Opportunities in Integrated Computational Materials Engineering (ICME) and the Materials Genome Initiative (MGI)

Dave McDowell, Executive Director
Institute for Materials
Georgia Institute of Technology

March 13, 2014
Materials Innovation Ecosystem @ GT

- Societal Impact – mobility, energy, health, infrastructure, communications, security
- Economic Impact – future workforce, 21st century economy

Over 200 materials-related faculty
Core Strength Snapshot: Materials@GT

- **Communications & Computing**
  - Novel graphene structures
  - Organic and inorganic photonics and electronics
  - Nanomaterials, nanostructured materials, and devices

- **Energy**
  - Electrodes for energy applications
  - Materials and interfaces for catalysis, separation, storage, and environmental applications
  - Elevated temperature, irradiated and corrosive environments
  - Materials for energy harvesting and self powered sensors

- **Mobility, Security, Infrastructure**
  - Lightweight materials
  - Materials for propulsion systems
  - Materials in extreme environments
  - Metamaterials
  - Forest biomass and lignocellulosic materials

- **Health**
  - Tissue repair and regeneration
  - Coatings to modulate bioresponses, and delivery of biotherapeutics
  - Bio-enabled materials synthesis and processing
  - Bio-inspired design

Materials modeling & simulation, design, data sciences, and informatics
Basis of Materials Genome Initiative

Both demand new science and technology development

http://www.whitehouse.gov/sites/default/files/microsites/ostp/materials_genome_initiative-final.pdf

White House OSTP

High Throughput

Materials Continuum Today
Material Structure as the Basis

**Structural Materials**

Properties (Materials Selection) - OLD

- Microstructure (Genome) - NEW

- Synthesis & processing

- Materials Development
- Materials Selection

- suppliers
- OEMs
- design engineers

- structure
- properties
- performance

- process
- goals/means (inductive)
- cause and effect (deductive)
- processing
Hierarchical Structure: Basis for Applications

IPST/IMat Workshop on Innovation in Lignocellulosic Materials

December 2013

M. Shofner, MSE

Forest-based nanomaterials

Different Structural Scales of Emphasis for Different Applications

Nanocellulose-Thermoset Composites

<table>
<thead>
<tr>
<th>Material</th>
<th>density (g/cm³)</th>
<th>Young's moduli (GPa)</th>
<th>Yield strength (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Carbon fiber</td>
<td>1.76</td>
<td>230</td>
<td>3.53</td>
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<tr>
<td>Glass fiber</td>
<td>2.58</td>
<td>73</td>
<td>3.45</td>
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<tr>
<td>Crystalline cellulose</td>
<td>1.6</td>
<td>110-220</td>
<td>7.5-7.7</td>
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CNCs
- lightweight
- renewability and sustainability
- high strength/high modulus

Forest Products Industry
19% mills closed since 2005
$9 Billion in lost wages

Forests Restoration
397 Million acres in need of mechanical thinning and profitable outlets

Natalie Girouard, ChBE
Dr. Carson Meredith, ChBE, IPST
Dr. Meisha Shofner, MSE, IPST
Dr. Greg Schueneman, FPL, Madison, WI

Moon et al., Chem Soc Rev, 2011

OPVs on Cellulose Nanocrystal (CNC) Substrates

Canek Fuentes-Hernandez, Kippelen research group

“Advanced” technology options
- Membranes
- Advanced Adsorbents
- Reactive Separations (e.g., Membrane Reactors)
- Others?

“Emerging” Materials for Separations and Catalysis
- Surface-Engineered Zeolites
- Mesoporous Silica
- Nanosized Layered Materials
- Metal-Organic Frameworks

Sankar Nair
Current Approach to Materials Development
(Poorly Connected Components with Limited Knowledge Transfer)

Contributions from Surya Kalidindi, IMat MGI Strategist

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<th>Synthesis and Processing</th>
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<td>Conventional Workflows (Slow, Empirical and Expensive)</td>
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Final Roller Pass
IMat Thrusts

Cross-cutting research program development and strategic industry engagement

Education and future workforce development, ICME/MGI relevant

Shared resources and materials data sciences infrastructure

Today we focus on this aspect in terms of vision and early progress in MatIN initiative
Materials Data is "Big Data"
- Volume
- Velocity
- Variety
- Veracity
- Value

How we handle significant numbers of very large datasets with different kinds of information and datastructures

Must be addressed first

How we interpret and use this information to accelerate materials development...
- Multiscale modeling
- Inverse design
- Verification and Validation
- Value of information for applications
- Assessment of horizontal product family transferability

VISION

Building & Infrastructure
Shipping containers
Biodevices
R&D Developments at Georgia Tech

Data Analytics Apps
Spatial correlation functions for microstructures; various tools

Reduced Order Modeling and Simulation, Inverse Design, V&V
Reduced order modeling and inverse design from research domain, e.g.,
• Materials Knowledge System
• Inductive Design Exploration Method – bottom up simulation, top-down design selection
• Combinatorial first principles search methods
• Multiscale uncertainty and V&V

S. Kalidindi, T. Fast, D. Turner, MINeD Group

• Veracity
• Value
Materials Data is “Big Data”
- Volume
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What MatIN does
- Shared data, codes and visualization
- Shared discussion
- Device agnostic, mobile (cell phones are fine)

What MatIN will do
- Query workflows
- Link with data analytics and M&S tools
- V&V and value assessment
MATIN-Facilitated Approach for Materials Development
(Intimately Connected Collaborative platform for Accelerated and Cost Effective Exploration of Materials and Process Design Spaces)

- Advanced Statistics
- Uncertainty Quantification
- Objective Decision Support Systems
- Data-driven
- Knowledge Mining using Machine Learning
- Computer Vision
- e-Collaborations
- Data Management
- Digital Capture, Curation, and Dissemination
- Automation

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**Value-Added Components to GT**

First “Data Registry”

First “Data Journal” (including DOI)

First Integrated Materials and Manufacturing Informatics Community (Leverages FLAMEL)

Meets Federal Data Management Plan Requirements

**Value-Added to Industry**

Internal Data Registry

Integrated Materials, Manufacturing, and Product Design Informatics

Archive and Identify Best Practices

Collaboration Productivity Management

Effective Cross-Disciplinary Teaming

Reduces Dependence on Domain Experts
Georgia Tech is Spearheading the Discussion of a National Materials Accelerator Network for MGI

National Academies’ Government-University-Industry Research Roundtable (policy and global affairs)

Creating a Materials Innovation Infrastructure: The Materials Genome Initiative and the Materials Innovation Accelerator Network
Wednesday, September 25, 2013
Dave McDowell – IMat
Cyrus Wadia, Assistant Director for Clean Energy and Materials R&D, White House OSTP
http://sites.nationalacademies.org/pga/guirr/index.htm

Spring 2014 GT MGI workshops:
• MGI regional – March 28 (GLC) – IMat host
• MGI materials accelerator network (Tentatively June 5-6) – IMat hosting with collaborators UW-Madison and Univ. Michigan

Register at www/materials.gatech.edu
MatIN Data Interactive Structure Demo

Tony Fast & Surya Kalidindi