Representing Material Structure

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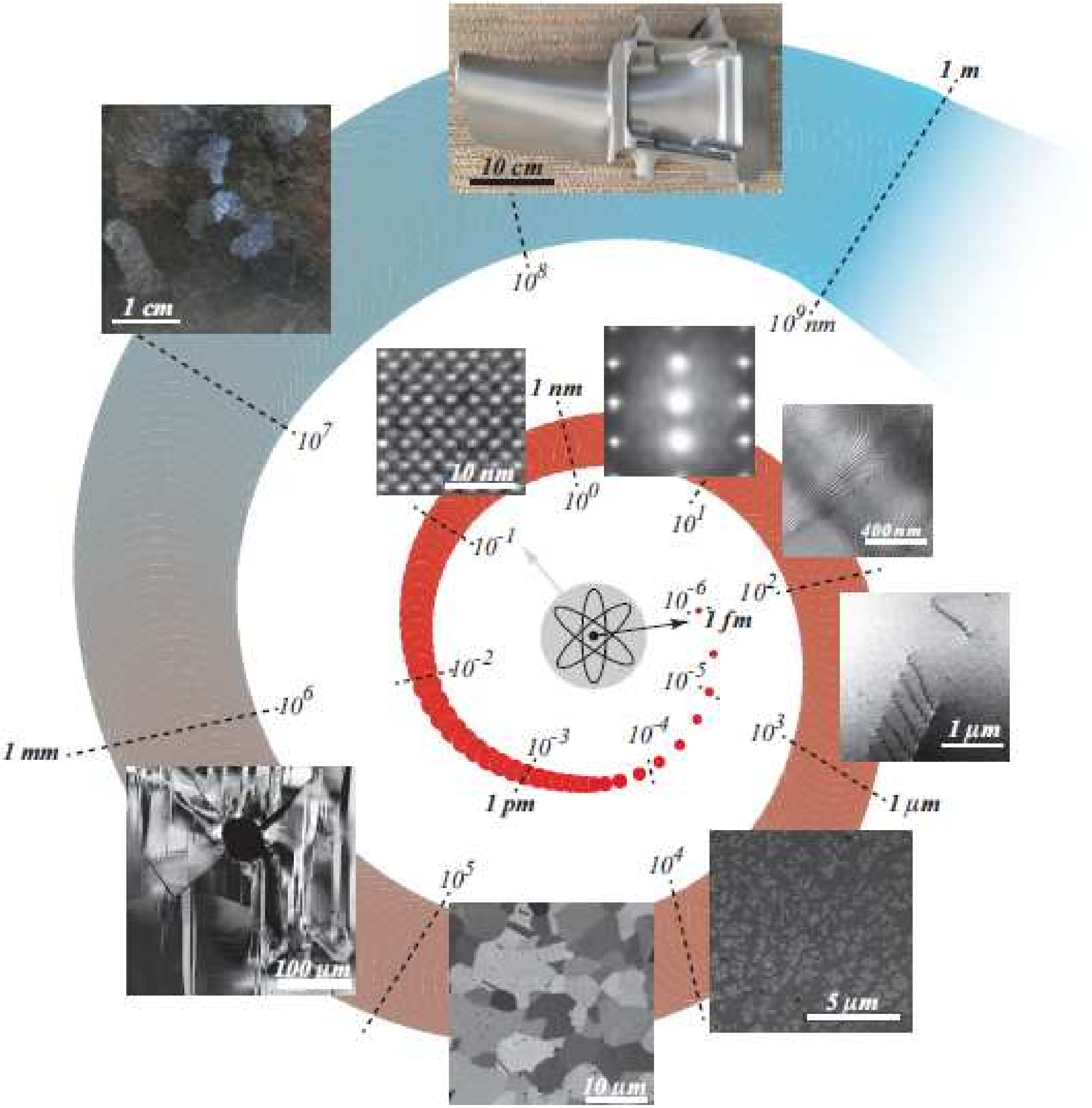
Funding: AFOSR-MURI, NIST

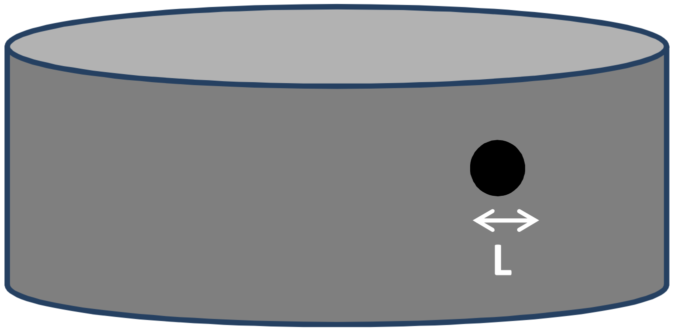
Hierarchical Material Structure



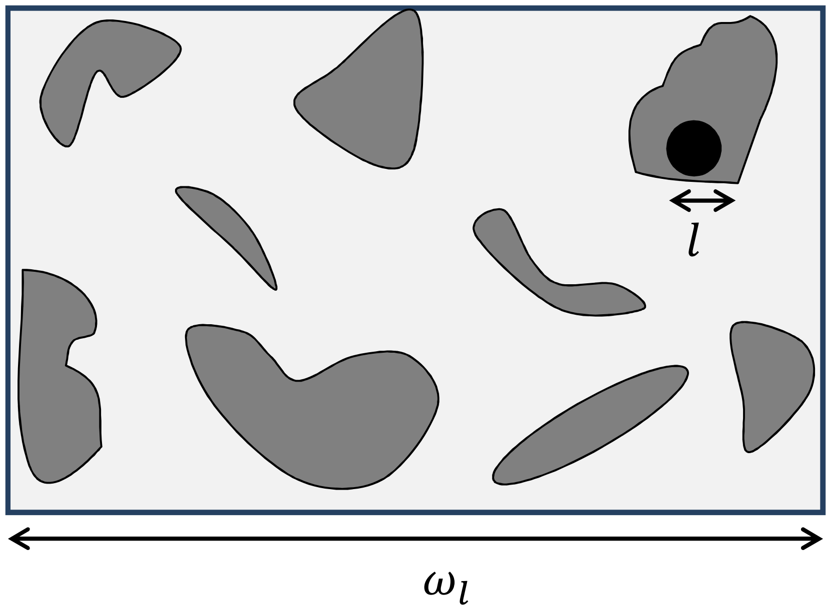
Kalidindi and DeGraef, ARMS, 2015

Well-Separated Length Scales and RVEs

Macroscale Object



Mesoscale Structure



<u>Key Assumptions</u>

- Homogenization length scales L and l exist (allows definition of material constitutive laws at these length scales)
- No major gradients occur at these length scales (fluctuations – even large ones – are allowed)
- ω_l: length scale of a representative (structure) volume element (RVE)
- Well-separated length scales: $l < \omega_l \ll L$

Challenges: Interfaces, Atomistics

Local States and Local State Spaces

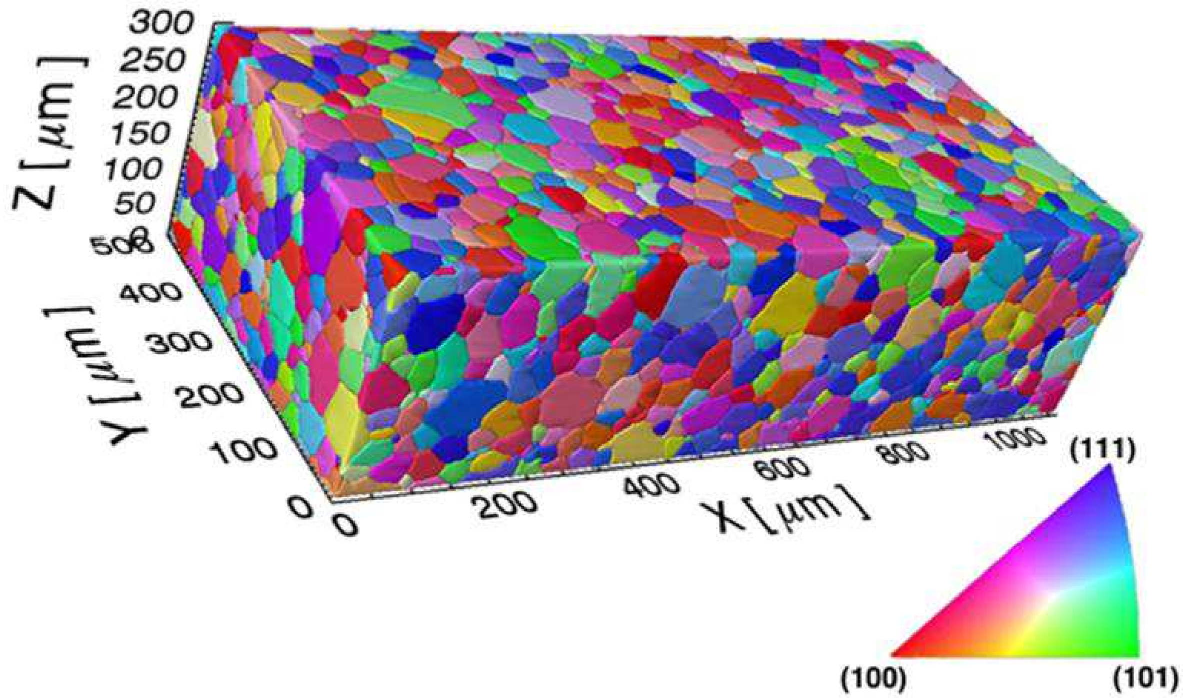
- Local State: a set of material structure attributes needed to completely specify all of the relevant material properties of interest at the selected length scale.

- Local State Space: the complete set of all theoretically possible local states one might expect to encounter in a given material system (including all the local states that may not even be present in a given sample of the selected material system)

Example: Multiphase Composites

$$h = (\rho, c_i)$$
$$H = \left\{(\rho, c_i) | \rho \in \{\alpha, \beta, \gamma, \dots\}, c_i \in C_i^{\rho}\right\}$$

Polycrystalline Microstructures



$$h = (\rho, c_i, g)$$

$$H = \left\{(\rho, c_i, g) \middle| \rho = (\alpha, \beta, \gamma, \dots), c_i \in C_i^{\rho}, g \in FZ_{\rho}\right\}$$

Microstructure Function

$$h(\boldsymbol{x}, t)$$

- Deterministic
- Impractical to implement in practice due to the resolution limits and uncertainty inherent to the characterization techniques used
- Does not allow for the presence of mixed local states (e.g., grain/phase boundary region)

Microstructure Function

$$m(h, \boldsymbol{x}, t) \text{ or } m(h, \boldsymbol{x})$$

- Defined as the probability density associated with finding local state h at the spatial location $\boldsymbol{x}$ at time t

- Captures the probability of finding one of the local states that lie within a small interval dh centered around h at a selected $\boldsymbol{x}$; $m(h, \boldsymbol{x})dhd\boldsymbol{x}$ would represent the probability and $m(h, \boldsymbol{x})$ the corresponding probability density

- Experiments typically produce only discretized information suitable to evaluating $m(h, \boldsymbol{x})$

Adams, Kalidindi & Fullwood, Butterworth-Heinemann, 2012

Digital Representations

- Information is stored in discrete units
- Many examples in images, music, and videos; has completely transformed these domains
- Involves discretization (sampling) and quantization (rounding)
- Most experimental materials datasets are already digitized
- Much less in materials simulation datasets – but there are good reasons to pursue digital representations
- Digital representations allow us to exploit the tools of digital signal processing (DSP)

Discretized Microstructure Function

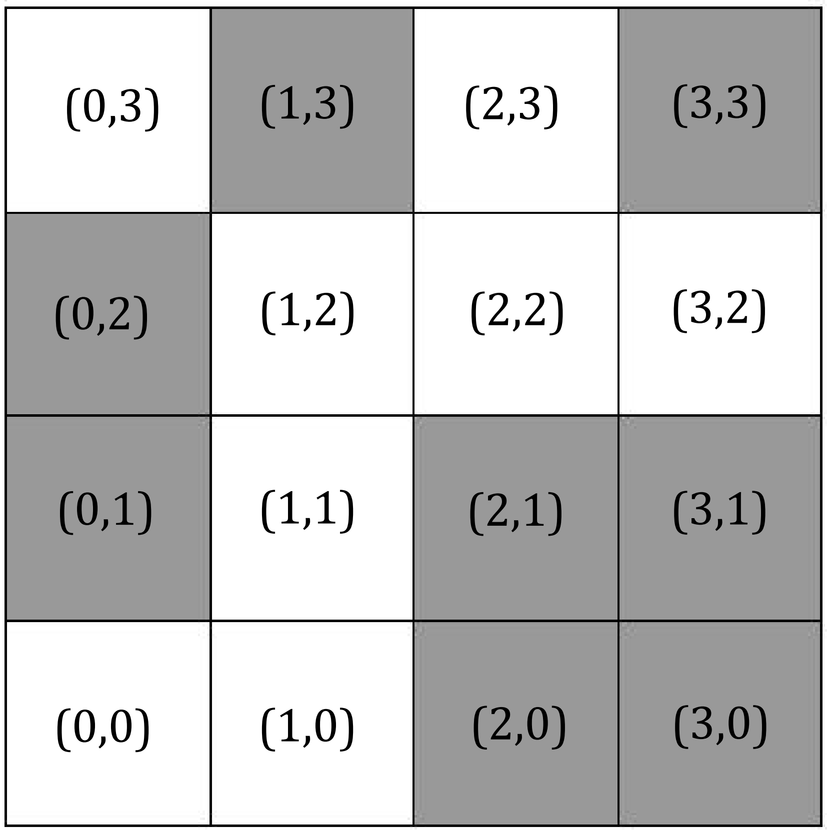
$m(h, \boldsymbol{x})$

$\{m_s^n | s = 0,1,2,\ldots, S-1; n = 1, 2, \ldots, N\}$

m_s^n represents the total volume fraction of all local states from bin *n* in the spatial bin *s*

$$\sum_{n=1}^{N} m_s^n = 1, \qquad 0 \leq m_s^n \leq 1$$

Discretized Microstructure Function



$$\boldsymbol{s} = (s_1, s_2)$$

$$m^1_{(1,2)} = 1, m^2_{(1,2)} = 0$$
$$m^1_{(2,1)} = 0, \ m^2_{(2,1)} = 1$$

Eigen microstructures

Discretized Microstructure Function

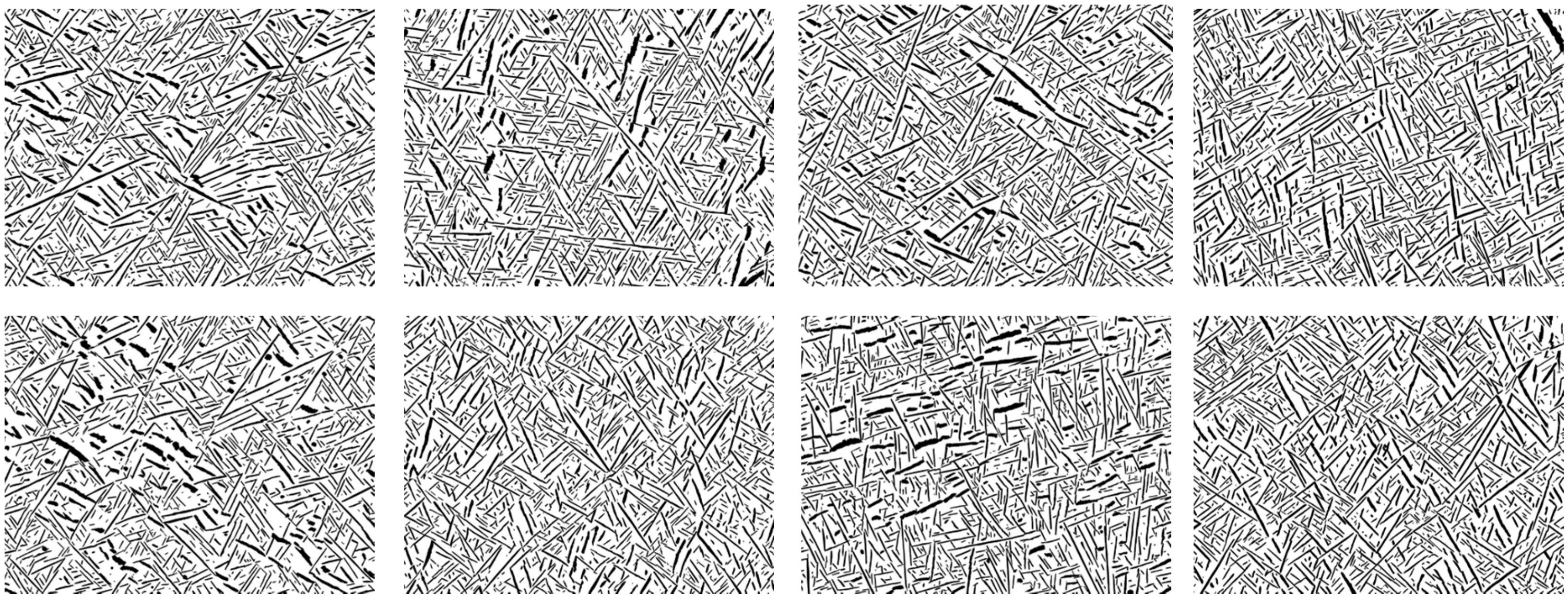
$$m(h, \boldsymbol{x}) \approx \sum_{\tilde{n}=1}^{N} \sum_{\boldsymbol{s}=\boldsymbol{0}}^{\boldsymbol{S-I}} m_{\boldsymbol{s}}^{n} \, \chi_n(h) \chi_{\boldsymbol{s}}(\boldsymbol{x})$$

$$m(h, \boldsymbol{x}) = \sum_{n=1}^{N} \sum_{\boldsymbol{k}=-\infty}^{\infty} M_k^n \, e^{\frac{i2\pi \boldsymbol{k}\cdot\boldsymbol{x}}{L}} \chi_n(h)$$

$$m(g, \boldsymbol{x}) = \sum_{\boldsymbol{s}=\boldsymbol{0}}^{\boldsymbol{S-I}} \sum_{\mu,n,l} M_{l\boldsymbol{s}}^{\mu n} \dot{T}_l^{\mu n}(g) \chi_{\boldsymbol{s}}(\boldsymbol{x})$$

$$m(c, \boldsymbol{x}) = \sum_{\boldsymbol{s}=\boldsymbol{0}}^{\boldsymbol{S-I}} \sum_{n} M_{\boldsymbol{s}}^{n} P^n(c) \chi_{\boldsymbol{s}}(\boldsymbol{x})$$

Microstructure Ensemble



$$\left\{ {}^{(j)}m_{\boldsymbol{s}}^{n};\ j = 1, 2, \ldots, J \right\}$$

a microstructure versus the microstructure

(SVE) (RVE)

Microstructure Statistics

$$m(h,\boldsymbol{x}) \approx \sum_{\tilde{n}=1}^{N} \sum_{\boldsymbol{s}=\boldsymbol{0}}^{\boldsymbol{S}-\boldsymbol{I}} m_{\boldsymbol{s}}^{n}\, \chi_n(h)\chi_{\boldsymbol{s}}(\boldsymbol{x})$$

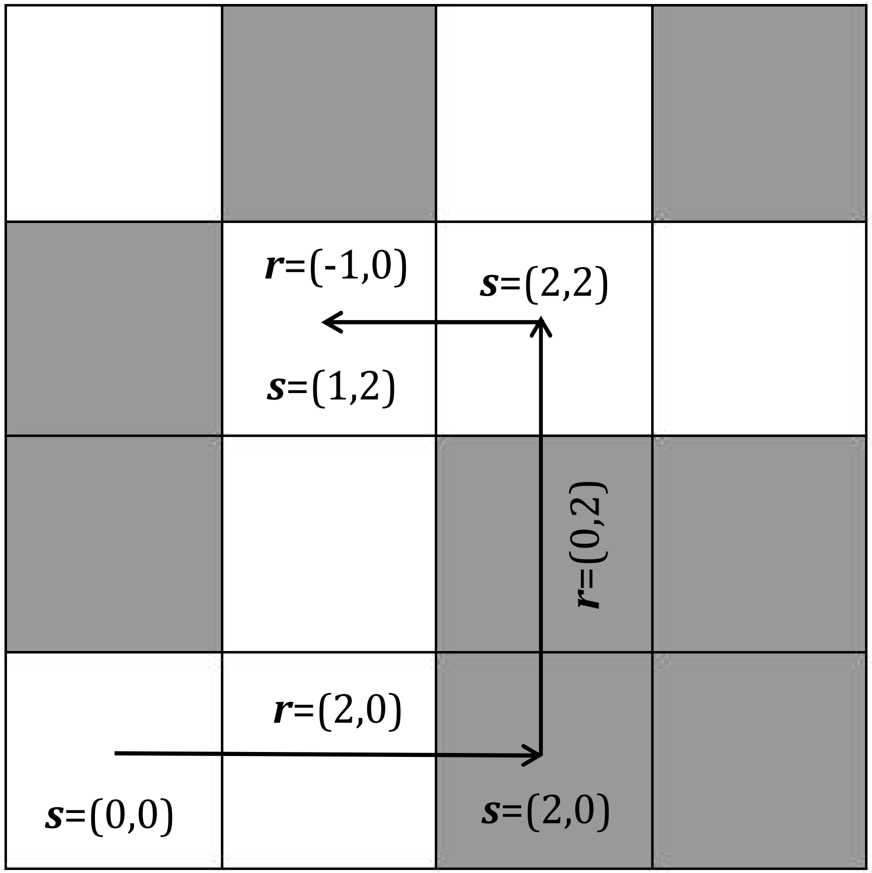
$$f_{\boldsymbol{s}}^{n} = \frac{1}{J}\sum_{j=1}^{J} {}^{(j)}m_{\boldsymbol{s}}^{n} \qquad j = 1, 2, \ldots, J$$

$$f^{n} = \frac{1}{S}\frac{1}{J}\sum_{\boldsymbol{s}}\sum_{j=1}^{J} {}^{(j)}m_{\boldsymbol{s}}^{n}$$

1-point spatial correlations or 1-point statistics

Microstructure Statistics

2-point spatial correlations or 2-point statistics



$$f_{\boldsymbol{rs}}^{np} = \frac{1}{J}\sum_{j=1}^{J} {}^{(j)}m_{\boldsymbol{s}}^{n}\ {}^{(j)}m_{\boldsymbol{s}+\boldsymbol{r}}^{p}$$

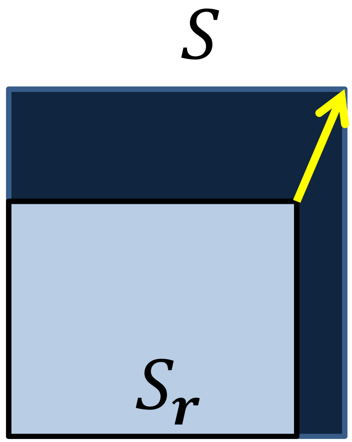
$$f_{\boldsymbol{r}}^{np} = \frac{1}{S_{\boldsymbol{r}}}\frac{1}{J}\sum_{\boldsymbol{s}}\sum_{j=1}^{J} {}^{(j)}m_{\boldsymbol{s}}^{n}\ {}^{(j)}m_{\boldsymbol{s}+\boldsymbol{r}}^{p}$$

$S_{\boldsymbol{r}}$ is the number of spatial bins that allow the placement of both ***s*** and ***s+r*** with the microstructure volume being studied

r indexes bins in vector space

Periodic Boundaries: $S_{\boldsymbol{r}} = S$

Microstructure Statistics



Non-periodic Boundaries

$$\boldsymbol{r} = r_1 i + r_2 j + r_3 k, \qquad S = S_1 S_2 S_3$$

$$S_{\boldsymbol{r}} = (S_1 - |r_1|)(S_2 - |r_2|)(S_3 - |r_3|)$$

$$f_{\boldsymbol{r}}^{np} = \frac{\sum_{s} \sum_{j=1}^{J} {}^{(j)}m_{s}^{n}\, {}^{(j)}m_{s+r}^{p}}{S_{r} J} = \frac{\#\ Successes}{\#\ Trials}$$

Redundancies in 2-pt. Statistics

$$f_{\boldsymbol{r}}^{np} = \left[\begin{pmatrix} f_{\boldsymbol{r}}^{11} & \cdots & f_{\boldsymbol{r}}^{1N} \\ \vdots & \ddots & \vdots \\ f_{\boldsymbol{r}}^{N1} & \cdots & f_{\boldsymbol{r}}^{NN} \end{pmatrix}\right]$$

$$f_{\boldsymbol{r}}^{np} = f_{-\boldsymbol{r}}^{pn} \qquad \sum_{p=1}^{N} f_{\boldsymbol{r}}^{np} = f^{n}$$

For a two-phase material, if $f_{\boldsymbol{r}}^{11}$ is known then $f_{\boldsymbol{r}}^{12}$, $f_{\boldsymbol{r}}^{21}$ and $f_{\boldsymbol{r}}^{22}$ can be calculated.

Niezgoda et al., Acta Materialia, 2008. **56**(18), p. 5285-5292: Only (N-1) independent correlations (using DFTs)

2-pt. Statistics Using DFTs

Implicitly assume periodic boundaries

$$f_{\boldsymbol{r}}^{np} = \frac{1}{S_{\boldsymbol{r}}} \sum_{\boldsymbol{s}} m_{\boldsymbol{s}}^{n} m_{\boldsymbol{s}+\boldsymbol{r}}^{p}$$

$$M_{\boldsymbol{k}}^{n} = \Im(m_{s}^{n}) = \sum_{\boldsymbol{s}=\boldsymbol{0}}^{\boldsymbol{S}-\boldsymbol{1}} m_{s}^{n} e^{2\pi i \boldsymbol{s}\cdot\boldsymbol{k}/S}$$

$$F_{\boldsymbol{k}}^{np} = \Im\left(f_{\boldsymbol{r}}^{np}\right) = \frac{1}{S} M_{\boldsymbol{k}}^{n*} M_{\boldsymbol{k}}^{p}$$

$$f_{\boldsymbol{r}}^{np} = f_{\boldsymbol{r}}^{np*} \Rightarrow F_{\boldsymbol{k}}^{np} = F_{(\boldsymbol{S}-\boldsymbol{1})-\boldsymbol{k}}^{np*}$$

Autocorrelations: $F_{\boldsymbol{k}}^{nn} = F_{\boldsymbol{k}}^{nn*}$

Plotting 2-pt. Statistics Using DFTs

$$M_{\boldsymbol{k}}^{n} = \Im(m_{\boldsymbol{s}}^{n}) = \sum_{\boldsymbol{s}=\mathbf{0}}^{\boldsymbol{S}-\mathbf{1}} m_{s}^{n} e^{2\pi i \boldsymbol{s}\cdot\boldsymbol{k}/S} \qquad \boldsymbol{s} = \mathbf{0}, \mathbf{1}, \dots, \boldsymbol{S} - \mathbf{1}$$

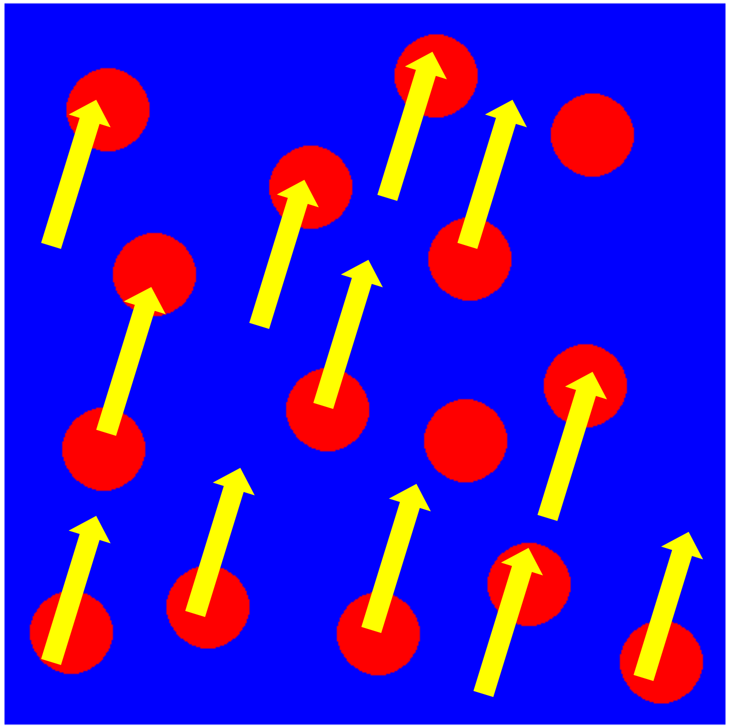
$$F_{\boldsymbol{k}}^{np} = \Im\left(f_{\boldsymbol{r}}^{np}\right) = \frac{1}{S} M_{\boldsymbol{k}}^{n*} M_{\boldsymbol{k}}^{p} \qquad \boldsymbol{r} = \mathbf{0}, \mathbf{1}, \dots, \boldsymbol{S} - \mathbf{1}$$

<u>Plotting:</u> $\boldsymbol{r} = -(\boldsymbol{S} - \mathbf{1})/2, \dots - \mathbf{1}, \mathbf{0}, \mathbf{1}, \dots, (\boldsymbol{S} - \mathbf{1})/2$

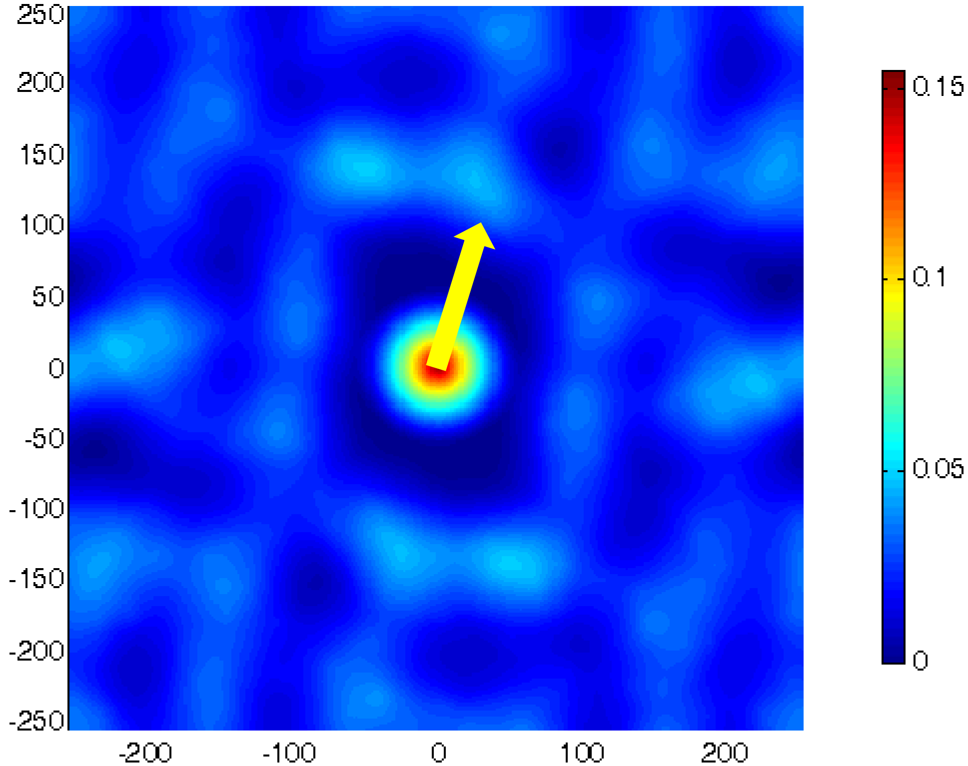
($\boldsymbol{r} = -\boldsymbol{S}/2, \dots - \mathbf{1}, \mathbf{0}, \mathbf{1}, \dots, \ \boldsymbol{S}/2$ when $\boldsymbol{S}$ is even)

$$f_{\boldsymbol{r}}^{np} = f_{\boldsymbol{r}+\boldsymbol{S}}^{np}$$

Plotting 2-Point Correlations



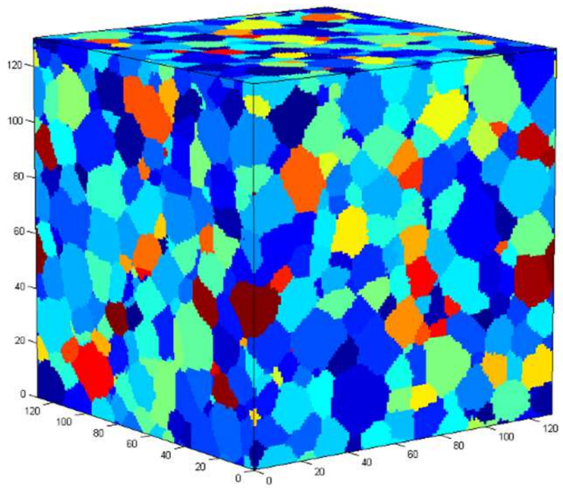
Microstructure

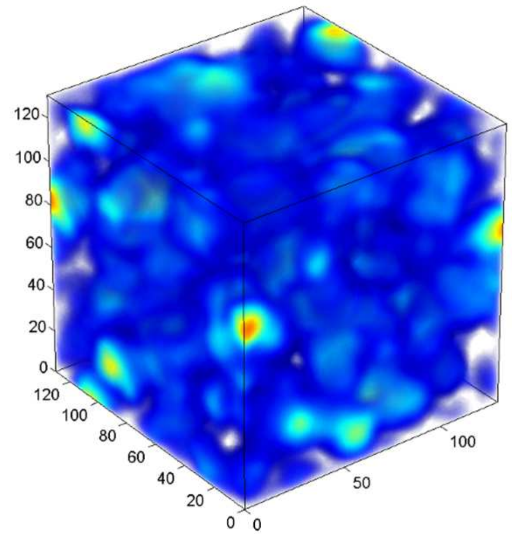


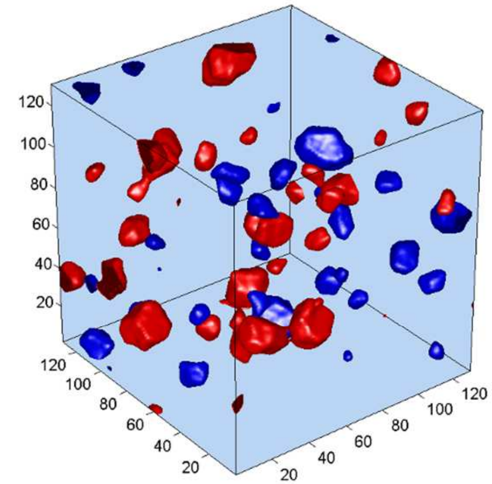
2-point auto correlation

- Image is converted into a smooth continuous pdf
- pdf allows easy statistical operations: mean, variance, …
- Dominant features of the pdf can be connected to properties and tracked in manufacturing processes

Reconstruction from 2-pt Statistics

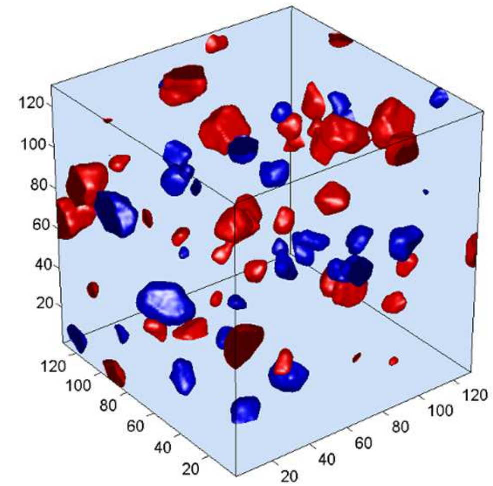






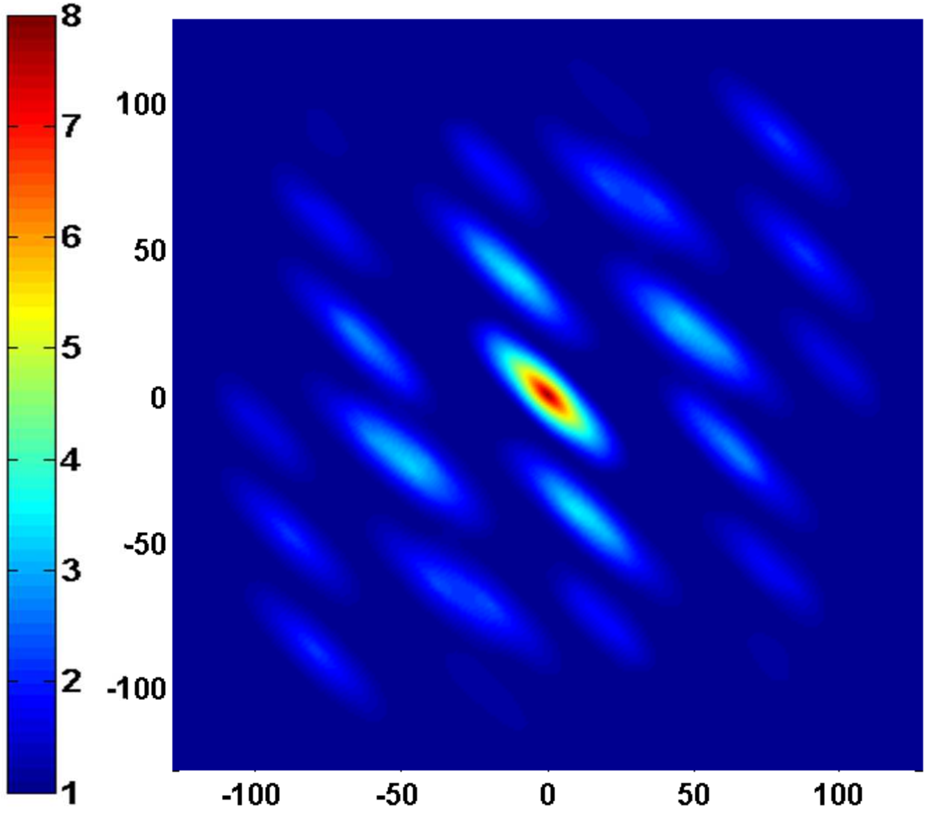
Original microstructure of 130x130x130 volume elements with orientation space binned into 512 distinct orientations. The far right shows bin 35 as blue and bin 5 as red in the original microstructure.

Bottom: Bins 35 and 5 are reconstructed exactly up to a linear shift!



Coherence Length

Coherence length (C) provides guidance on scan sizes



$$\lim_{|\mathbf{r}| \to C} \frac{f_2\left(h, h' \middle| \mathbf{r}\right)}{f(h)\, f(h')} = 1$$

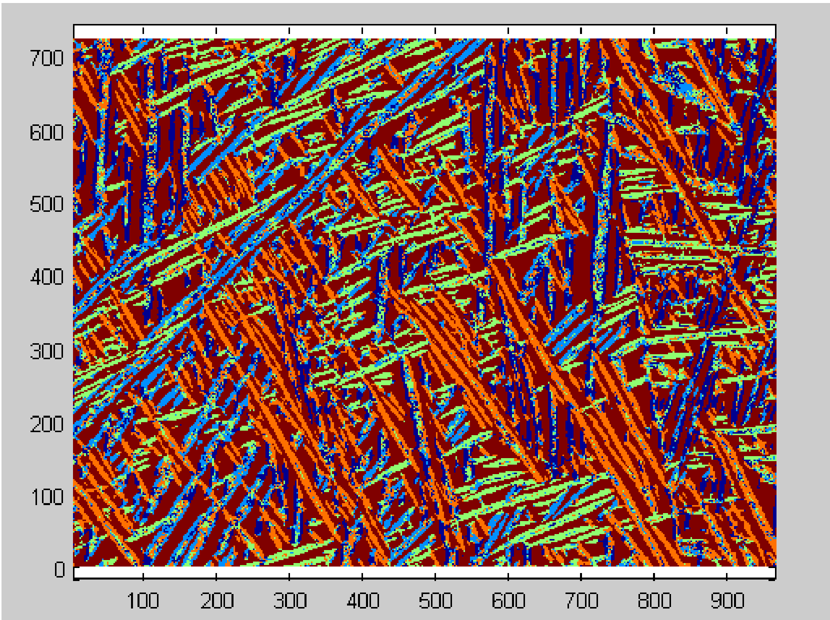
<u>Example Digitally Created Microstructure:</u>

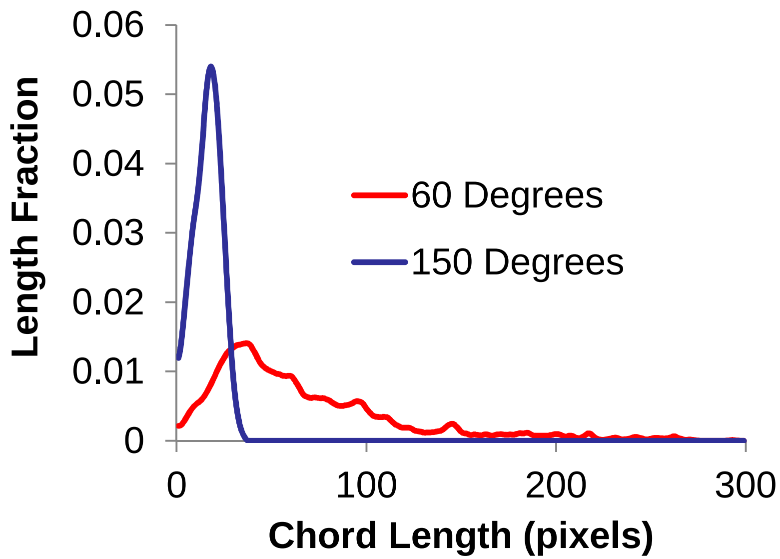
Average Feature Size ~ 15 pixels

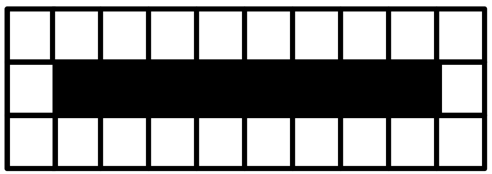
Coherence Length for Auto-correlation ~ 125 pixels

Features of Interest

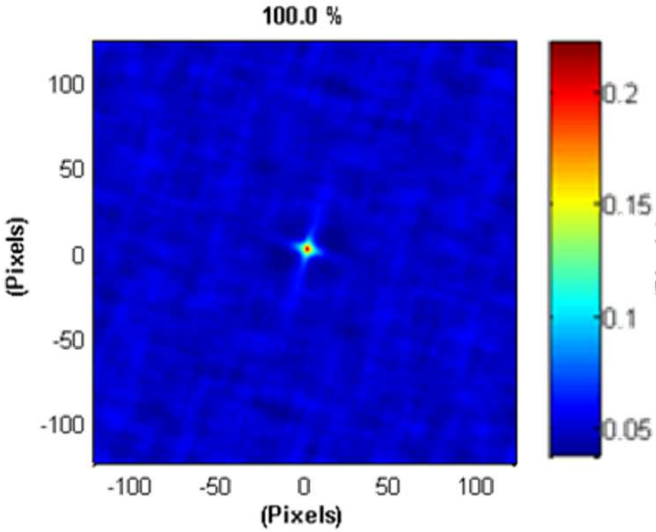
Many local features of interest can be identified based on concepts of n-point statistics

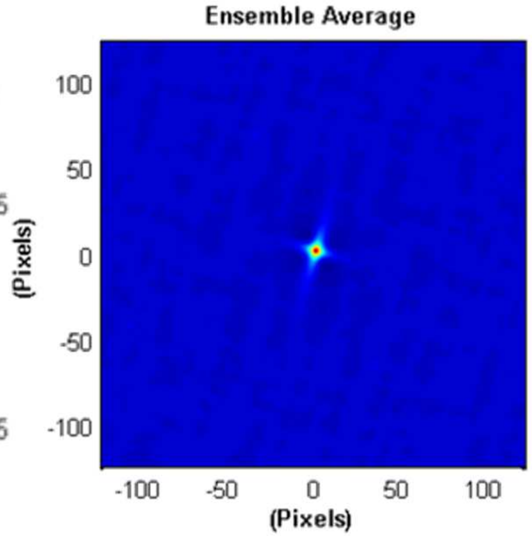


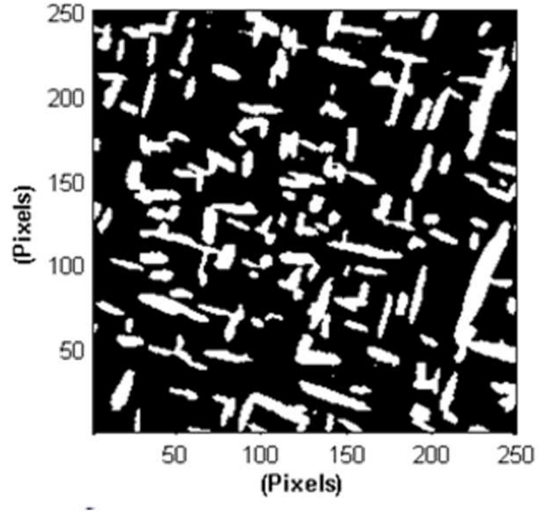


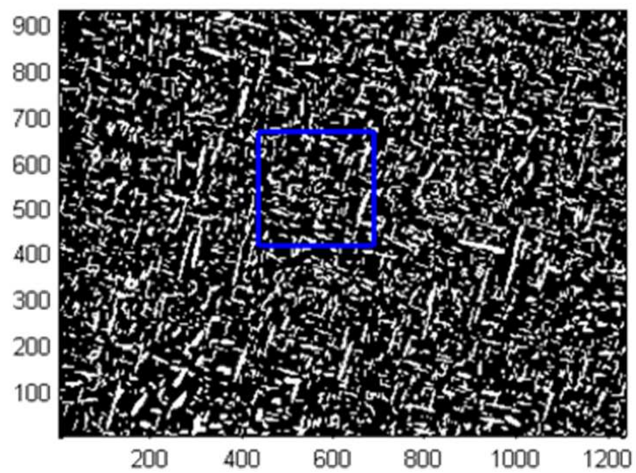


RVE









Elastic Modulus

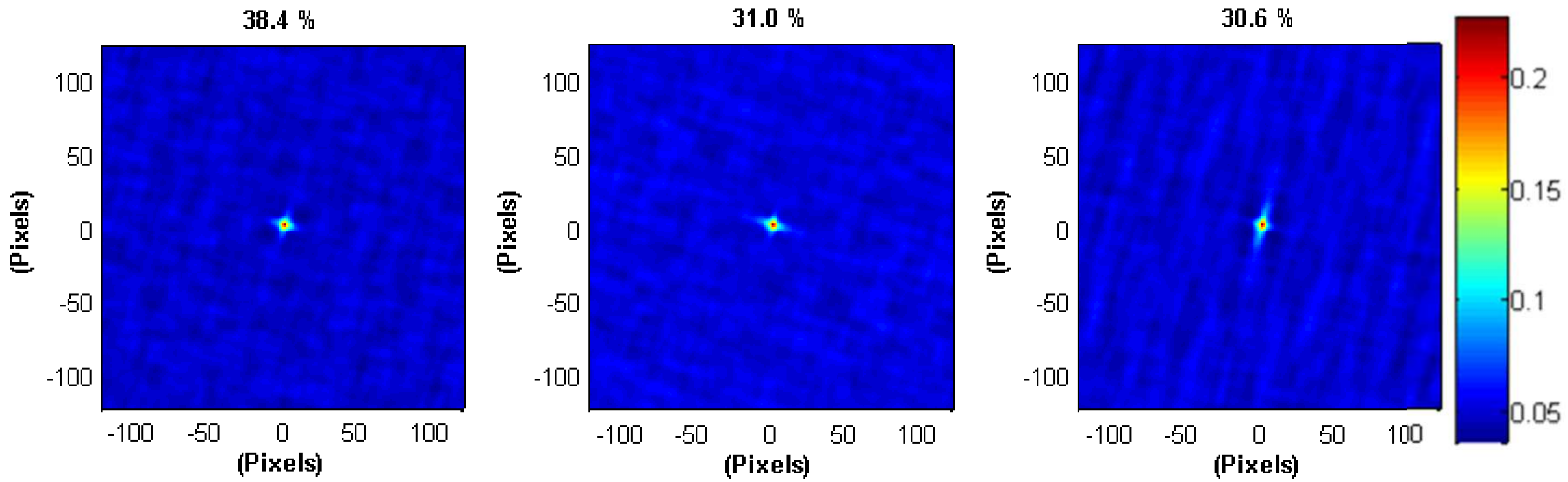
RVE: 111 GPa
Sample: 111 GPa

Critically Stressed Volume Fraction

RVE: 0.0866
Sample: 0.0897

3% Error

Weighted SVE Sets

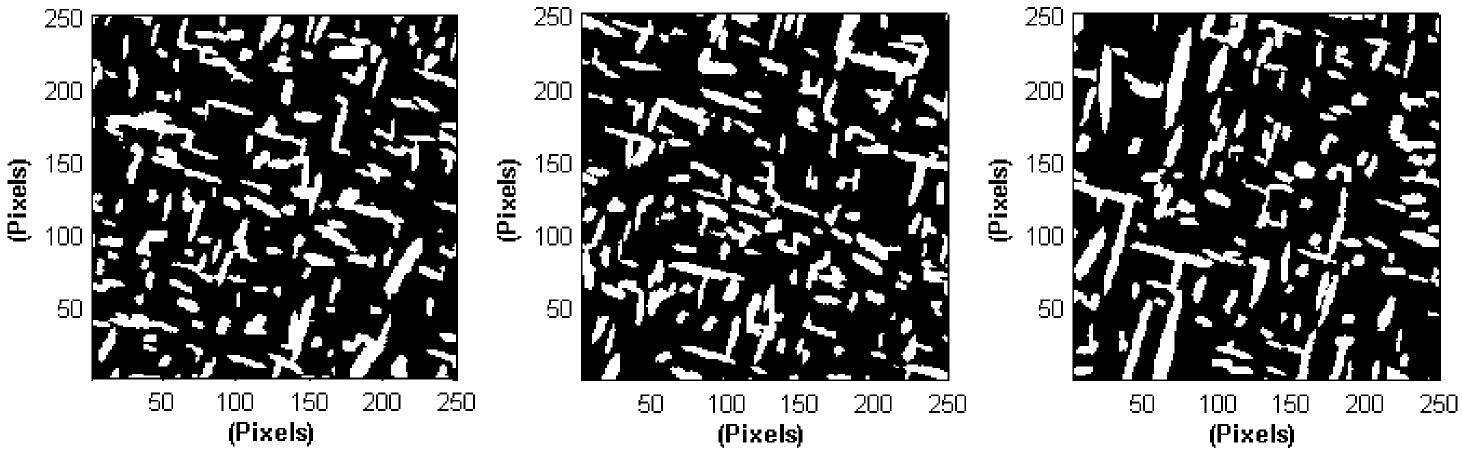


Critically Stressed Volume Fraction in Sample = 0.0897

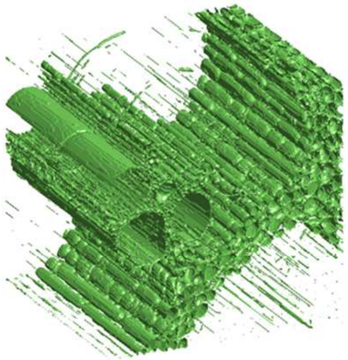
0.0810
9.9% Error

0.0909
1.3% Error

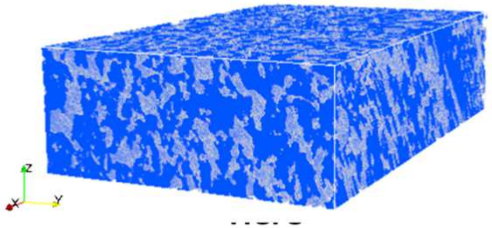
0.0974
8.6% Error



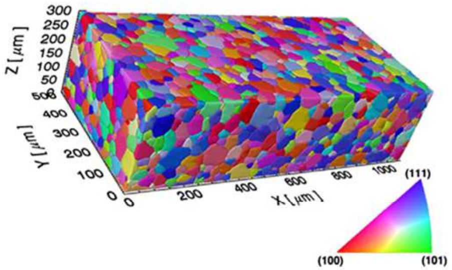
Microstructure Representation



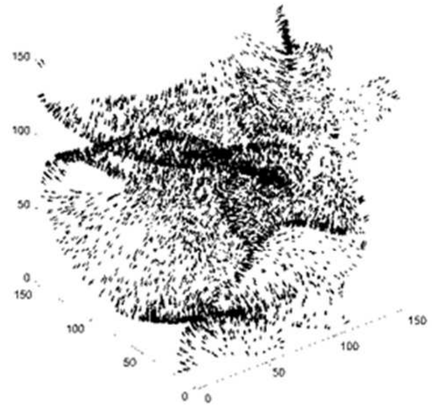
Bamboo
X-Ray Tomography



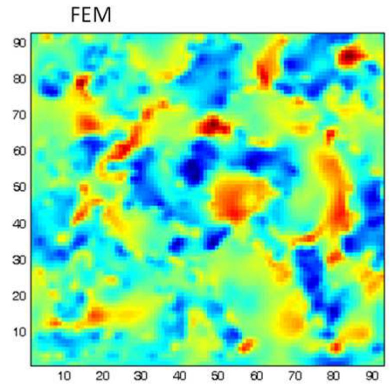
Fuel Cell Micro Porous Layer
FIB SEM



Beta Titanium
Mechanically Polished SEM+EBSD

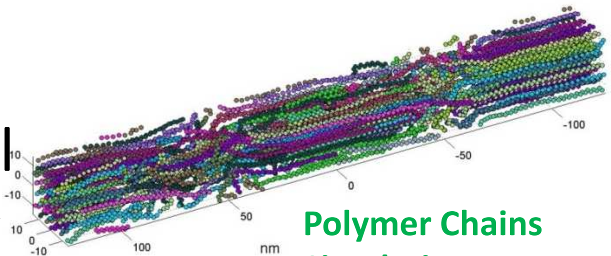


Surface Curvature data



Strain Distribution Simulation Data

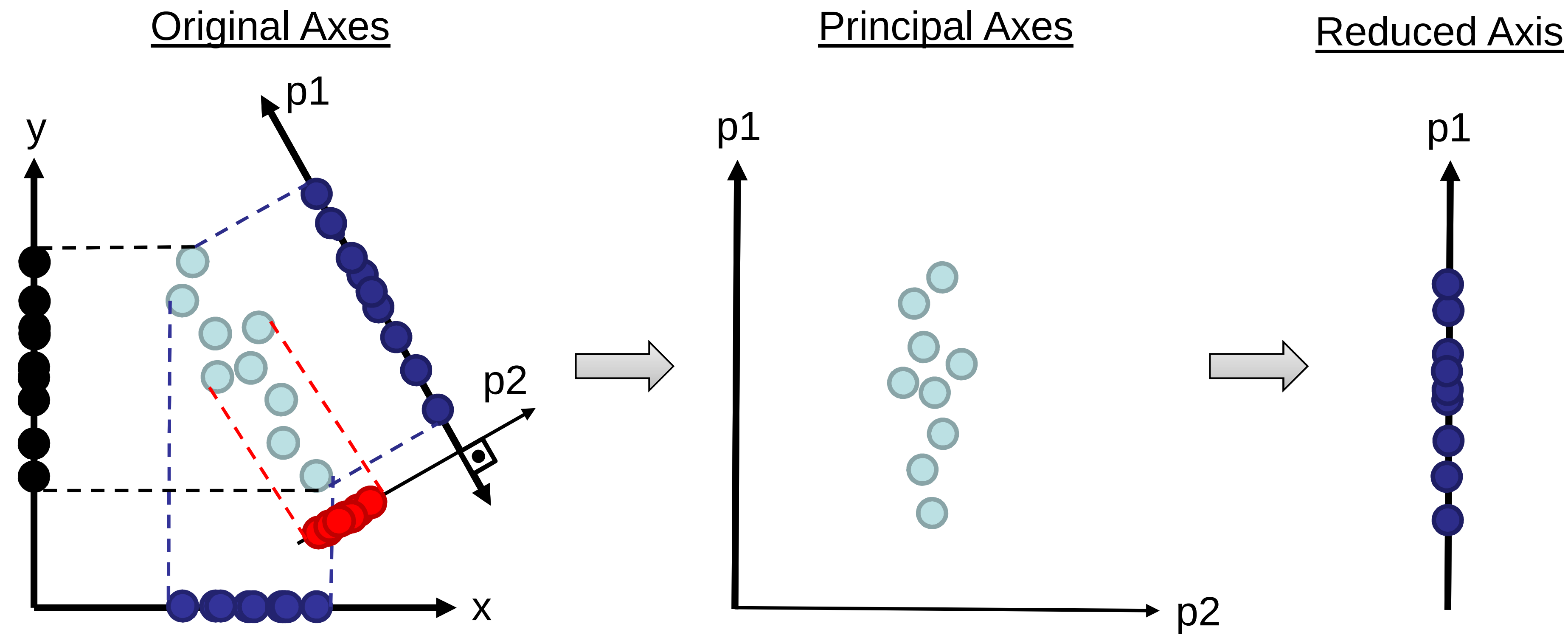
- Thinking of microstructure as a **digital signal** allows a generalized treatment at multiple hierarchical length/structure scales: m_s^h
- Intuitive measures of microstructure: average grain size, average spacing, ODF, MODF, ...
- Naturally organized extensible measures of microstructure: **n-point statistics**
- **Data Analytics**: seek objective low-dimensional representations for process-structure-property relationships



Polymer Chains Simulation Data

Dimensionality Reduction

Intuition and/or Known Physics and/or Data Driven



- Axes prioritized based on variance in the data
- Unsupervised (i.e., uninformed) and Independent

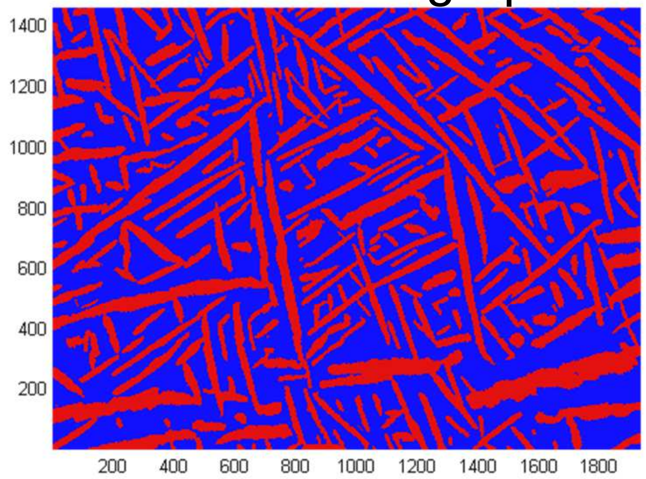
PC Scores as Microstructure Measures

Hypothesis: PCA weights of *n*-point statistics provide objective measures of microstructure

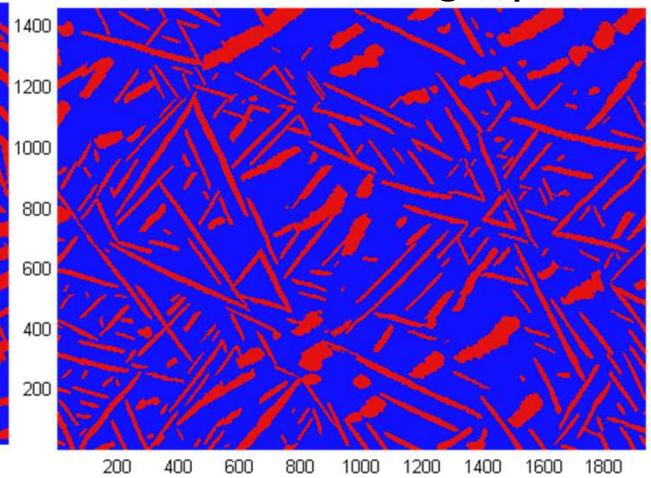
$$f_r^{(j)} = \sum_{k=1}^{\min((J-1),R)} \alpha_k^{(j)} \varphi_{kr} + \bar{f}_r$$

Microstructure Databases

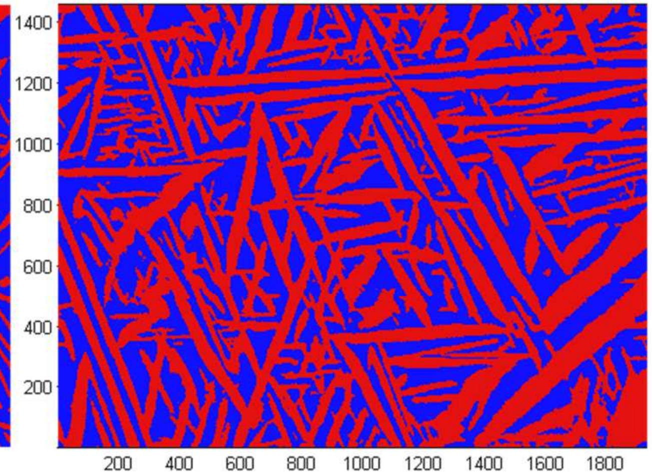
HT1-20 micrographs

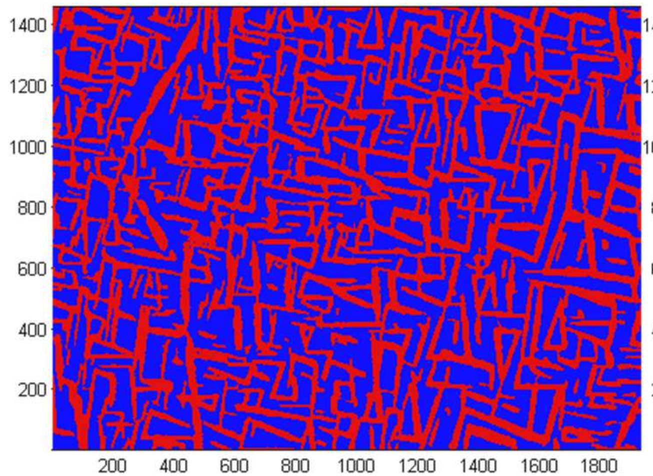


HT2-28 Micrographs

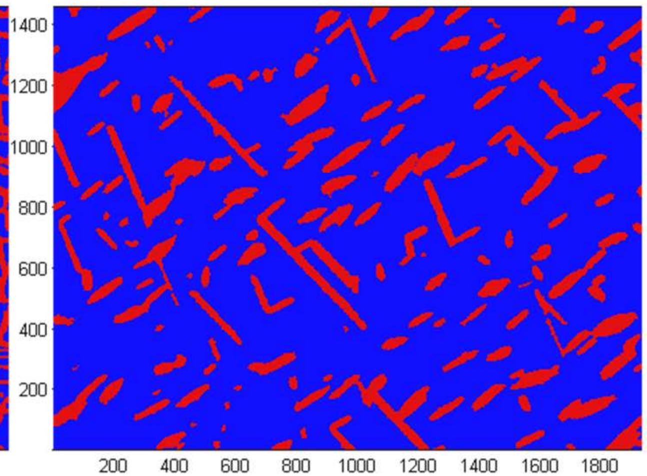


HT3-32 micrographs





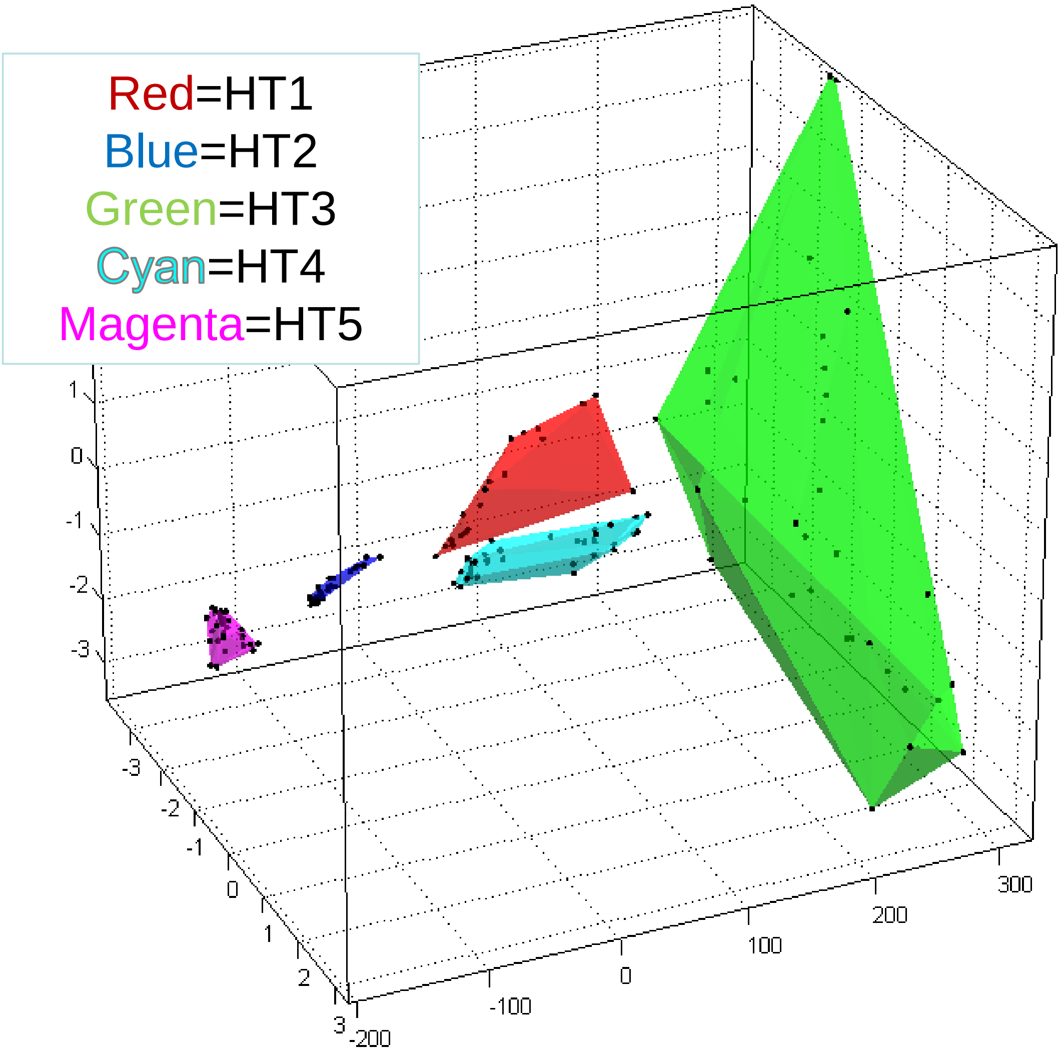
HT4-36 micrographs



HT5-32 micrographs

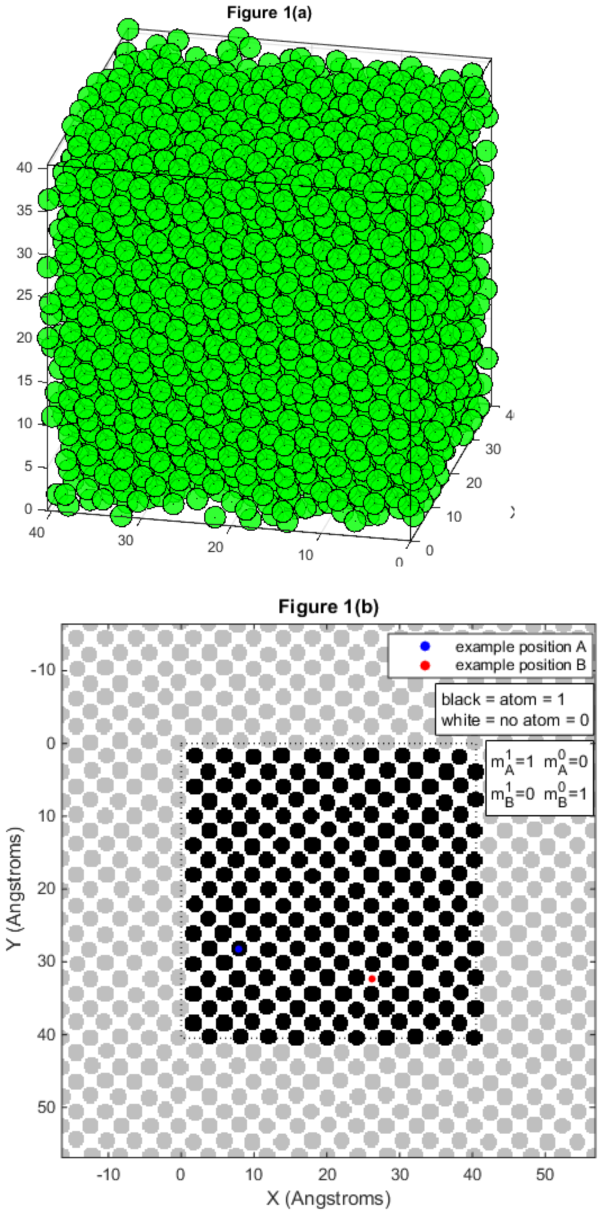
Data from
H. Fraser's
group at
OSU

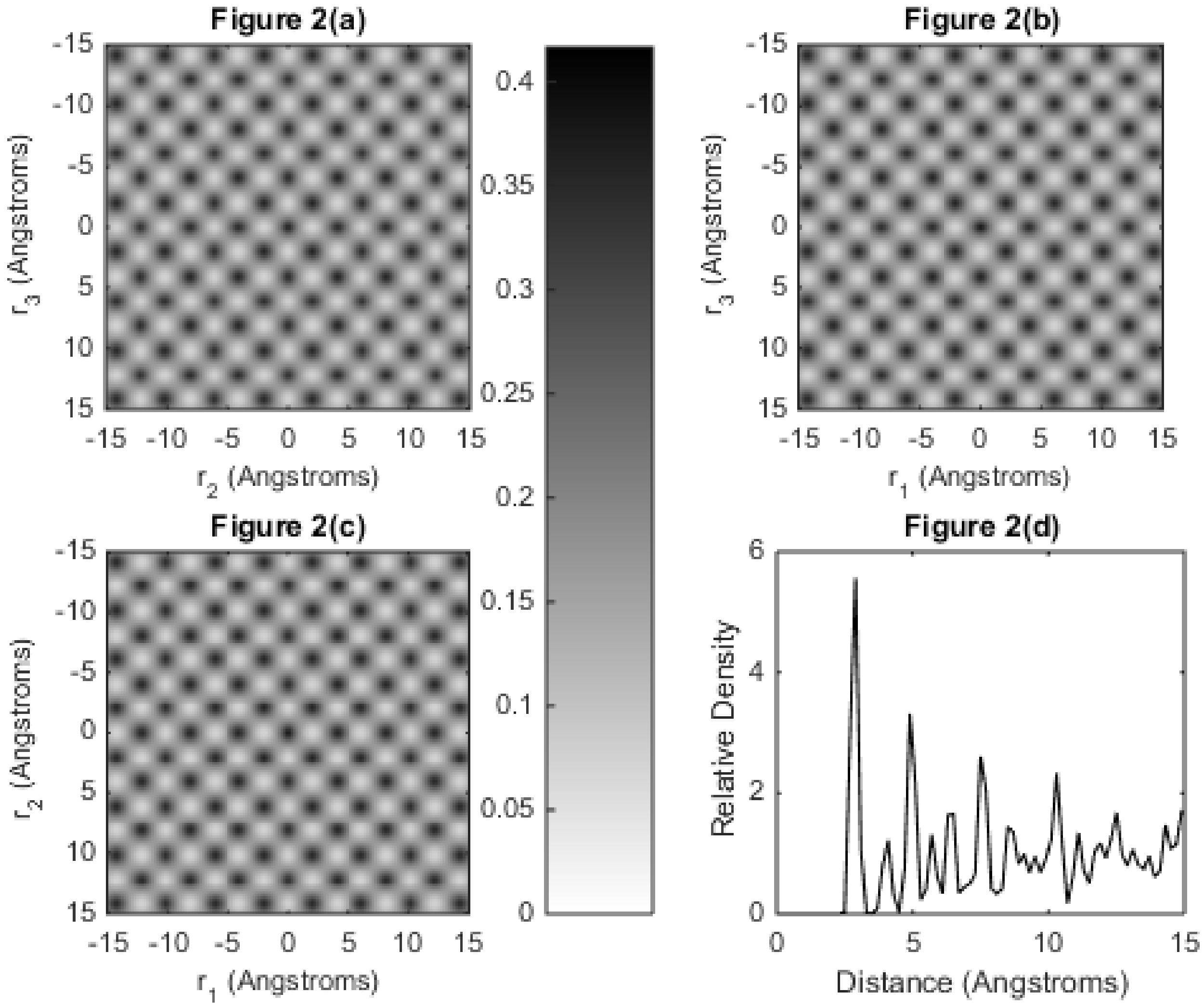
Microstructure Databases



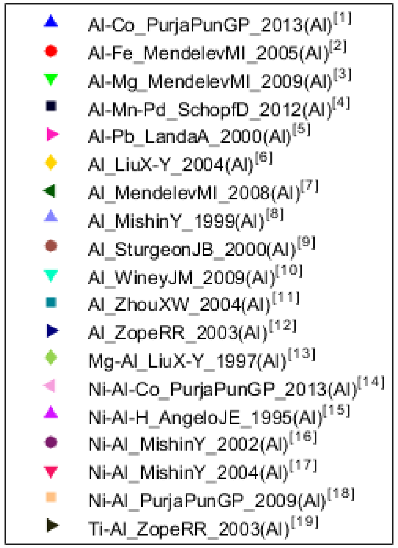
- Each point corresponds to a microstructure dataset.
- Datasets from the same heat treatment are shown as a hull.
- Volume of the hull can be related directly to the variance in structure between datasets.
- Euclidean distance is a metric of similarity or difference between samples
- Quality control applications

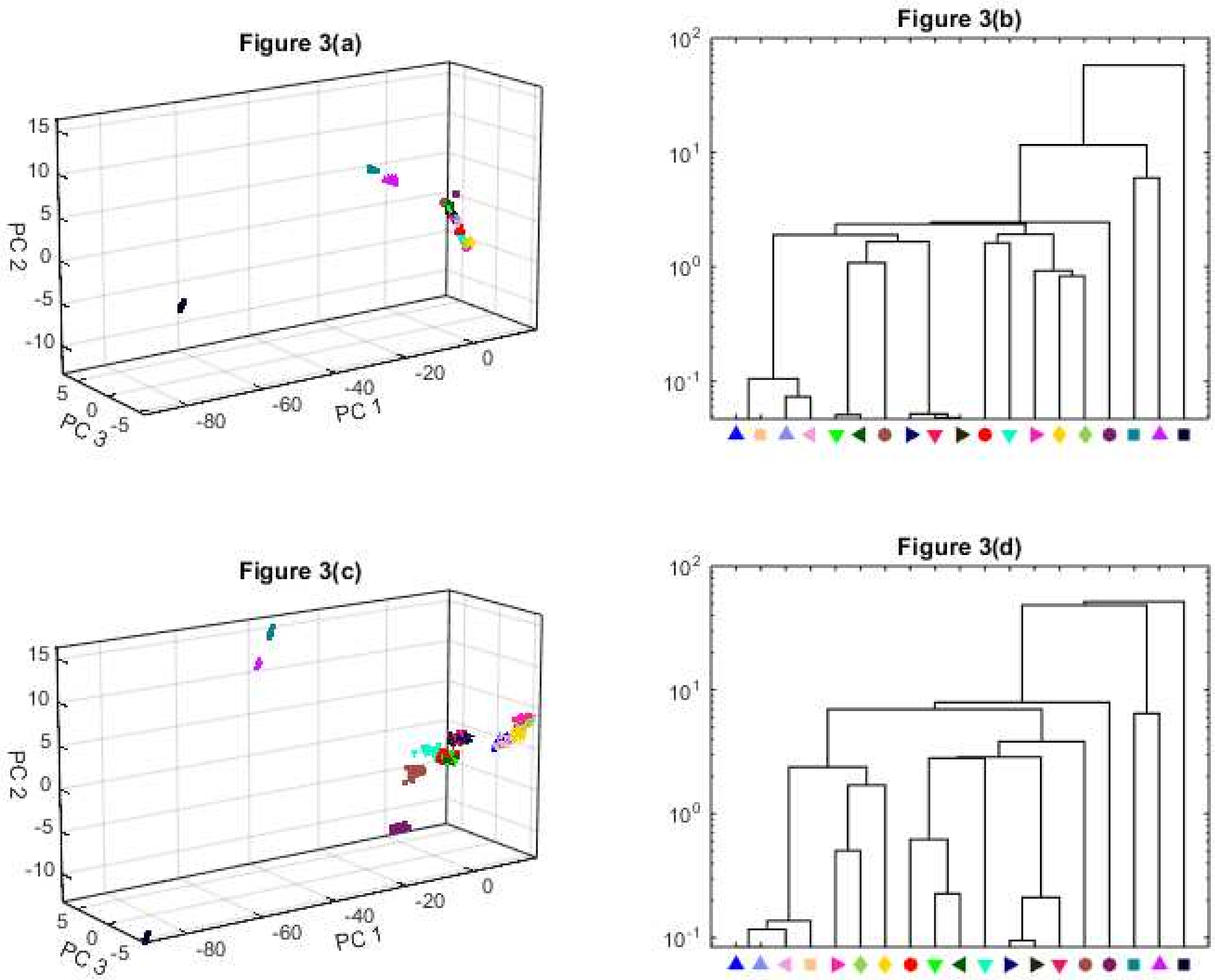
Microstructure Databases





Unsupervised Classification of Different Potentials Based on Atomic Structure

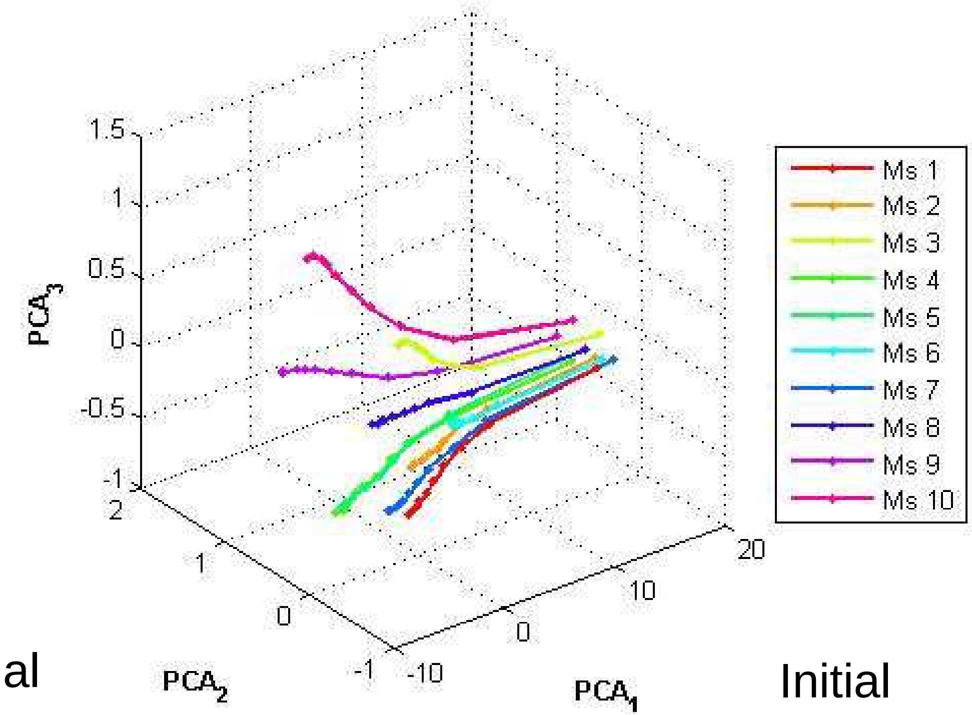




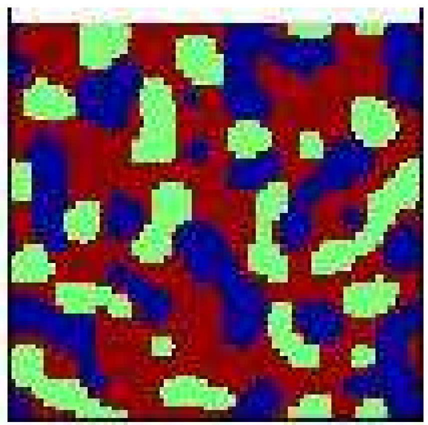
Collaboration with Becker and Trautt (NIST)

Visualization of 4-D Microstructure Datasets

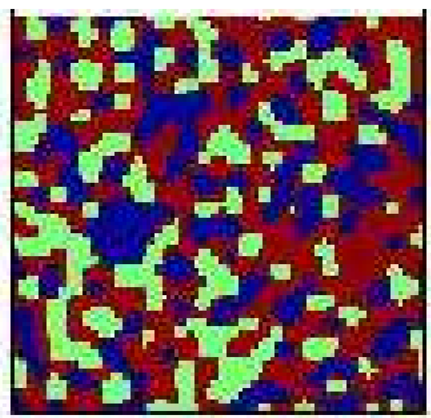
Datasets from phase-field simulations of microstructure evolution (3-D space + time)



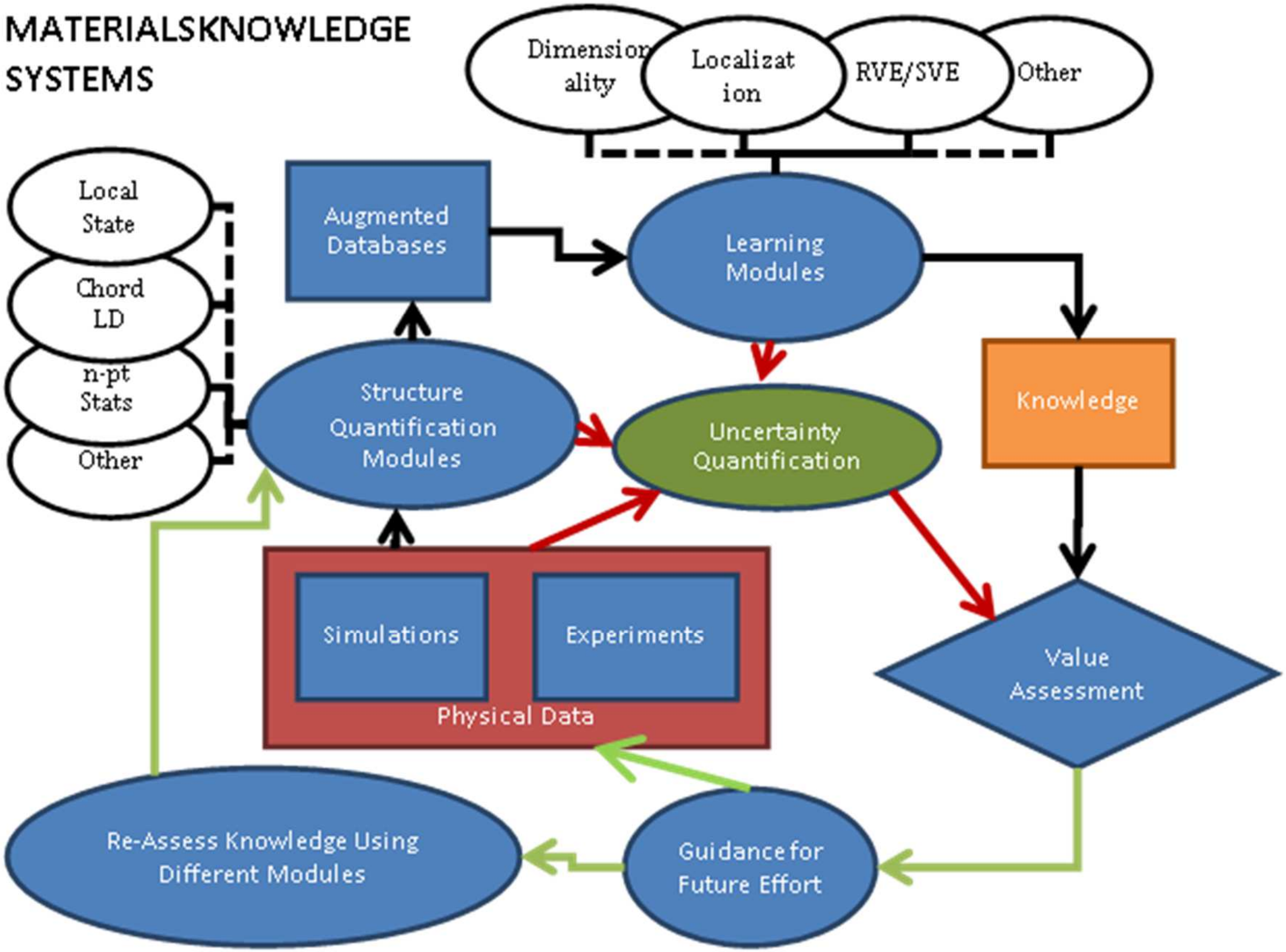
Final



Initial



Overall Framework



Code Repositories

- **Spatial Statistics**
  http://tonyfast.com/SpatialStatisticsFFT/

- **PyMKS**
  http://openmaterials.github.io/pymks/index.html