Materials Genome Initiative

&

Integrated Computational Materials Science and Engineering

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Integrity ★ Service ★ Excellence

Approved for public release, distribution is unlimited (88ABW-2014-5912)
Challenge: US losing market lead in Advanced Technology Products

U.S. Trade Balance for Advanced Technology Products

- 11% of U.S. GDP
- 12 million U.S. jobs
- 57% of U.S. Exports

Source: Census Bureau
A Widening Valley of Death?
For Materials Transition

Typical Development Times for New Materials (& Processes) for Jet Engines

I. Modification of an existing material for a non-critical component
   – Approximately 2-3 years

II. Modification of an existing material for a critical structural component
    – Up to 4 years

III. New material within a system that we already have experience
    – Up to 10 years

IV. New material class
    – Up to 20 years, and beyond

However, the jet engine design cycle has decreased by 50% over the past ~10 years

Courtesy C. Haubert & J.C. Williams, GE Aviation, circa 2009
Engineered Materials as a Commodity

Materials Engineers engaged in R&D in US Primary Metal Industry

Source: Globalization of Materials R&D: Time for a National Strategy, NRC, 2004
Increased System Expectations

Average USAF Aircraft Age in 2013

Source: Air Force Magazine, May 2013

Reduce maintenance costs now; prognostics for future systems
Growth in Materials Information

162,000 materials science & engineering journal articles published in 2012

Source: Thomson Reuters Web of Knowledge℠
Imperatives & Opportunities

Strengthen US Industrial base by:

• Improve cost, schedule & materials solutions for system design
• Enhance capability to develop, manufacture & design systems
• Increase fidelity of system life-cycle performance predictions
• Leverage global investment in creating materials knowledge
Changing the Materials Life Cycle

**PAST**
- Sequential
- Qualitative
- Empirical
  - Ad Hoc
- Fragmented Data (in a drawer)
- Disjoint Processes
- Material & Process Specifications

**FUTURE**
- Integrated Approach
- Digital Data & Processes
- Flexible Interfaces across Engineering
- Shared Knowledge
- Retained Knowledge
- Plug & Play Modularity for tools and data
“Integrated Computational Materials Engineering (ICME) is the integration of materials information, captured in computational tools, with engineering product performance analysis and manufacturing-process simulation.” ...NRC (2008)

• MGI and ICMSE are a paradigm shift in capability and culture:
  – Quantitative & Predictive Tools
  – Combined Computation and Experiment
  – Addresses complete materials life cycle
  – Integrated with system design framework

Goal: A model-based definition of materials & processes
1. Develop a Materials Innovation Infrastructure
2. Achieve National goals in energy, security, and human welfare with advanced materials

2. Equipping the next generation materials workforce
MGI Strategic Plan

1. Enable a Paradigm Shift in Culture

2. Integrate Experiments, Computation, and Theory

3. Facilitate Access to Materials Data

4. Equip the Next-Generation Materials Workforce

Elements of the Materials Innovation Infrastructure (MGI)

Materials discovery - first principles and atomistics

High throughput computation

Process models for manufacturing and scale-up

Verification and Validation - Experiment/Model coupling

Synthesis and processing, including high throughput

Sensors and in situ measurements; automation

Materials characterization and microstructure representation

Computational Tools

Experimental Tools

Digital Data

Multiscale Modeling
- process-structure
- structure-property

UQ and uncertainty management

Designer materials knowledge systems and representation

Databases, data sciences and material informatics

Systems design and MDO
- Design exploration
- Detail design

Distributed collaborative networks

Expanded by D.L. McDowell, Georgia Tech, from OSTP MGI White Paper
AFRL ICMSE Approach

- Foundational Engineering Problem 1
- Foundational Engineering Problem 2
- Invention/Development 1
- Invention/Development 2
- Experimental Techniques
- Efficient Modelling
- Data Standards & Structure
- Uncertainty Quantification, Verification & Validation
- Infrastructure
Basic science
Largely government funded

Commercialization
private sector owned/funded

Advanced Materials
& Manufacturing Federal Funding

Basic

$100M

$10M

$1M

$100K

Annual Budget

DOE Energy Innovation Hub

National Network for Manufacturing Innovation

MGI infrastructure to bridge basic research to commercialization

MGI Funding ~ $125 million per year
Established Office of Data and Informatics
Goal: To Enable & Enhance Data Exchange
- building databases and possible federated databases and repositories
- developing tools for capture, mining, analytics
- developing standards for ontologies and metadata

Partnering is key to make materials data accessible on the scale that it happens in biology
NIST CENTER OF EXCELLENCE IN MGI

CHIMaD
THE CENTER FOR HIERARCHICAL MATERIALS DESIGN

Peter Voorhees, Greg Olson, Northwestern University
Juan de Pablo, University of Chicago

$5M/y for 5y

• To foster hierarchical materials discovery, in accordance with the goals of MGI and NIST
• To serve, with NIST, as a national resource for verified codes and curated databases to enable proliferation of a materials-by-design strategy
• To foster the next generation of computational tools, databases and experimental techniques
• To provide opportunities to transition new breakthroughs in advanced materials to industry

Seed Project: Low D nanoelectronics
Goal: to understand and realize p-type and n-type doping in the low-dimensional limit

CNT-MoS$_2$ p-n heterojunction
(Hersam, Lauhon, PNAS, 2013)
Enabling Multi-Scale Management

Multi-scale hierarchical management can occur with sufficient MSE guidance of links between scales and knowledge of digital representation.

In construct of Objects with Attributes, higher-scale objects can have Attributes of lower-scale information.

Computational management tools for structure hierarchy do not exist today.
Abstract Hierarchical Scheme

GEOMETRY, LABELING, STATISTICS

Object–Attribute construct generalizes storage of digital, spatial information
An App Suite for Materials

SIMPL
- Manages Current Object Versions
- Brokers Application Interaction
- Controls I/O
- Manages Digital History of Data

* Blue boxes represent a suite of applications for specific processes
* Red arrows represent the transfer of information to/from SIMPL to Application
* Central box represents SIMPL as a broker/manager between applications
* Images are example outputs from existing applications for specific processes

SIMPL is material independent; Apps may be material & data-type dependent
Foundational Engineering Problems

Objectives

• Develop & establish **pervasive ICMSE technologies, methodologies, & protocols** portable to other applications of interest

• Demonstrate a **digital framework** linking processing, property, structure relationships for material design to account for processibility, manufacturability, system performance and sustainability

• **Demonstrate reduced cost & development** time can be delivered using ICMSE on high return on investment components

• **Identify infrastructure/technology gaps** to be solved by the community

• **Strengthen ICMSE competency & infrastructure** within the supplier base
Residual Stress Engineering in Ni Structures

- Residual stress represents pervasive issue to metals industrial base
- Significant “tech pull” from OEM designers and materials suppliers
- Significant potential impact:
  - Increased design efficiency
  - Reduced scrap at production and depot
  - Life extension of legacy components

Integrated Computational Methods for Composite Materials (ICM2)

Objective: Develop a digital framework that links material processing, property, and structure relationships to account for engine and airframe processibility, manufacturability, system performance and sustainability
ICME Development of 3GAHSS

Apply ICME techniques to design steel chemistry, processing, and manufacturing for a body or chassis structure with 35% weight reduction at a cost of less than $3.18 per pound saved

- Connect experimental and modeling techniques across many length scales
- Identify steels exceeding 800MPa/1200MPa/30% and 1200MPa/1500MPa/25% (Tensile/Ultimate/Elongation)

DOE funding: $6M (1 award)

Predictive Engineering Tools for Injection Molded Long Carbon Fiber Composites

Validate existing models for carbon fiber length and orientation in complex, 3D injection molded parts
- Integrate current state-of-the-art predictive tools and validate performance against experimental results
DOE funding: $1M/$740k (2 awards)
PNNL and partners, ORNL and partners

Advanced Alloy Development for Automotive and Heavy Duty Engines

Apply ICME to develop new Al (LD) and Fe (HD) alloys to enable higher peak cylinder pressures and improve efficiency
DOE funding: $3.3M/$3.5M/$3.5M/$3.5M (4 awards)
Ford and partners, GM and partners, ORNL and partners, Caterpillar and partners
NNMI: starts with materials

- **Additive Manufacturing (DOD)**
  - $50M fed, $60M match
  - Lead: Nat’l Center for Defense Manufacturing and Machining
  - Hub Location: Youngstown, OH
  - Partners: >100

- **Power Electronics (DOE)**
  - $70M fed, $70M match
  - Lead: NC State University
  - Hub Location: Research Triangle, NC
  - Partners: 17 industry, 5 university, 3 other

- **Digital Manufacturing (DOD)**
  - $70M fed, $24M match
  - Lead: UI Labs
  - Hub Location: Chicago
  - Partners: 41 industry, 23 university/labs, 9 other

- **Lightweight/ Modern Metals (DOD)**
  - $70M fed, $70M match
  - Lead: EWI
  - Hub Location: Detroit
  - Partners: 34 industry, 9 university/labs, 17 other

- **Adv. Composites Manufacturing (DOE)**
  - $70M fed
  - Proposals under evaluation

- **Integrated Photonics Manufacturing (DOD)**
  - $100M fed
  - Proposals due December 19th

- **Solicitation TBA (DOD)**

- **Solicitation TBA (DOE)**
Data-Driven Materials Development
New Cast & Wrought Disk Alloy, R65

ICMSE Case Study
Rolls Royce Plc

“Scrap avoidance/reduction for unit cost/quality”

“Distortion modeling/near net shape for unit cost/quality”

“ICME & PHM for improved life calculation accuracy”

“Integrated design-make for performance & manufacturability”

“Material modeling for reduced development time”

“Tuned residual stress & material properties for performance/life”

Process modeling for right first time manufacture

Bolcavage et al. Integrating Materials and Manufacturing Innovation 2014, 3:13
ICMSE Case Study

Rolls Royce Plc

Reduction in casting scrap
>> US$5M p.a.

Decreasing forging machining costs
50% cost reduction

Distortion prediction of forged parts
resulting in less scrap, fewer concessions
99.98% Right First Time

“ICME & PHM for Improved Life calculation accuracy”

Increasing tensile strength
~ 5% on forged/formed parts

Significant reduction (by 90%) of forming trials (powder HIP process)

Optimization of parts in furnaces to increase utilization; increasing stock-turn and lowering costs.

Bolcavage et al. Integrating Materials and Manufacturing Innovation 2014, 3:13
Verification and validation of ICME methods and models for aerospace applications

Bradford Cowles\(^1\), Dan Backman\(^2\) and Rollie Dutton\(^3\)

Abstract

Integrated Computational Materials Engineering (ICME) has revolutionized the design and materials processing, microstructure development, and manufacturing processes in aerospace. However, the scale of model applicability is limited by the output uncertainty, and identifying potential sources of model applicability is crucial. In this paper we provide a summary of the ICME Tool Maturity Model (TMM) previously developed for the verification and validation of ICME models.

ICME Model Verification and Validation Checklist

M1: ICME Model Development
- Developed mathematical model and initial computational model
- Conducted sensitivity studies to assess inputs, internal parameters & BC/ICs
- Performed UQ to determine output uncertainty based on inputs uncertainty
- Participate in system level uncertainty propagation analysis activities
- Established detailed experimental approach to support model development
- Established plan to measure internal parameters, inputs, and outputs
- Conducted experiments to measure internal parameters, inputs, and outputs
- Applied UQ to assess accuracy and variation for experimental results

M2: Experimental Support of Model Development and UQ
- Established experimental approach to support model development & UQ
- Determined experimental methods and sources of uncertainty
- Experiments conducted and UQ applied to determine uncertainty of results
- Assess data and uncertainty in support of system level validation

M3: Model Verification
- Established model verification plan
- Identified verification benchmark model and/or data
- Checked and executed computational model to identify/fix coding problems
- Compared model results against benchmark(s)
- Identified and repaired computation model deficiencies

M4: Model Validation
- Established overall validation plan
- Defined and executed experimental plan for validation
- Analyzed results using UQ methods
- Defined and executed modelling plan for validation
- Analyzed results using UQ methods
- Applied UQ methods to determine model accuracy & range of applicability
- Completed activities and support to system level validation
Digital Twin Aircraft

- Configuration Control
- Inspections
- Usage
- Models
- Computation / Data
- Materials State Awareness
- Fleet & Tail # Lifecycle Management
A-10 Current NLign Deployment

- A-10 NLign current structure for ASIP support
  - Full 3D model with part tree
    - Basic 3D model functions
  - Serialized component tracking
    - Component hour tracking for major assemblies
  - Analysis support data
    - Analysis mapped visually onto 3D model
      - Clean metadata with AC (X,Y,Z)
      - Supporting documents ‘one-click’ away
  - Maintenance inspection data
  - Test and Teardown data
    - Each crack mapped onto 3D model
      - Supporting crack data ‘one-click’ away
  - All data verified for quality
Link Back to NDI Data

Summary

• Tremendous community-wide challenges and opportunities that require augmented approaches to materials science & engineering to integrate with structural design

• Requires coupling between experiment, computation and data and a seamless link to structural design

• “New” technology gaps defined by integration, VVUQ, high throughput experimentation and computation, data management, reuse and integration, and infrastructure

• MGI & ICMSE will be a long-term commitment to change the way in which we approach materials science and engineering

• Materials, manufacturing, structural design & sustainment all migrating toward the same end point—digitally enabled, integrated engineering
Key Technical Challenges

• Improved physical understanding and models to relate processing, structure, property and performance of materials

• Integration across vast time and length scales, and with other engineering disciplines

• Application of verification, validation and uncertainty quantification methodologies

• Novel and high throughput experimental techniques

• Acceptance of digital materials data as a valuable research & engineering asset, and standard means of information flow

• A materials information infrastructure to support research and engineering including informatics techniques
Progress Toward the Vision

Success depends on your perspective

Increasing fidelity and integration, decreasing uncertainty
Software Overview

Collect-Organize-Archive-Analyze

Map ultrasound C-Scan to 3-D model with trending (colored dots) to find problem areas

Map digital radiography to 2-D model with trending and show trending results (colored dots) to identify problem areas

Analyze

- Reporting
- Visualization
- Trending
- Coverage checking
- Analysis integration

Integrated reporting Tools
- Scatter plots
- Histograms
- Bar charts
- Line charts
- Excel Export

Map eddy current C-scan to model to check for inspection coverage

Repair design tool shows multiple layers of data

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