Digitization of Materials Innovation in support of Advanced Manufacturing

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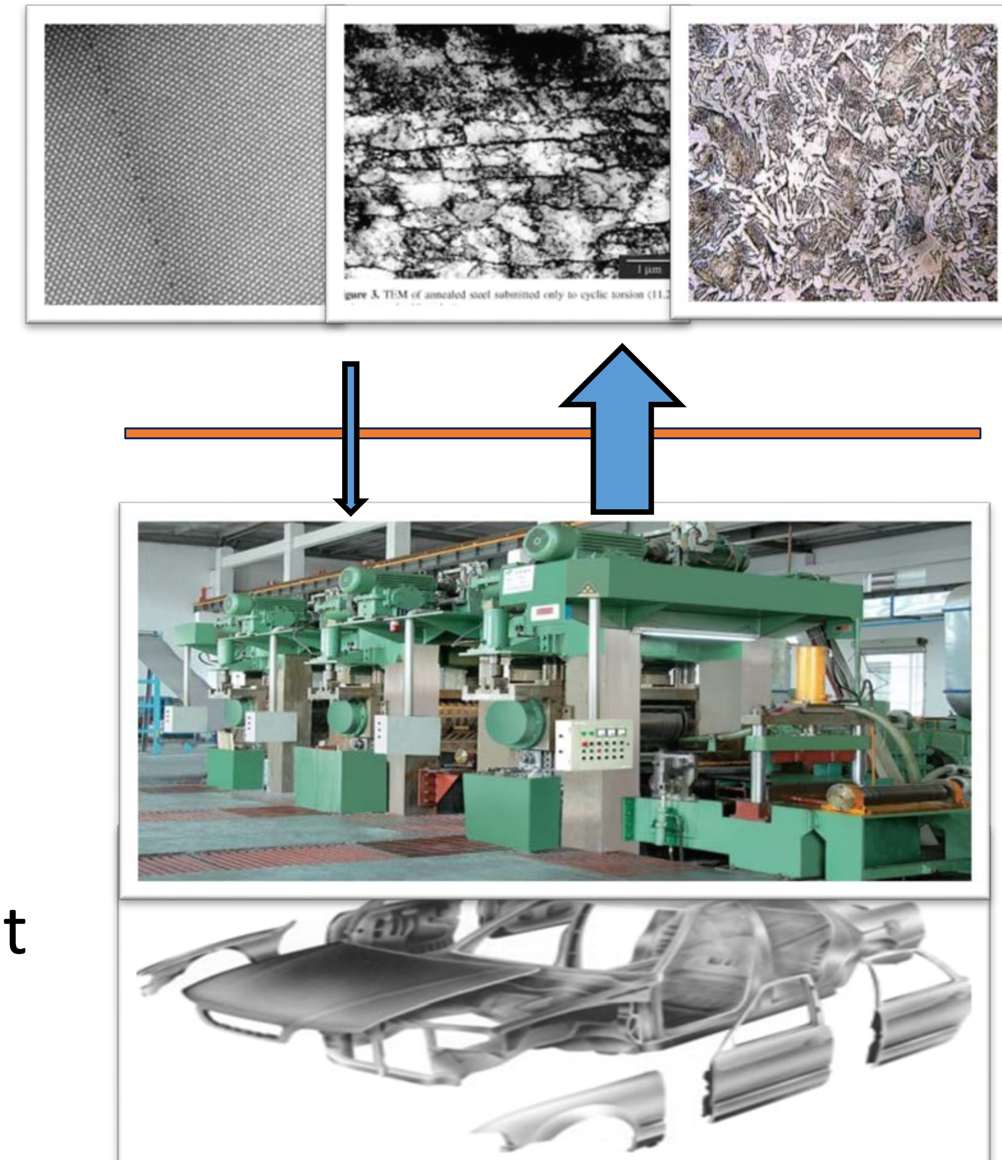
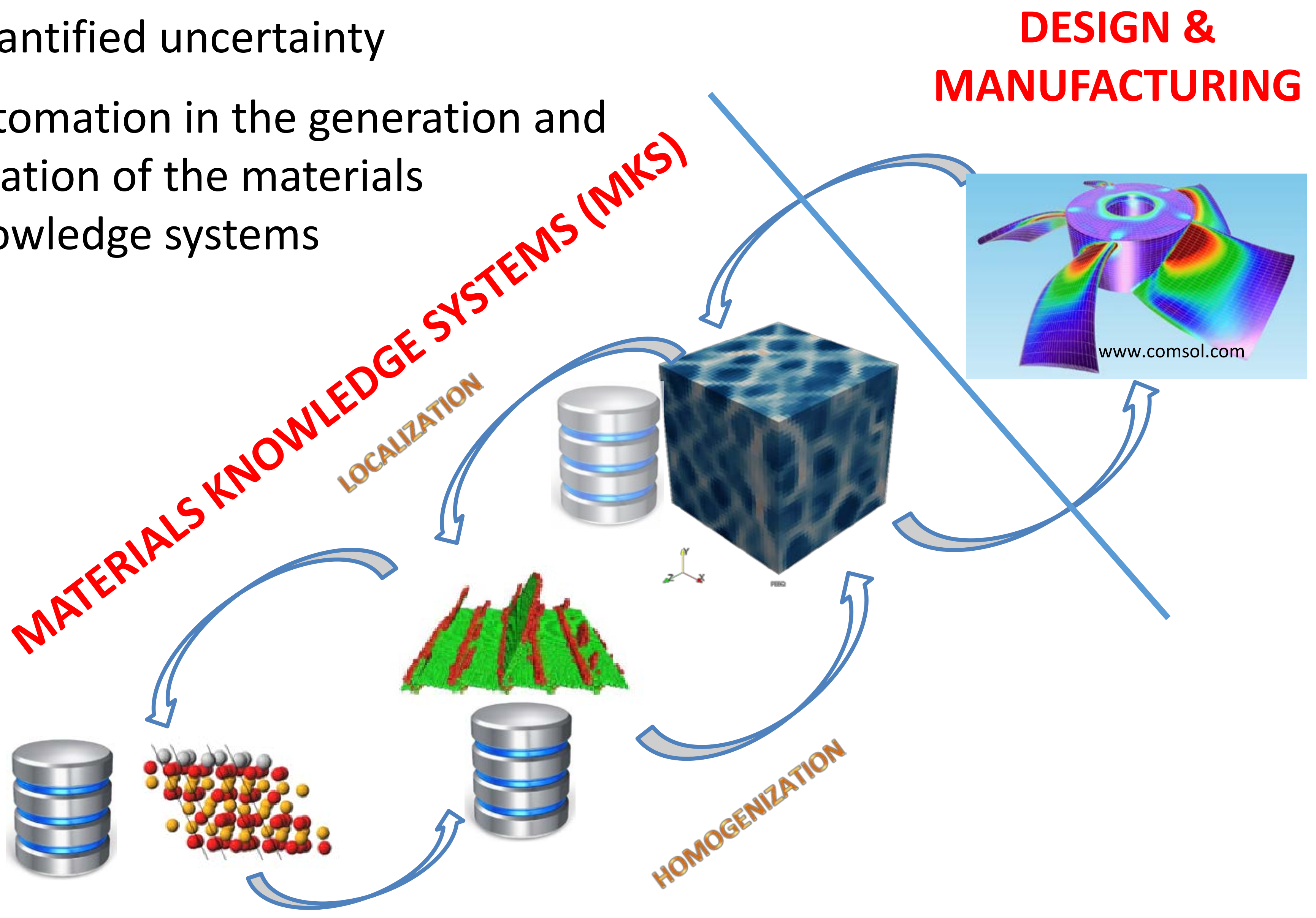
Materials-Manufacturing Nexus: Valley of Death

Reduced-order, uncertainty-quantified, Process-Structure-Property (PSP) models (i.e., core materials knowledge) predicting multiscale multiphysics material's responses are critically needed for successful extension of the digital thread of manufacturing to fully exploit the unimaginably large materials design space.



Materials Innovation Supported by Knowledge Systems

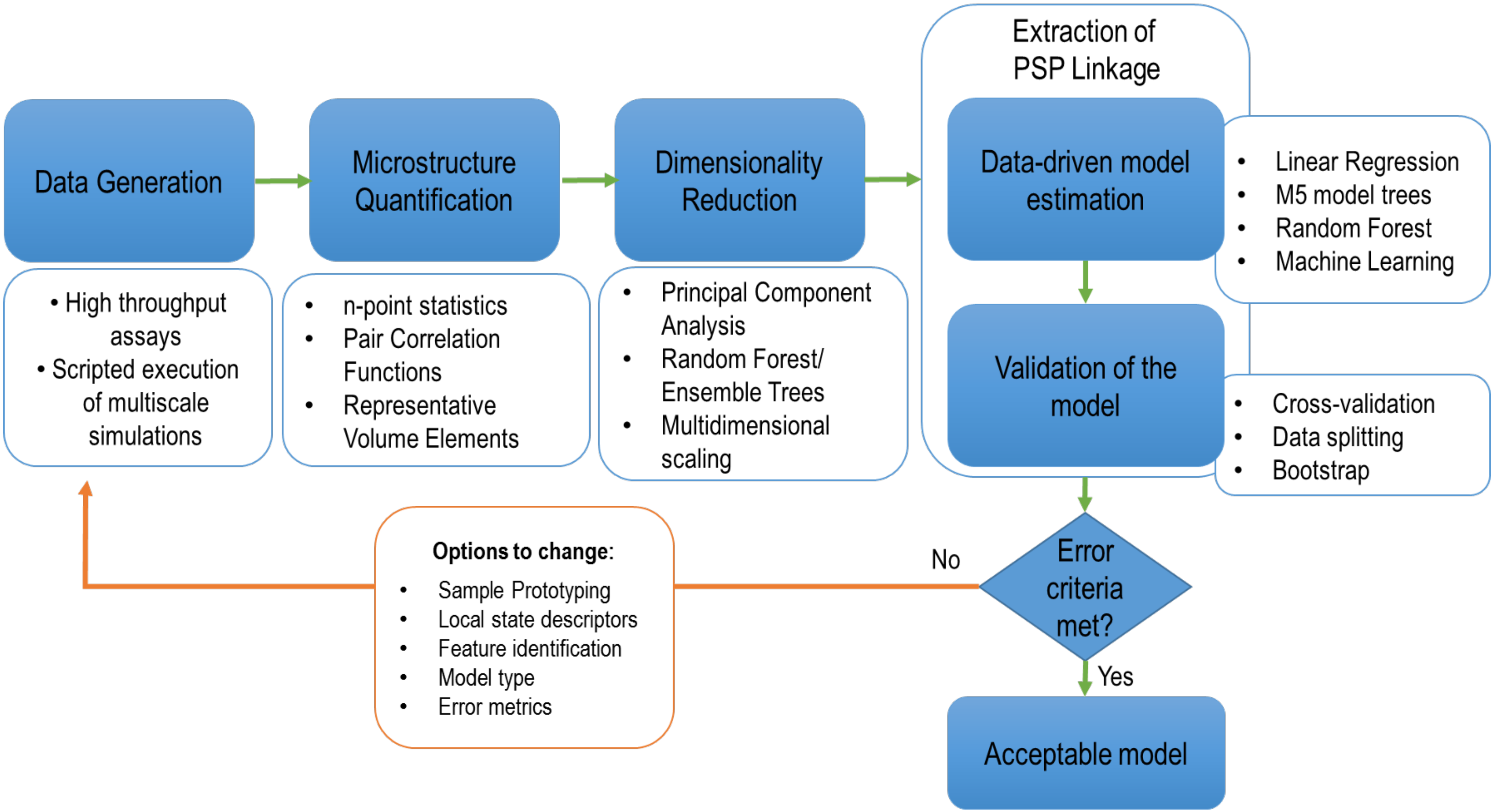
- Pre-computed knowledge systems
- Quantified uncertainty
- Automation in the generation and curation of the materials knowledge systems



Critically Needed Foundational Elements

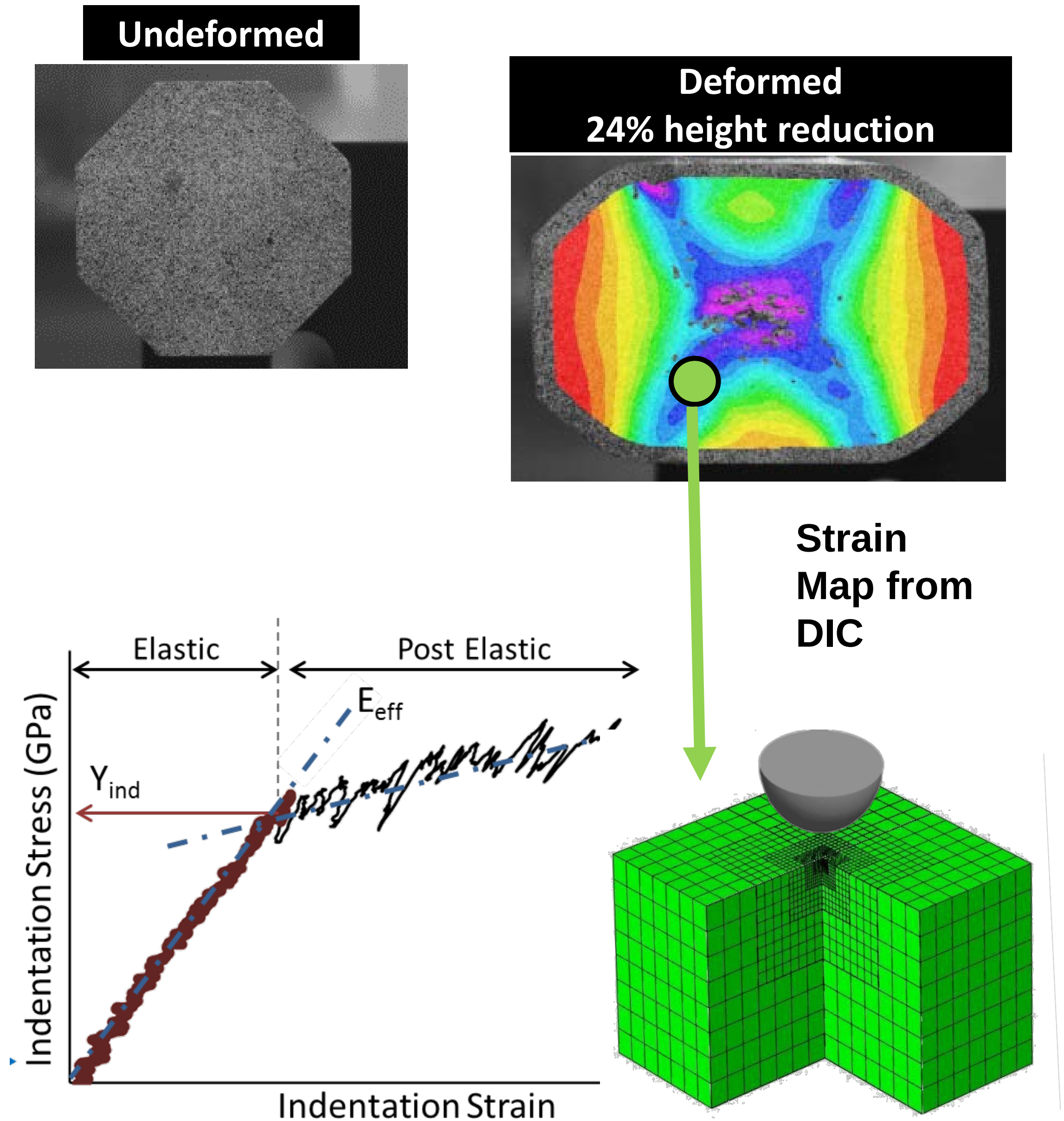
- Data/Metadata lifecycle design, automation and deployment
- Statistical quantification of material structure over a hierarchy of length scales (e.g., using n-point spatial correlations) and their high-value low-dimensional representations (e.g., using PCA)
- High-throughput experimental assays aimed at rapid exploration of the multiscale multiphysics process-structure-property linkages of high value to advanced manufacturing
- Low-dimensional representations of governing physics in capturing high-fidelity process-structure-property linkages using a combination of physics-based approaches (e.g., Green's function based approaches) supported by machine learning approaches
- Objective fusion of information extracted from experiments and simulations based on a consideration of the implicit uncertainty associated with the data to facilitate rapid and robust exploration of the extremely large materials design space

Templated Workflows for Extracting PSP Linkages

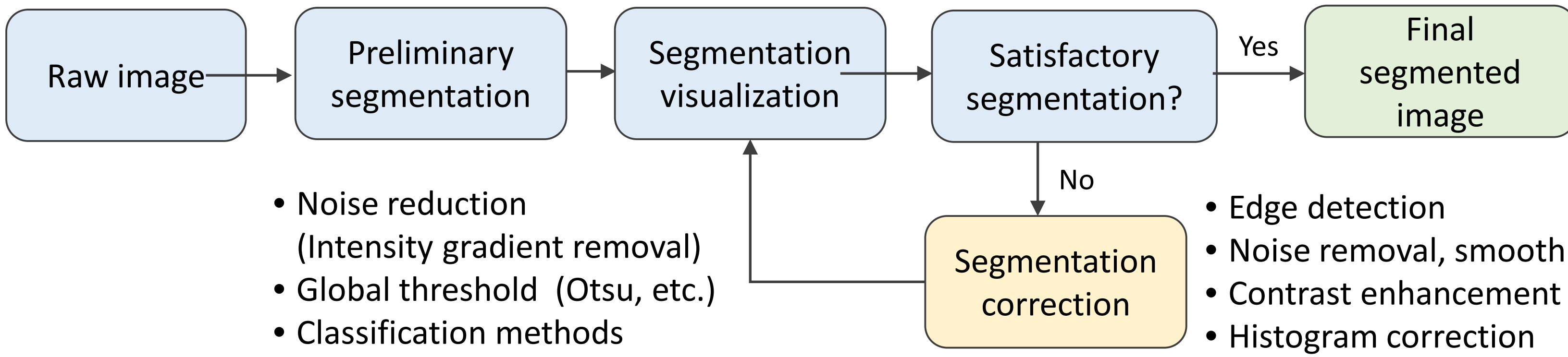


High Throughput Experimental Assays for PSP Linkages

- 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

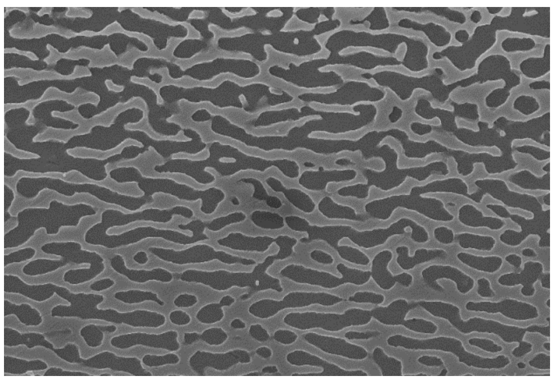


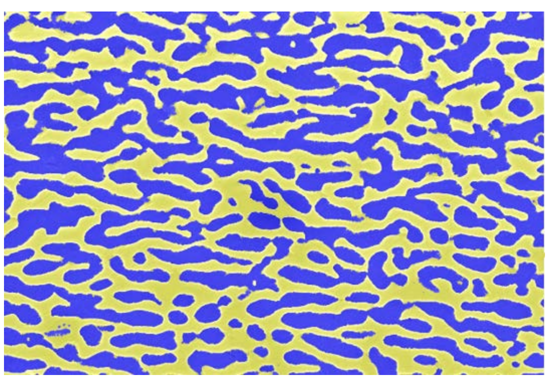
Automated Image Analyses

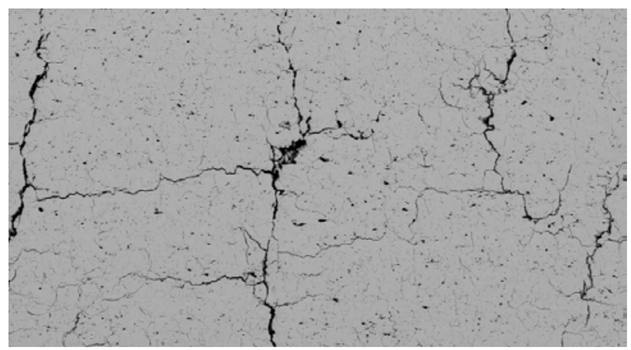


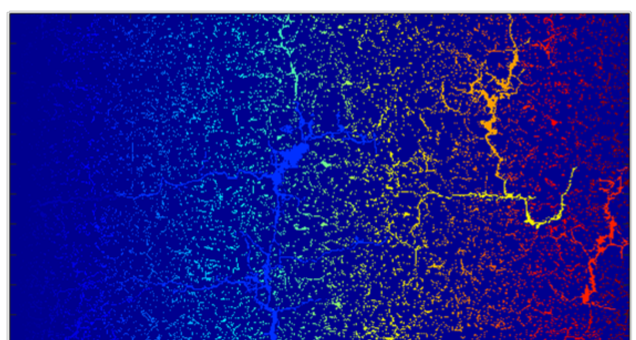
- Noise reduction
  (Intensity gradient removal)
- Global threshold (Otsu, etc.)
- Classification methods
  (Gaussian mixture, k-means, etc.)

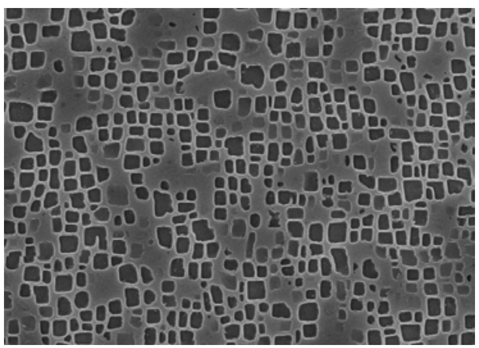
- Edge detection
- Noise removal, smoothing
- Contrast enhancement
- Histogram correction
- Intensity Gradient Removal
- Morphological filters







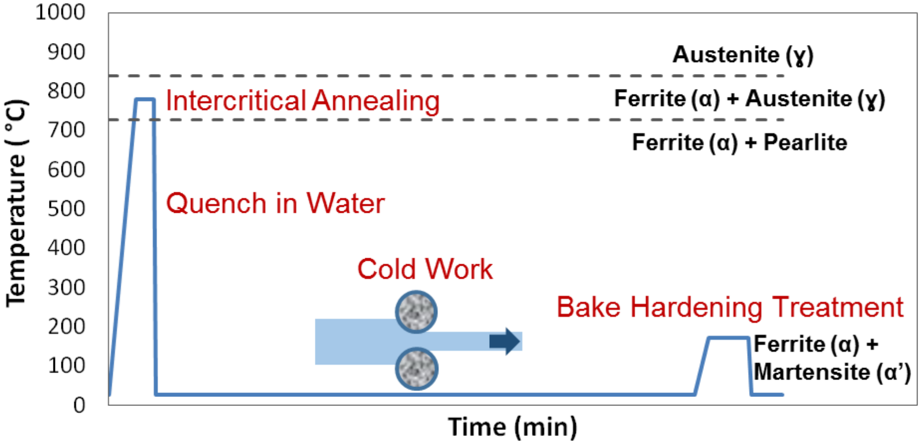




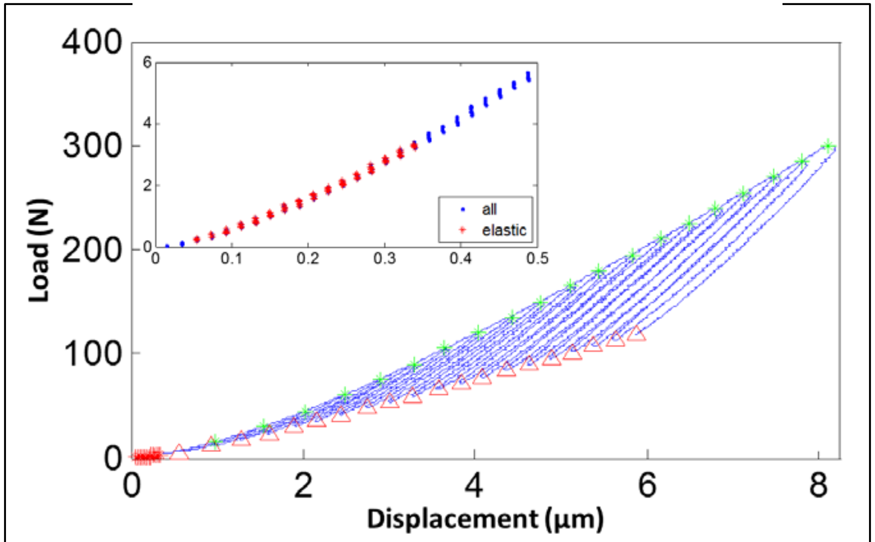
Example: PSP Linkages in DP Steels

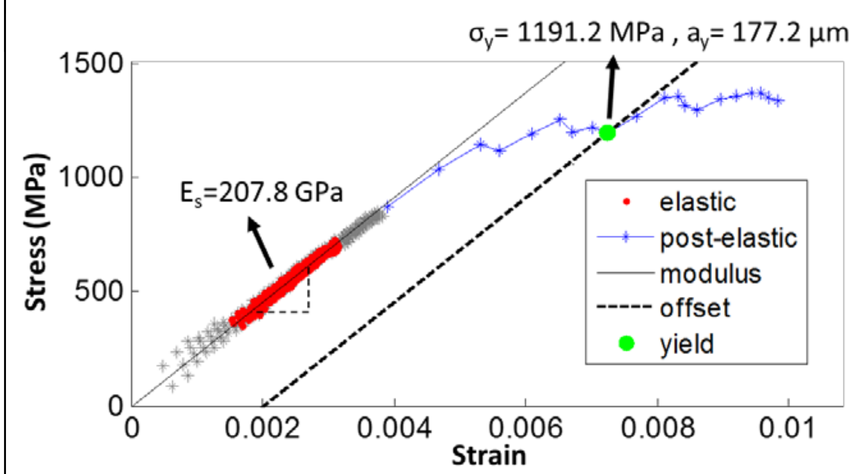
Khosravani et al., *Acta Materialia*, **123**, pp. 55-69, 2017

Thermo-mechanical Processing

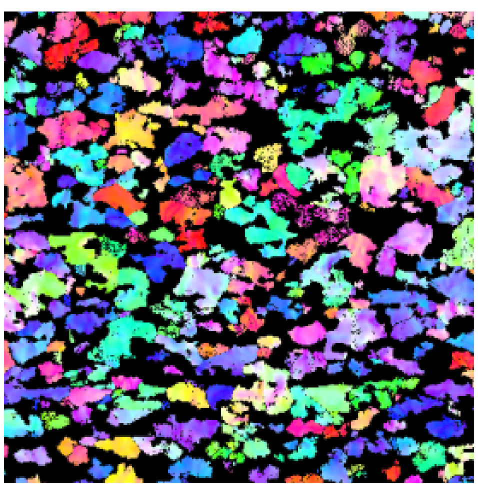


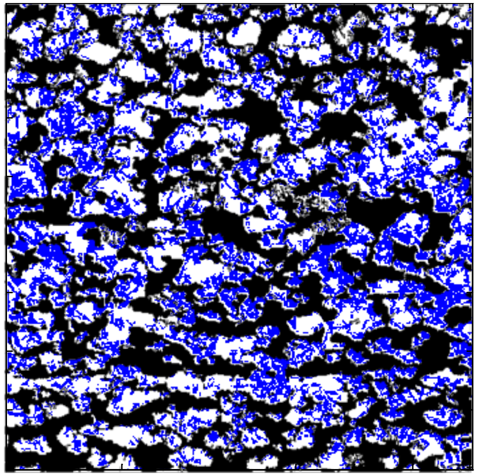
Mechanical Characterization





Structure Characterization





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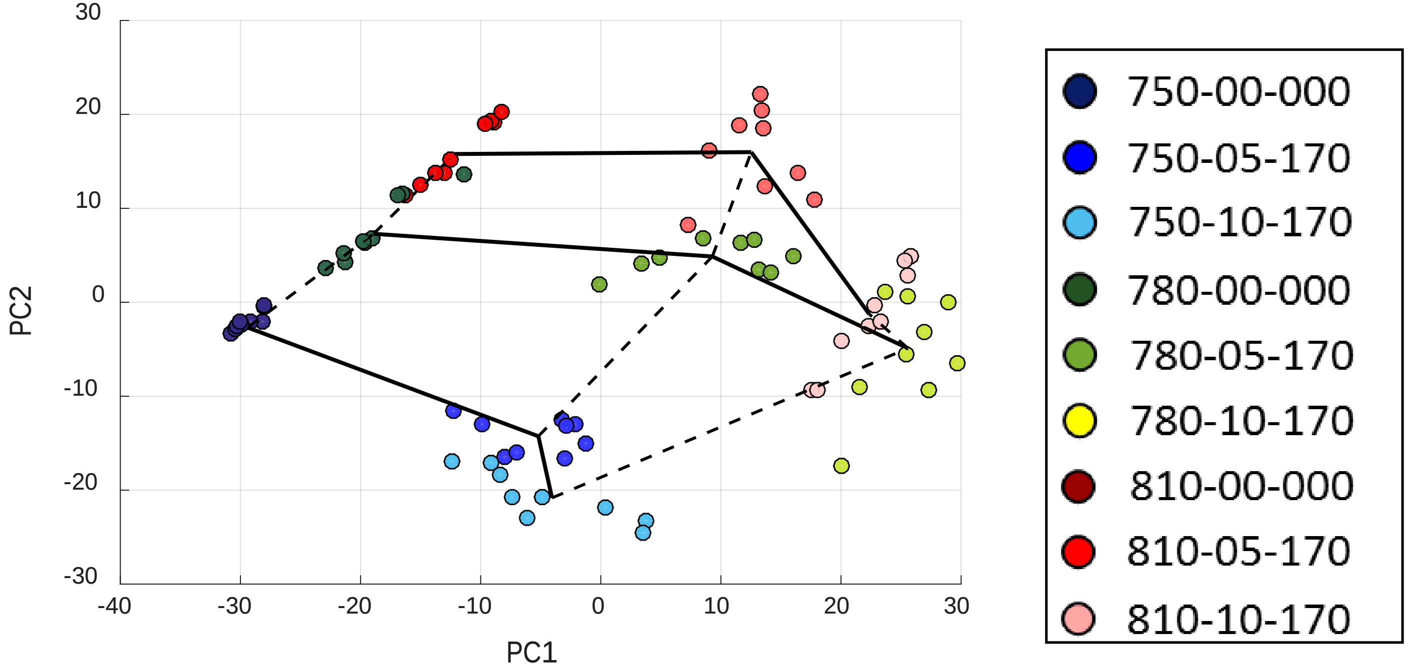
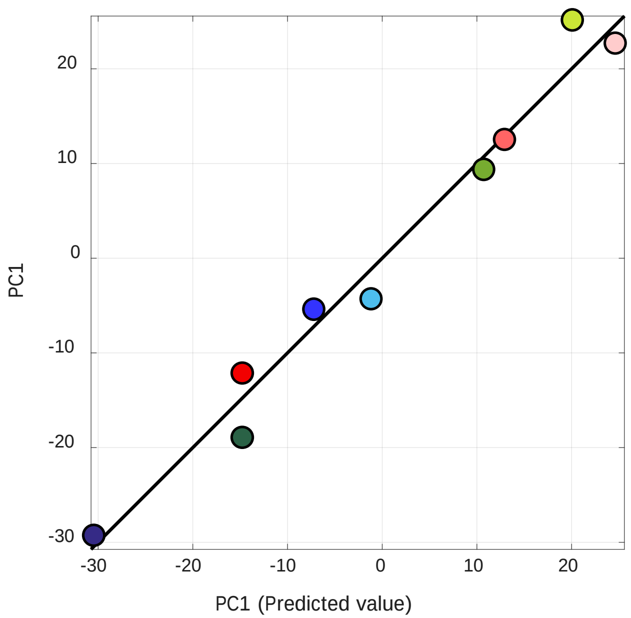
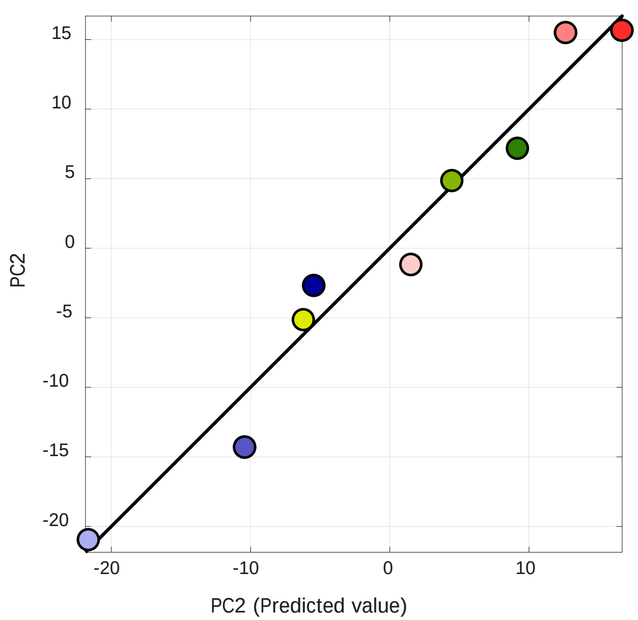
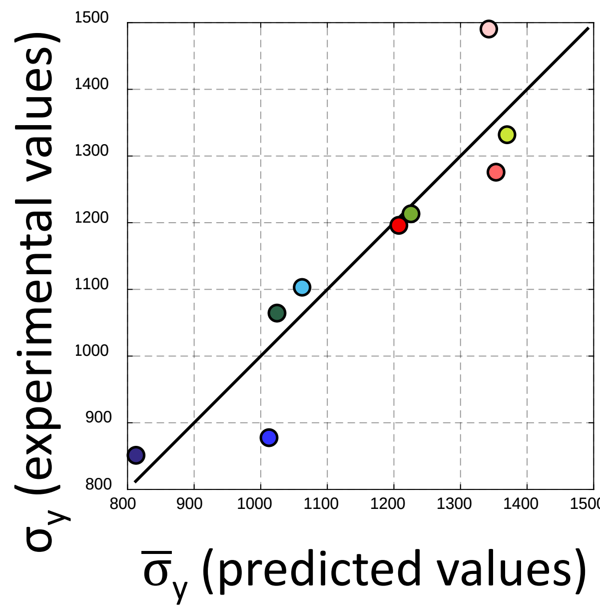


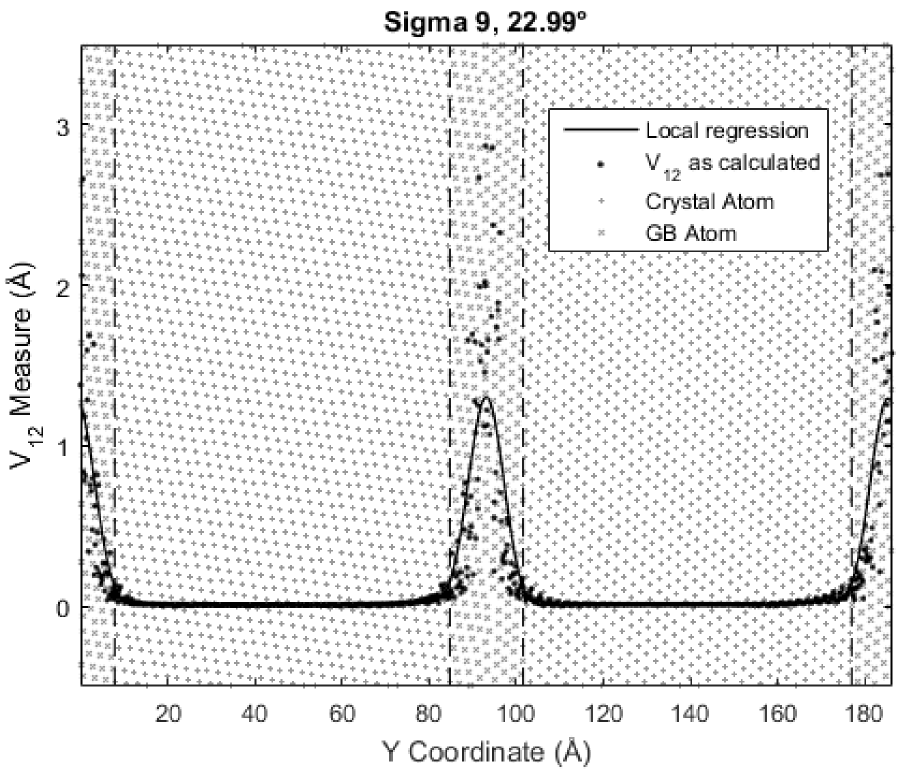


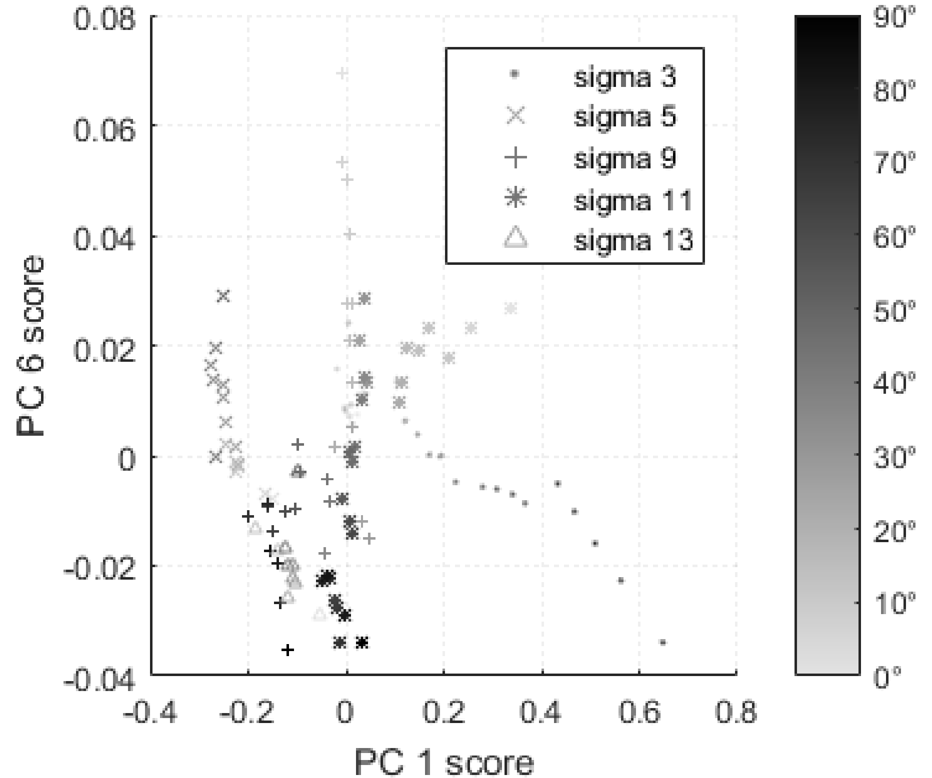




Example: PSP Linkages from MD/MM Simulations

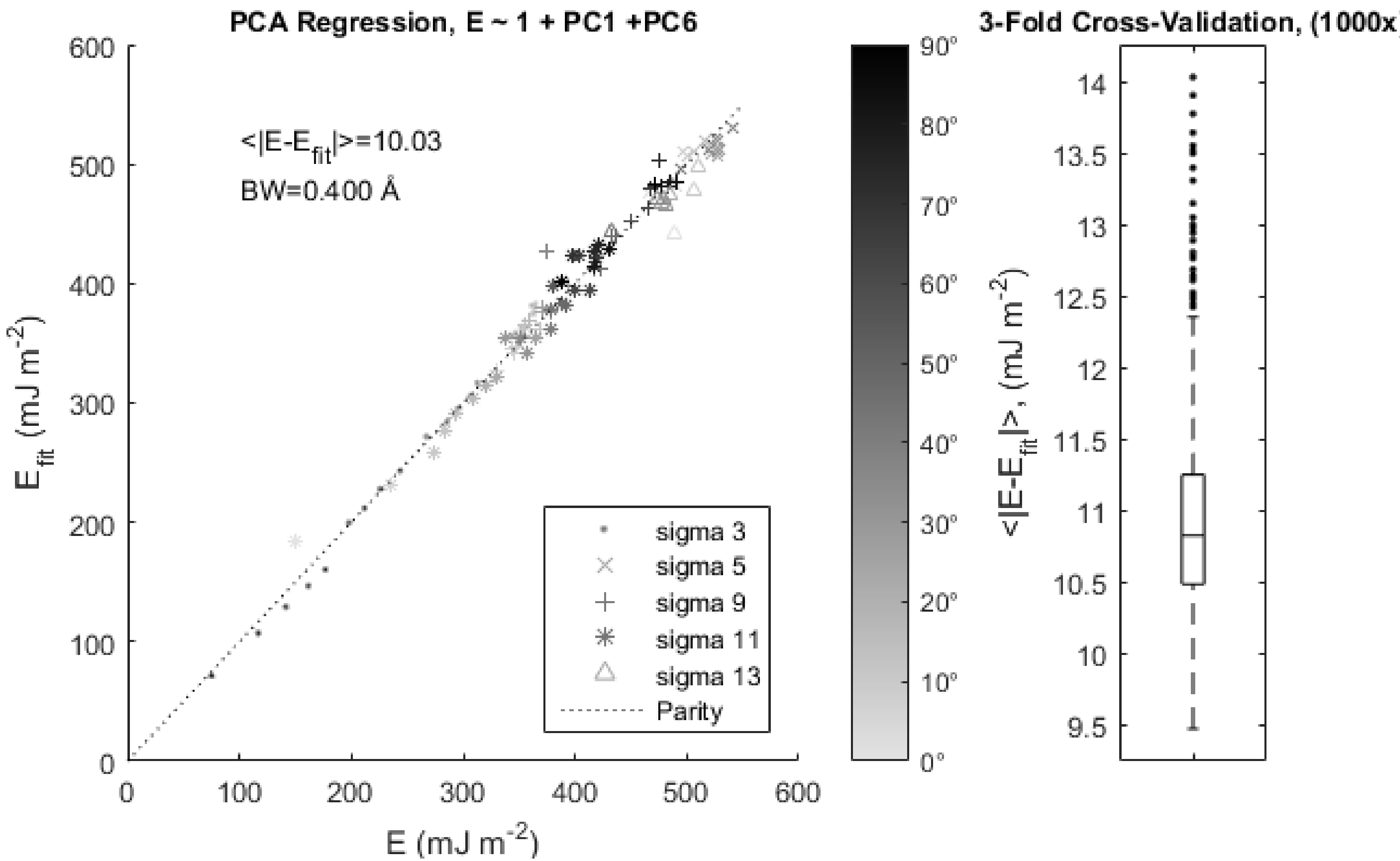
<u>Tschopp et al., IMMI, 2015</u>: 106 Datasets; Energy-minimized Al GBs; Σ 3,5,9,11,13; Inclination angle 0-90°



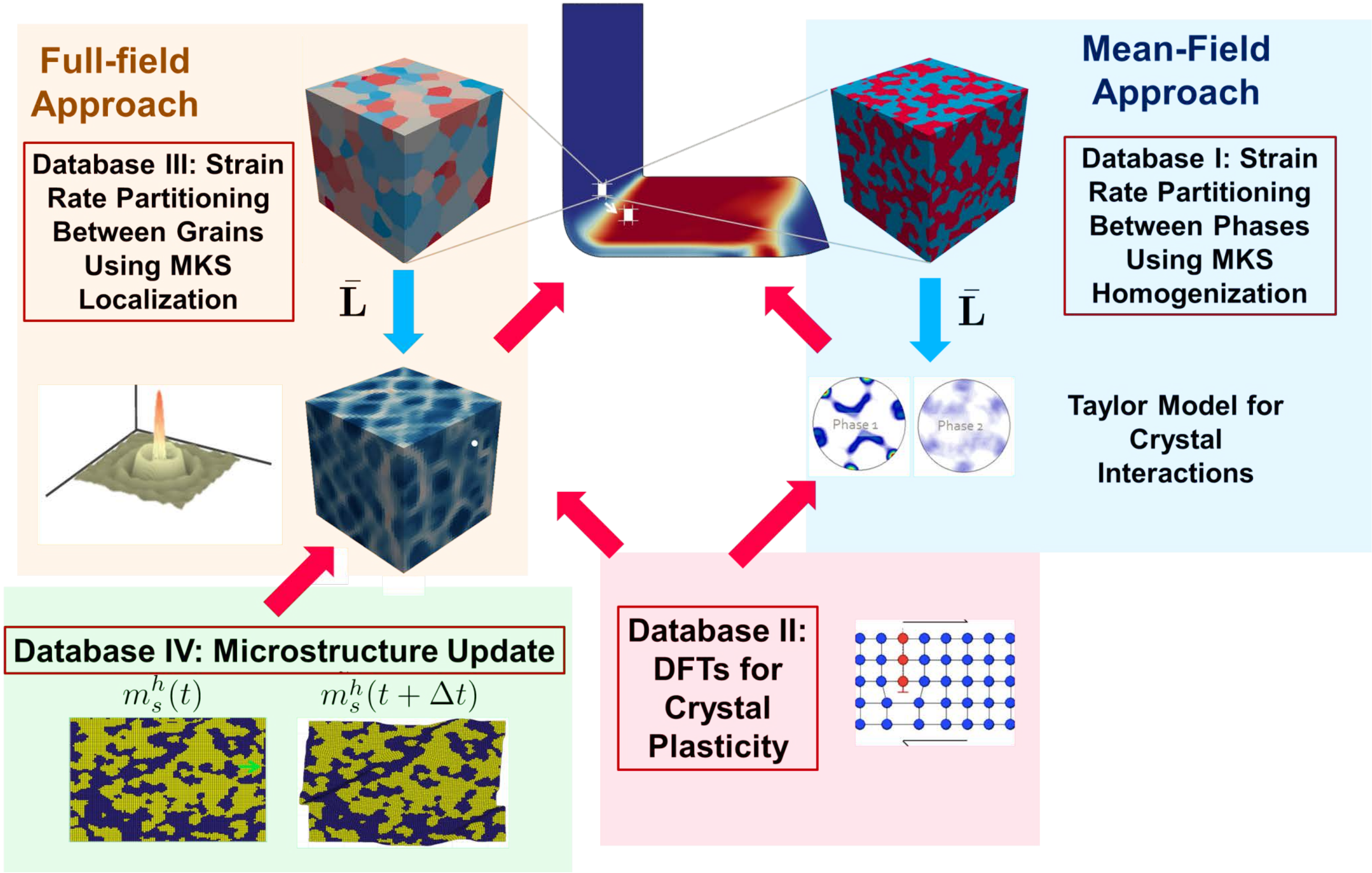


<u>Workflow:</u> Identify GB atoms; Calculate pair correlation functions; Predict GB energy using PCA regression

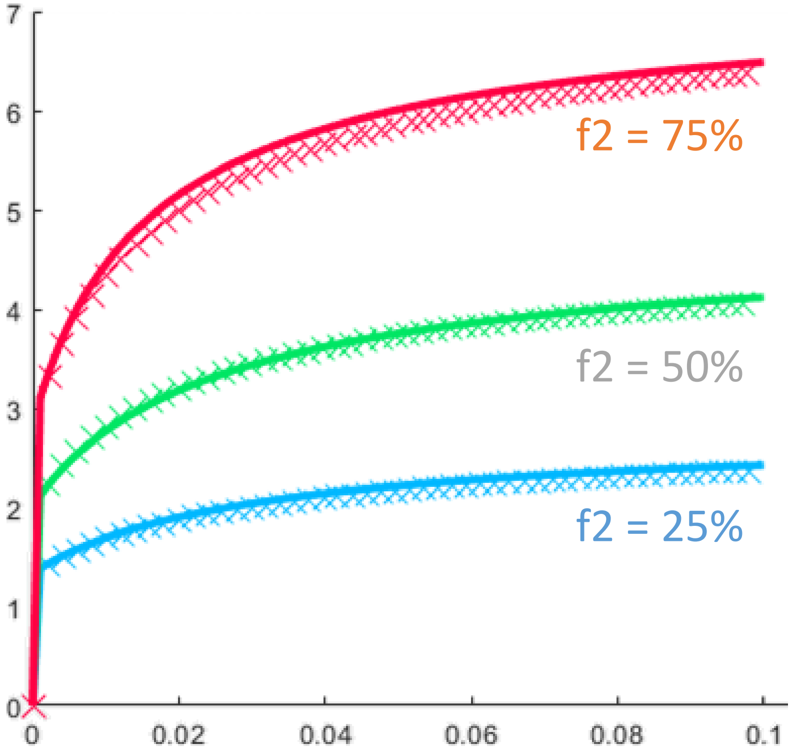
Example: PSP Linkages from MD/MM Simulations



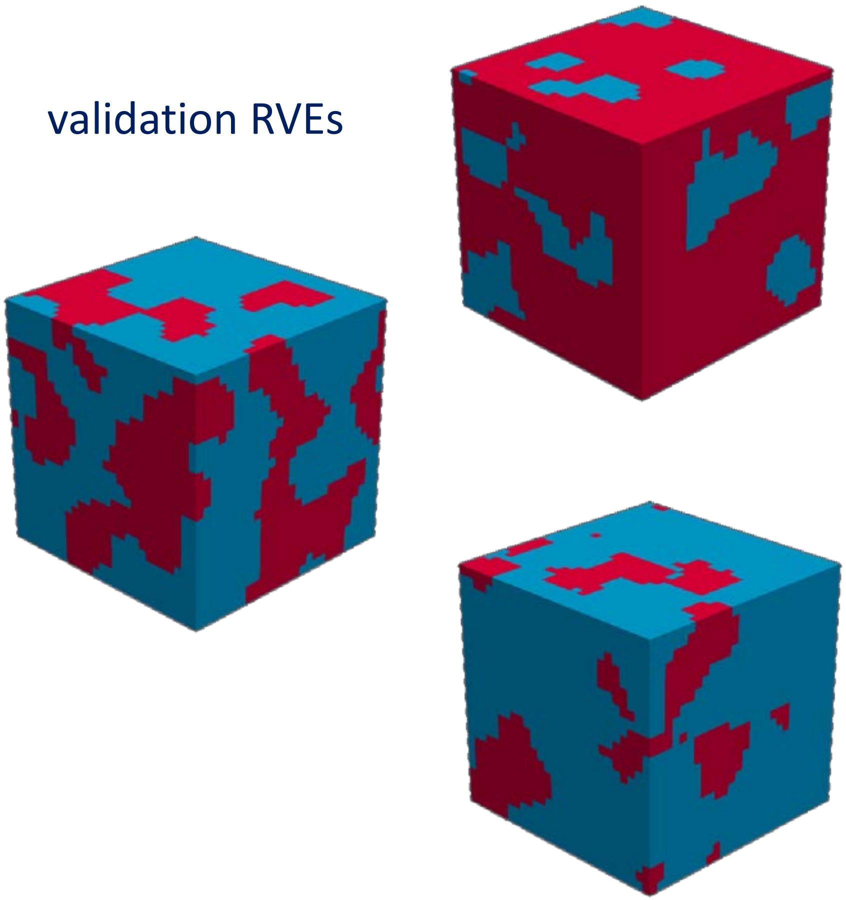
Example: Multiscale Plasticity Models



Prediction of Composite Stress-Strain Responses



validation RVEs



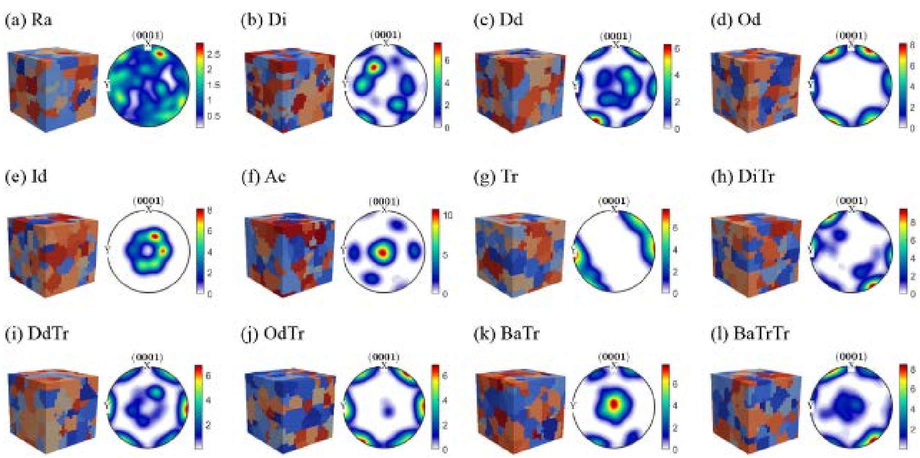
CPU Time

MKS **0.5 s**

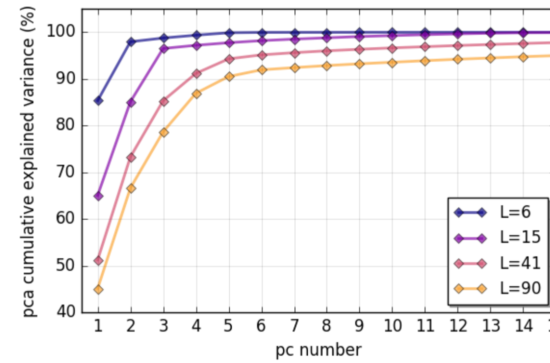
FEM up to ~24 hrs

Structure-Property Linkages: α-Ti Polycrystals

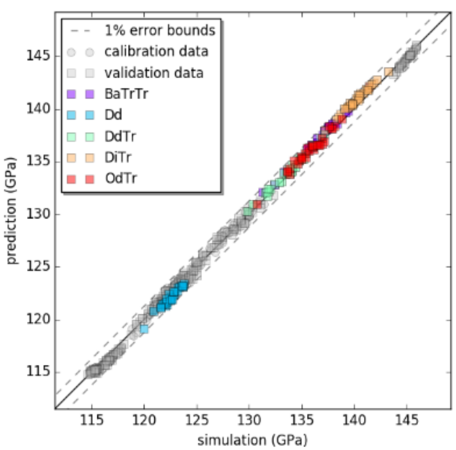
Paulson, Priddy, McDowell, Kalidindi, Acta Materialia, 129, 2017



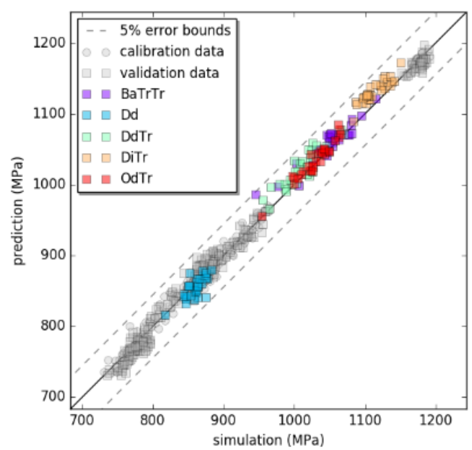
Reduced-order microstructure representation

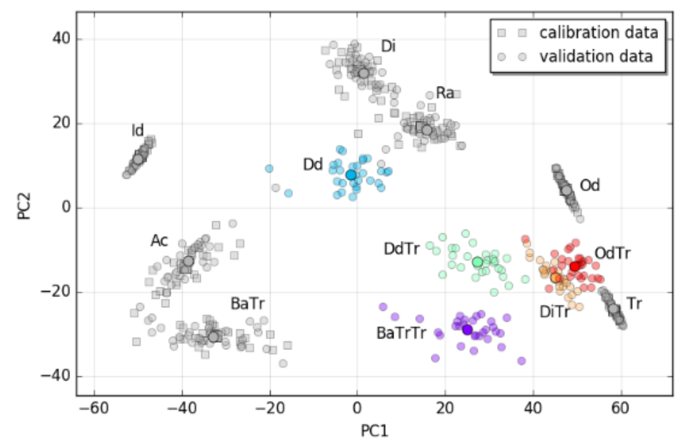


E_{eff}



σ_y

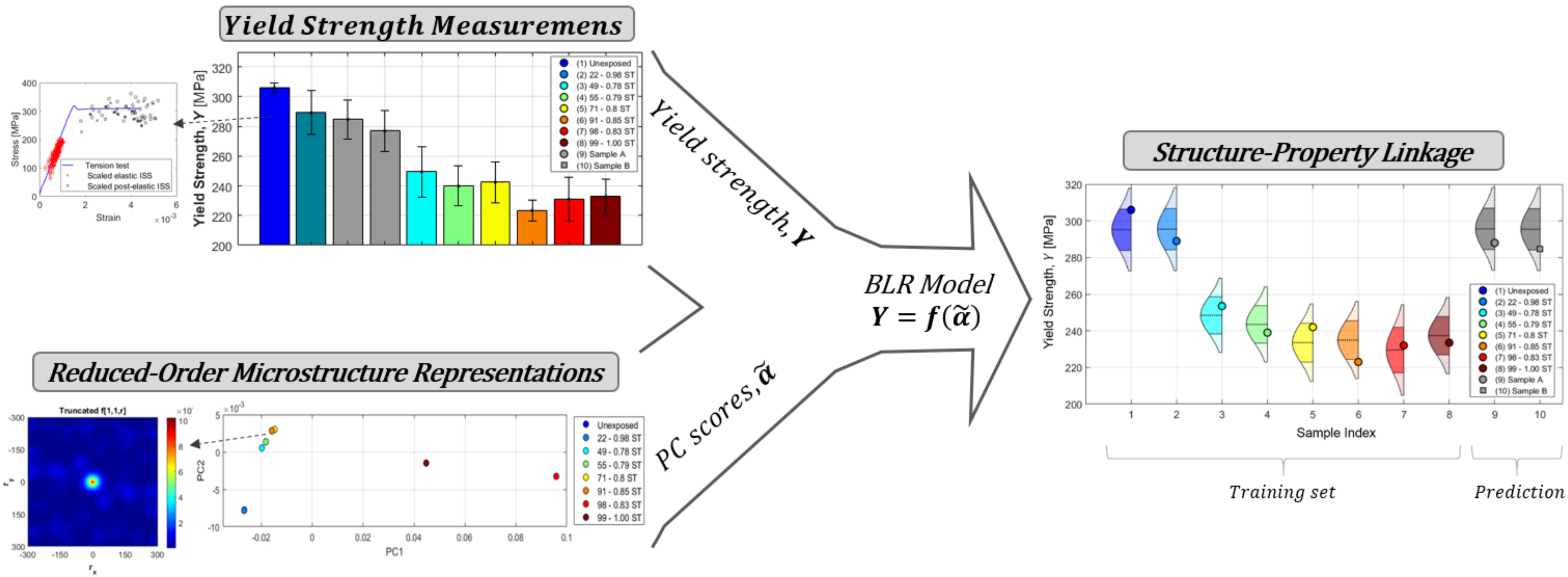




New protocol is **10,000x faster** than traditional protocols in prediction of σ_y

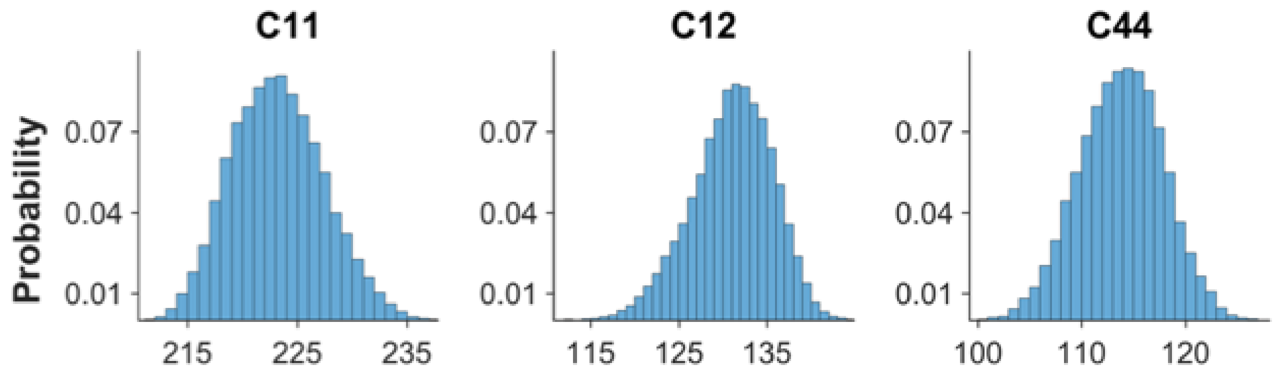
Application: Steel Scoops Excised from High-Temperature Exposed Components

A. Iskakov, Y. C. Yabansu, S. Rajagopalan, A. Kapustina, S. R. Kalidindi, *Acta Materialia*, **144**, pp. 758-767, 2018

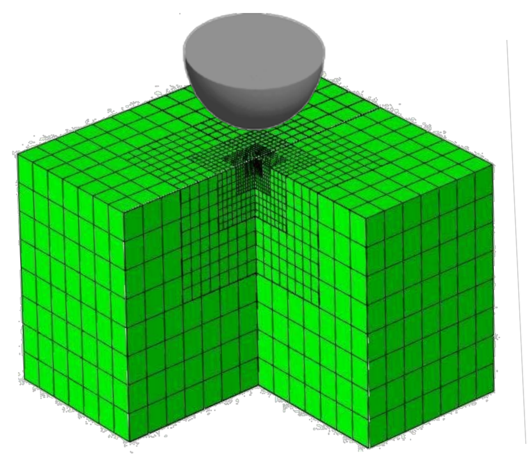


Application: Extraction of Intrinsic Material Properties from Indentation Experiments

Orientation ($\varphi_1, \Phi, \varphi_2$)	Experimental E_{eff}, GPa
339.8, 54.4, 46.1	202.9
103.7, 121.6, 49.9	199.3
232.5, 53.1, 324.0	197.7
83.2, 125.4, 30.4	195.9
3.0, 41.3, 76.4	194.0
194.7, 79.7, 317	191.1
50.0, 38.1, 250.1	190.5
114.2, 85, 173.5	173.2
170.0, 102.6, 357.9	178.3
163.6, 78.8, 168	181.2
259.9, 238.0, 145.8	189.6



	C11	C12	C44
Mean (GPa)	223.20	131.04	113.84
STDEV	4.19	4.61	4.03



Summary Outlook and Keys to Success

- Broader acceptance of data science as a powerful scientific toolset by the materials research community
- Education and training (including re-training) of materials workforce in the emerging data and informatics toolsets
- Design, launch, and adoption of modern materials innovation cyberinfrastructure employing automated and autonomous explorations
- Launch of materials-centered e-science and/or e-collaboration online communities that bring together experts from materials science and engineering, manufacturing science and engineering, computational science and engineering, data sciences, informatics, statistical sciences, and computer science