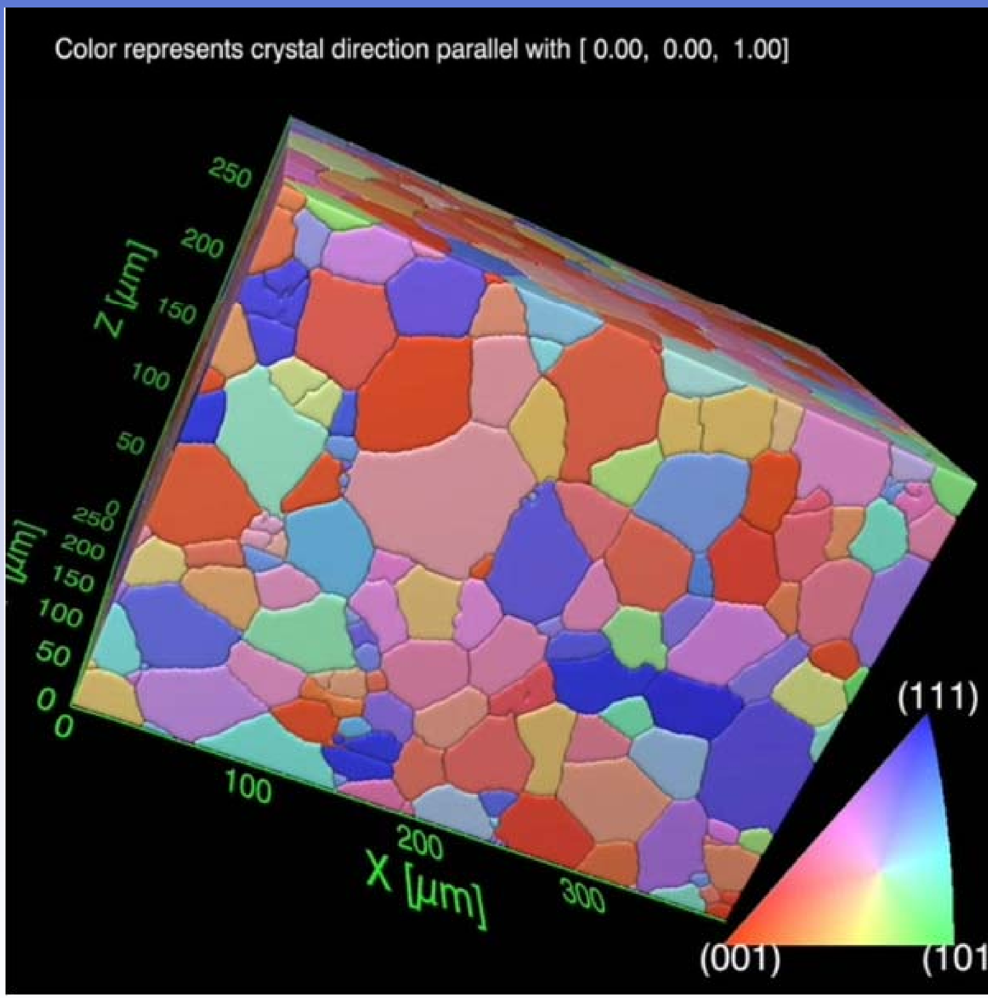


- Initial problem set up
  - Working with **Northwestern & Questek**, decided on Ti-modified 4330 steel
  - Significant ancillary data (properties, microstructure, etc.) and experience



(wt%)	C	Si	Cr	Mo	Ni	Cu	Ti	V	P	S	Fe
Mod. 4330	0.29	1.52	1.91	0.38	0.19	0.14	0.042	0.11	0.012	0.005	Bal.

3D Reconstruction: β-Titanium Grains in Ti21S

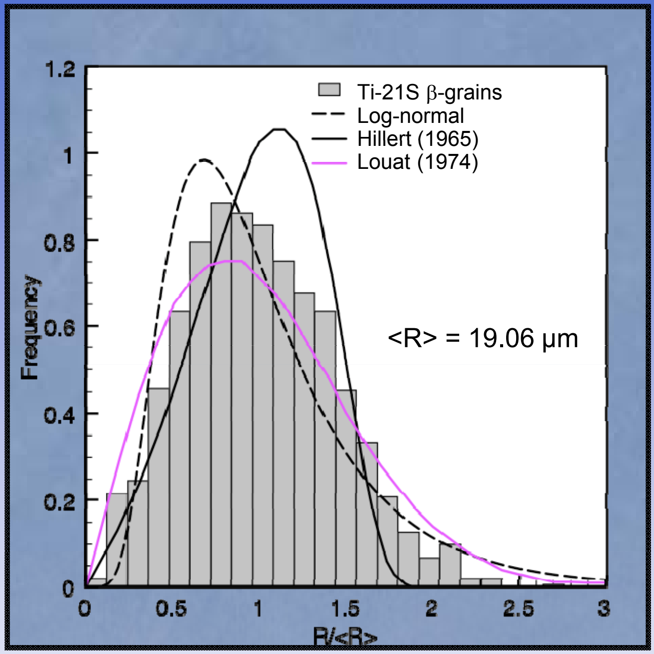


- 200 sections, with 20 EBSD sections for full 3D crystallography: “3D - EBSD”
- IDL scripts (D. Rowenhorst) for 3D visualization,quantitative analyses
  - also interfacial texture analysis code of **Rohrer et al., CMU**
- Subset only shown here ~1000 grains (300 internal)
- Full data set > 4300 grains (2100 internal, unbiased)

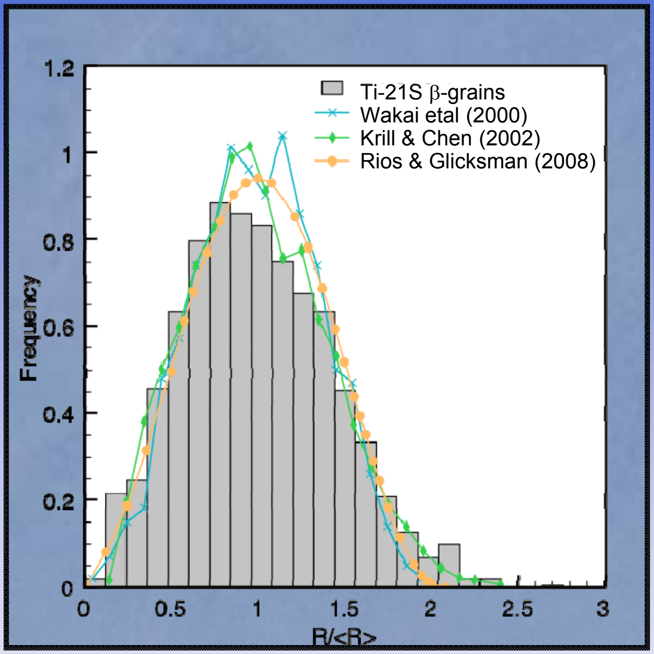
TMS

Quantitative 3D Analyses, Direct Comparison to Predictive Models - Critical Validation for ICME Tools

Grain Size Distributions



vs traditional GG models

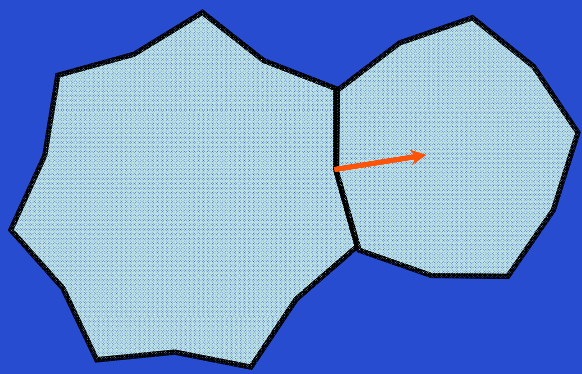


vs newer models

- Direct comparison with recent theories & computational models
- More recent simulations, models match distribution much better
- Some variations near tail of distribution
  - Important for fatigue nucleation, etc.

TMS

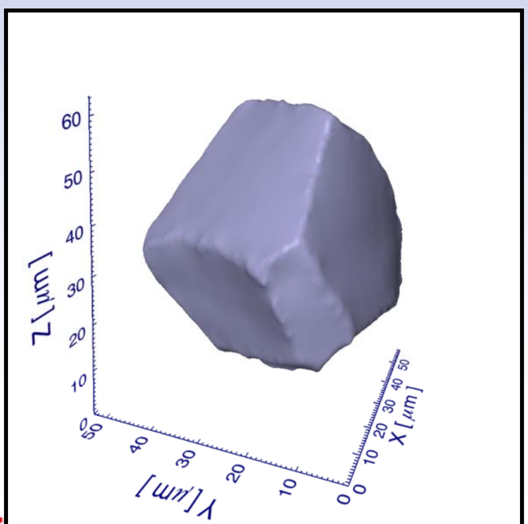
Curvature Driven Grain Growth



$$\mathbf{v} \cdot \mathbf{n} = -M\gamma H$$

Mean Curvature: $H = \left(\frac{1}{R_1} + \frac{1}{R_2}\right)$

$$\frac{\partial V}{\partial t} = -M\gamma \int_{Faces} H \, dS$$

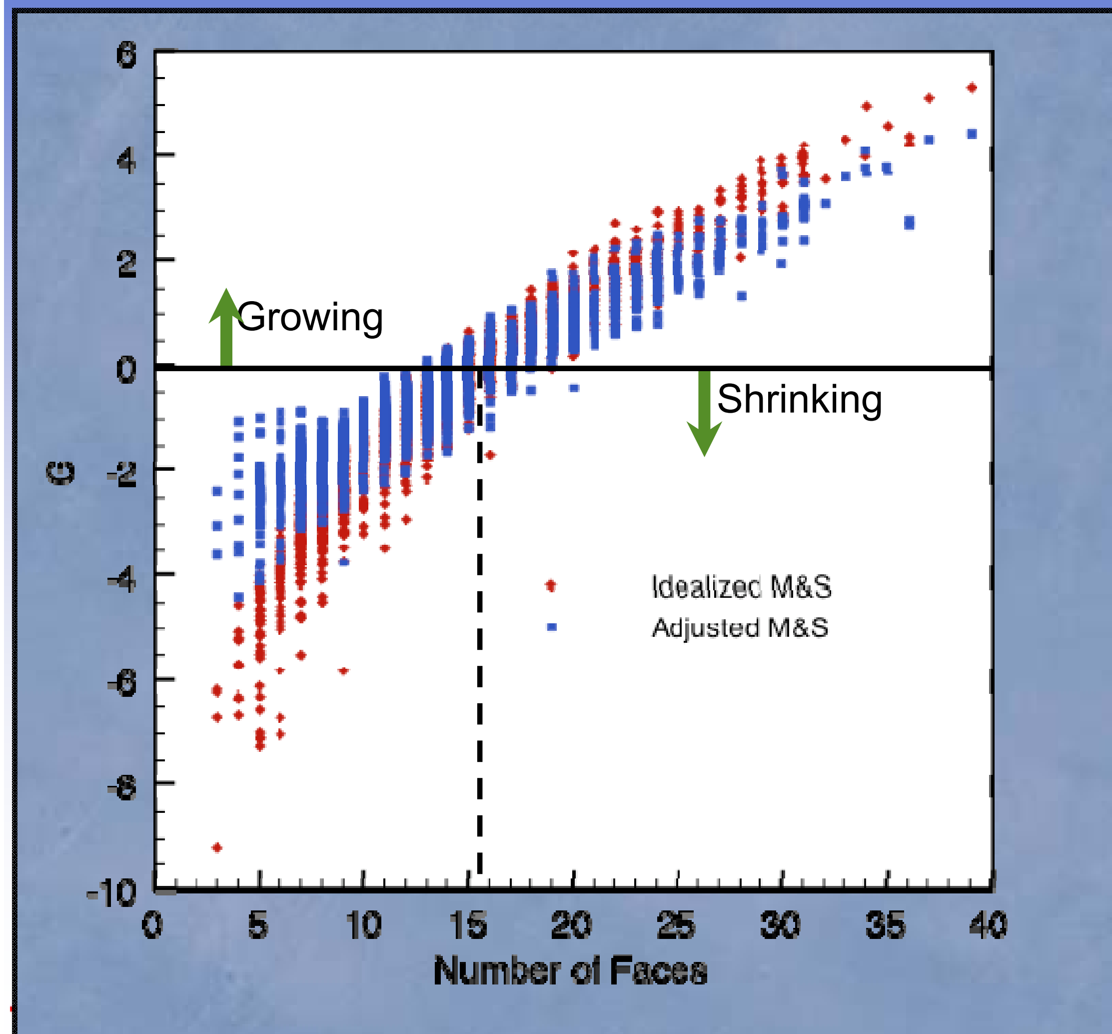


Growth rate of a grain is proportional to integral mean curvature for all grain faces, not including curvature at triple junctions

Grain Face Integral Mean Curvature

$$\frac{\partial V}{\partial t} = M\gamma V^{1/3}\mathcal{G}$$

$$\mathcal{G} = -\int_{\mathrm{Faces}} \frac{H}{V^{1/3}} dS$$



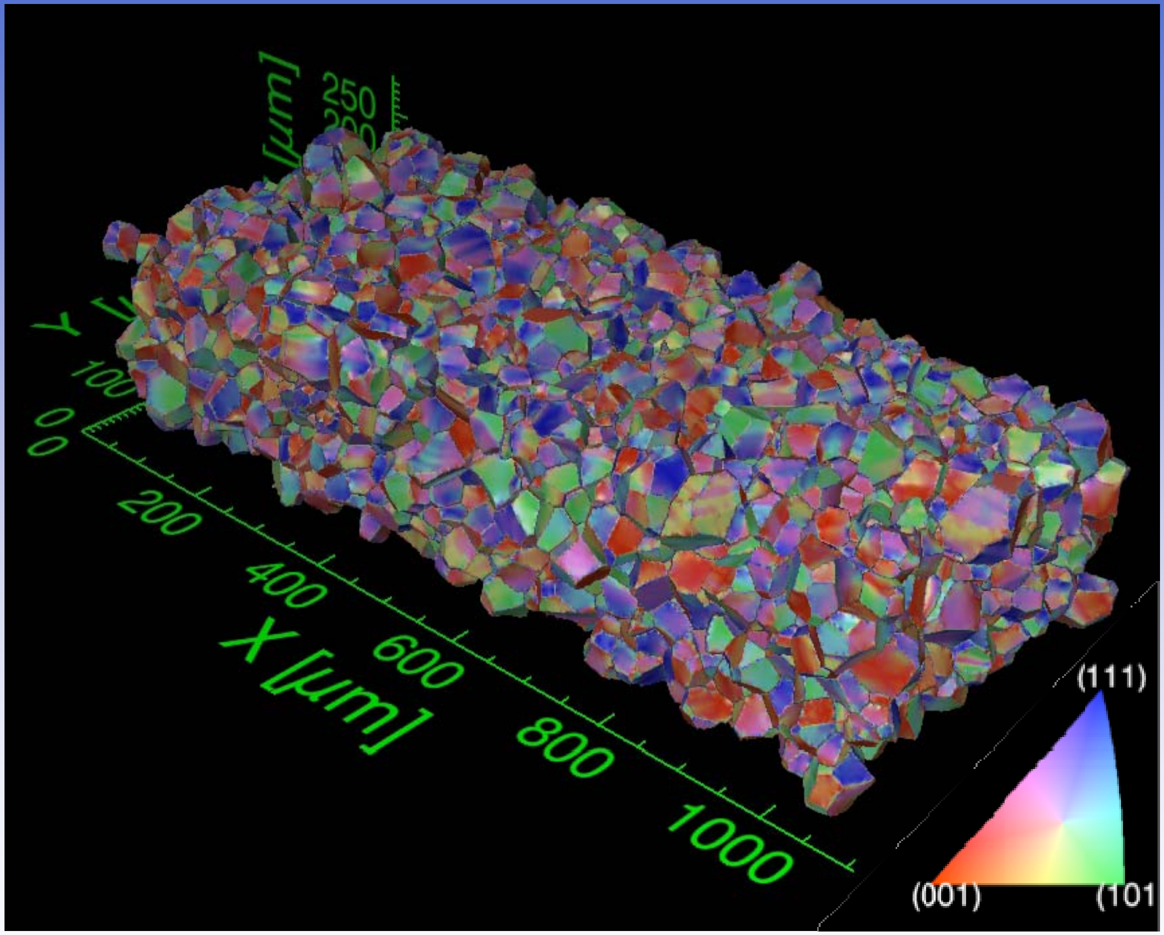
- Cross-over point for shrinking/growing occurs at ~15.5 faces; not at the average F (13.7) or predicted zero mean curvature shape
- Showed this was due to complex grain interactions with nearest neighbors not fully accounted for
- Critical for enhancement/ validation of grain evolution models for ICME predictive modules

G is size-independent growth rate

Also Include Full Crystallography and Interfacial Texture

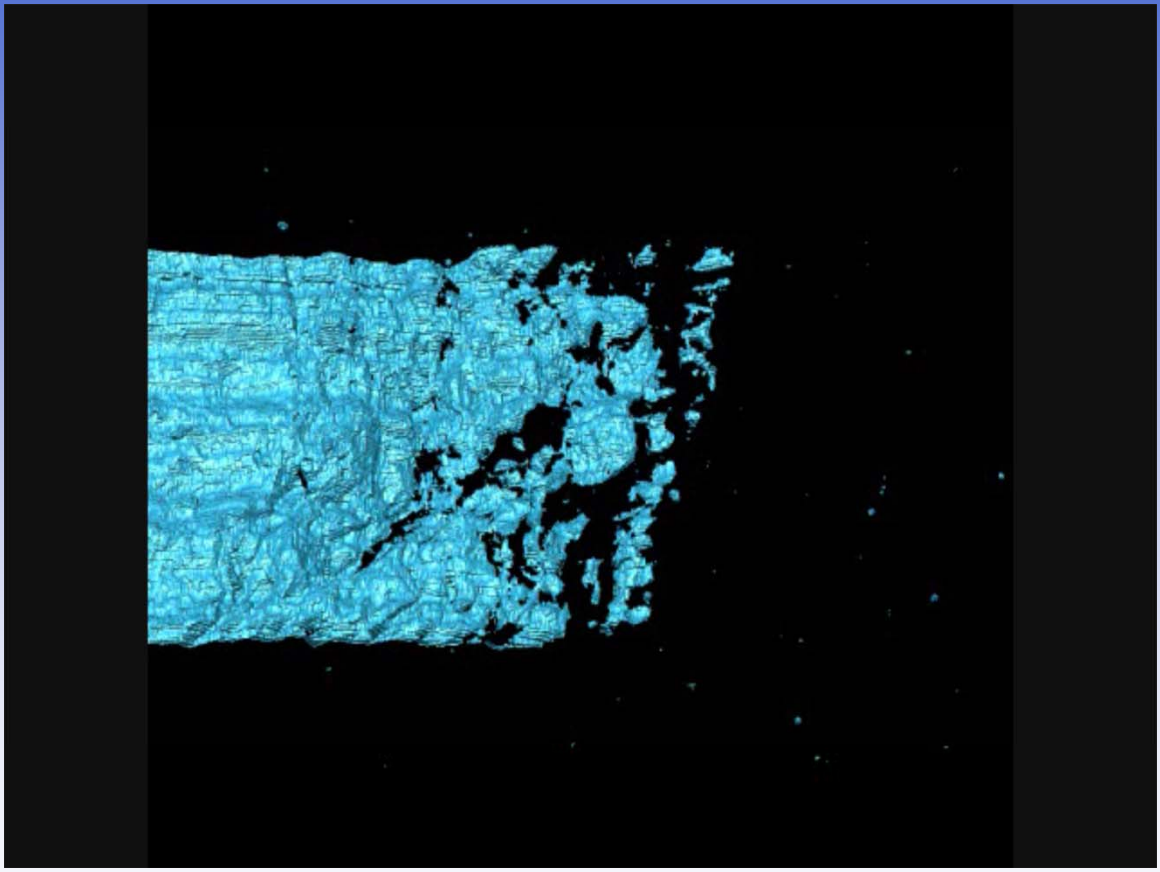
These same techniques can be used on the aggregate structure to get information about the 3D <u>interfacial</u> texture

Each point on the interface is colored by its crystallographic normal



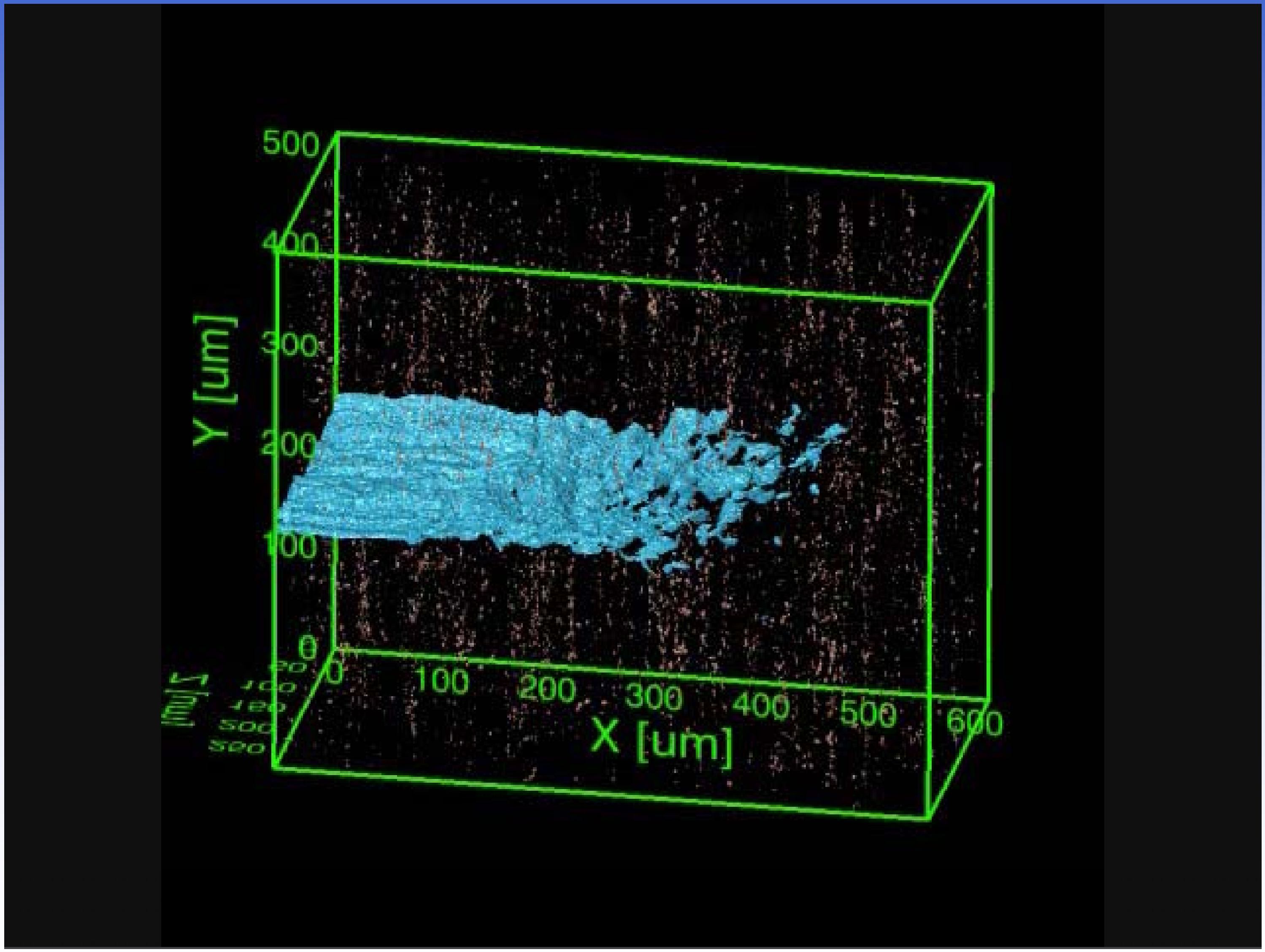
Have quantified facet distributions using CIND (<u>C</u>rystallographic <u>I</u>nterface <u>N</u>ormal <u>D</u>istribution) and Interfacial Texture Analyses developed at **CMU**

Mod4330 – Crack Reconstruction

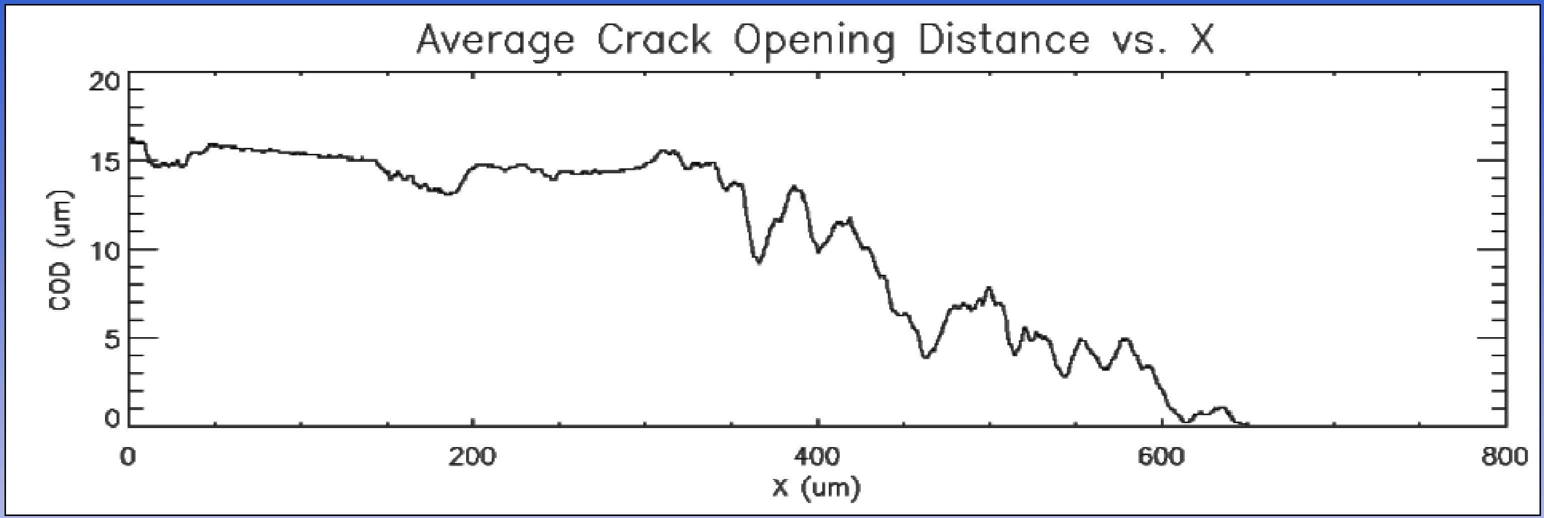


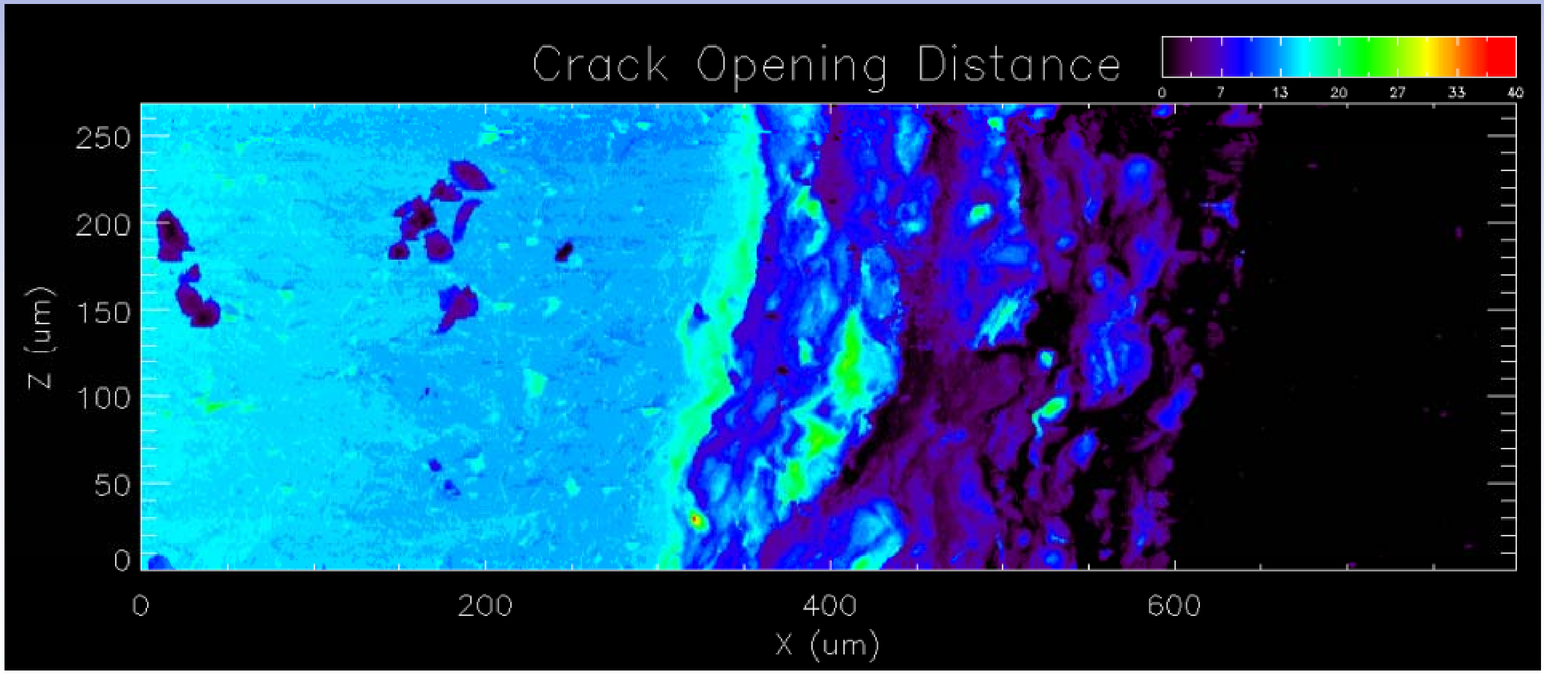
Volume: 1096 x 831 x 150 μm^3

Full Reconstruction Including TiN Particles



3D Quantification (Chan & Olson, Northwestern)





TMS

Courtesy S. Chan

Primary Particle Statistics

	CT#1 (low res.)	CT#3 (high res.)	FSL (M. Echlin)
Particle Density (#/m^3)	1.29×10^{13}	10.9×10^{13}	2.84×10^{13}
Volume Fraction (%)	0.176 0.088	0.050 0.039	0.028 0.016
Mean Diameter (μm)	4.86	1.79	2.12
Mean Nearest-Neighbor Distance (μm)	15.8 22.6	6.7 10.8	10.0 17.4

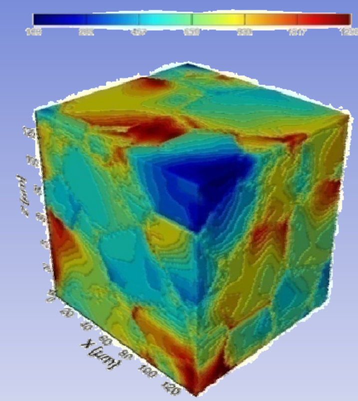
Calculated values as a function of radius and particle density, from J.S. Wang

TMS

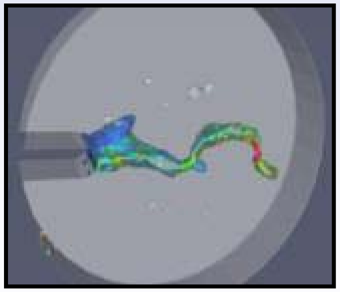
Courtesy S. Chan

How These 3D Microstructural Data Have Been Employed in Computational Models

- 3D β grain structure in Ti-21S
  - Simulation of response to mechanical loading: FEM modeling (Geltmacher et al. - **NRL**; Dawson - **Cornell**)
  - Simulation of response to thermal exposure: Phase Field modeling (Voorhees et al. - **Northwestern**)



- 3D reconstruction of crack, voids, inclusions in Ti-modified 4330 steel
  - Multi-scale ductile fracture modeling (Liu & Olson – **Northwestern**)

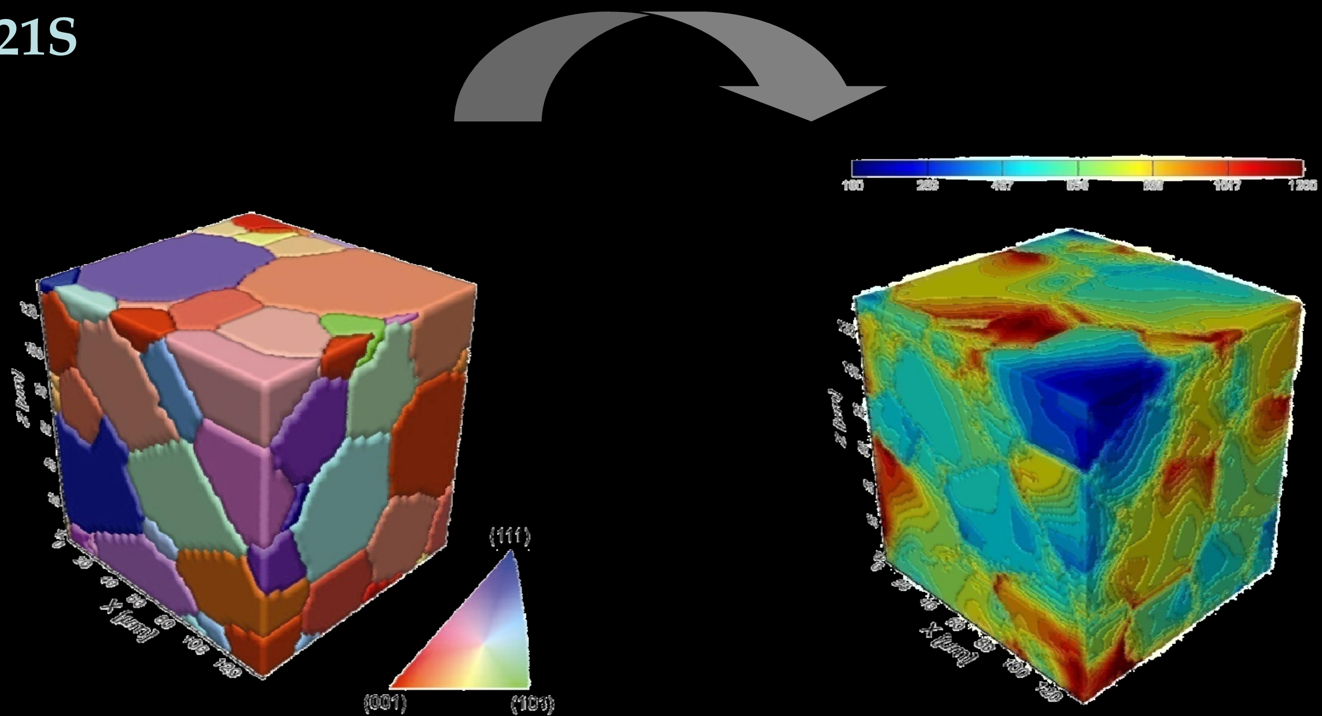


TMS

"Image-Based" FEM Simulations - β Ti Alloy
(Geltmacher, Lewis, Qidwai, NRL)

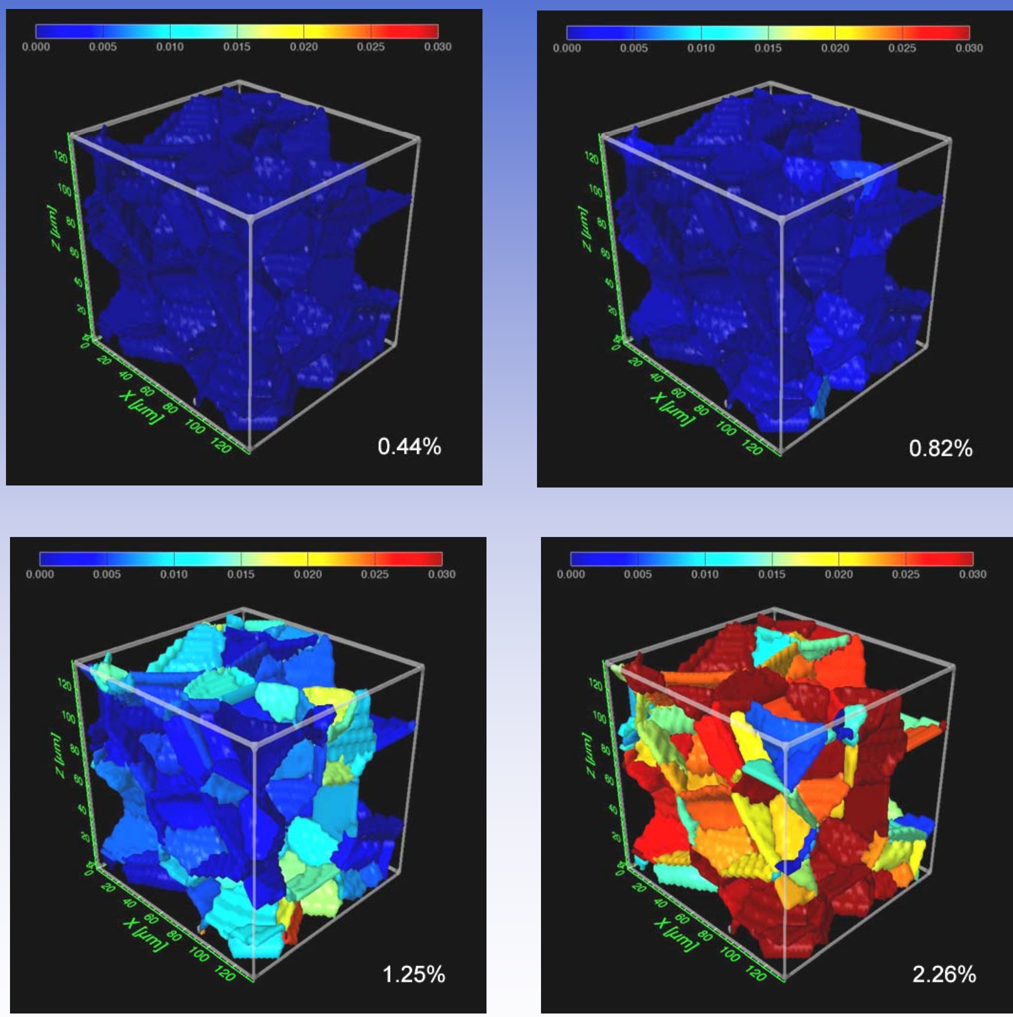
Real 3D Microstructure input into FE Model

Ti- β21S

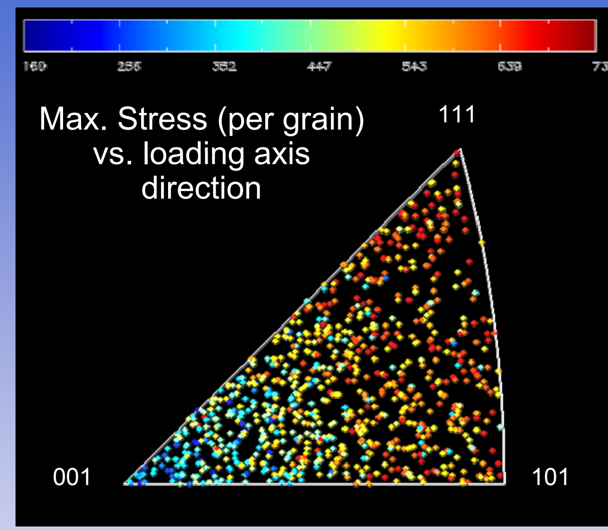


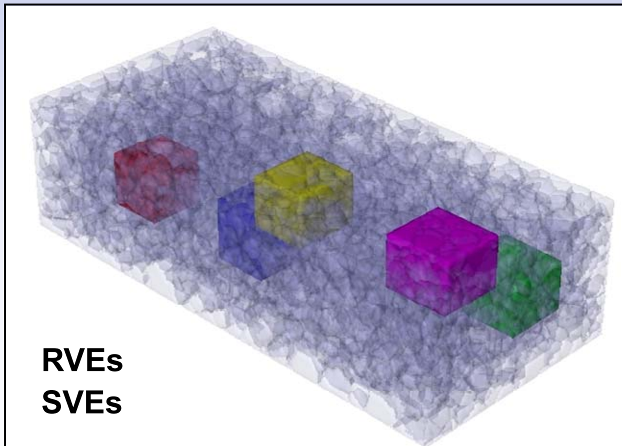
Reduced dataset of 92 grains—16 internal—spanning 136 x 128 x 137 μm^3.

Mechanical Response: Visualization at GBs, Stress vs. Crystallography, etc.

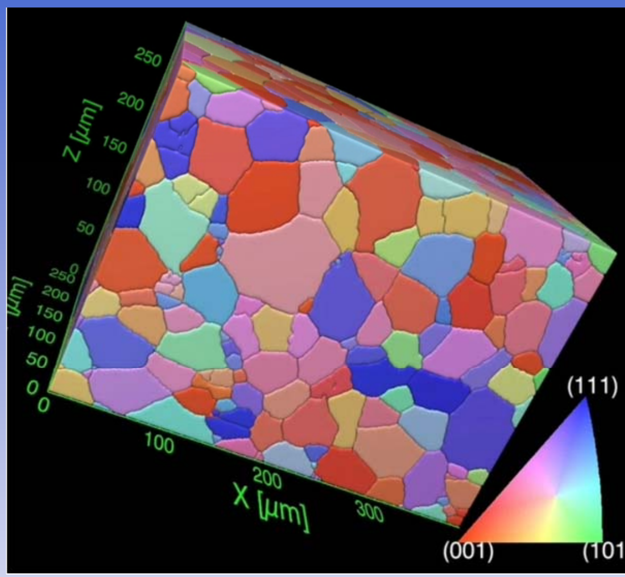


mean cumulative shear strain on grain boundaries (vs. applied strain)

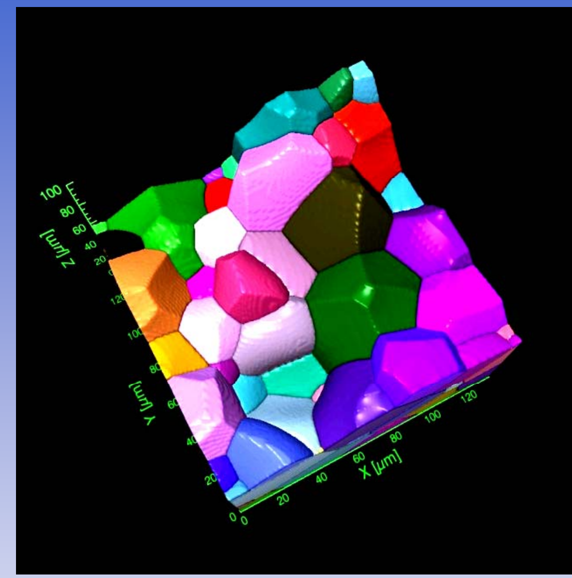




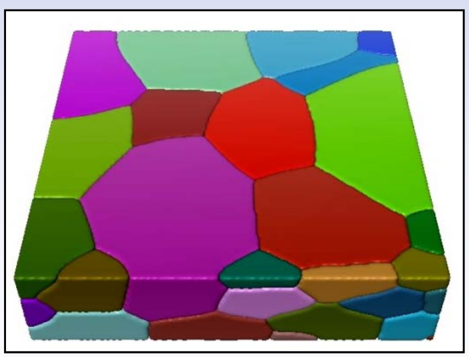
Predictive Phase Field Simulations of Grain Growth - Using 3D Experimental Input
(with McKenna & Voorhees, Northwestern)



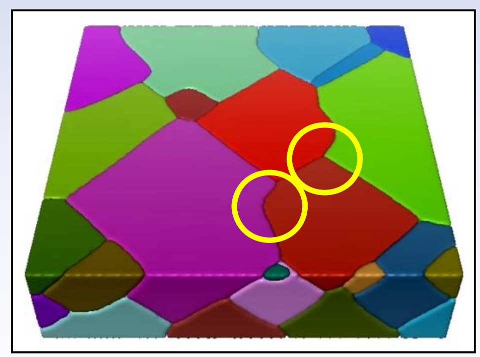
NRL β 21-S Serial Sectioning
3D Reconstructions



3D Phase-field Model (Northwestern)
- Material Response to Thermal Exposure



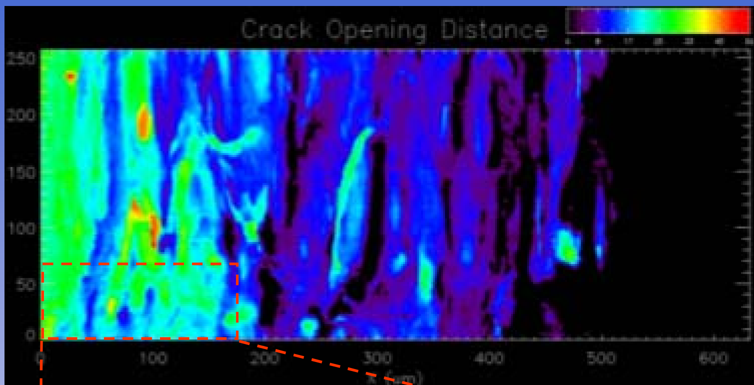
Isotropic model



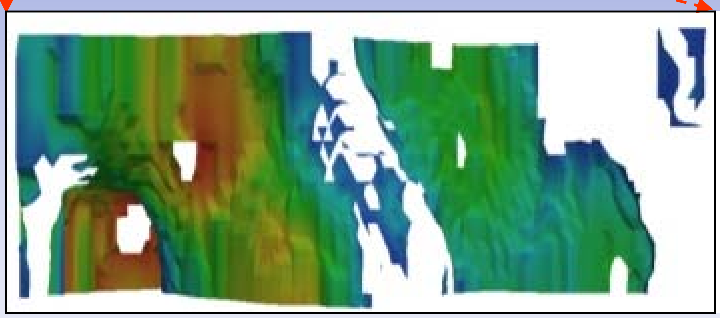
Anisotropic model

Collaborating with Risoe Nat. Lab., made first direct comparisons vs. time

Using 3D Steels Data in Multiscale Fracture Models



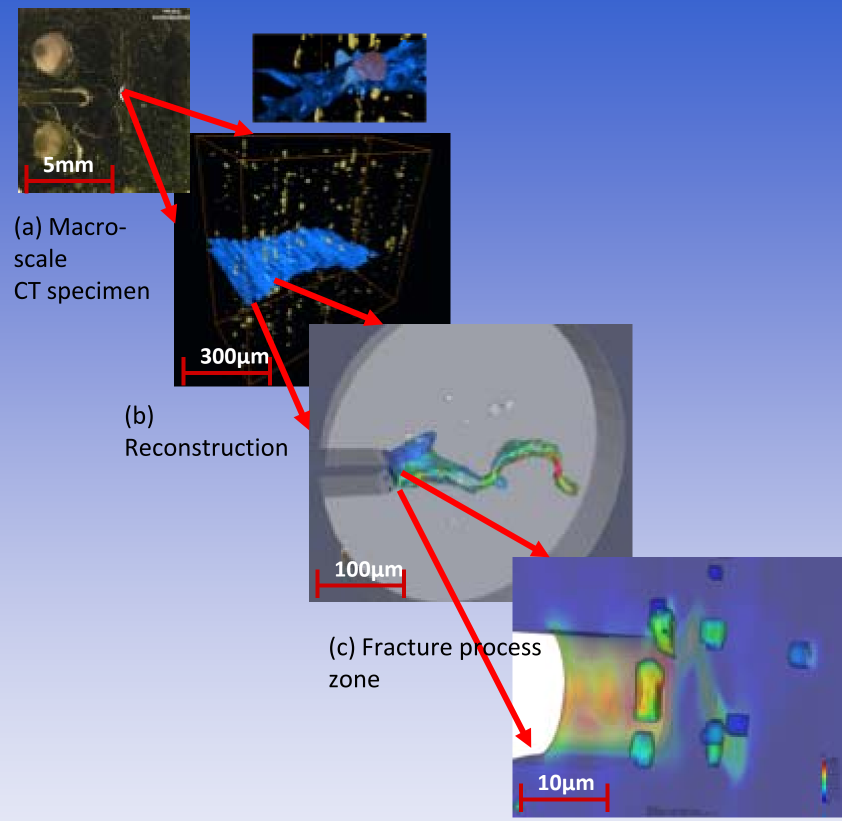
Experiment



Simulation （ preliminary result ）

Step 1: validation

Courtesy S. Chan



Step 2: prediction

- Results used as input into Multi-scale fracture modeling of Profs. Liu & Olson (**Northwestern**)
- For use in **Questek** materials and manufacturing design models

TMS

Manufacturing Emphasis: Corporations & Other Gov. Agency Interactions

- Applied our characterization and computational suite of tools to Navy problems
- Have worked extensively with a number of groups
  - **Government**: Navy MANTECH, ONR, NSWC, two Navy MANTECH centers - NCEMT (CTC) & NJC (EWI)
  - **Industry/Companies**: Electric Boat, Newport News Shipyard, American Tank and Fabrication, Questek
- Only recently though have begun to more intimately integrate across organizations, and amongst experimental and computational tools
- Now primed to meld together 3D experimental and computational efforts with more applied manufacturing efforts - employing 3D suite of tools developed under D3D

Role of Materials Societies in ICME

TMS
LEARN • NETWORK • ADVANCE

Serving the Computational Materials Science and Engineering Community

The Minerals, Metals, and Materials Society (TMS) has been recognized in the recent National Academies report for its efforts to support the emerging area of Integrated Computational Materials Engineering.
Key areas of activity and future plans are described below.

Networking and Conference Programming

MS&T'08:
- Discovery and Optimization of Materials Through Computational Design
- Modeling of Multi-Scale Phenomena in Materials Processing

2009 TMS Annual Meeting:
- Computational Thermodynamics and Kinetics
- Open Source Tools for Materials Science and Engineering
- Progress in Computational Materials Science and Engineering Education
- Synergies of Computational and Experimental Materials Science

MS&T'09:
- Discovery and Optimization of Materials Through Computational Materials Design
- Integrated Computational and Experimental Investigations on Microstructure Evolution of Coarsening Systems
- Microstructure Characterization, Analyses, and Design

2010 TMS Annual Meeting:
- Three-Dimensional Materials Science VI
- Computational Thermodynamics and Kinetics
- The Vasek Vitek Symposium on Crystal Defects, Computational Materials Science and Applications
- Stochastic Methods in Materials Research

Roundtables/Workshops:
- Computational Materials Design: Experience and Perspectives: A lunch time seminar presented with Penn State's CCMD at MS&T'09.
- Materials Digital Laboratory Roundtable Luncheon Workshop: ICME, MatForge, & Gibbs: Presented with the Center for Materials Informatics at Kent State University at the 2009 TMS Annual Meeting and MS&T'09

TMS2010
139th Annual Meeting & Exhibition

MS&T'09®

Knowledge Dissemination through Technical Publications

JOM:
- 3-D Characterization: Methods and Applications December 2006
- Integrated Computational Materials Engineering November 2006
- "Materials Informatics" March 2008 and January 2009

Conference Proceedings:
- Integrated Computational Materials Engineering: Lessons from Many Fields
- Advances in Computational Materials Science and Engineering Methods
- Computational Thermodynamics and Phase Transformations
- Multiphase Phenomena and CFD Modeling and Simulation in Materials Processes

Kn KNOWLEDGE
Your Materials Books and More e-Store!
TMS KNOWLEDGE RESOURCE CENTER
http://knowledge.tms.org

Online Resources

Integrated Computational Materials Engineering Digital Resource Center at Materials Technology@TMS
- Literature resources
- Database resources
- Software/code resources
- Discussion Board

MATERIALS TECHNOLOGY@TMS
MaterialsTechnology.org

Creating a Professional Home for ICME

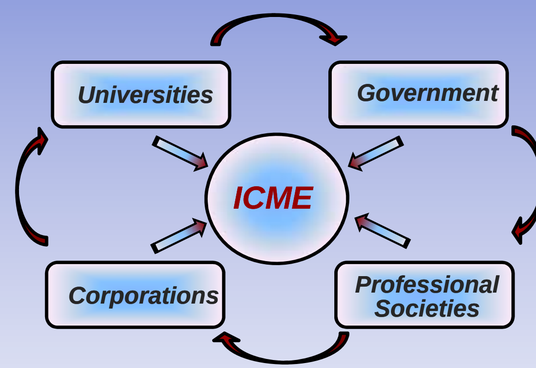
TMS is establishing a standing ICME committee as part of its technical committee structure that will serve to continue and accelerate the momentum.

In addition, the Board authorized further activities to support four specific areas:
- Knowledge Dissemination
- Collaborative Networking
- Academic Activities
- Continuing Education

Your Professional Partner for Career Advancement.

Role of Materials Societies in ICME, and in Implementation of ICME in Academia

- ICME committee of TMS
  - Very active committee
  - Members across four organization spectrum (many are here)



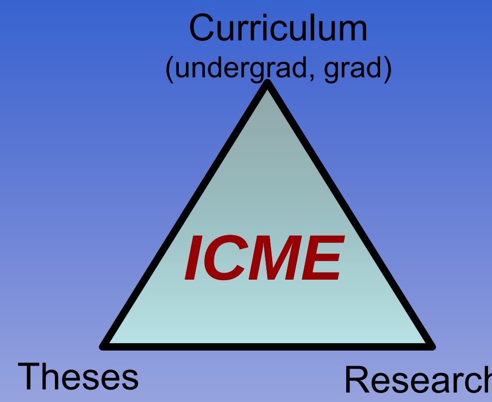
- Conference Programming (subcommittee)
  - **1st World Congress on ICME (July 2011)** - see next slide
  - **TMS Annual meeting (March 2011)** - *ICME: Overcoming Barriers and Streamlining the Transition of Advanced Technologies to Engineering Practice* (5 sessions)

1st International Congress on ICME

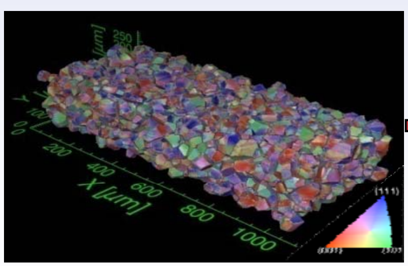
- Advance notice: ***First International World Congress on Integrated Computational Materials Engineering (ICME 2011)***
- July 10-14, 2011 (save the date) – Seven Springs, Pennsylvania
- Have commitments from a number of top level keynote speakers, and an International Advisory Committee representing > 15 countries
- Will involve leading modelers and experimentalists in the field
- GRC like setting and schedule:
  - Sunday (pm): Opening Keynote presentation
  - Monday: Modeling Processing-Structure Relationships
  - Tuesday: Modeling Structure-Property Relationships
  - ***Wednesday (am): ICME in Education***
  - Wednesday (pm): Information Infrastructure
  - Thursday (am): Success Stories
- ICME in education obvious major component
  - Strong UMC presence expected
  - One talk – out brief from this UMC meeting?
- Abstract call: July 2010 (deadline Nov. 1)

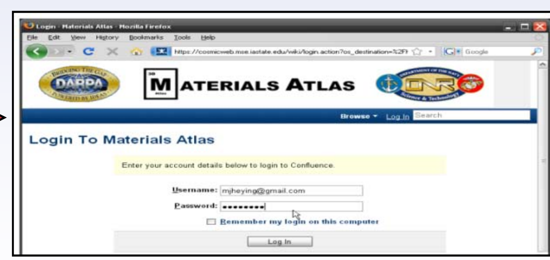
Role of Materials Societies…..

- ICME Education subcommittee
  - Initiate continuing education opportunities
  - Symposia (coordinate with programming subcommittee)
  - Liaison with TMS Education Committee
  - Planning 2012 TMS Annual meeting symposium

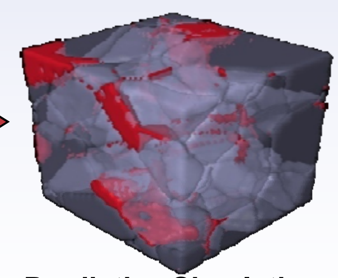


- Facilitate development of Information Infrastructure (“Cyber-infrastructure”)
  - As computational capabilities increase and data set sizes grow (3D, terabytes), information infrastructure is critical
  - Should be included in computational materials education


Experimental Studies



Materials Atlas


Predictive Simulations

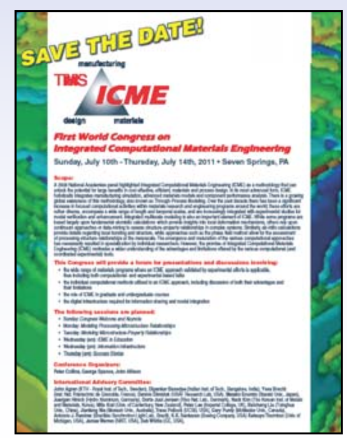
Role of Materials Societies…..

Publications

- JOM
  - 2006: 3D Characterization: Methods and Applications
  - 2006: Integrated Computational Materials Engineering
  - 2008: Materials Informatics
  - 2009: Survey on CMSE in undergrad. education (Thornton)
  - 2011: Enabling ICME: Successful Transition of Advanced Technologies to Engineering Practice (Me Li, ICME Comm.)

- Metallurgical and Materials Transactions
  - Current planning (T. Pollock, J. Allison, ICME Committee) on special ICME issue

- Conference proceedings
  - 1st International Congress on ICME (2011)
  - Others….



Role of Materials Societies…..

Online Digital Resources/Communities

Under Banner of Materials Technology@TMS

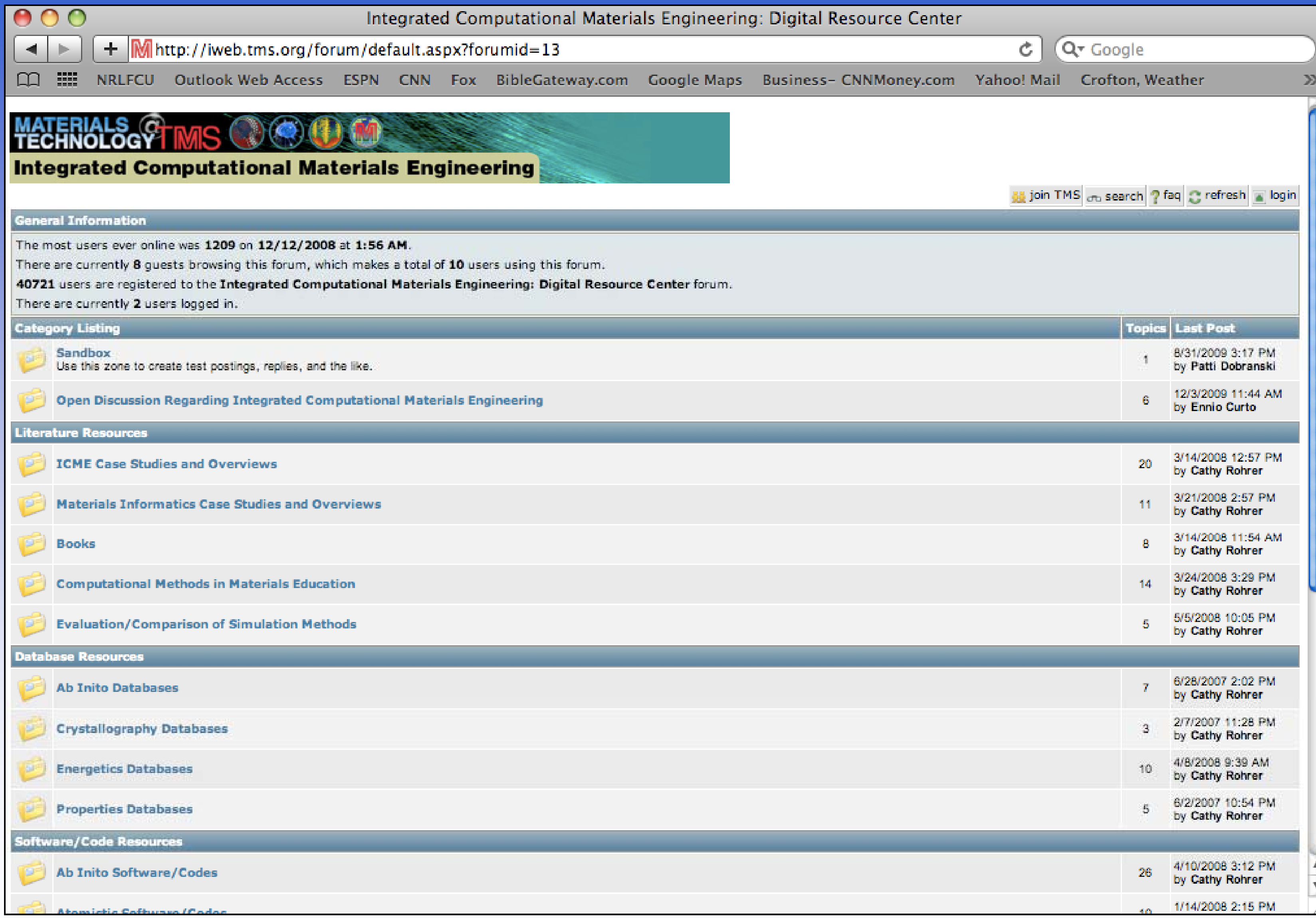
- ICME Digital Resource Center:

http://iweb.tms.org/forum/default.aspx?forumid=13

- Materials Education Community:

http://materialstechnology.tms.org/EDU/home.aspx

ICME Digital Resource Center


Integrated Computational Materials Engineering: Digital Resource Center

http://iweb.tms.org/forum/default.aspx?forumid=13

NRLFCU Outlook Web Access ESPN CNN Fox BibleGateway.com Google Maps Business- CNNMoney.com Yahoo! Mail Crofton, Weather

MATERIALS TECHNOLOGY @ TMS

Integrated Computational Materials Engineering

join TMS search faq refresh login

General Information

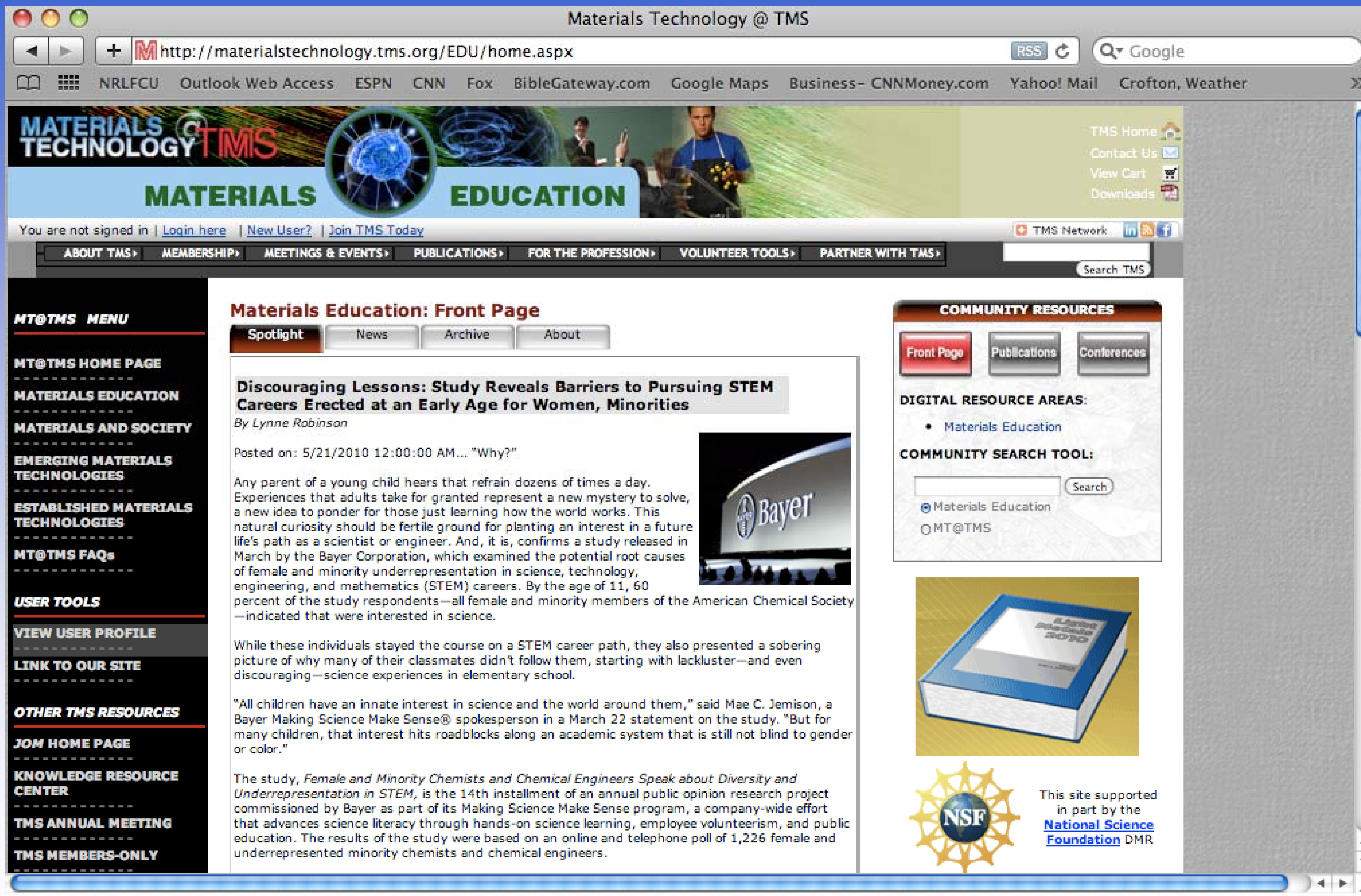
The most users ever online was **1209** on **12/12/2008** at **1:56 AM**.
There are currently **8** guests browsing this forum, which makes a total of **10** users using this forum.
40721 users are registered to the **Integrated Computational Materials Engineering: Digital Resource Center** forum.
There are currently **2** users logged in.

Category Listing	Topics	Last Post
Sandbox Use this zone to create test postings, replies, and the like.	1	8/31/2009 3:17 PM by Patti Dobranski
Open Discussion Regarding Integrated Computational Materials Engineering	6	12/3/2009 11:44 AM by Ennio Curto
Literature Resources		
ICME Case Studies and Overviews	20	3/14/2008 12:57 PM by Cathy Rohrer
Materials Informatics Case Studies and Overviews	11	3/21/2008 2:57 PM by Cathy Rohrer
Books	8	3/14/2008 11:54 AM by Cathy Rohrer
Computational Methods in Materials Education	14	3/24/2008 3:29 PM by Cathy Rohrer
Evaluation/Comparison of Simulation Methods	5	5/5/2008 10:05 PM by Cathy Rohrer
Database Resources		
Ab Inito Databases	7	6/28/2007 2:02 PM by Cathy Rohrer
Crystallography Databases	3	2/7/2007 11:28 PM by Cathy Rohrer
Energetics Databases	10	4/8/2008 9:39 AM by Cathy Rohrer
Properties Databases	5	6/2/2007 10:54 PM by Cathy Rohrer
Software/Code Resources		
Ab Inito Software/Codes	26	4/10/2008 3:12 PM by Cathy Rohrer
Atomistic Software/Codes	10	1/14/2008 2:15 PM

http://iweb.tms.org/forum/default.aspx?forumid=13

TMS

Materials Education Community at Materials Technology@TMS



http://materialstechnology.tms.org/EDU/home.aspx

TMS

Role of Materials Societies…..

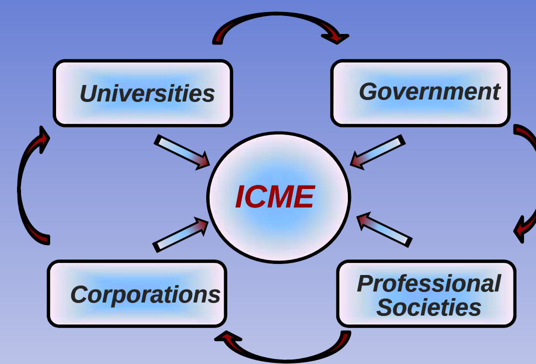
- Development of short courses, summer schools
  - Currently coordinating with K. Thornton, U. of Michigan (also chairs the TMS ICME committee)
  - Leverage TMS's access to the community, experience, and expertise
  - Please see me if you have ideas/plans, and want to coordinate with TMS

- UMC members, and appropriate faculty - consider active involvement in (and leveraging through) the committees, programs, and venues mentioned here
  - Can significantly affect Computational Materials Science and Engineering education through many of these activities
  - If not currently a member, you can enroll easily/quickly at:

    http://www.tms.org/Society/ProfMembership.aspx

TMS Contacts

- TMS Technical Director - George Spanos (gspanos@tms.org):
  - Coordinating all ICME activities
  - TMS board identified ICME as a major growth area for TMS, and the Materials Community
  - Bringing together TMS members from the four "foundational groups" for these many activities

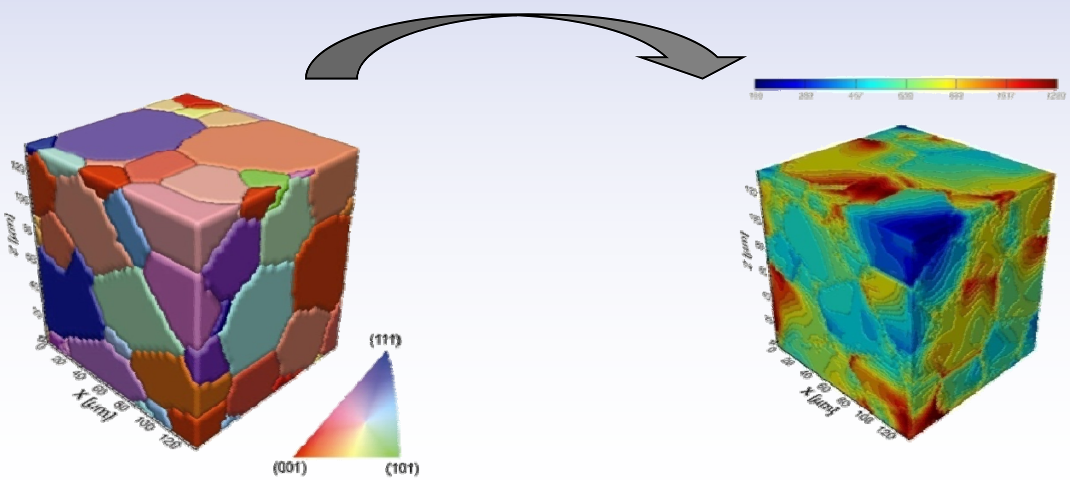


- Director of Professional Development & Publications - Bob Makowski (makowski@tms.org)
  - Spearheading efforts on professional growth
  - TMS contact on UECC (Undergraduate Education Coordinating Committee - ABET)

Take Away Point from NRL/TMS Experience

- Any ICME approach must involve a significant experimental component for validation, accuracy, and efficiency of computational models
  - Experiments and computational modeling must be intimately integrated
  - "Image-based" modeling methodology
  - Should be preformed in three dimensions, for accuracy and robustness

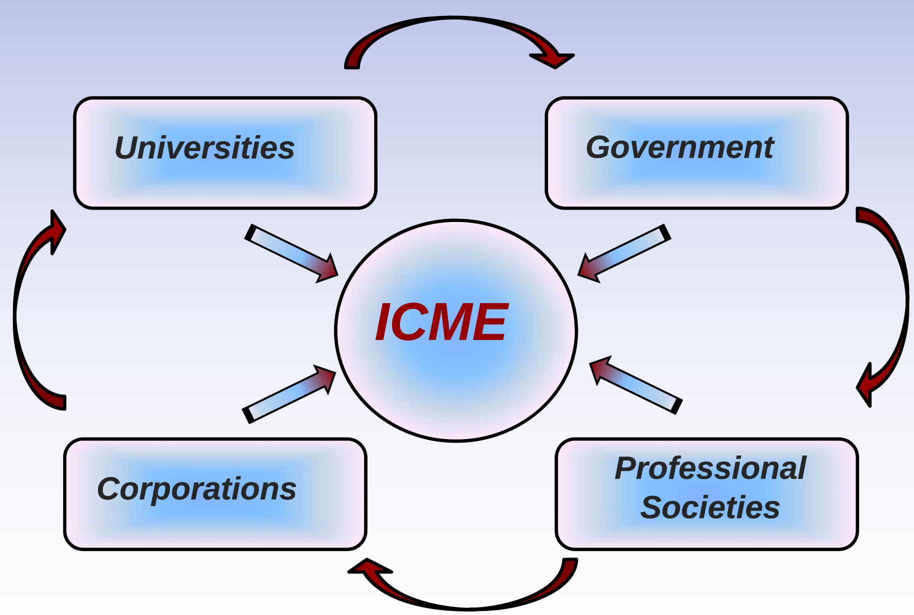
- This intimate synergy between 3D experiment and 3D computational modeling *must be considered, and should become a part of any curriculum in computational materials science and engineering, as well as in university-based research related to ICME*



TMS

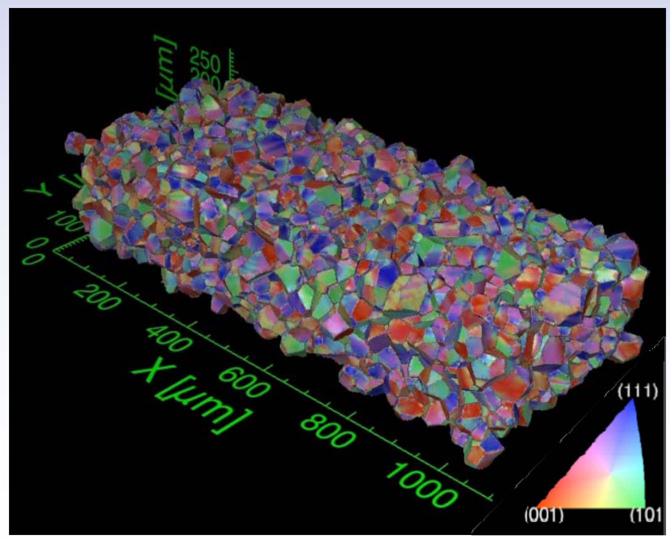
Take Away Point - #2

- Any ICME approach (tool development) must involve significant leveraging across many programs, organizations
- Simply too much work to be done for any one organization to handle
- Need to take advantage of each one's strength, experience
- This multidisciplinary, multi-organizational methodology *should be considered upstream, in any curriculum related to ICME, as well as in university-based research in ICME*



Suggestions For Future Directions of Research and Education in 3D Analyses and ICME Tools

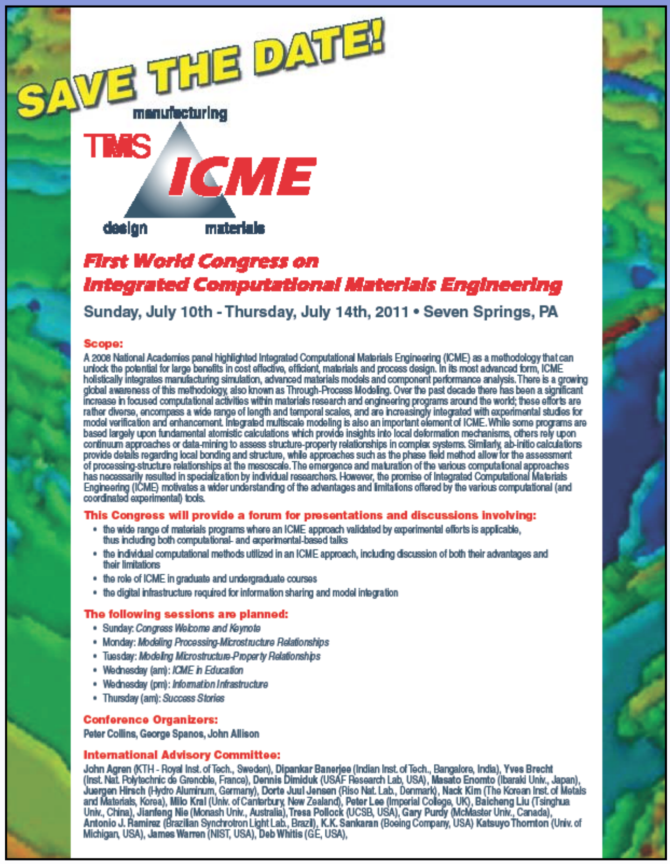
- *Quantitative, 3D* analyses (well beyond "visualization" stage)
  - Statistically relevant data sets: >1000 internal/unbiased grains
- Time evolution of microstructure
  - Image-based *simulations* (predictive)
  - In-situ and ex-situ 3D *experiments*
- Continue to develop 3D experimental, analysis, and modeling techniques in critical areas
  - serial sectioning, FIB, SEM/EBSD, X-ray, computational modeling
- ICME: Model Validation and Enhancement via 3D experiments is critical
- Must embed these tools into alloy/ process design cycle (ICME)
  - Leverage with other programs, multiple collaborators
- Archiving and mining 3D data:
  - Web-based Materials Atlas



1st International Congress on ICME (ICME 2011)

- July 10-14, 2011 (save the date) – Seven Springs, Pennsylvania
- Have commitments from a number of top level keynote speakers, and an International Advisory Committee representing > 15 countries
- Will involve leading modelers and experimentalists in the field
- GRC like setting and schedule:
  - Sunday (pm): Opening Keynote presentation
  - Monday: Processing-Structure Relationships
  - Tuesday: Structure-Property Relationships
  - **Wednesday (am): ICME in Education**
  - Wednesday (pm): Information Infrastructure
  - Thursday (am): Success Stories
- ICME in education obvious major component
  - Strong UMC presence expected
- Abstract call: July 2010 (deadline Nov. 1)

❖Hardcopies of Advance Flyer Available Here



SAVE THE DATE!

manufacturing
TMS
ICME
design materials

First World Congress on Integrated Computational Materials Engineering

Sunday, July 10th - Thursday, July 14th, 2011 • Seven Springs, PA

Scope:

A 2008 National Academies panel highlighted Integrated Computational Materials Engineering (ICME) as a methodology that can unlock the potential for large benefits in cost effective, efficient, materials and process design. In its most advanced form, ICME holistically integrates manufacturing simulation, advanced materials models and component performance analysis. There is a growing global awareness of this methodology, also known as Through-Process Modeling. Over the past decade there has been a significant increase in focused computational activities within materials research and engineering programs around the world; these efforts are rather diverse, encompass a wide range of length and temporal scales, and are increasingly integrated with experimental studies for model verification and enhancement. Integrated multiscale modeling is also an important element of ICME. While some programs are based largely upon fundamental atomistic calculations which provide insights into local deformation mechanisms, others rely upon continuum approaches or data-mining to assess structure-property relationships in complex systems. Similarly, ab-initio calculations provide details regarding local bonding and structure, while approaches such as the phase field method allow for the assessment of processing-structure relationships at the mesoscale. The emergence and maturation of the various computational approaches has necessarily resulted in specialization by individual researchers. However, the promise of Integrated Computational Materials Engineering (ICME) motivates a wider understanding of the advantages and limitations offered by the various computational (and coordinated experimental) tools.

This Congress will provide a forum for presentations and discussions involving:

- the wide range of materials programs where an ICME approach validated by experimental efforts is applicable, thus including both computational- and experimental-based talks
- the individual computational methods utilized in an ICME approach, including discussion of both their advantages and their limitations
- the role of ICME in graduate and undergraduate courses
- the digital infrastructure required for information sharing and model integration

The following sessions are planned:

- Sunday: *Congress Welcome and Keynote*
- Monday: *Modeling Processing-Microstructure Relationships*
- Tuesday: *Modeling Microstructure-Property Relationships*
- Wednesday (am): *ICME in Education*
- Wednesday (pm): *Information Infrastructure*
- Thursday (am): *Success Stories*

Conference Organizers:

Peter Collins, George Spanos, John Allison

International Advisory Committee:

John Agren (KTH - Royal Inst. of Tech., Sweden), **Dipankar Banerjee** (Indian Inst. of Tech., Bangalore, India), **Yves Brecht** (Inst. Nat. Polytechnic de Grenoble, France), **Dennis Dimiduk** (USAF Research Lab, USA), **Masato Enomto** (Ibaraki Univ., Japan), **Juergen Hirsch** (Hydro Aluminum, Germany), **Dorte Juul Jensen** (Riso Nat. Lab., Denmark), **Nack Kim** (The Korean Inst. of Metals and Materials, Korea), **Milo Kral** (Univ. of Canterbury, New Zealand), **Peter Lee** (Imperial College, UK), **Baicheng Liu** (Tsinghua Univ., China), **Jianfeng Nie** (Monash Univ., Australia), **Tresa Pollock** (UCSB, USA), **Gary Purdy** (McMaster Univ., Canada), **Antonio J. Ramirez** (Brazilian Synchrotron Light Lab., Brazil), **K.K. Sankaran** (Boeing Company, USA) **Katsuyo Thornton** (Univ. of Michigan, USA), **James Warren** (NIST, USA), **Deb Whitis** (GE, USA),