Georgia Institute of Technology

Integration of Materials Knowledge into Design: Challenges and Opportunities

Surya R. Kalidindi

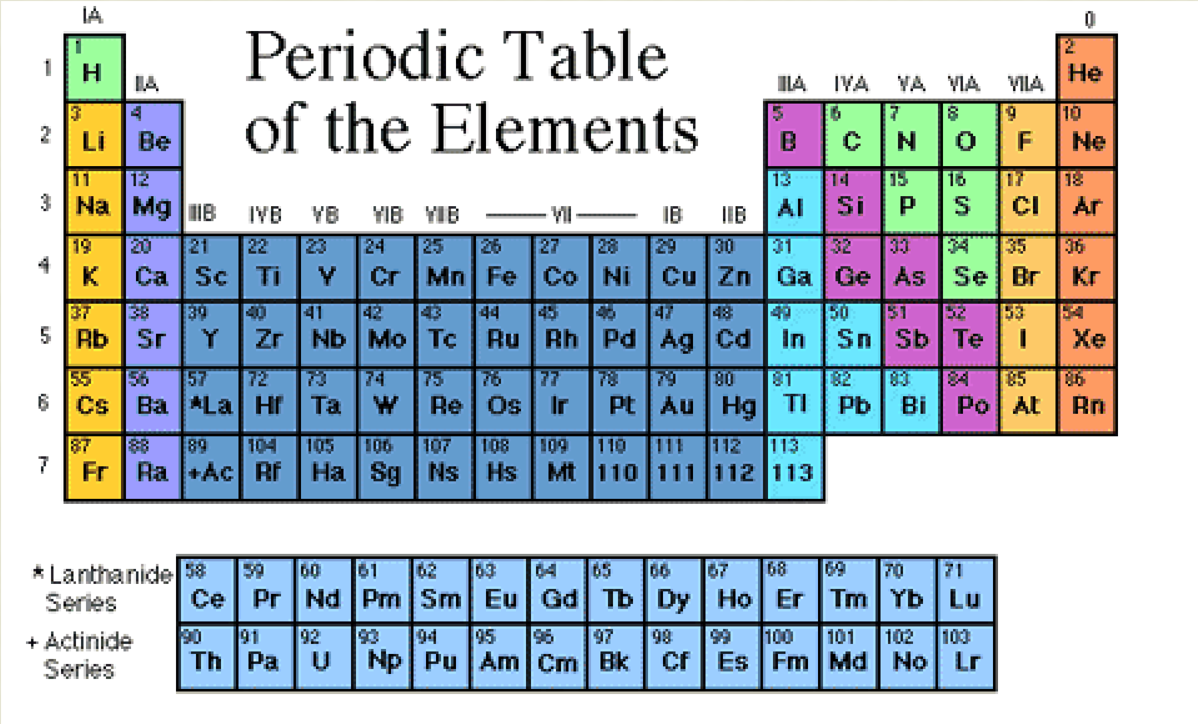
Funding: NSF, AFOSR-MURI, NIST

MINED

Material $\neq$ Just Chemistry

- Different forms of carbon exhibit vastly different mechanical properties (e.g., graphite is one of the softest materials while diamond is one of the hardest materials)
- Fiber composites exhibit properties that can be an order of magnitude different in directions parallel and perpendicular to the fibers
- For the same nominal chemistry, the mechanical properties of interest in advanced metals (e.g., steels, Al alloys) can be altered by 100-200% by controlling the amount and distribution of constituent phases in the material hierarchical internal structure

Atomic Structure

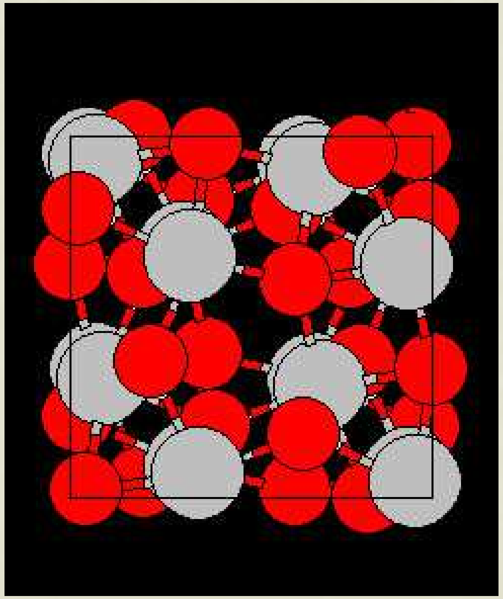


1 Å	1 nm	1 µm	1mm	1 cm	1 m

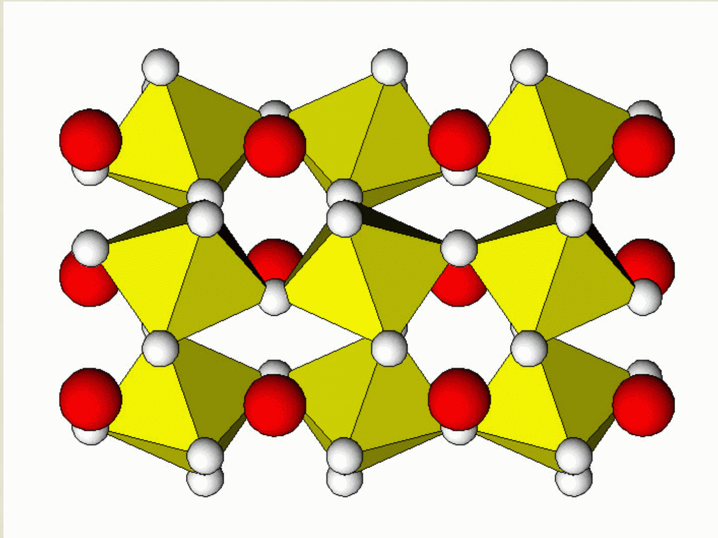
Molecular Structure

$2\,Al + 3\,O \rightarrow Al_2O_3$

Metal + gas → ceramic



Many combinations are possible with 2, 3 or more elements

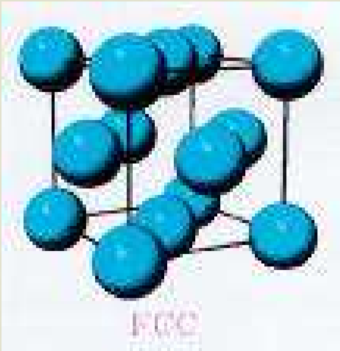


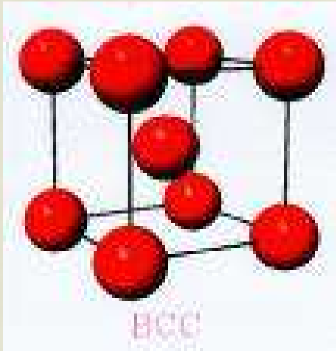
Perovskite: $LaScO_3$

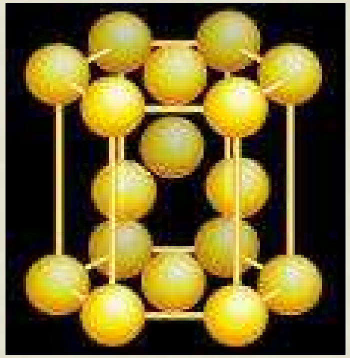
1 Å	1 nm	1 µm	1mm	1 cm	1 m

Molecular Structure

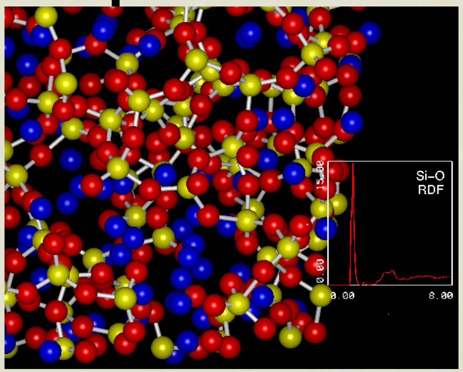
- Crystalline materials: Metals, ceramics

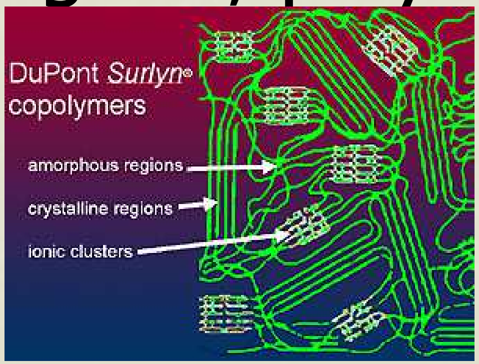






- Amorphous materials: glass, polymers

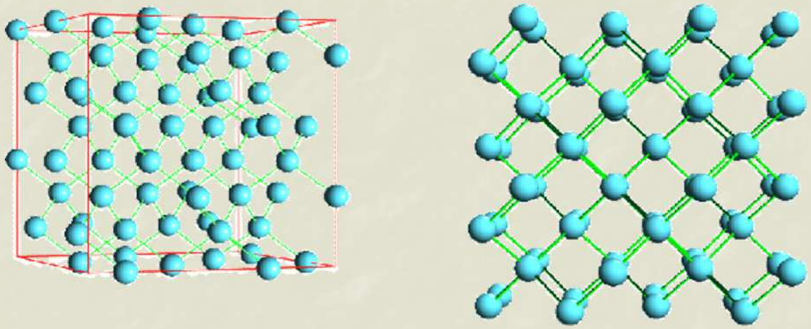




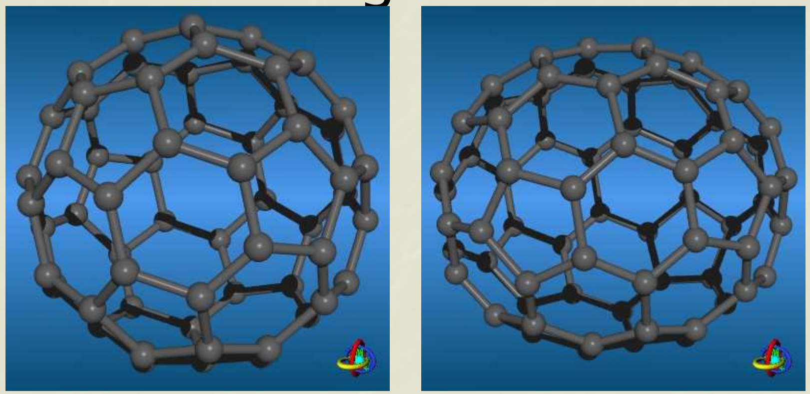
1 Å	1 nm	1 µm	1mm	1 cm	1 m

Molecular Structure

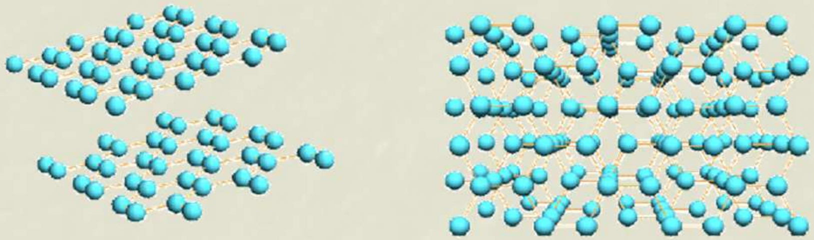
Carbon exists under several forms. The properties of carbon vary depending on its atomic arrangement.



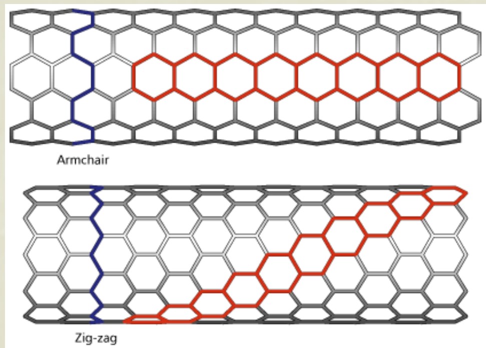
Diamond structure



Fullerenes C60 and C70



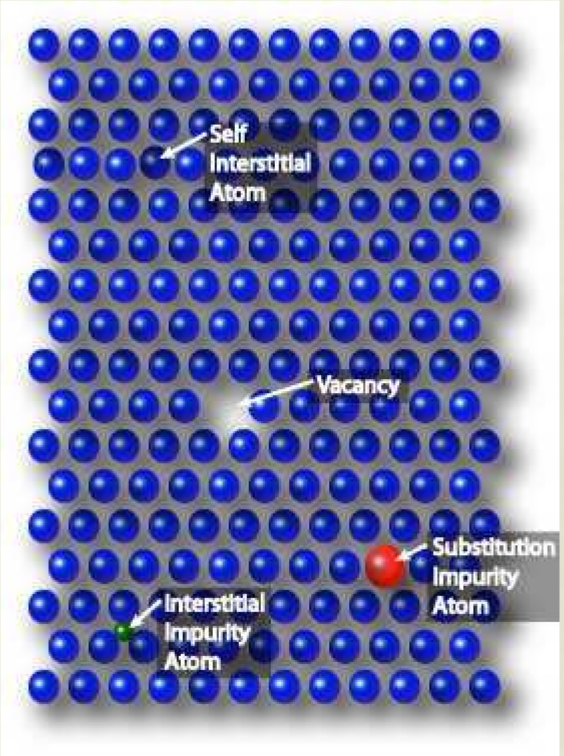
Graphite structure

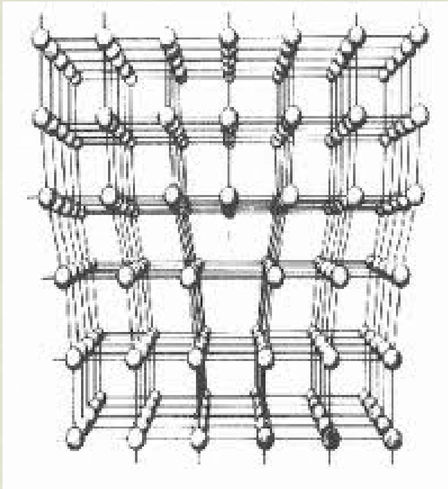


Carbon nanotubes

1 Å	1 nm	1 µm	1mm	1 cm	1 m

Defects in Crystal Structure





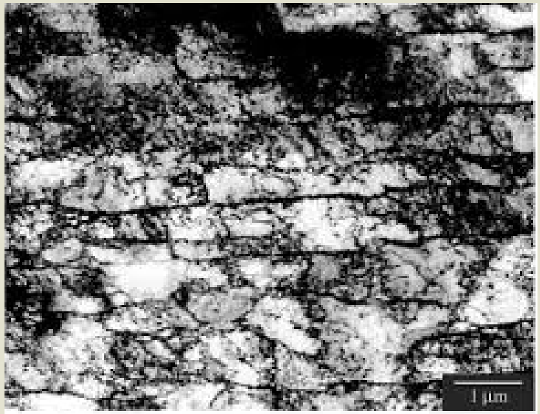
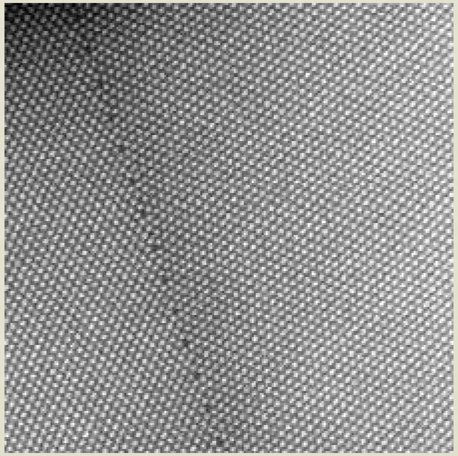


Figure 3. TEM of annealed steel submitted only to cyclic torsion (11.2% strain per cycle, 10 cycles).

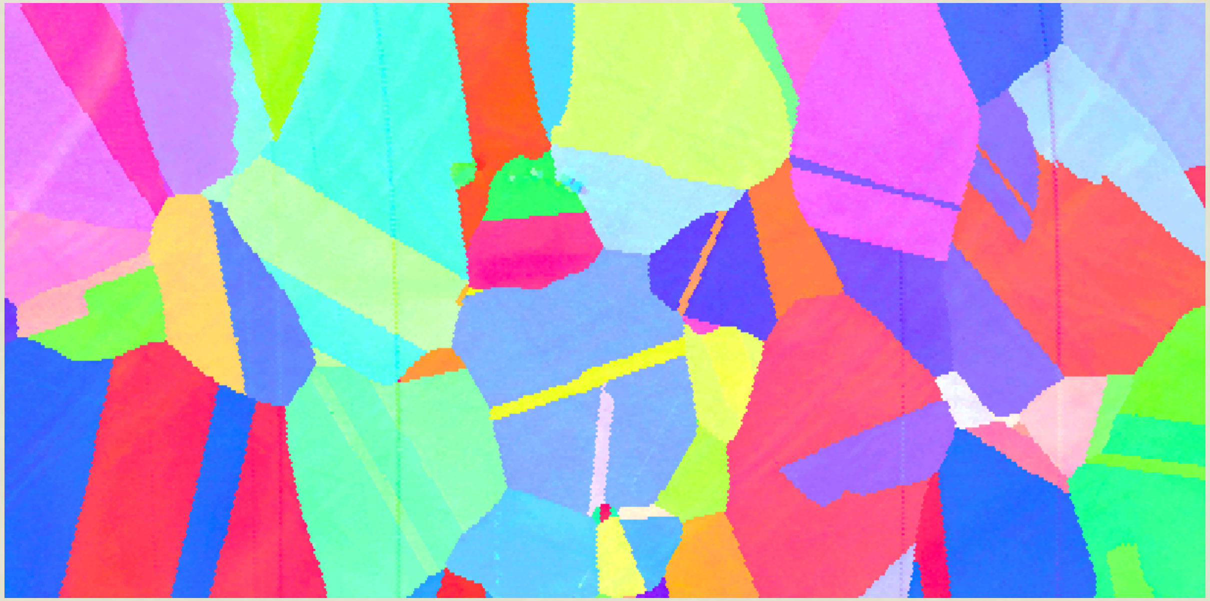


Theoretical strength of perfect crystals is about 3-4 orders of magnitude larger than those typically measured in experiments.

1 Å	1 nm	1 μm	1mm	1 cm	1 m

Microstructure

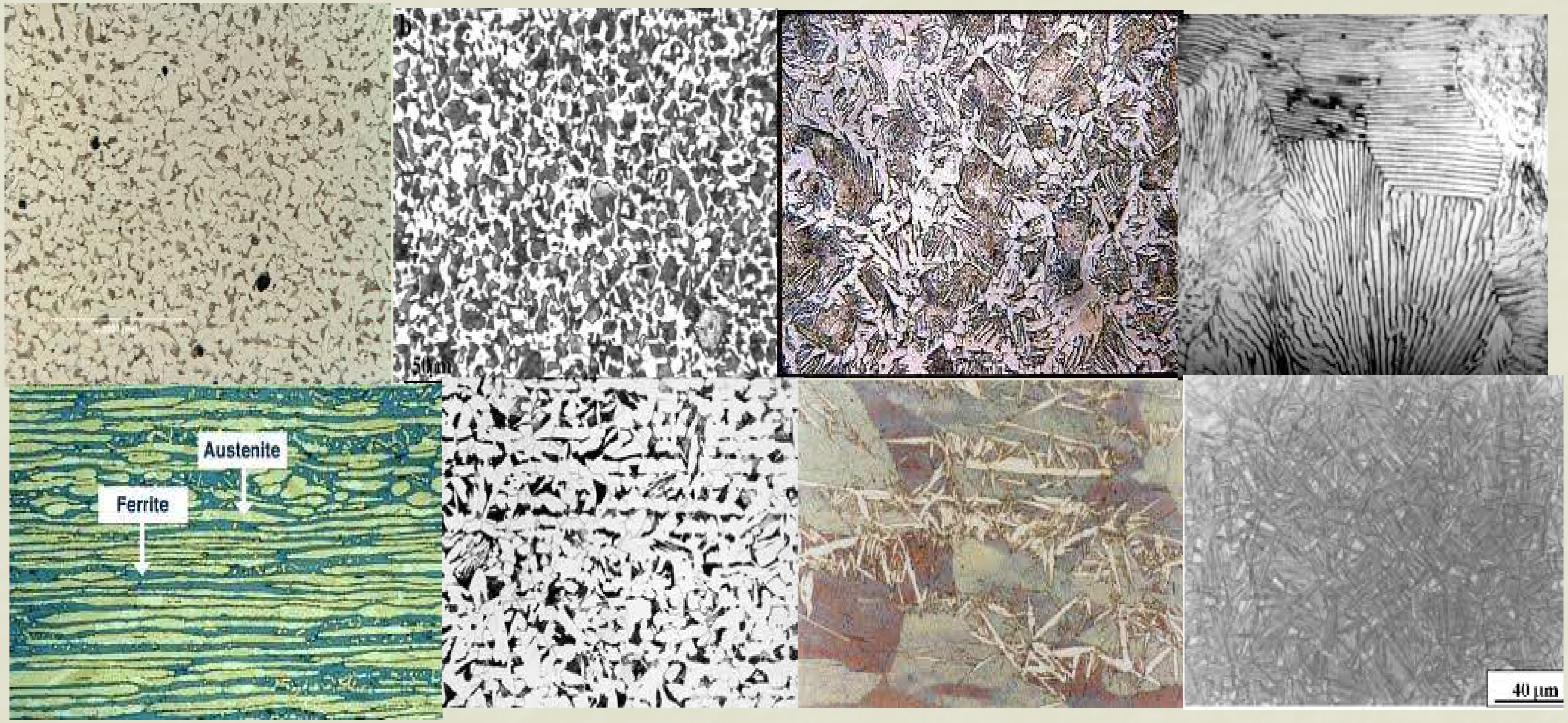
Crystalline materials are usually not made of a single crystal but of a arrangement of different crystals. Different phases can be present.



Orientation map of an Copper sample

1 Å	1 nm	1 µm	1mm	1 cm	1 m

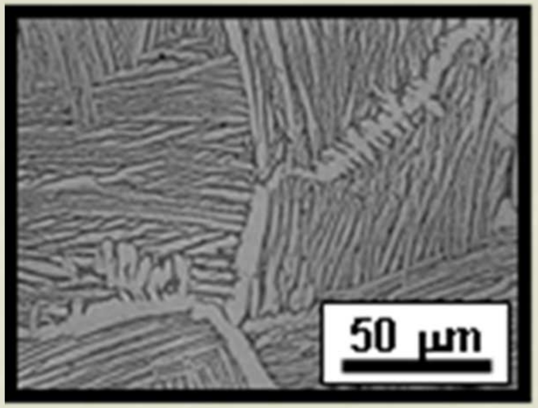
Microstructure



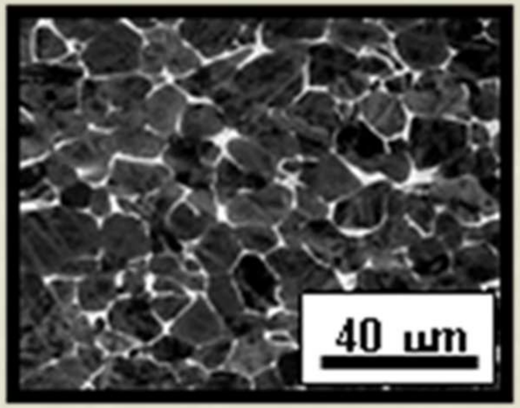
Examples of Microstructures in Steels

1 Å	1 nm	1 µm	1mm	1 cm	1 m

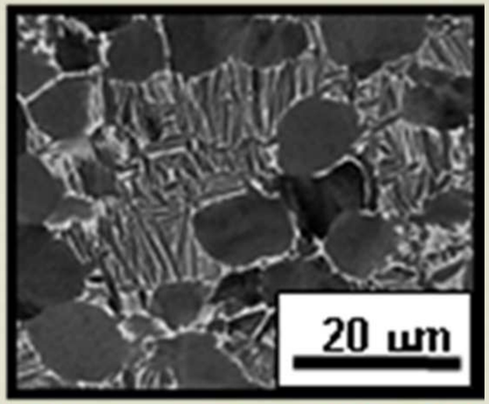
Microstructure



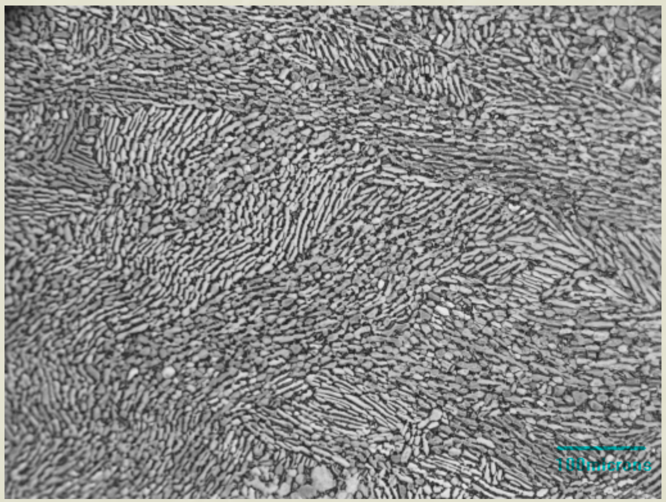
(a)

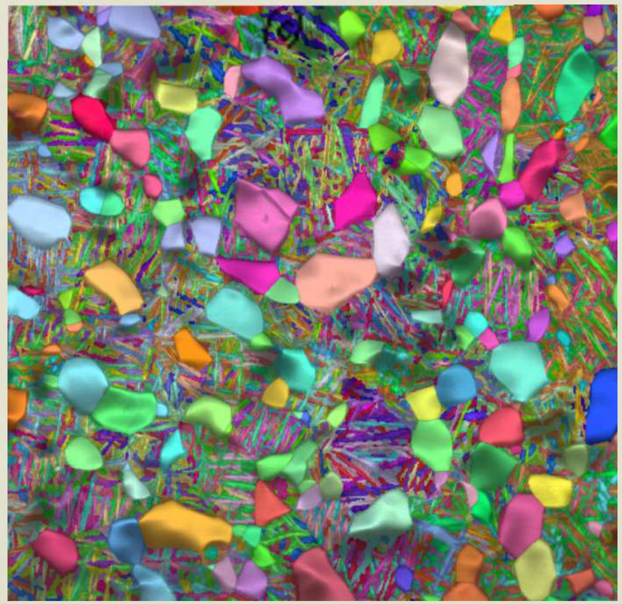


(b)



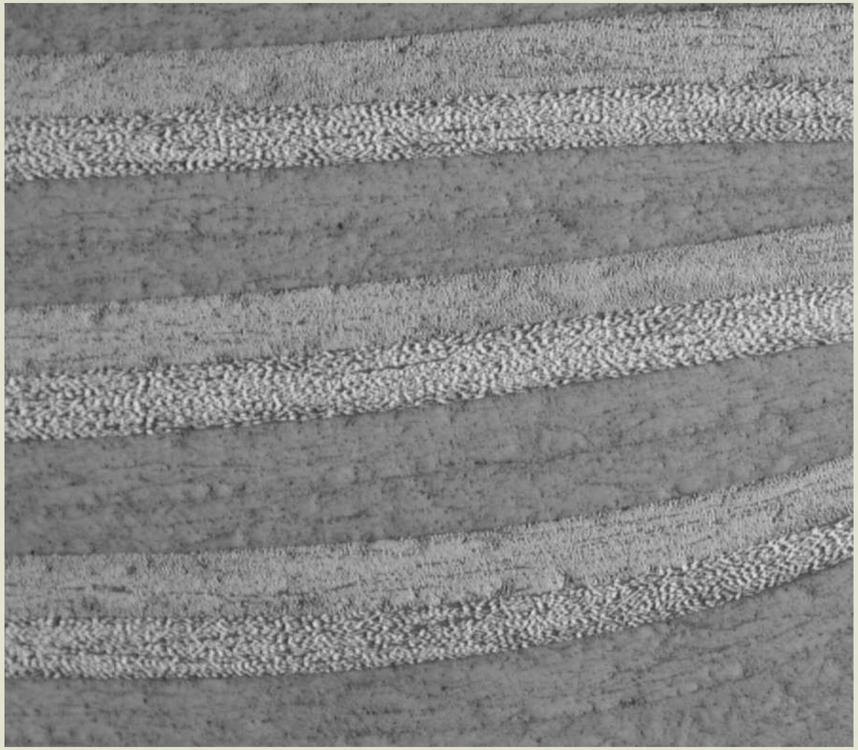
Ti Alloys

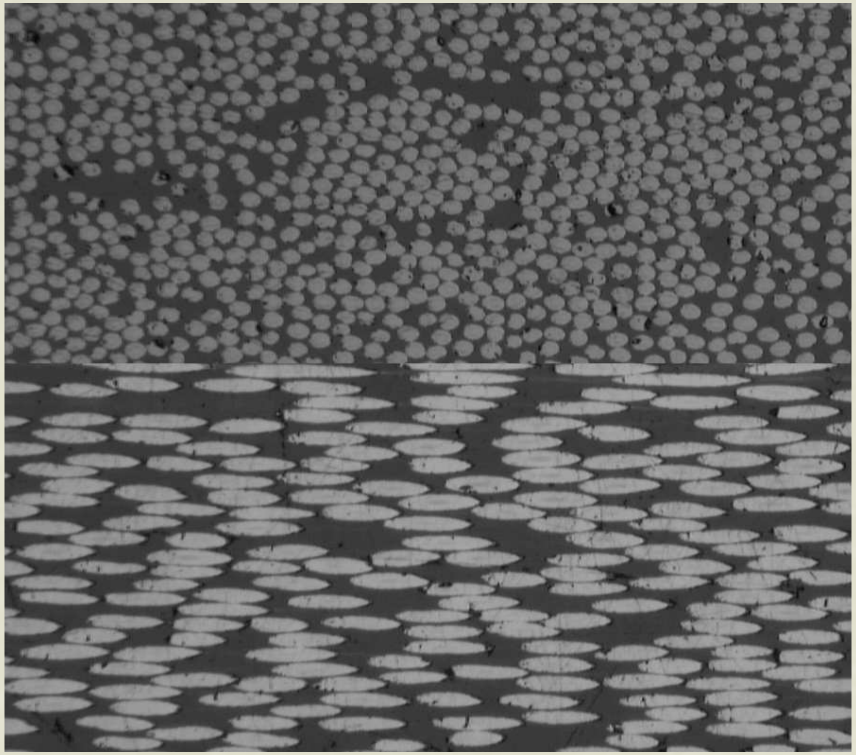




1 Å	1 nm	1 µm	1mm	1 cm	1 m

Microstructure



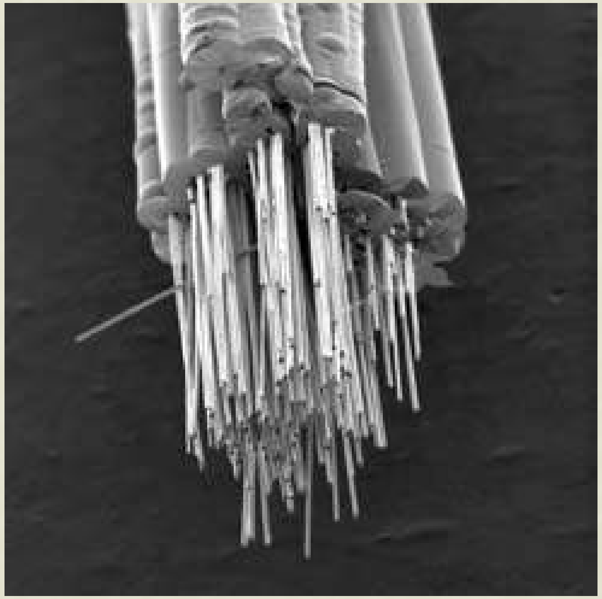


Typical laminate carbon epoxy lay-up showing layers of fibers with different orientations and close-ups of two layers (right). Filament diameter is approximately 7 microns.

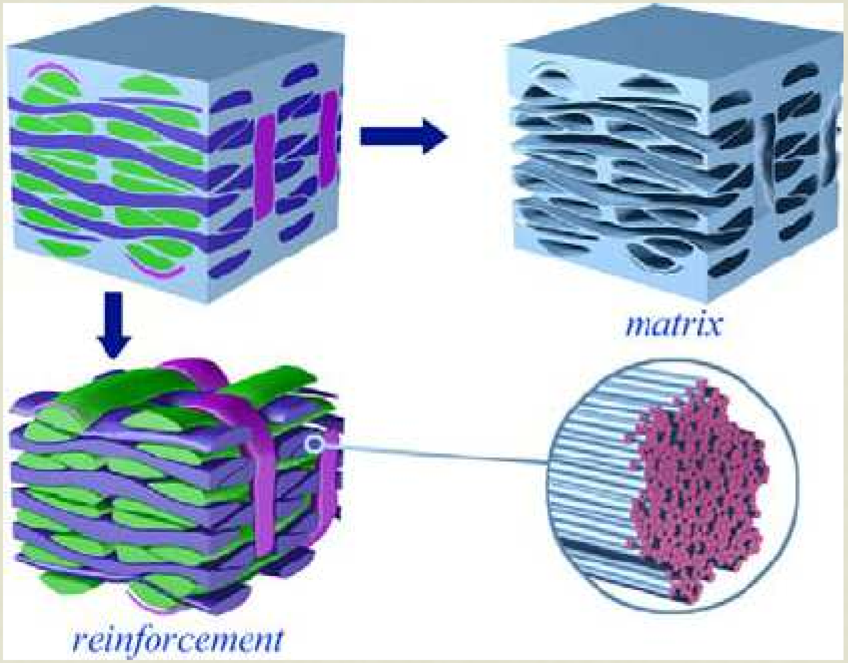
1 Å	1 nm	1 µm	1mm	1 cm	1 m

Microstructure

Composite materials are made of several materials, each one having its own properties.



Ceramic Fiber/Ceramic Matrix Composite

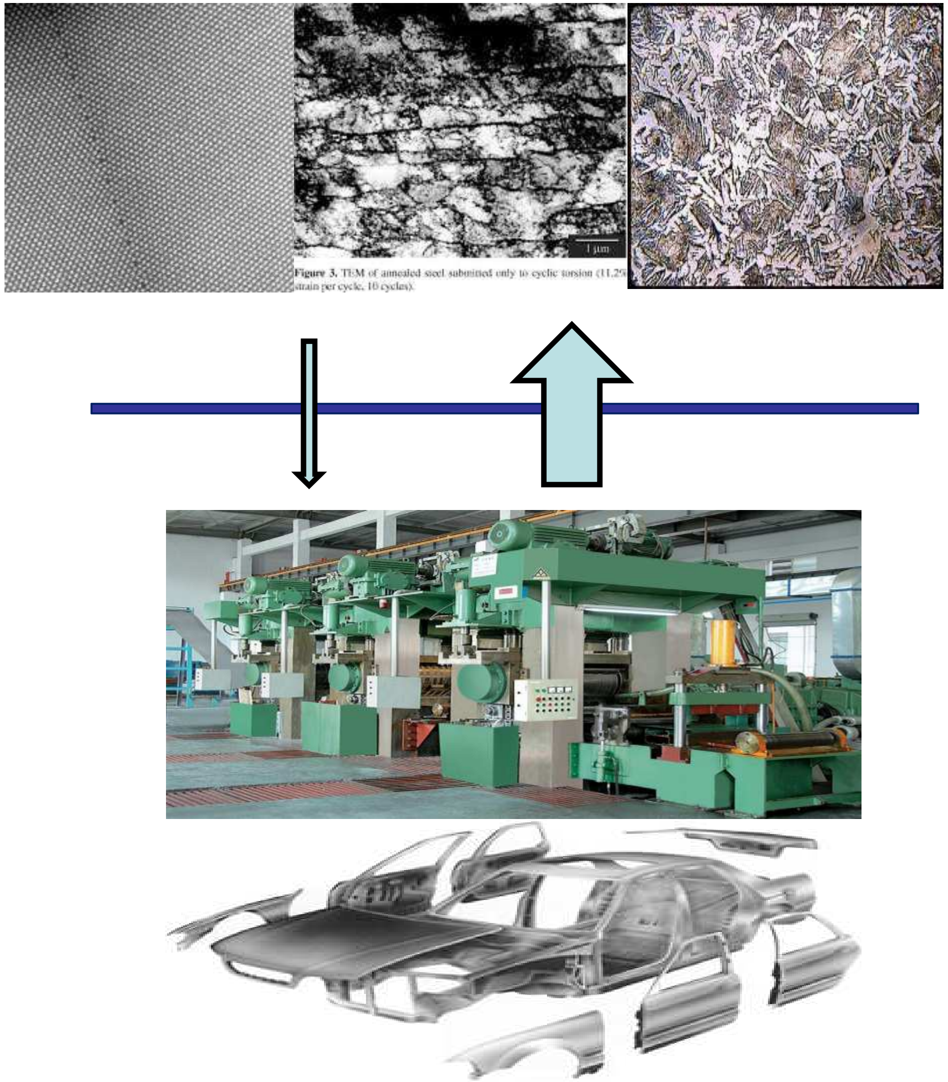


Woven Composite

1 Å	1 nm	1 µm	1mm	1 cm	1 m

Materials - Manufacturing & Design

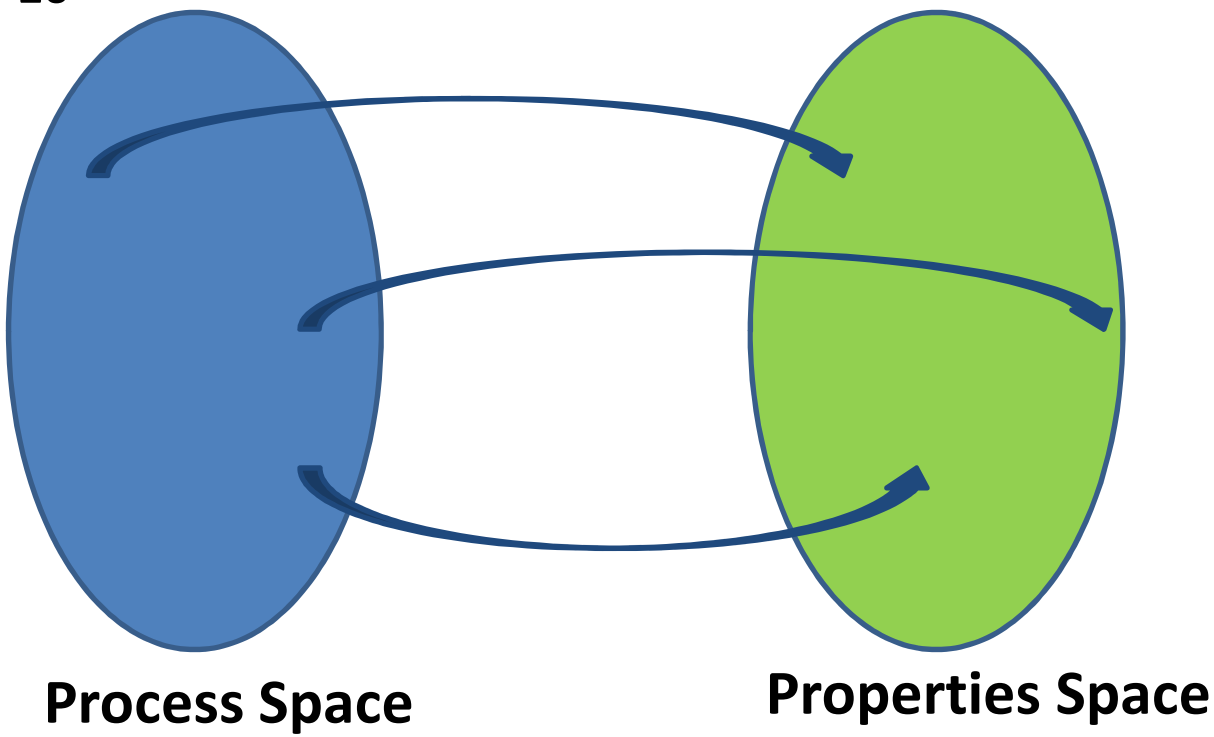
- Science vs. Engineering Focus
- Inconsistent innovation strategies
- Diverse physics at different length/ structure scales
- Vast differences in how knowledge is captured and structured for re-use



Manufacturing Process Development

HP1: P1+P2+P5+P2+P10

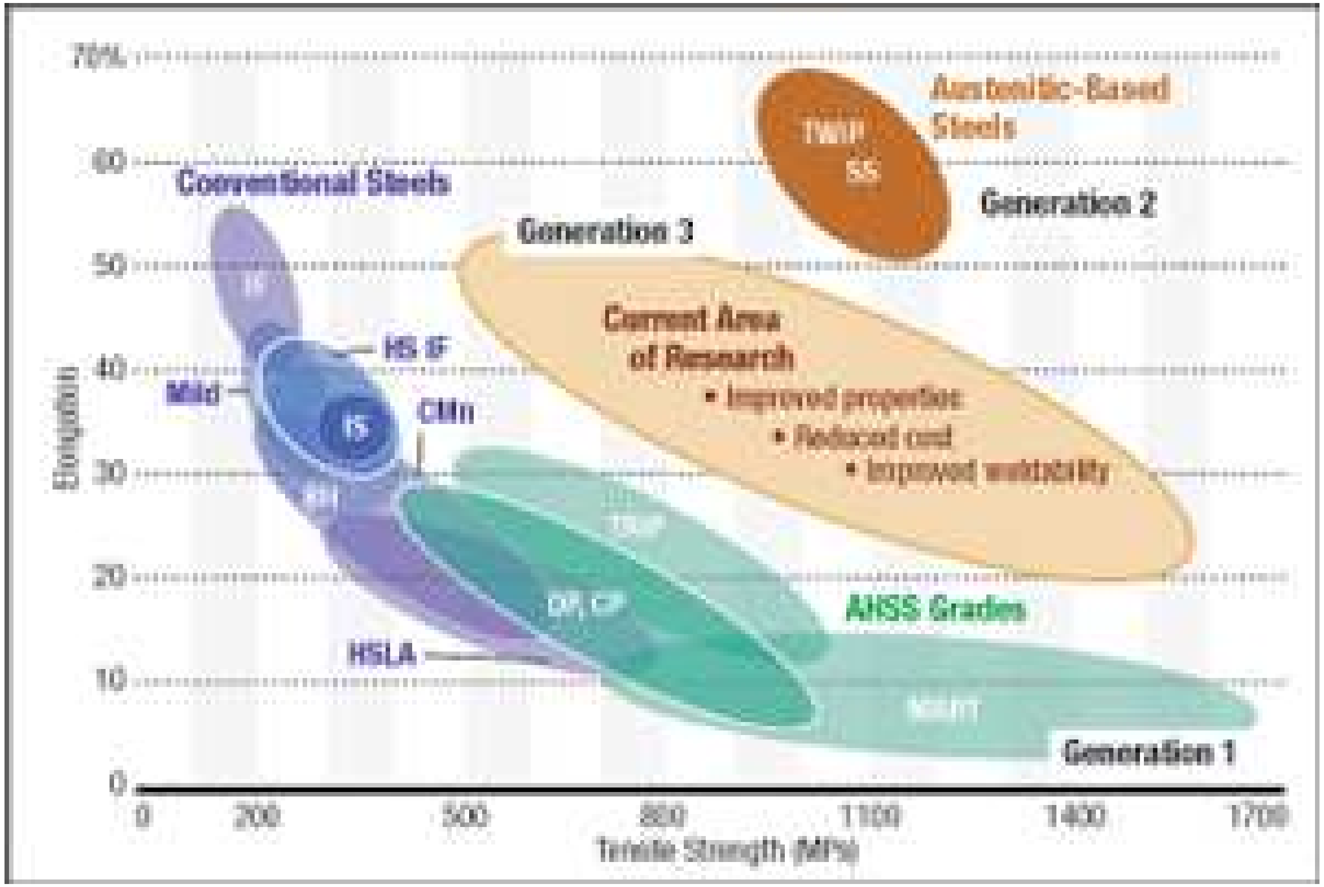
HP2: P1+P6+P2



An element of process space is a hybrid process, which is made up of a <u>sequence</u> of unit manufacturing processes

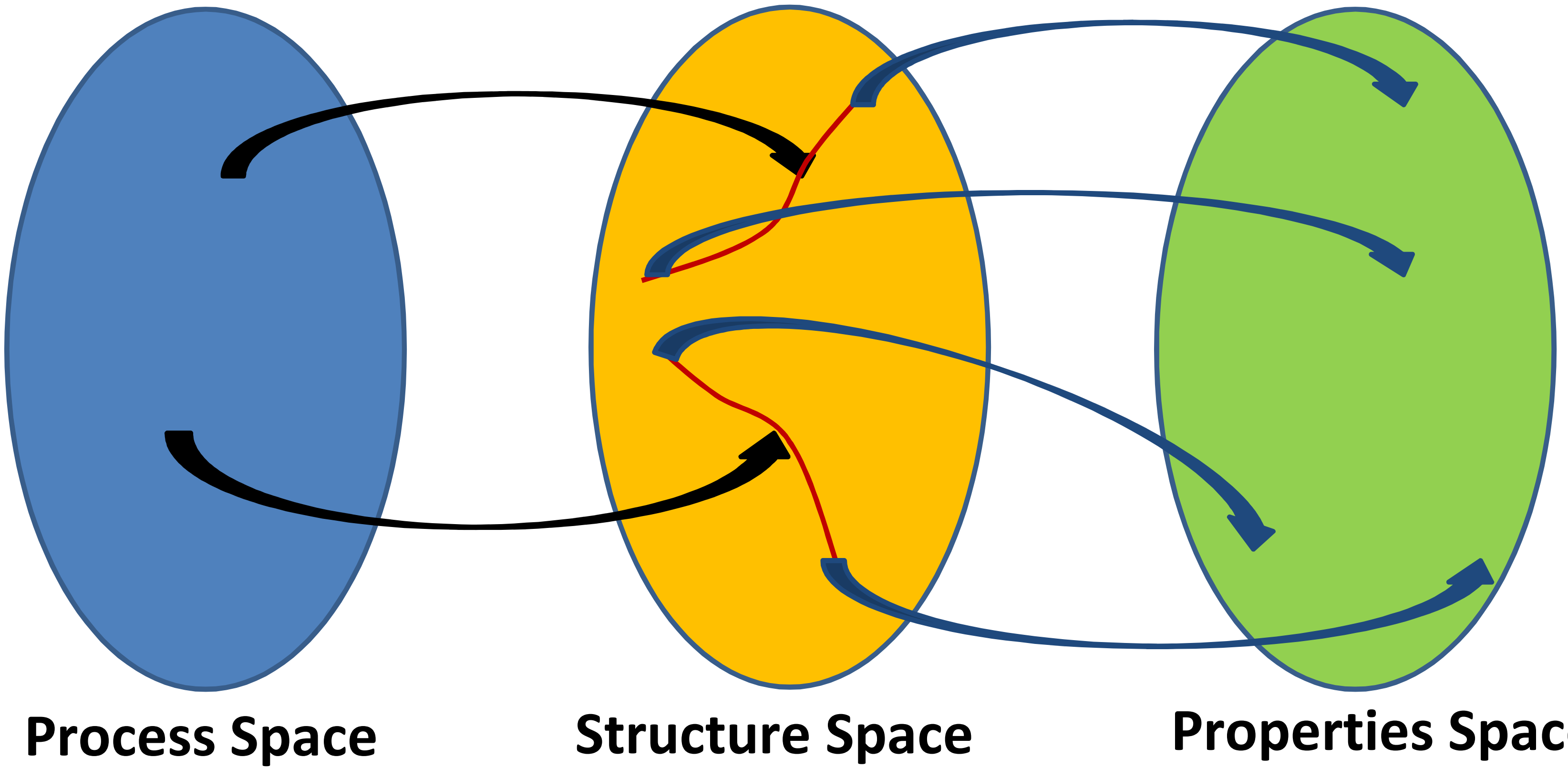
Interpolations in process space cannot often be interpreted

Example: Advanced High Strength Steels



- Explorations in the composition and process space are highly inefficient
- Properties are intrinsically related to hierarchical material internal structures

Core Materials Knowledge: Process-Structure-Property (PSP) Linkages



- Each material structure is associated with only one value of a property
- Each hybrid process can be depicted as a pathline in the structure space
- If formulated as reduced-order linkages, it will be possible to address inverse problems of materials and process design

Central Challenges in Formulating PSP Linkages

- Rigorous mathematical framework for quantification of material structure across all material types
  - ❖ Multiple length/structure scales
  - ❖ Raw data obtained as images from a variety of machines (microscopes, spectroscopes, etc.)
  - ❖ Each micrograph represents a sampling of the material structure: RVE, rare events, etc.
  - ❖ Rigorous protocols for high value, low-dimensional, representations are essential

Central Challenges in Formulating PSP Linkages

- Homogenization and Localization theories
  - ❖ Analytical or closed-form solutions exist only for a limited number of materials phenomena
  - ❖ Most physics-based multiscale materials models demand significant computational resources
  - ❖ Involve large numbers of unknown parameters and model forms $\Rightarrow$ Uncertainty Management
  - ❖ Standardized workflows do not exist for extracting reduced-order PSP linkages from available multiscale materials datasets

Central Challenges in Formulating PSP Linkages

- Organized aggregation, curation, and dissemination
  - ❖ Current efforts occur in siloes based on different materials types, different length scales (or physics), different protocols
  - ❖ Inadequate exchange of information between materials and design/manufacturing communities
  - ❖ Nucleate, sustain, and grow e-science communities that take advantage of recent advances in data sciences and informatics

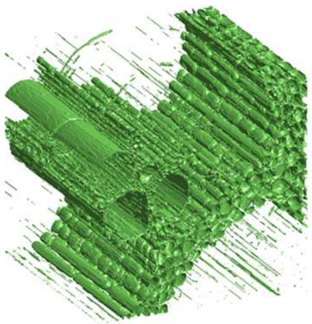
Novel Framework for Microstructure Quantification

Step 1: Convert microstructure image into a digital signal (digital data)

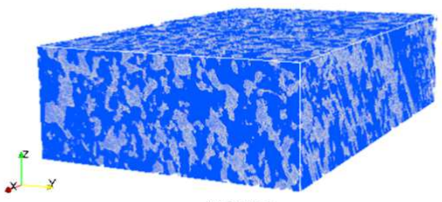
Step 2: Compute n-point spatial correlations (capture important features identified by known physics)

Step 3: Obtain low dimensional structure measures using principal component analyses (dimensionality reduction)

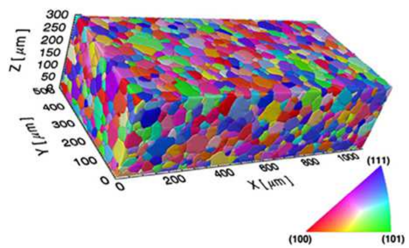
Step 4: Utilize structure measures in learning PSP linkages



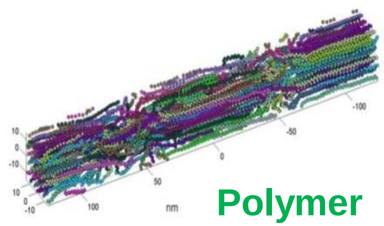
Bamboo
X-Ray
Tomography



Fuel Cell Micro Porous Layer
FIB SEM



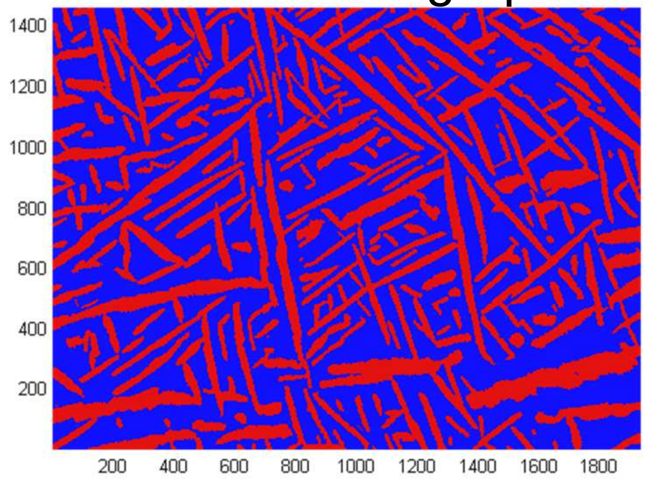
Beta Titanium
Mechanically Polished
SEM+EBSD



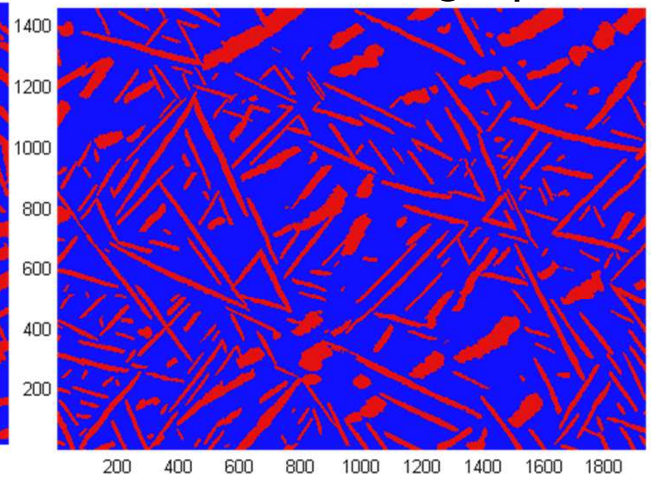
Polymer
Chains
Simulation
Data

Application: Microstructure Classification

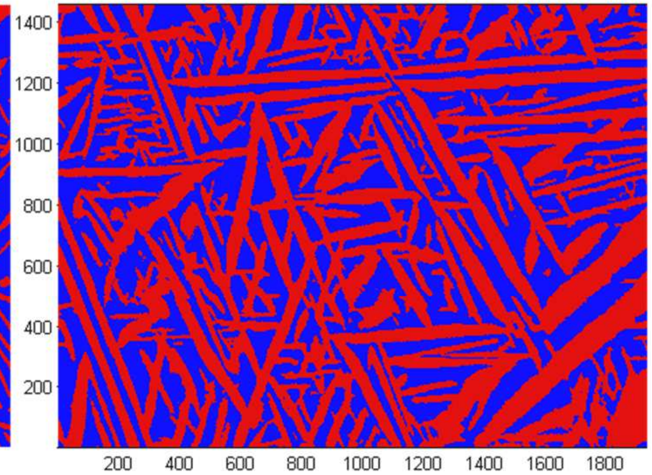
HT1-20 micrographs

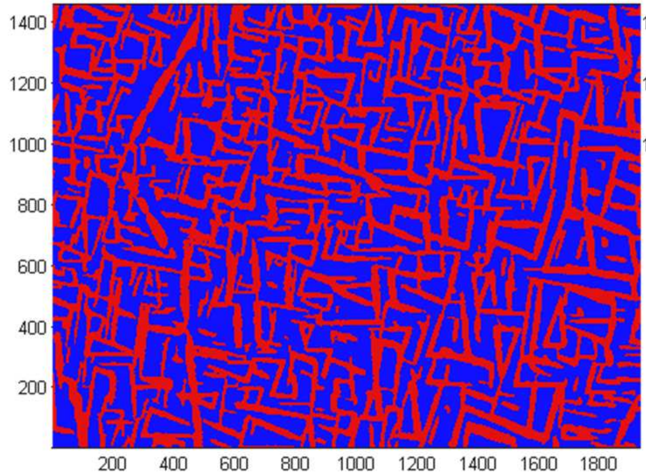


HT2-28 Micrographs

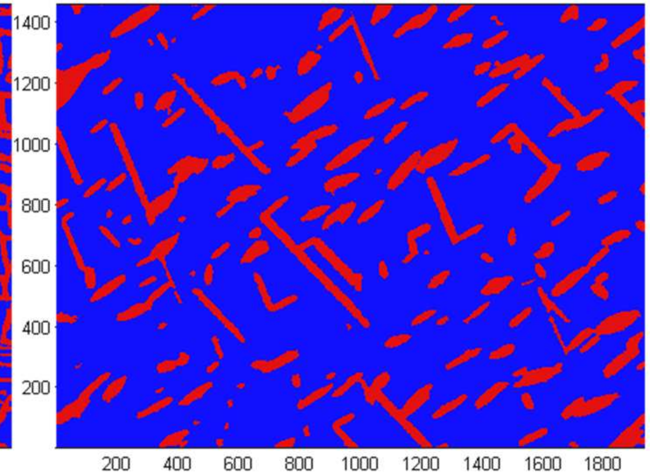


HT3-32 micrographs





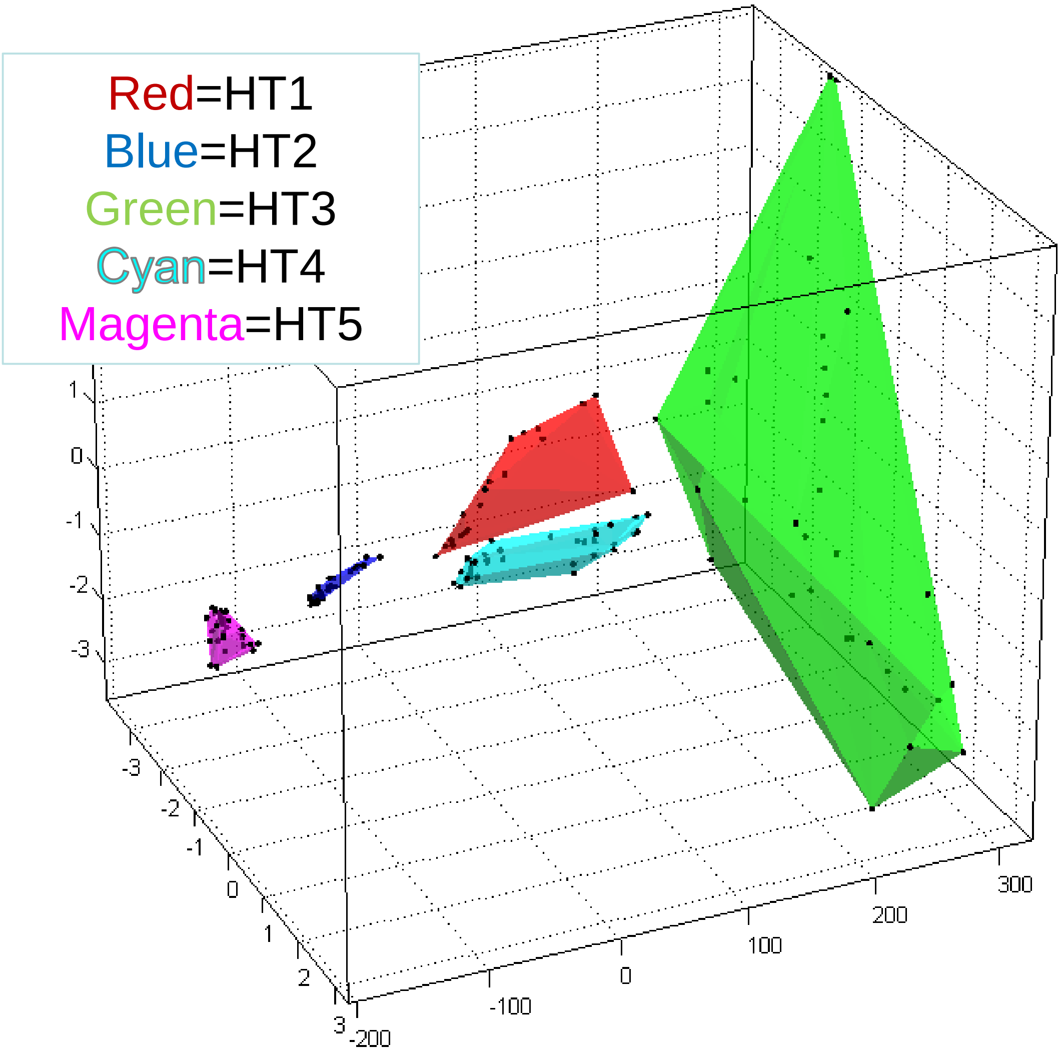
HT4-36 micrographs



HT5-32 micrographs

Data from
H. Fraser
(OSU)

Application: Microstructure Classification

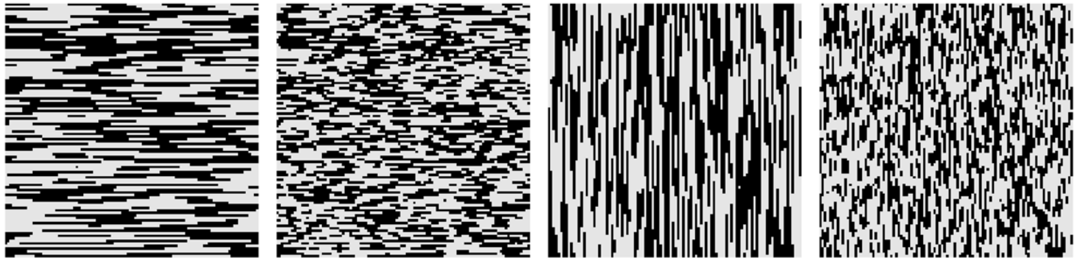


- Each point corresponds to a microstructure dataset.
- Datasets from the same heat treatment are shown as a hull.
- RVE corresponds to the centroid of the volume.
- Volume of the hull can be related directly to the variance in structure between datasets.
- Quality control applications.

Templated Structure-Property Linkages

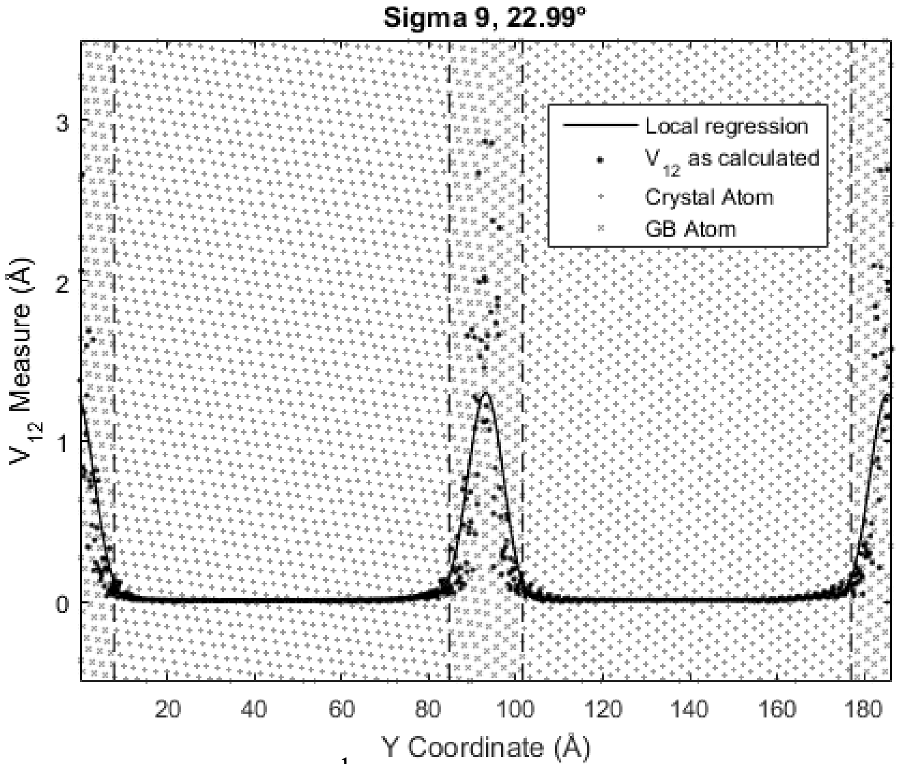
- 800 3-D microstructures
- Each microstructure quantified using PCs of 2-pt statistics
- Property evaluated using FE model
- Polynomial Fit for P-S linkage

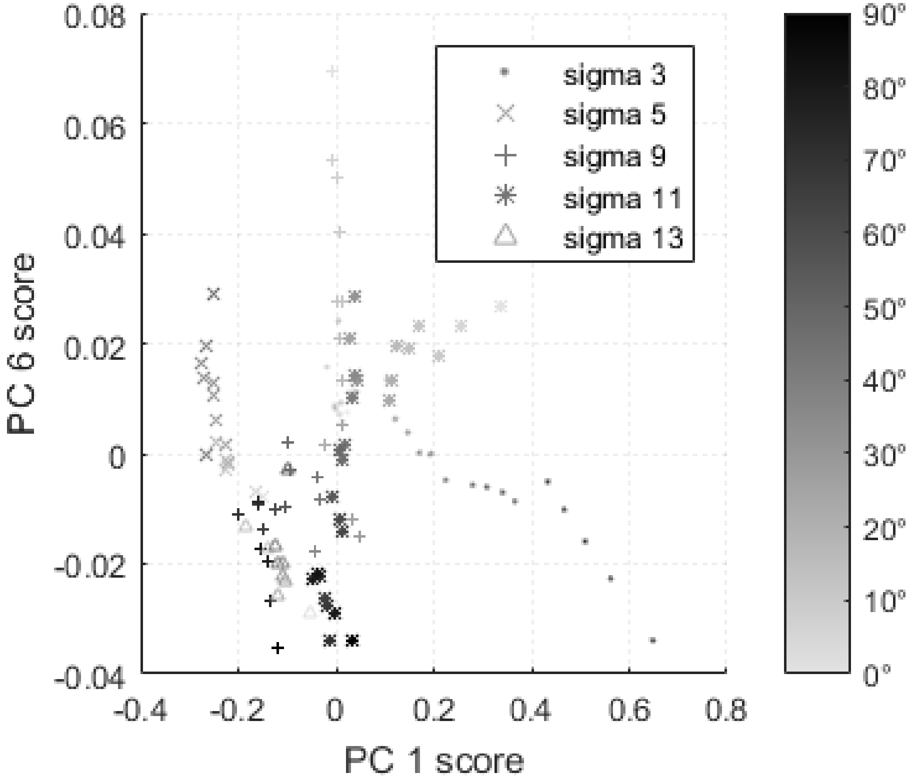
Mined New Knowledge is highly reliable, very accessible, and has high re-usability



Grain Boundary Regions

Tschopp et al., IMMI, 2015: 106 Datasets; Energy-minimized Al GBs; Σ 3,5,9,11,13; Inclination angle 0-90°

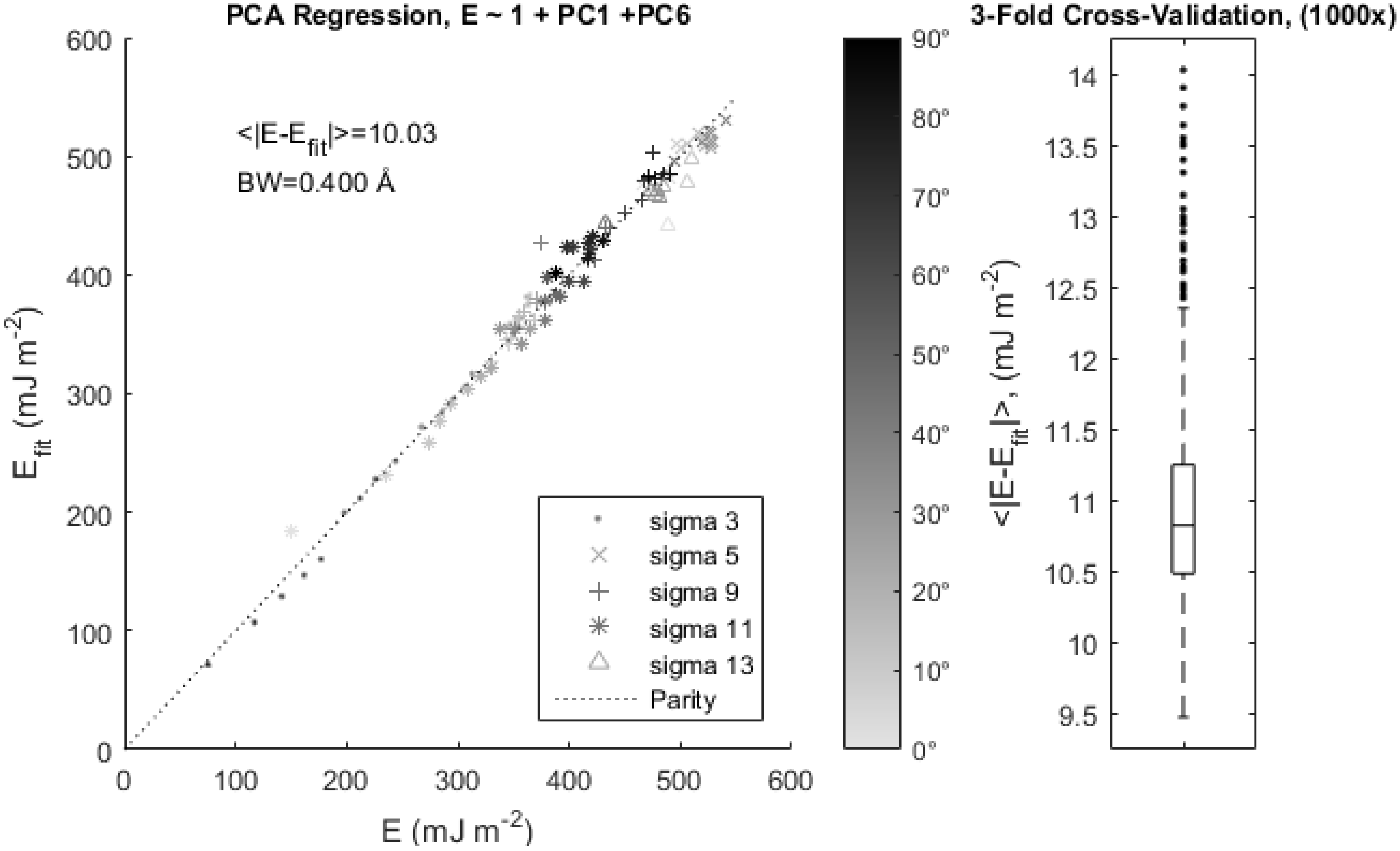




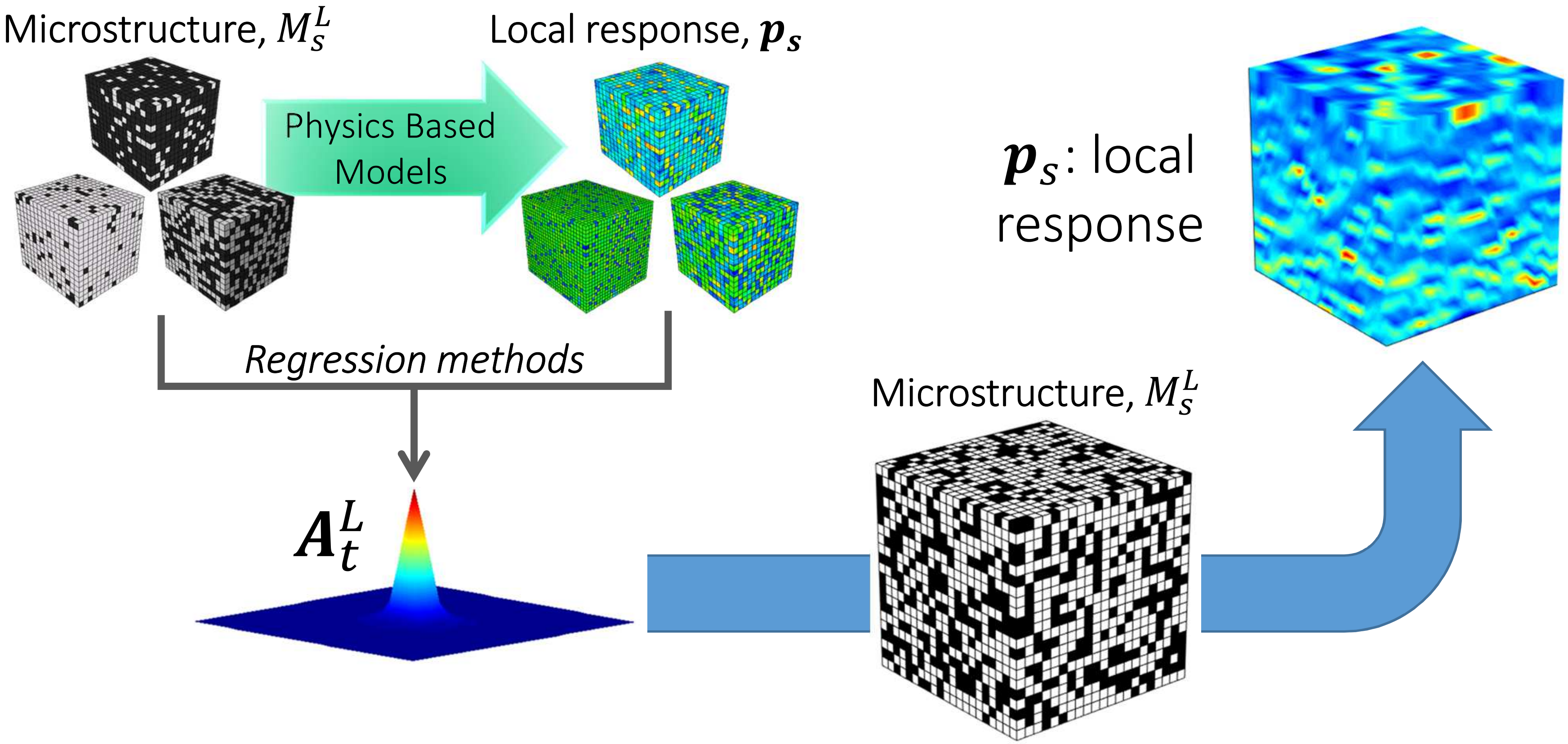
$$V_k = \sum_{i=1}^{k} \left| D_i - D_{i,perfect} \right|$$

Workflow: Identify GB atoms; Calculate pair correlation functions; Predict GB energy using PCA regression

Grain Boundary Structure-Energy Linkages



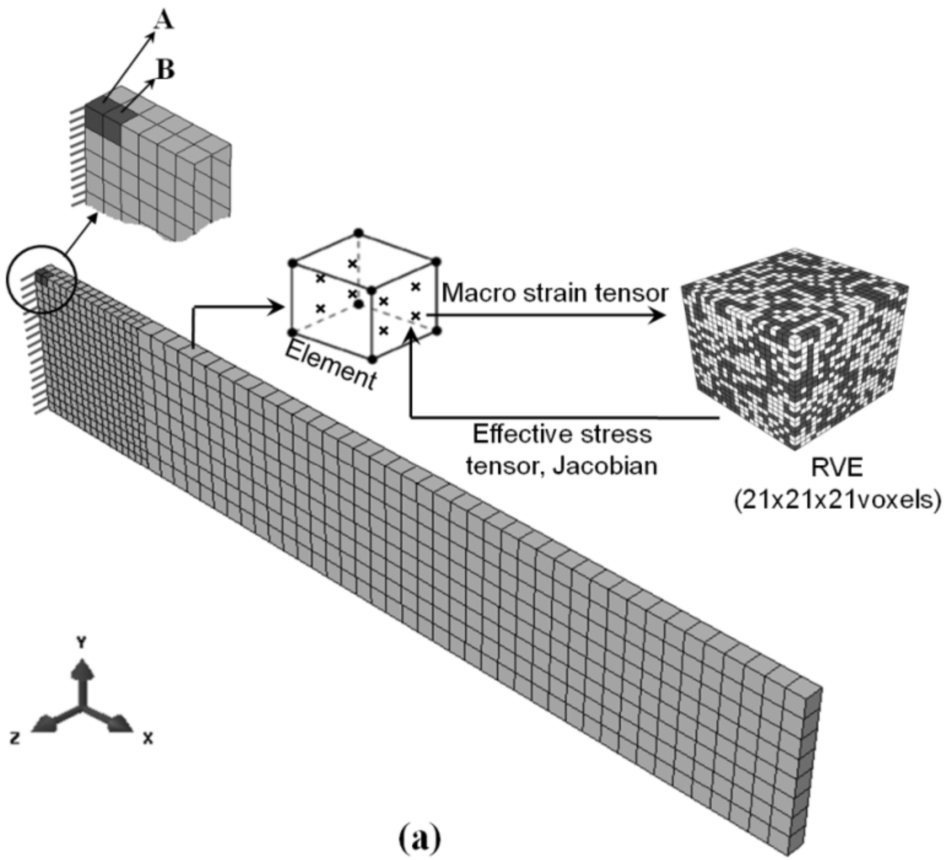
Metamodels for Localization



$$\boldsymbol{p}_s = \left(\sum_{L} \sum_{t=1}^{S} \frac{\Delta}{N_L} A_t^L M_{s+t}^L + \sum_{L} \sum_{L'} \sum_{t=1}^{S} \sum_{t'=1}^{S} \frac{\Delta^2}{N_L N_{L'}} A_{tt'}^{LL'} M_{s+t}^L M_{s+t+t'}^{L'} + \cdots \right) \langle \boldsymbol{p} \rangle$$

Strategy: New Representations of Physics + Data Science

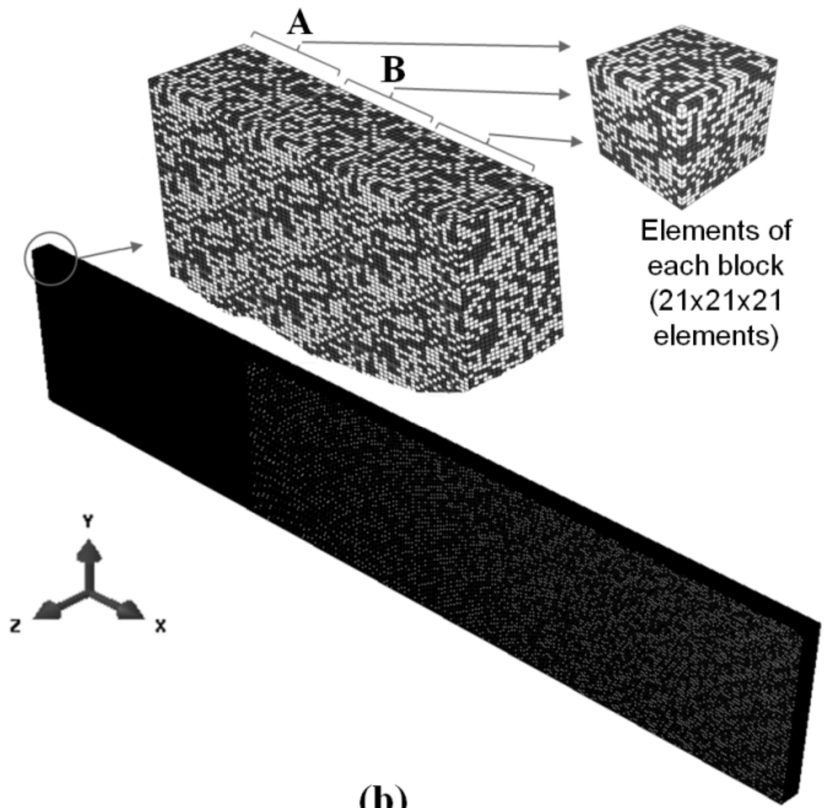
Practical Multiscaling Using MKS-FE



(a)

637 C3D8 Elements

(55 s on a standard desktop computer with 2.6 GHz CPU and 4 GB RAM)

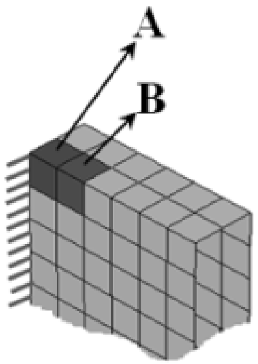


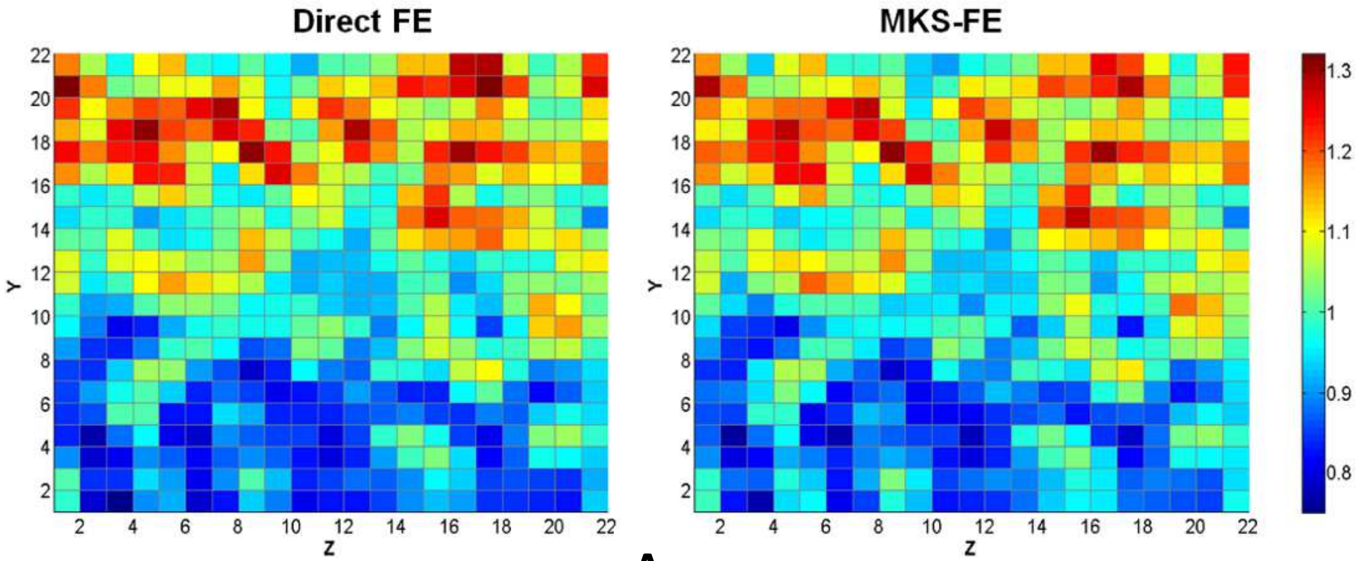
(b)

5,899,257 C3D8 Elements

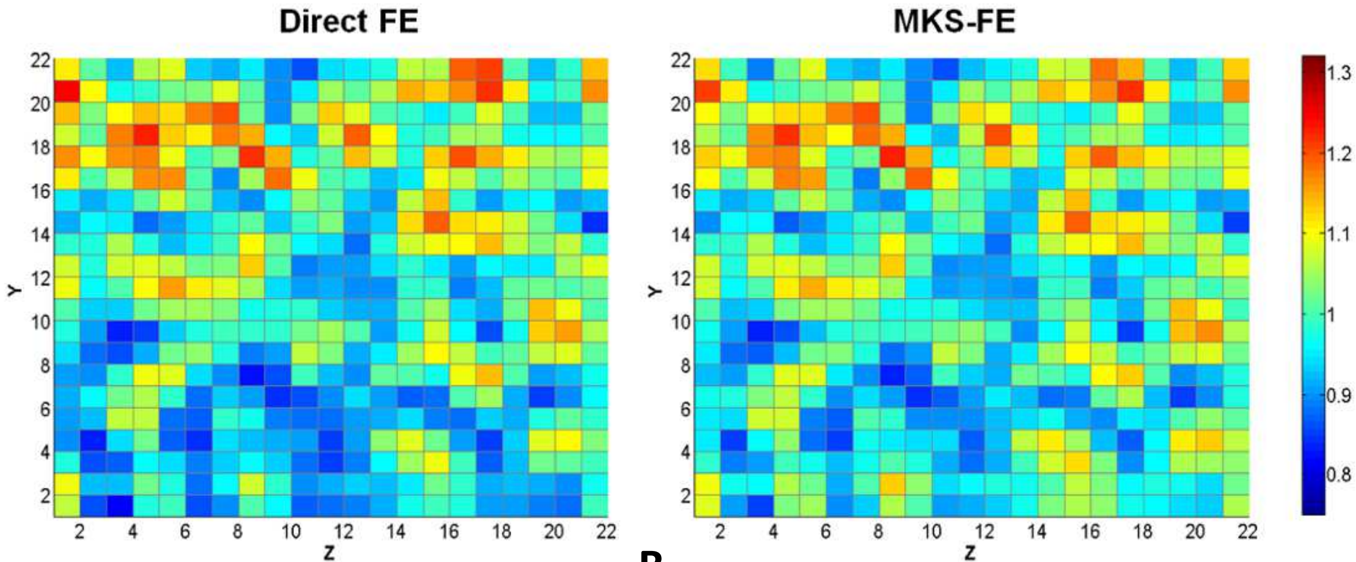
(15 hrs when using 64 processors on a supercomputer)

MKS-FE Simulations



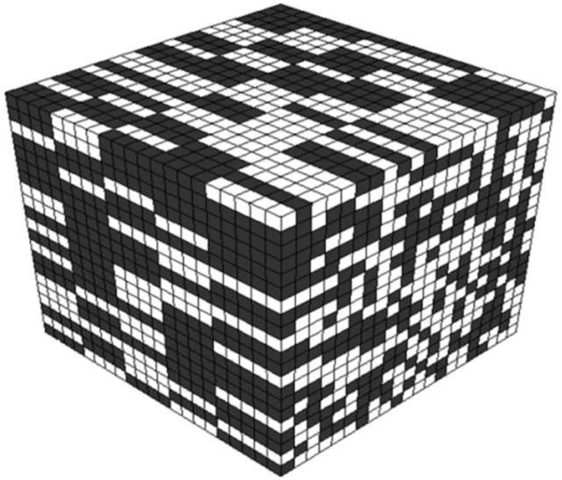


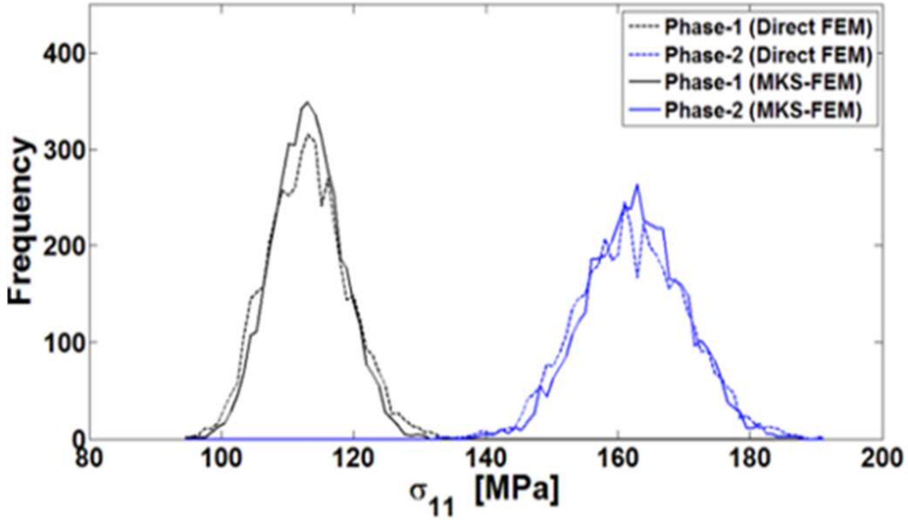
A

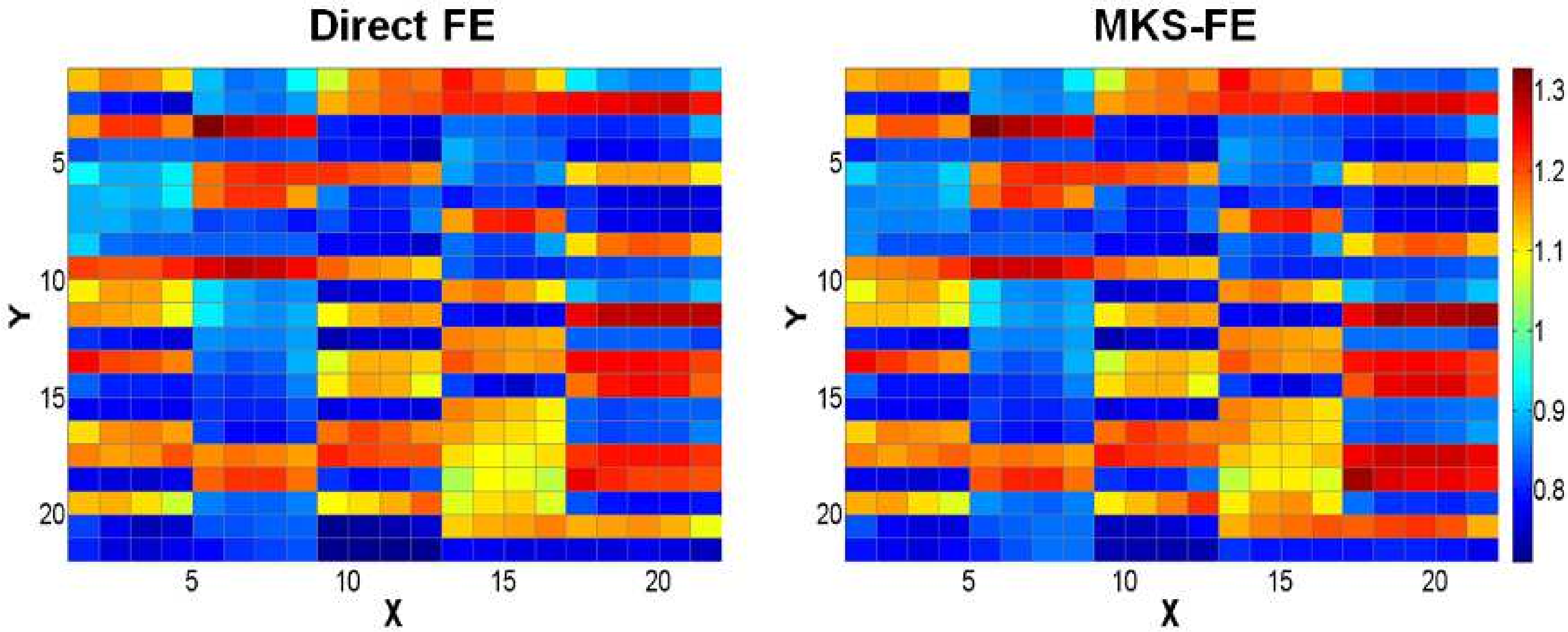


B

MKS-FE Simulations

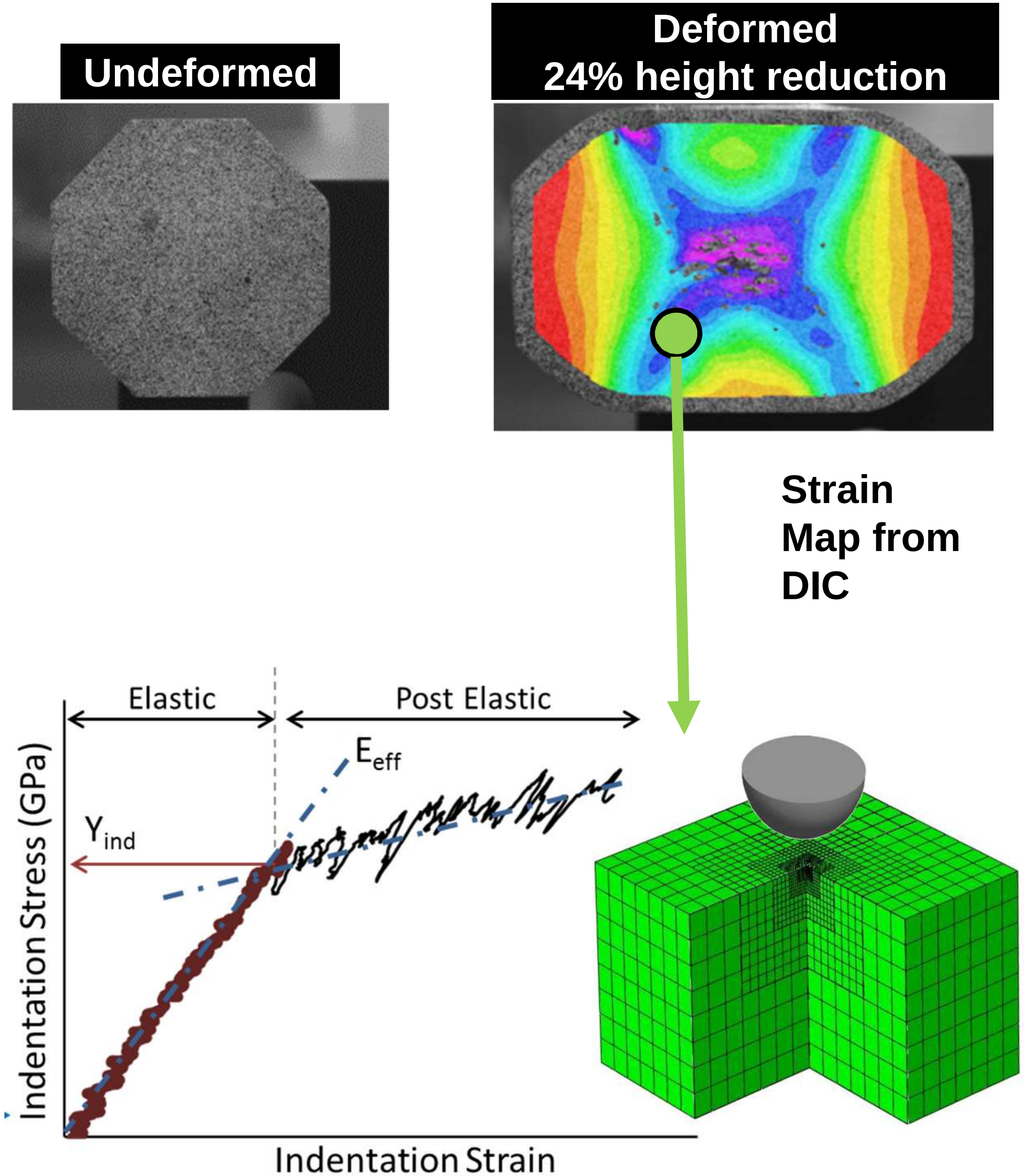


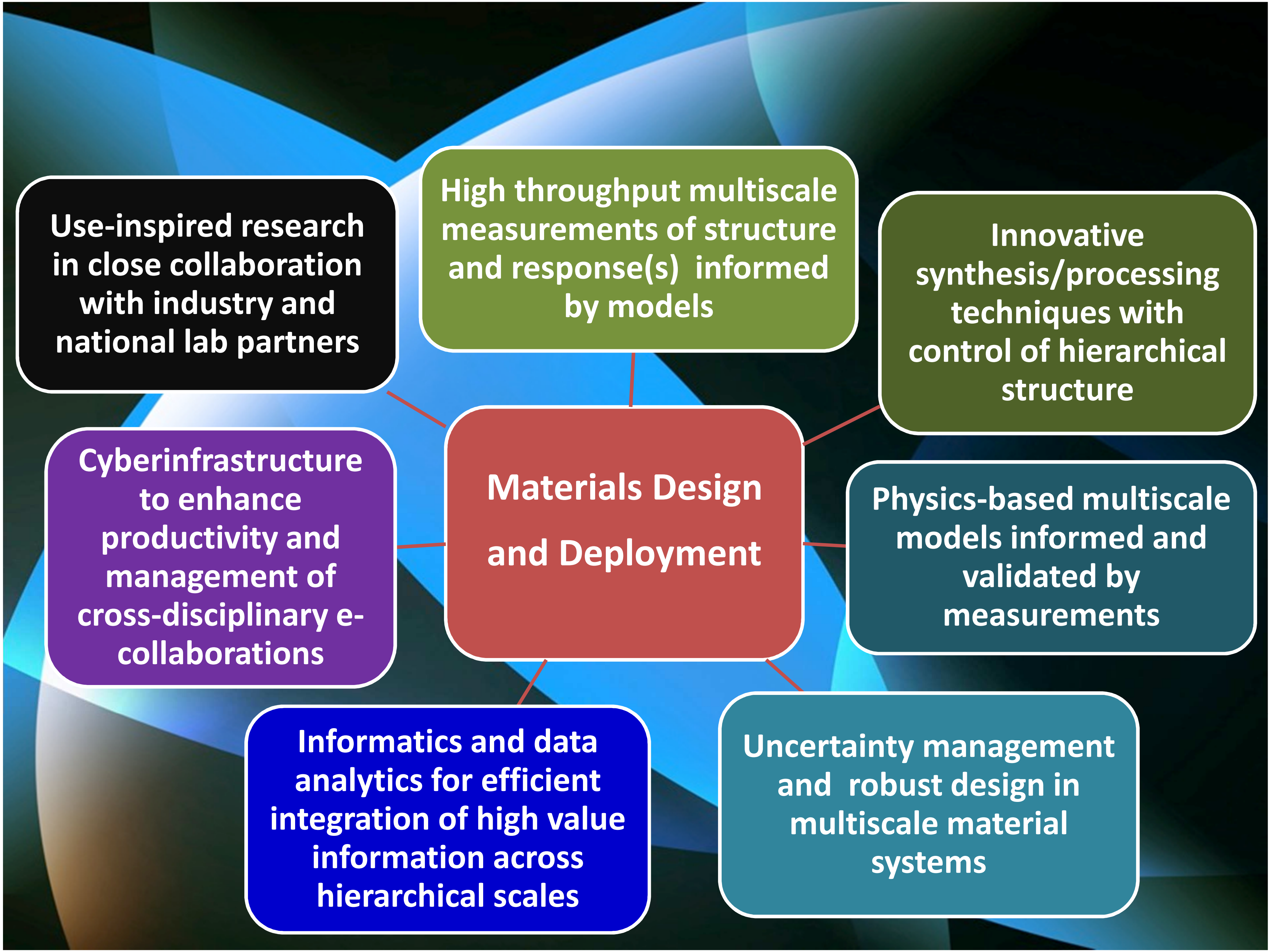




High Throughput Measurements Science

- High throughput prototyping of high value microstructures through controlled thermal and/or mechanical gradients
- Instrumented indentation is capable of providing quantitative stress-strain responses at length scales ranging from 50 nms to 500 microns




Use-inspired research in close collaboration with industry and national lab partners
High throughput multiscale measurements of structure and response(s) informed by models
Innovative synthesis/processing techniques with control of hierarchical structure
Cyberinfrastructure to enhance productivity and management of cross-disciplinary e-collaborations
Materials Design and Deployment
Physics-based multiscale models informed and validated by measurements
Informatics and data analytics for efficient integration of high value information across hierarchical scales
Uncertainty management and robust design in multiscale material systems