Design of Emerging Engineered Material Systems

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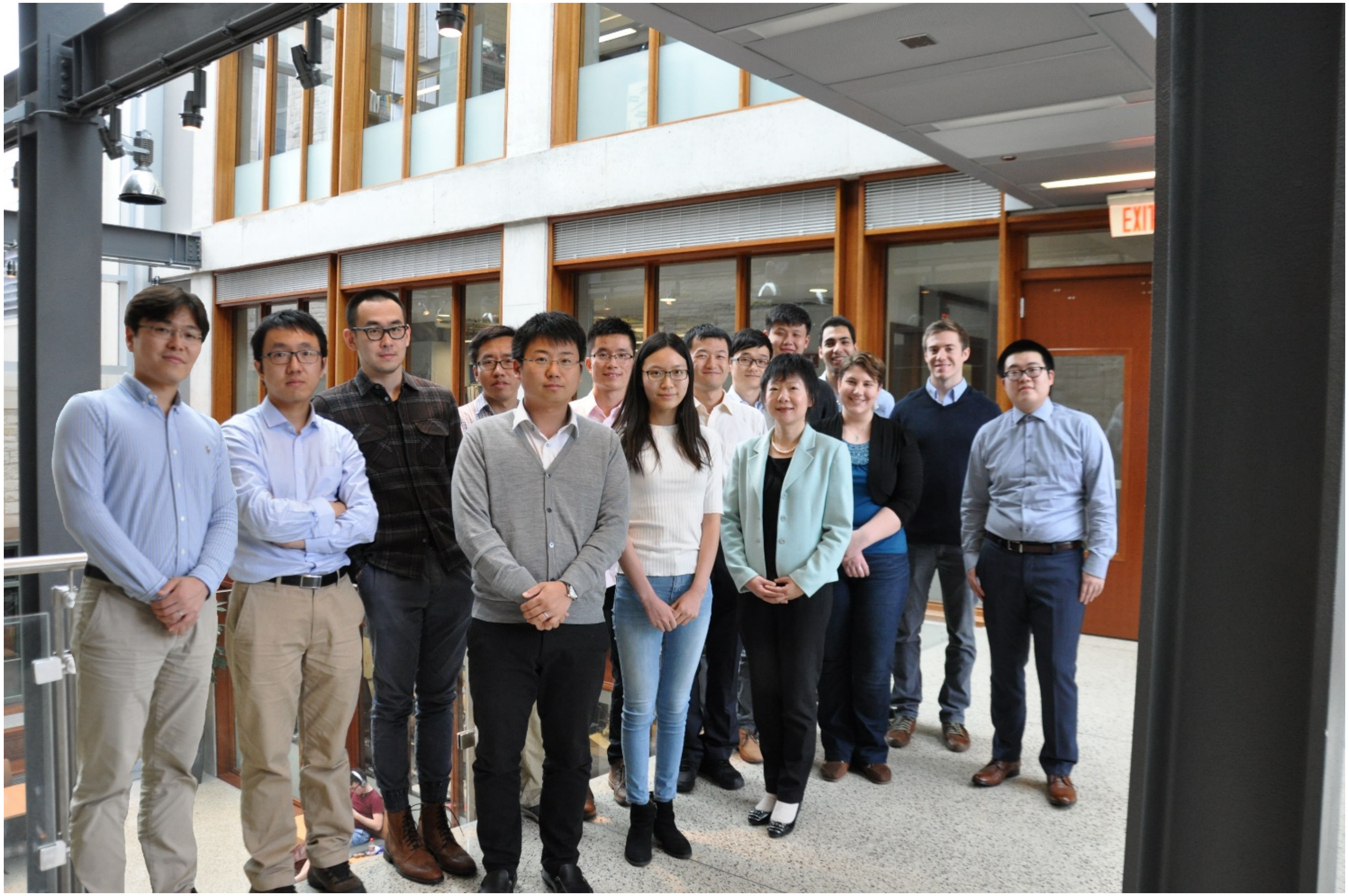
Integrated DEsign Automation Laboratory (*IDEAL*)

http://ideal.mech.northwestern.edu/

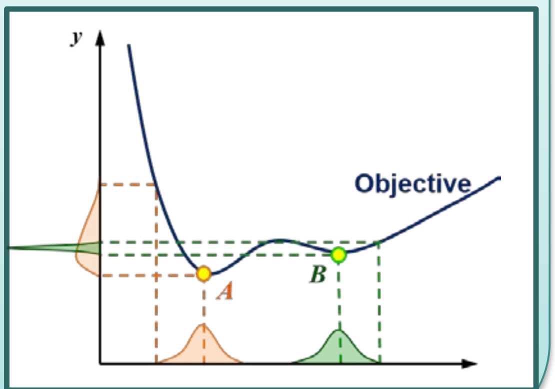
Integrated DEsign Automation Laboratory (IDEAL)

Develop advanced computational and statistical techniques to support engineering design, manufacturing, and product realization.



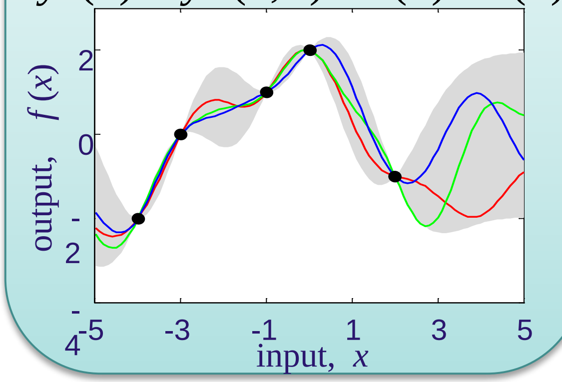
Major Research Areas

Design under Uncertainty

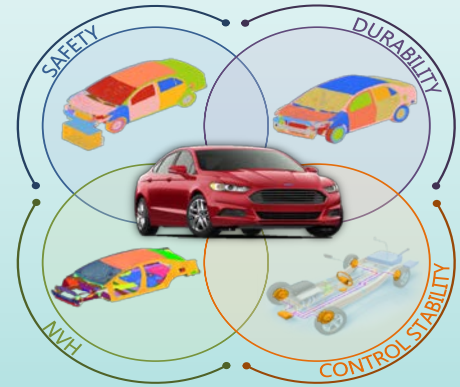


Uncertainty Quantification

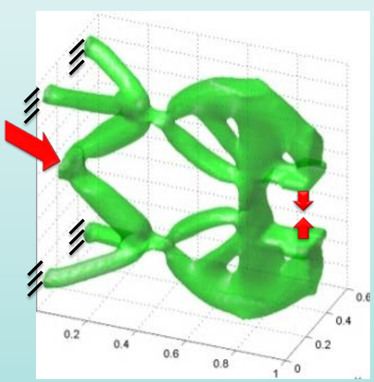
$$y^e(\mathbf{x}) = y^m(\mathbf{x}, \boldsymbol{\theta}) + \delta(\mathbf{x}) + \varepsilon(\mathbf{x})$$



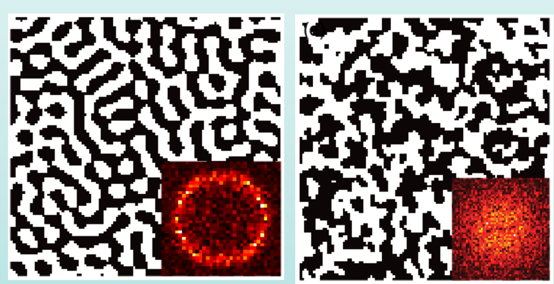
Multidisciplinary Design Optimization



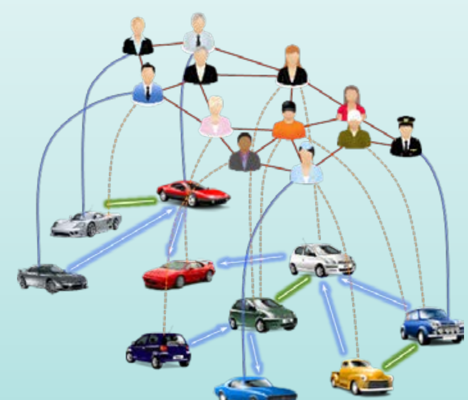
Robust Shape & Topology Optimization



Design of Emerging Material Systems



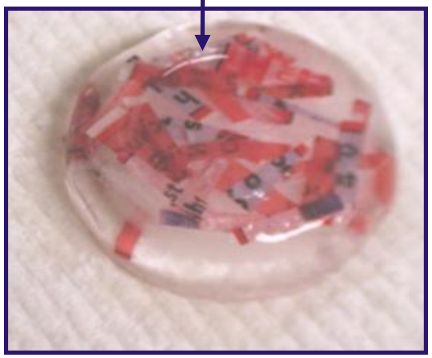
Enterprise-Driven Decision Based Design



Opportunity in Materials Design

Ice

“Reinforced” Ice



Dropped

Dropped

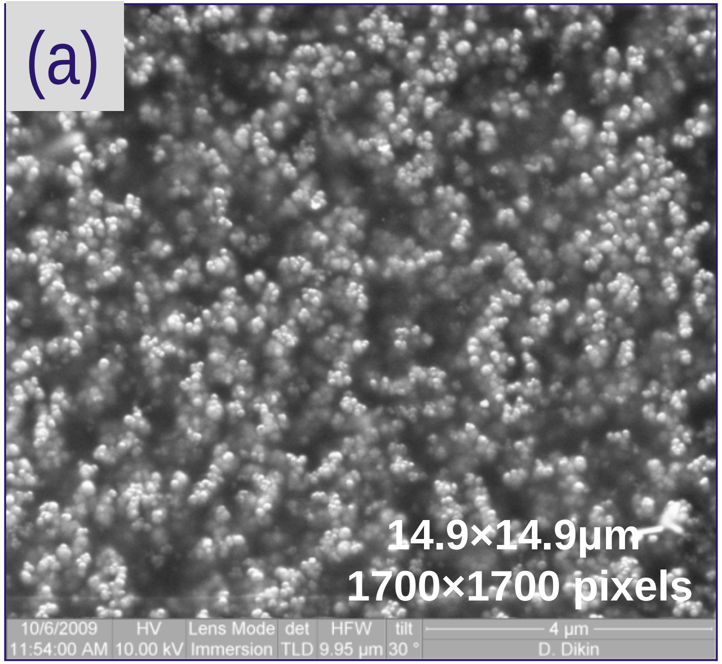
Courtesy of Y-H Chung

Advanced Materials System

- New materials
- Multiple material constituents
- Superior properties

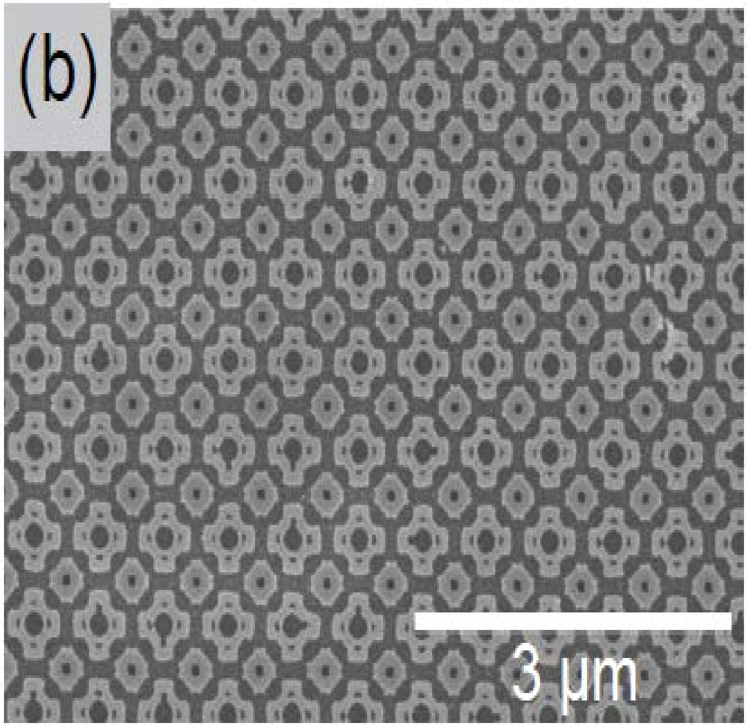
Two Types of Nanostructured Materials Design

Microstructural Morphology



Polymer Nanocomposites

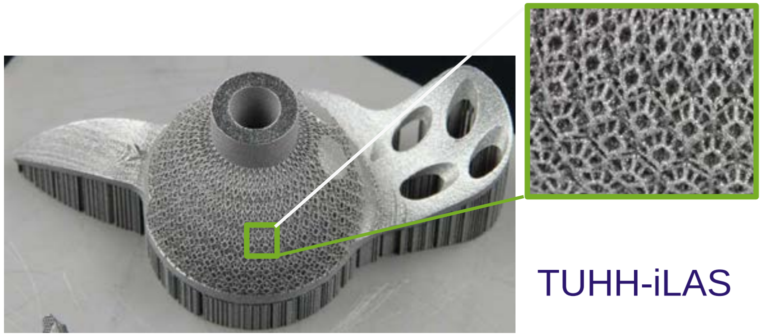
Metamaterial Topology



Thin-Film Solar Cell

Multiscale Structures from Additive Manufacturing

TUHH-iLAS

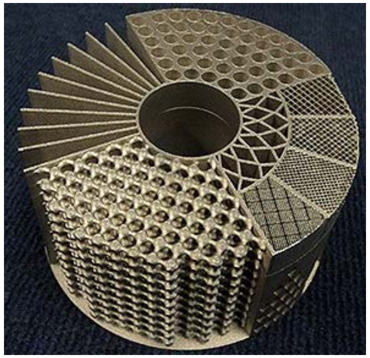


TUHH-iLAS

Sophisticated macro structures enabled by additive manufacturing

Benefits of multiscale latticed structures:

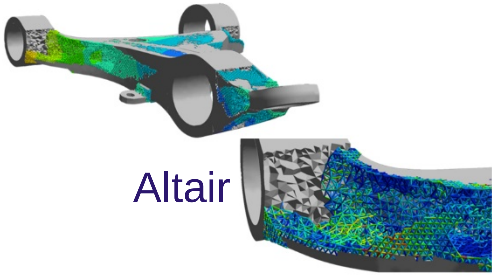
- Additional weight reduction
- Increased surface area
- Desired permeability
- Another design dimension



Lockheed Martin

Lattice materials by additive manufacturing

Altair



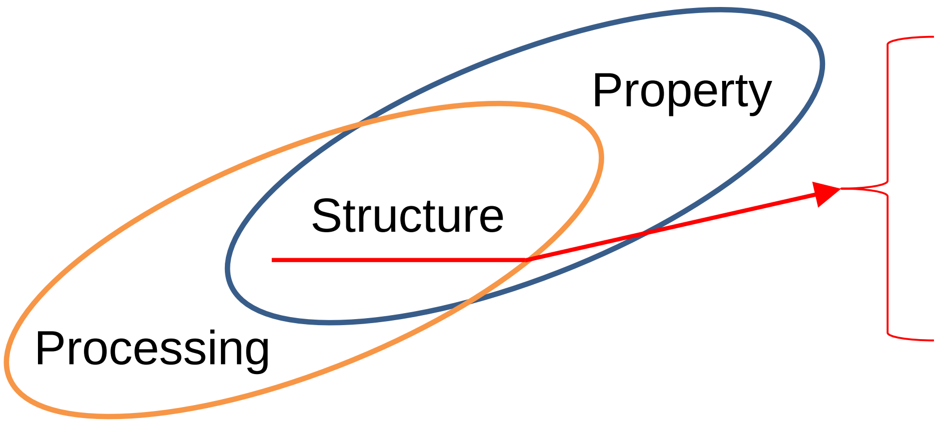
CAESS

GKN Aerospace

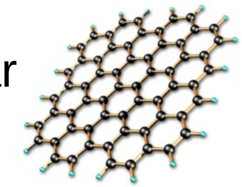
Paradigm Shift: Microstructure-Mediated Design

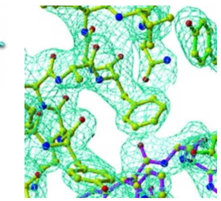
Microstructural Materials:

Spatial arrangement of local microstructure features at various constituent length scales highly influence overall properties

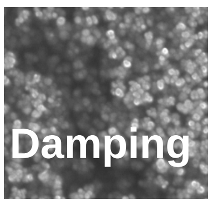


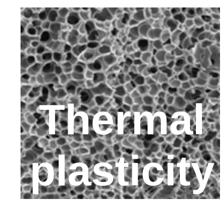
Atomic/molecular level





Micro level





Computational "Microstructure-mediated" design
(McDowell, D. L., Olson, G., B., 2008)

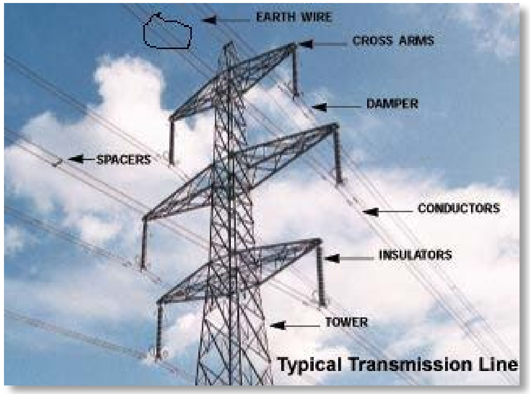
- Advanced simulation
- Material Informatics
- System Design Methodologies

Integrated DEsign Automation Laboratory

Design of Polymer Nanodielectric Systems (NSF/DEMS, Chen-Brinson-Schadler)

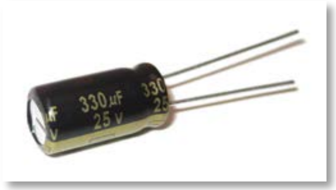
Application of Dielectric Material

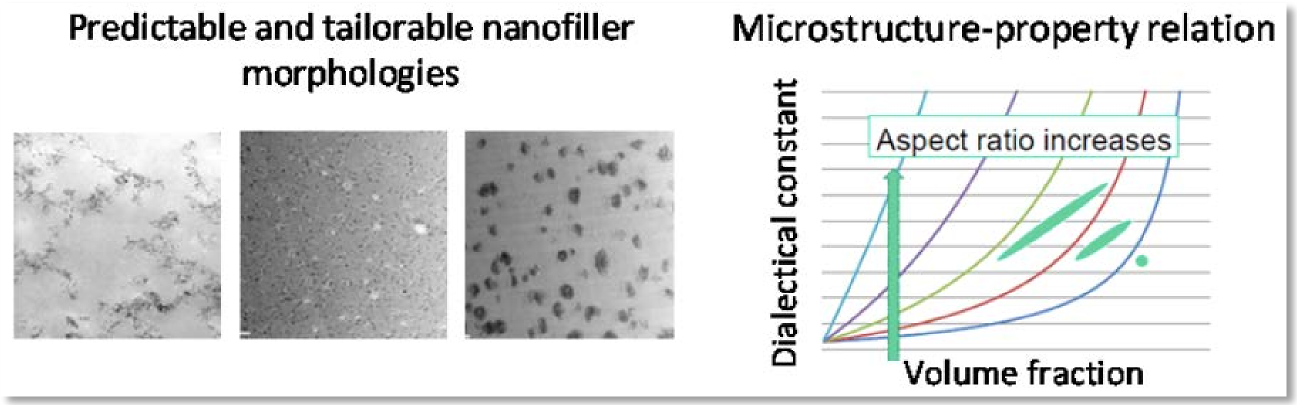
- Wires and cables that carry electrical current
- Insulation in heavy machinery
- Insulation material in capacitors

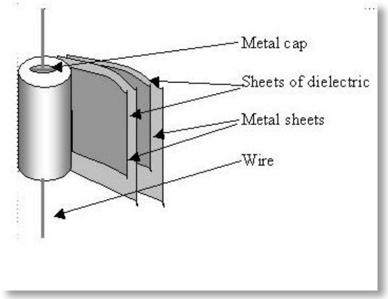


Design Criteria

- High dielectric constant, low dielectric loss
- High breakdown strength (complicated physical model)
- High strength endurance

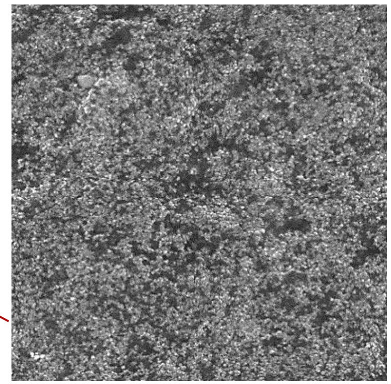




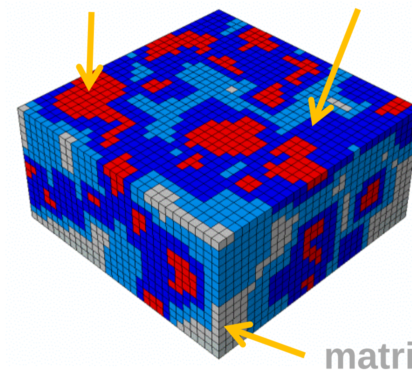


Design of Tire Polymer Nanocomposite (Goodyear)

GOODYEAR

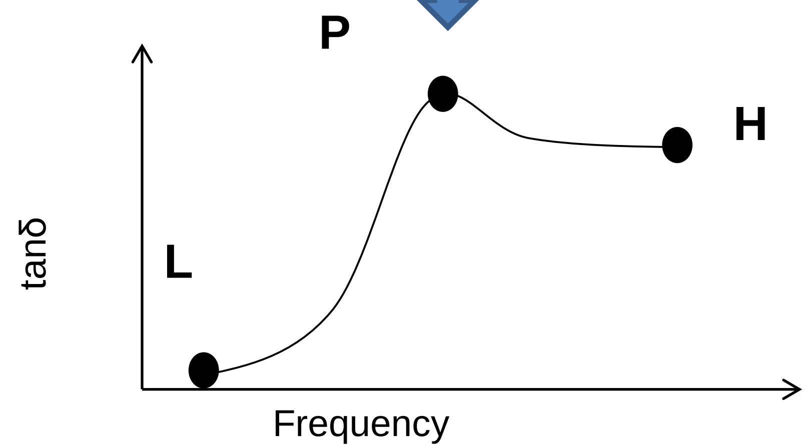


FEA Model



Design Objective

- ❑ Min L (Min wear)
- ❑ Max P (Max wet traction)
- ❑ Max H (Min rolling resistance)



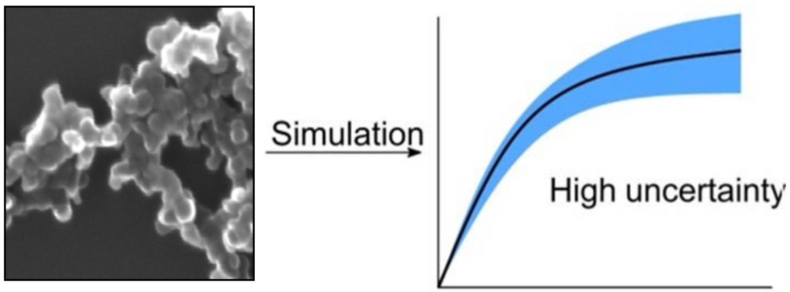
Design Challenges

- **Complexity**: multidisciplinary, multiscale materials-structure system, expensive simulations
- **Stochasticity**: uncertainties induced by materials structural heterogeneity, manufacturing imperfection, and lacking of knowledge
- **Manufacturability**: mapping between processing and structure; manufacturability constraints; top-down vs bottom-up processes
- **Material Informatics**: exploration of vast materials database & computational models

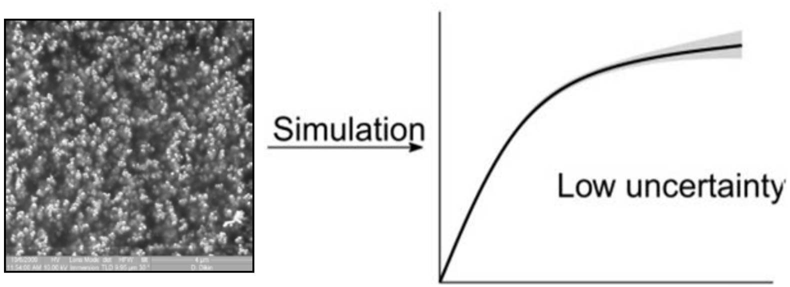
Need for Stochastic Characterization and Prediction

- Smaller volume element ⟶ larger uncertainty in constitutive relations

Statistical Volume Element (SVE)

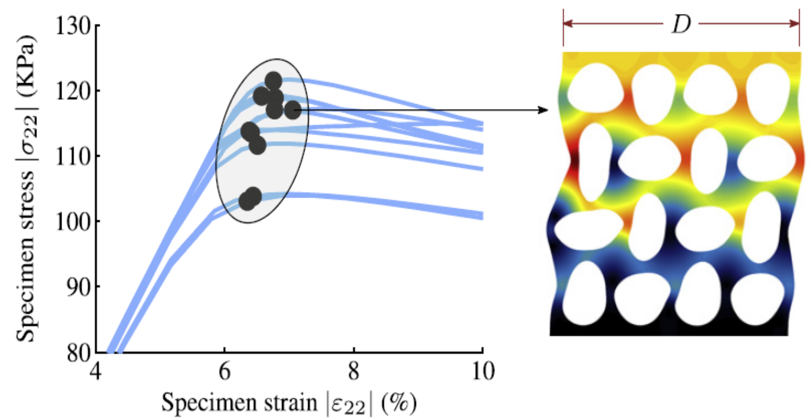


Representative Volume Element (RVE)



- The uncertainty of certain behavior (fracture, failure, fatigue, etc.) is large.
- Cell averaging is not applicable.

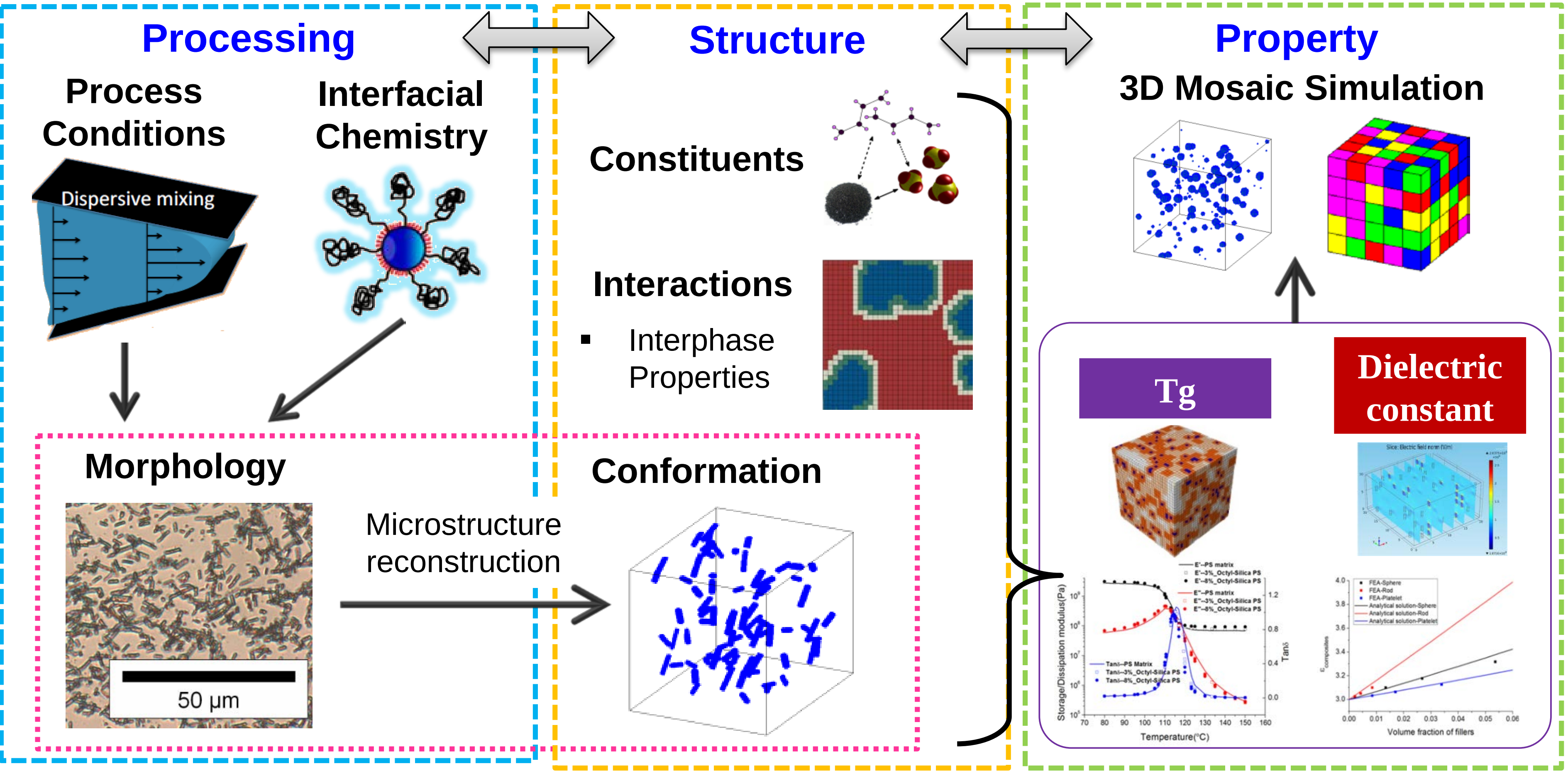
Example: microbuckling



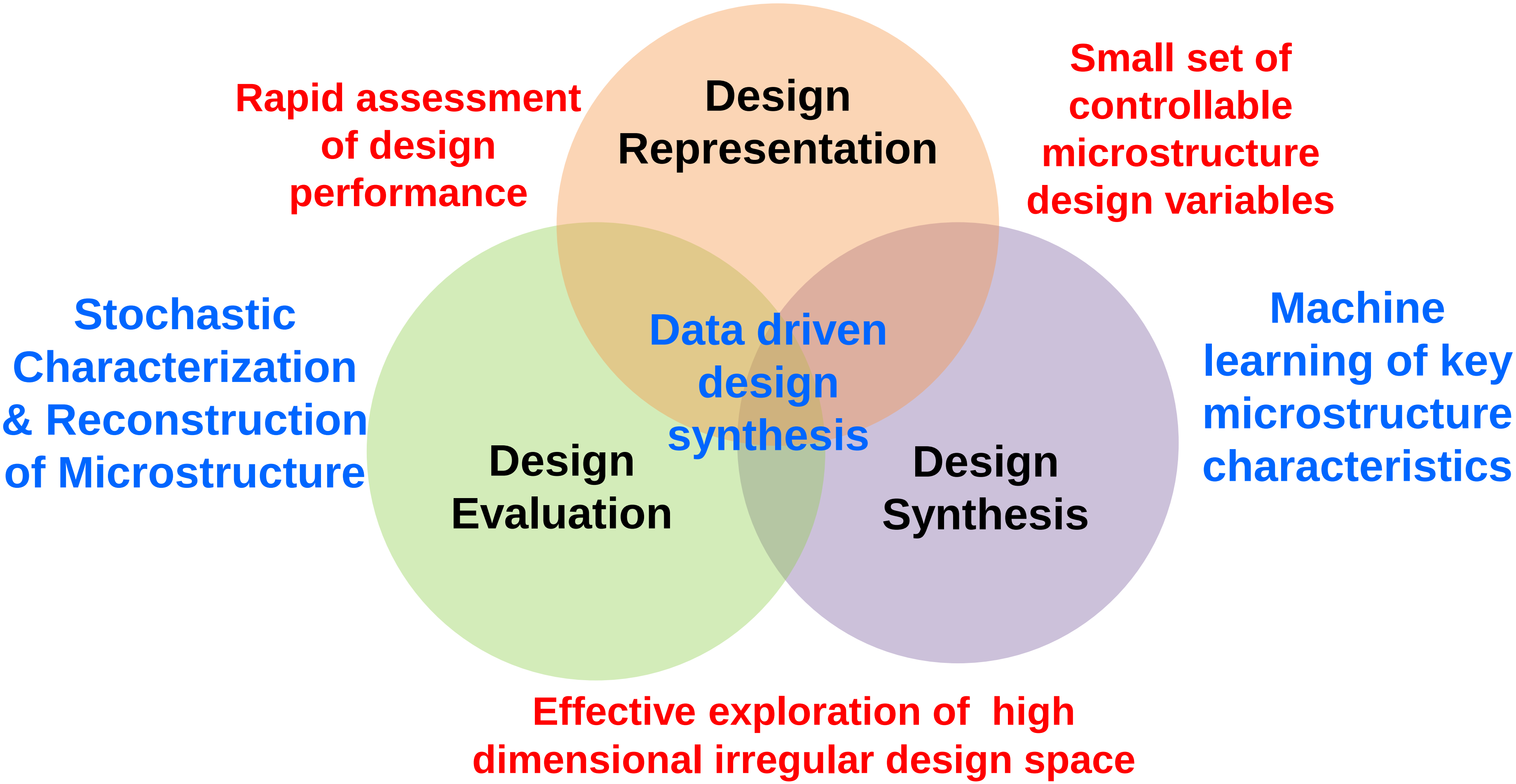
Greene, M. S., **Xu, H.**, Tang, S., Chen, W., Liu, W. K., "A generalized uncertainty propagation criterion from benchmark studies of microstructured material systems", *Computer Methods in Applied Mechanics and Engineering*, 254, pp 271-291, 2012.

Greene, M.S. et al. *CMAME* 2011.

Processing-Structure-Property Relation Chain



Research Issues in Microstructure Design

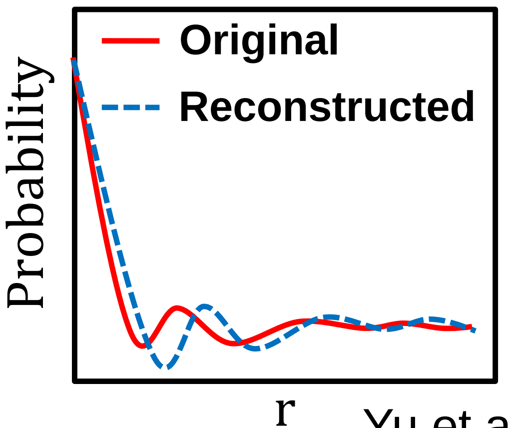


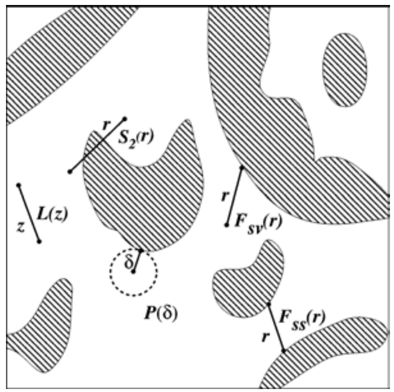
Statistical Characterization and Reconstruction

Correlation Functions:

Ch.: Morphology → Probability space

Rec. : Matching via iterative pixel swapping



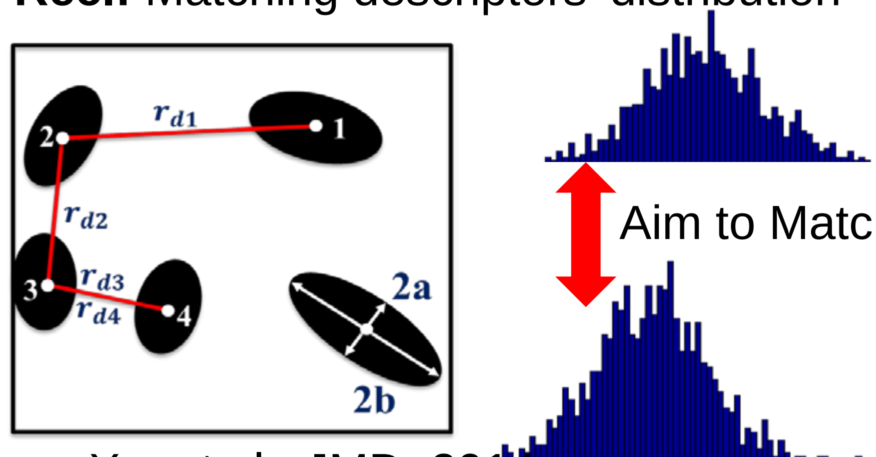


Yu et al., CAD, 2013

Descriptor-Based:

Ch.: Distribution of physical descriptors

Rec.: Matching descriptors' distribution

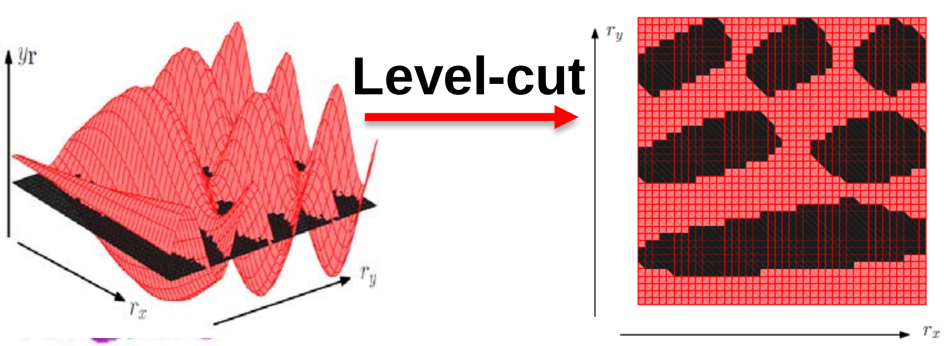


Xu, et al., JMD, 2014

Random Field (RF):

Ch.: Modeling the RF of the morphology

Rec.: Level-cutting the RF

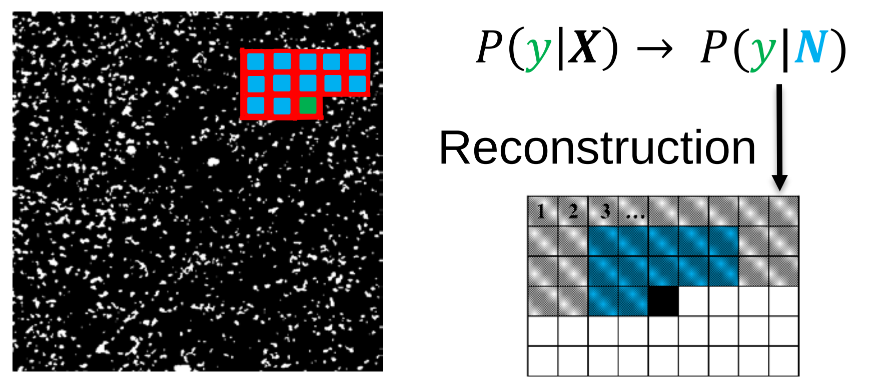


Jiang et al, J. Microsco, 2014

Supervised Learning:

Ch.: Morphology → Conditional probability

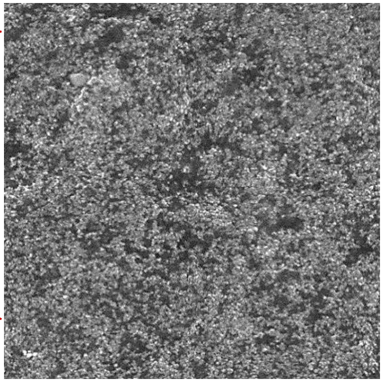
Rec.: Sampling from the conditionals



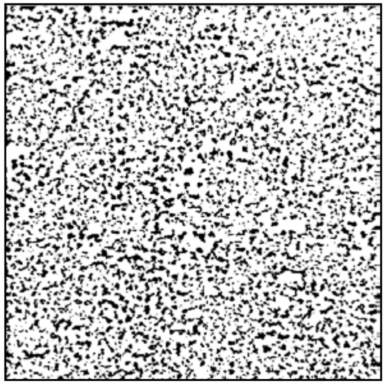
Original Image (**X**) Bostanabad, et al, 2015

Correlation Function-based Characterization

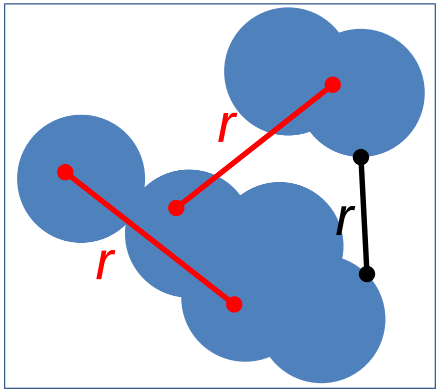
Original Image

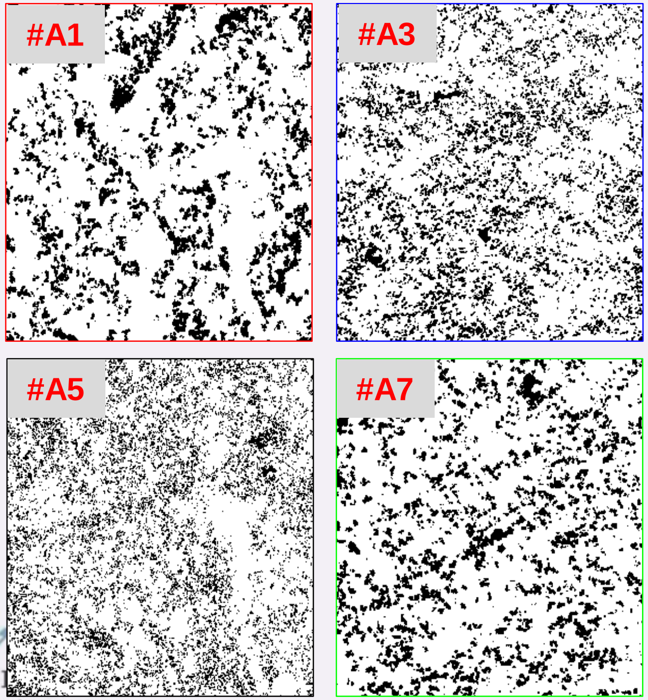


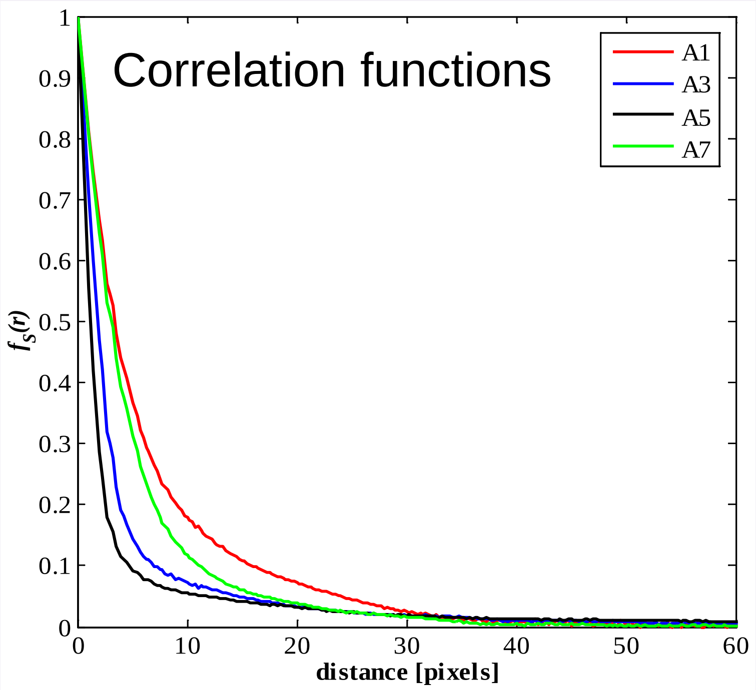
Binarization



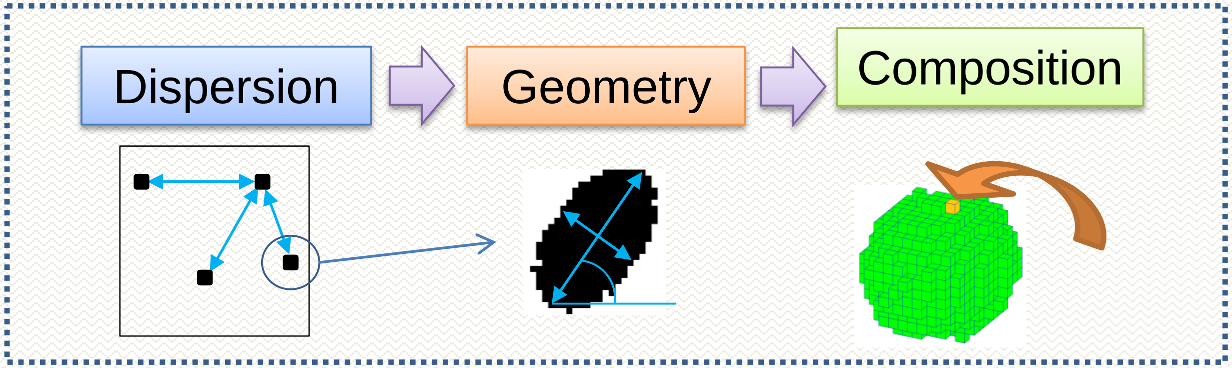
Characterization





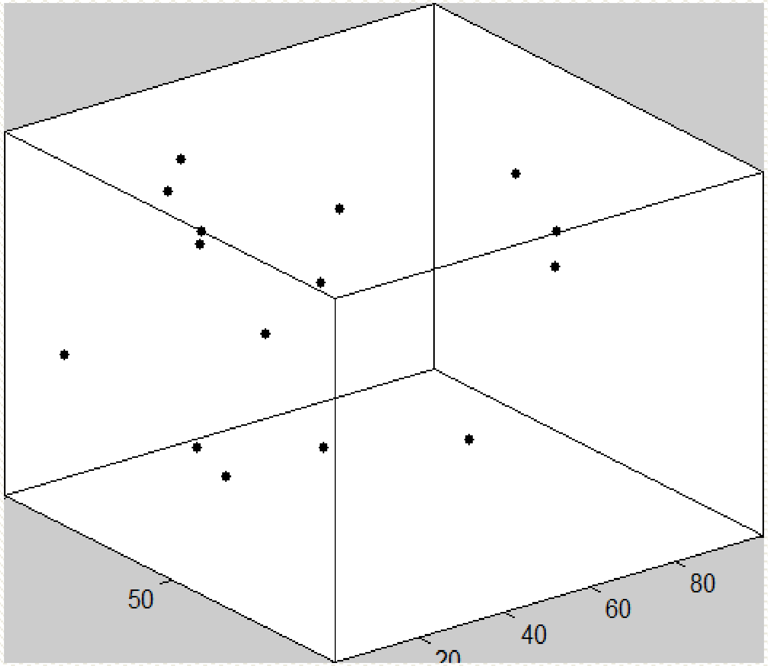


Descriptor-based Reconstruction



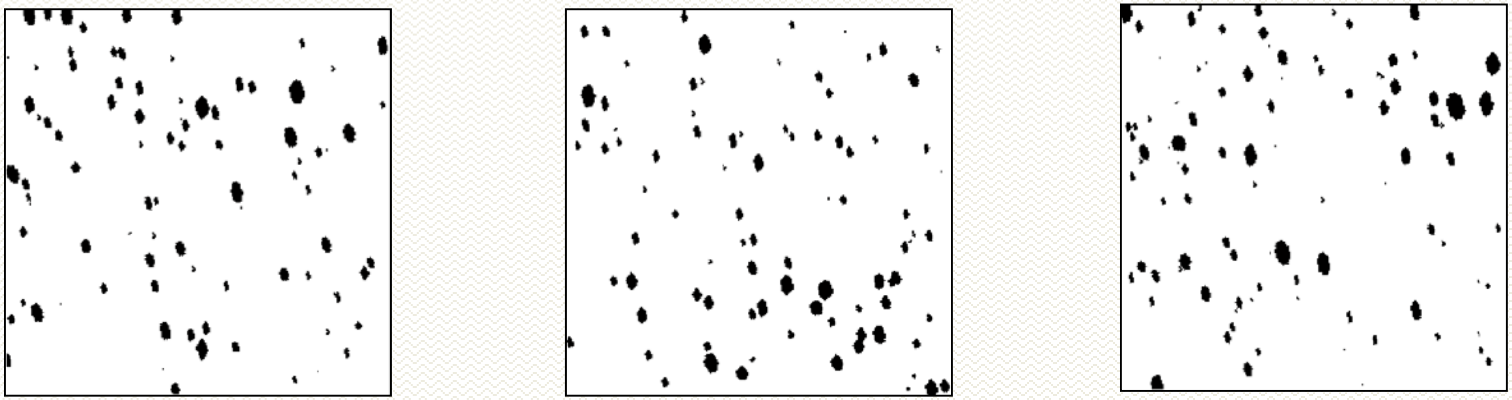
Computational Cost Comparison		
Size (voxel)	Correlation Function	Descriptor
100^3	170 hr	< 3 min
300^3	Memory issue	< 2 hr

- ❑ Low computational cost
- ❑ High accuracy
- ❑ Clear physical meaning

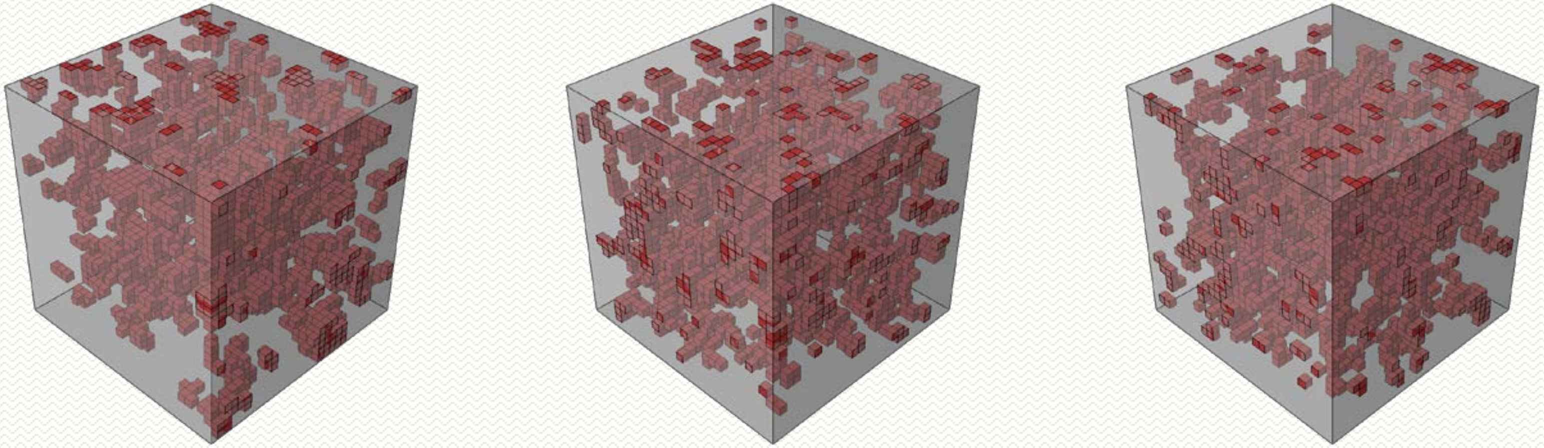


Statistically Equivalent Microstructures

❖ Stochastic reconstruction of 2D isotropic structure



❖ Stochastic reconstruction of 3D isotropic structure

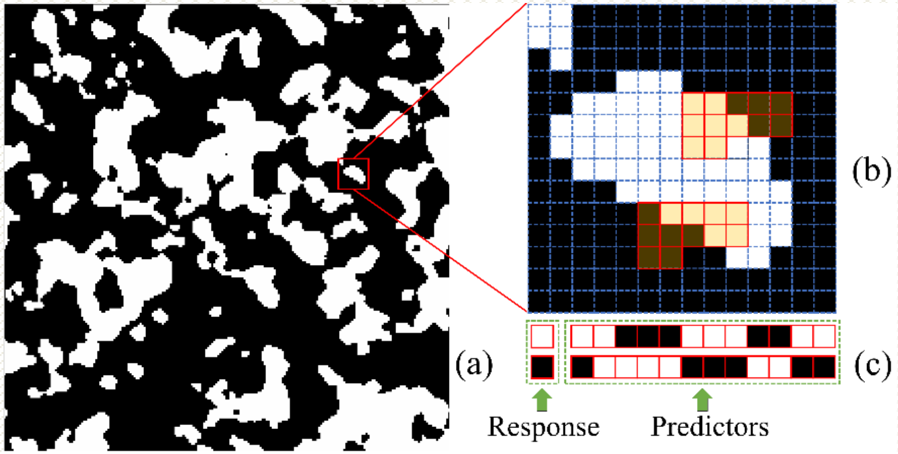


Characterization and Reconstruction (C&R) via Supervised Learning

GOAL: Development of a Generic and Model-based C&R Method

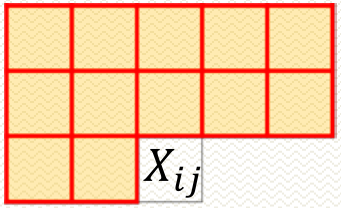
Bostanabad R., et al. *Acta Materialia*, DOI. 10.1016/j.actamat.2015.09.044, 2015.

- **Characterize** by learning the full joint distribution of the constituents
- **Reconstruct** by sampling from the learned distribution



$$f(\boldsymbol{X}) = f(X_{11})f(X_{12}|X_{11})f(X_{13}|X_{11},X_{12})\cdots f\left(X_{n_1n_2}|X_{11},X_{12},\dots,X_{n_1(n_2-1)}\right)$$
$$= f\left(X_{11}|\boldsymbol{X}^{(<11)}\right)f\left(X_{12}|\boldsymbol{X}^{(<12)}\right)f\left(X_{13}|\boldsymbol{X}^{(<13)}\right)\cdots f\left(X_{n_1n_2}|\boldsymbol{X}^{(<n_1n_2)}\right)$$

Where $\boldsymbol{X}^{(<ij)}$ is the set of all the pixels in $\boldsymbol{X}$ ordered before X_{ij}.



$\boldsymbol{M}_{ij}$: Neighborhood of X_{ij}

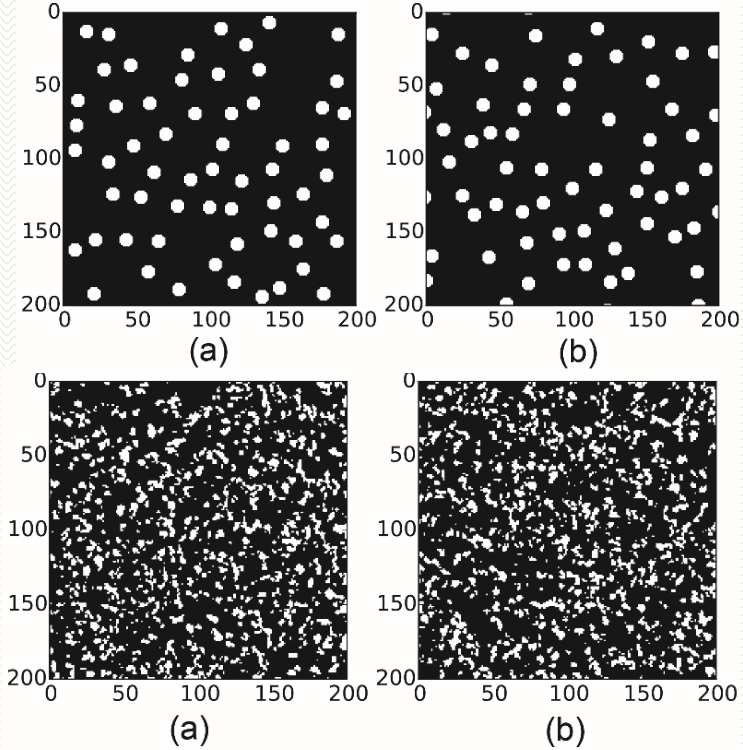
To make the approximation of $f(\boldsymbol{X})$ tractable, $\boldsymbol{X}$ is assumed to be a form of stationary Markov random field (MRF):

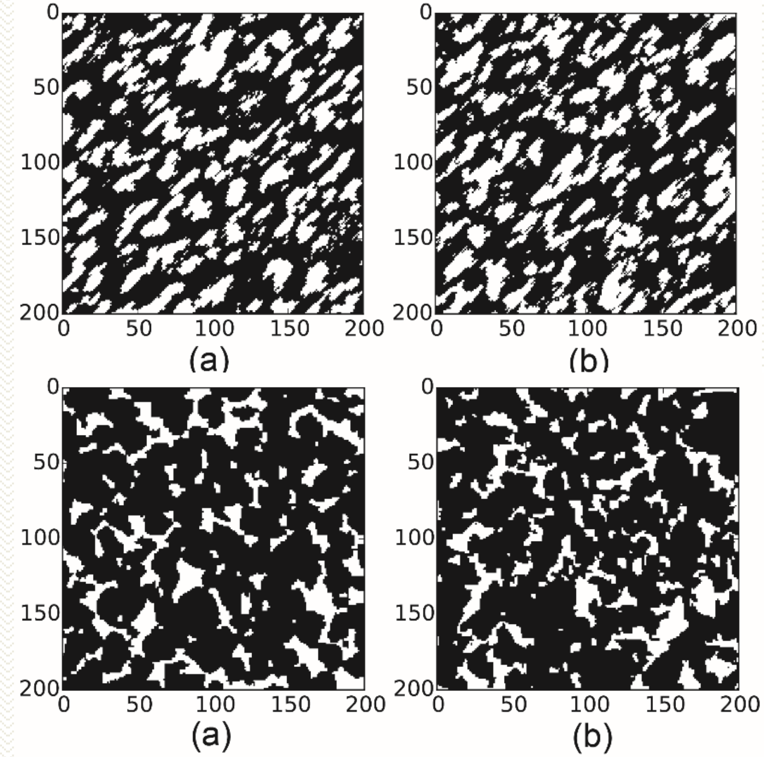
- **Locality:** $f\left(X_{ij}|\boldsymbol{X}^{(<ij)}\right) = f(X_{ij}|\boldsymbol{M}_{ij})$ for a sufficiently large (causal) neighborhood $\boldsymbol{M}_{ij}$.
- **Stationarity:** $f(X_{ij}|\boldsymbol{M}_{ij})$ does not depend on pixel location (i,j).

NORTHWESTERN UNIVERSITY

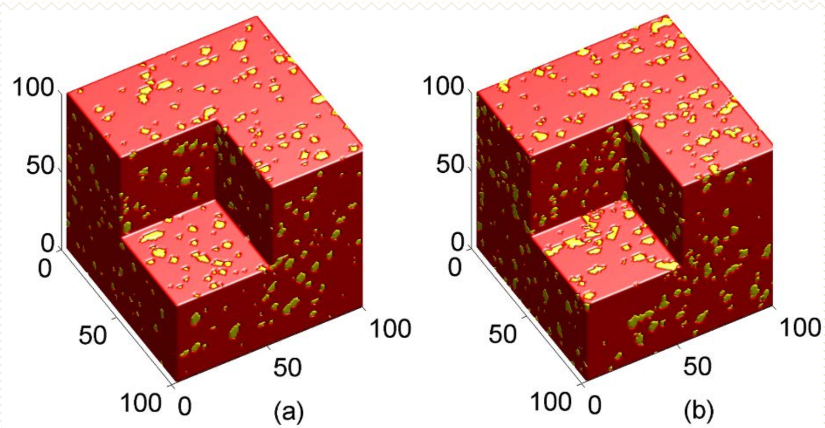
Applications to Various Material Systems

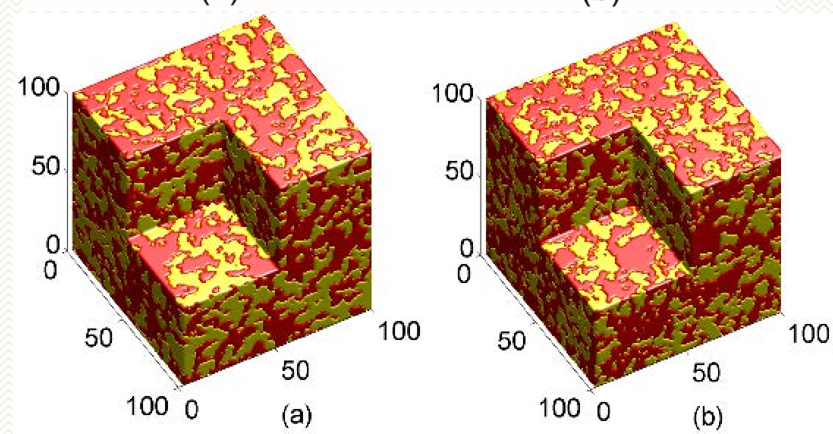
2D





3D

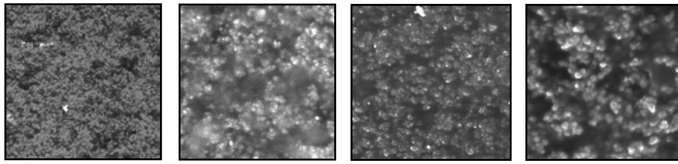




(a) Original image, (b) Reconstructed

Machine Learning for Identifying Key Descriptors

Microstructure samples



FEA ***or*** **Literature Search**

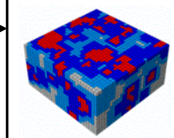
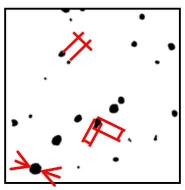
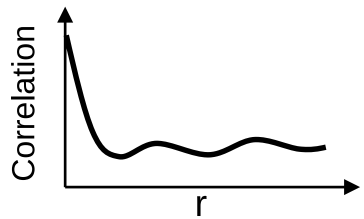


Image Analysis

Descriptors



Correlation functions



Material properties

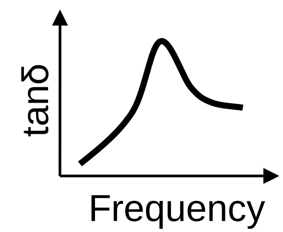


Image-based Analysis

(1) <u>Correlation-based feature selection</u>: eliminate redundant descriptors by correlation analysis

(2) Correlation function-based supervised learning

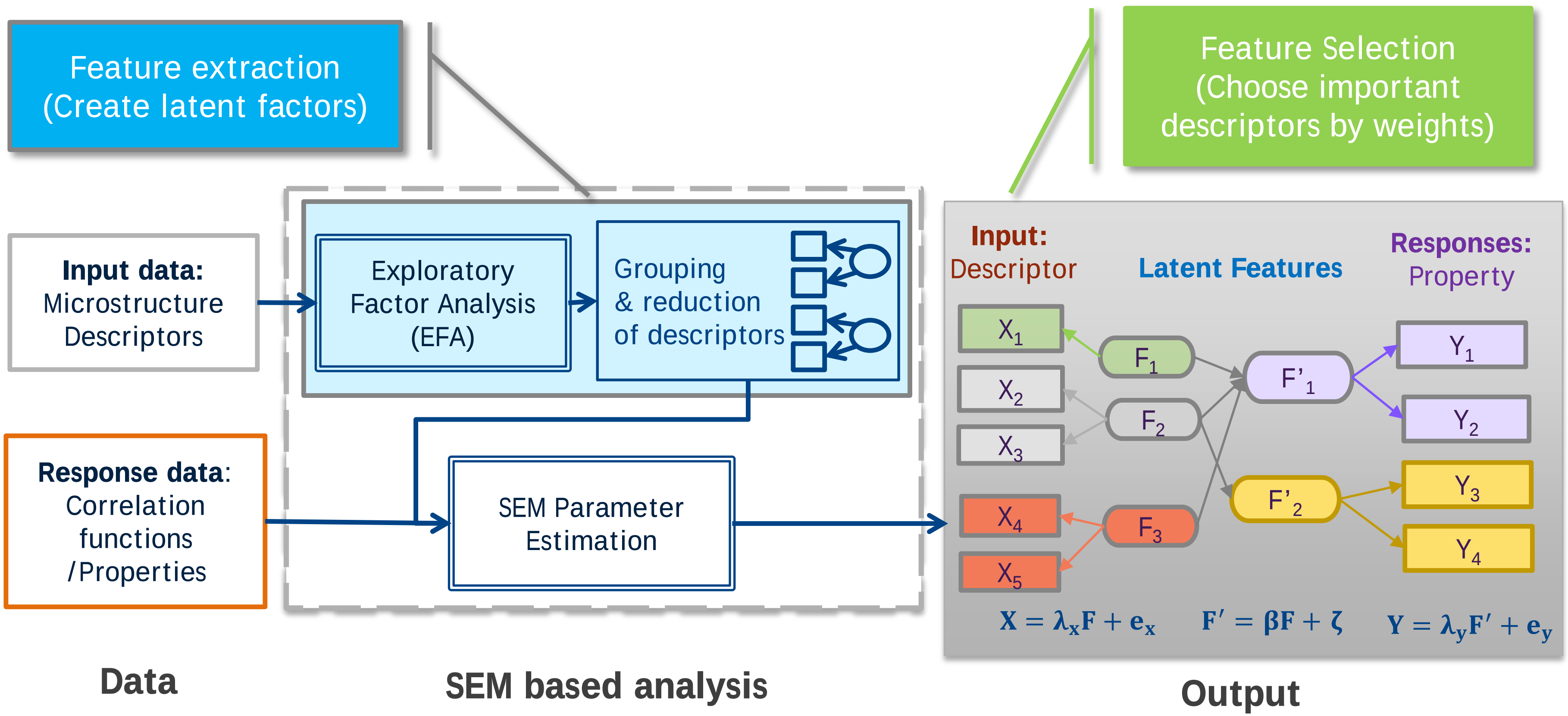
(3) Property-based supervised learning

Supervised Learning

Xu et al. JMD, 2014

Structural Equation Model (SEM) for Key Descriptor Identification

- **Reduce dimension by discovering latent microstructure features**



Zhang, Y., TMS IMMI, 2015

Reduced Descriptor Set for Tire Material

Initial Statistical Descriptor Set (56)

Composition	❑ VF
Dispersion	❑ Nearest boundary distance ❑ Nearest center distance ❑ Local VF of Voronoi cells ❑ Cluster number ❑ Filler Surface Area ❑ Matrix Surface Area ❑ Orientation
Geometry	❑ Pore size ❑ Area ❑ Equivalent Radius ❑ Compactness ❑ Aspect ratio ❑ Roundness ❑ Eccentricity ❑ Rectangularity ❑ Tortuosity

Key Descriptor set

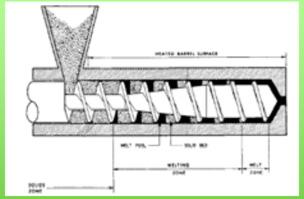
↓

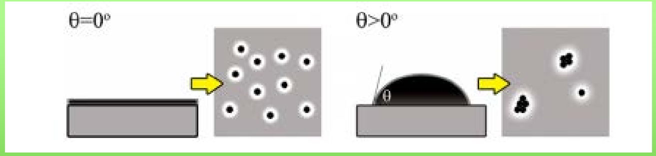
Microstructure Design Variables:

- ❑ Cluster number N
- ❑ Volume fraction VF
- ❑ Elongation ratio e_l
- ❑ Nearest distance r_d

Design Evaluation: Processing-Structure Mapping

Single Screw Extrusion



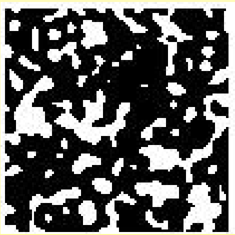


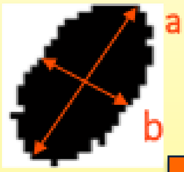
Descriptors: Processing energy E_γ

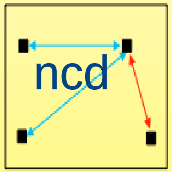
Interfacial energy W_{PF}/W_{FF}

Microstructure Dispersion

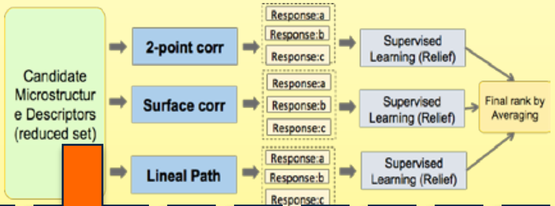
Physical Descriptors







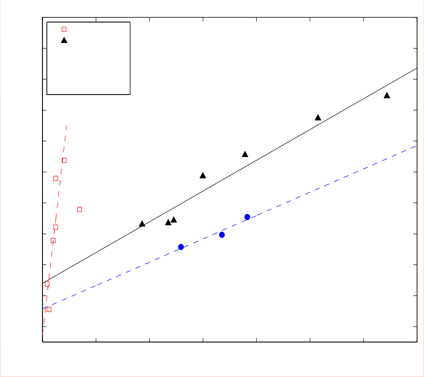
Key descriptors learnt via supervised learning



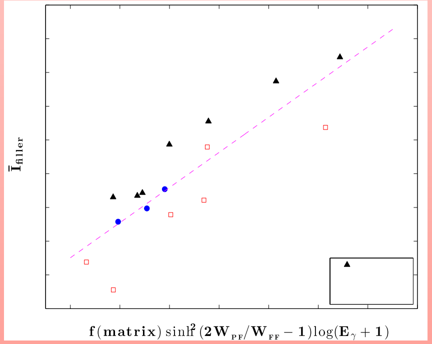
Descriptor:

Normalized interfacial area I_{filler}

Processing-structure Relationship



Matrix-specific Model



Generalized Model

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Hassinger I., Li X., et al, J. Mater. Sci, 2016

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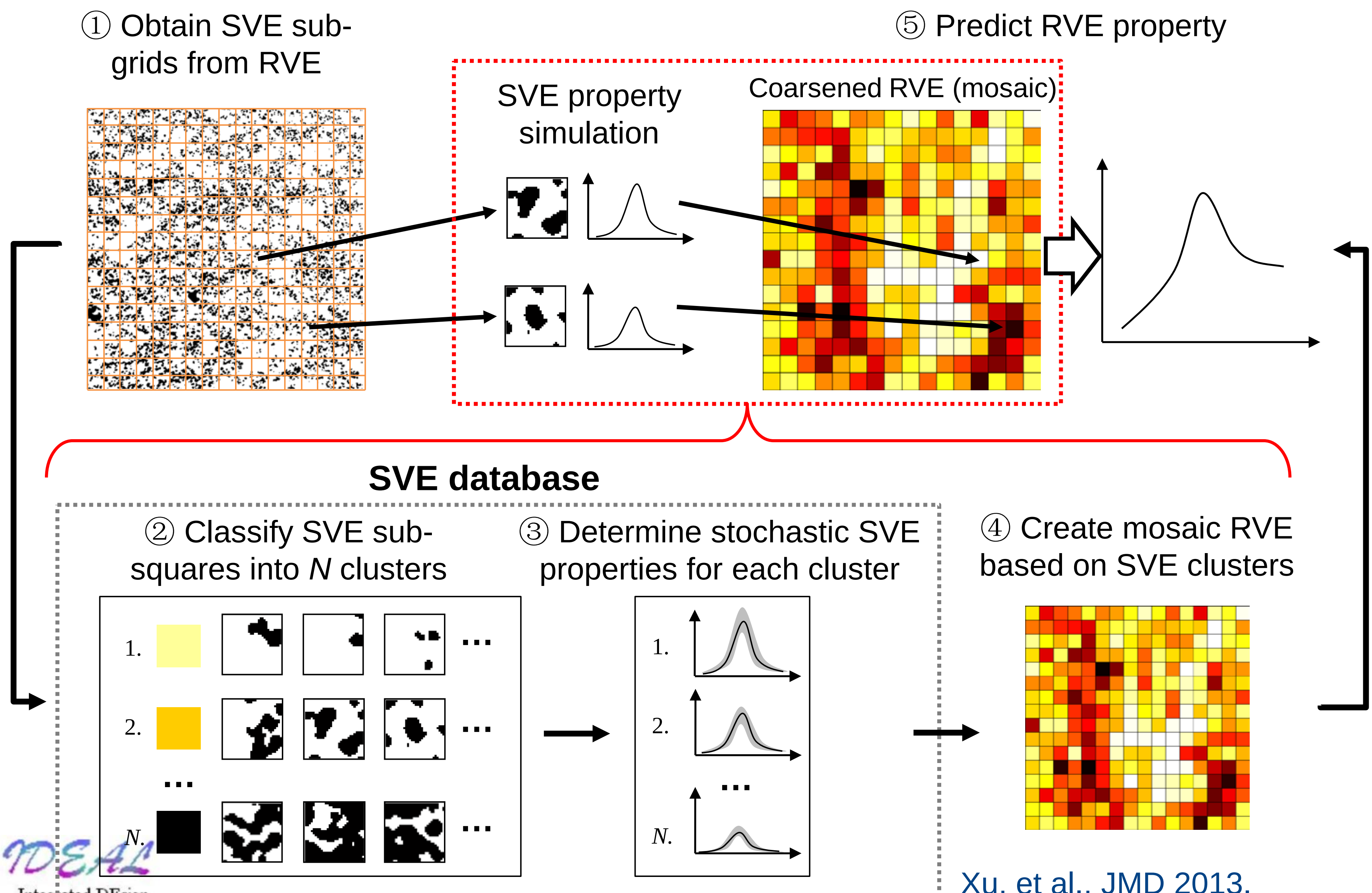
Design Evaluation: Mosaic Approach for Structure-Property Evaluations



Xu, et al., JMD 2013.

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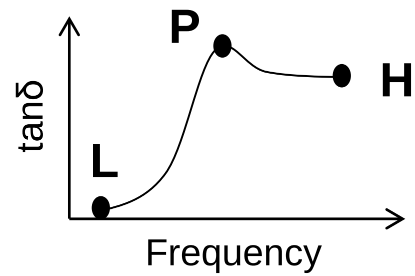
Data Driven Design Synthesis

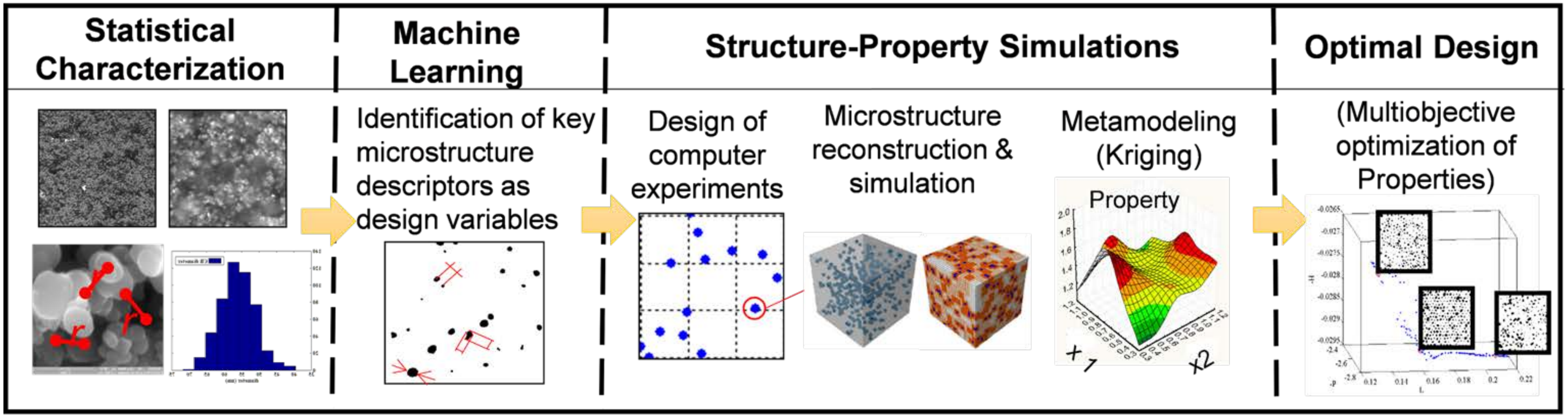
Microstructure Design Variables:

- ❑ Cluster number *N*
- ❑ Volume fraction *VF*
- ❑ Elongation ratio e_l
- ❑ Nearest distance r_d

Design Objective (multi-objective optimization):

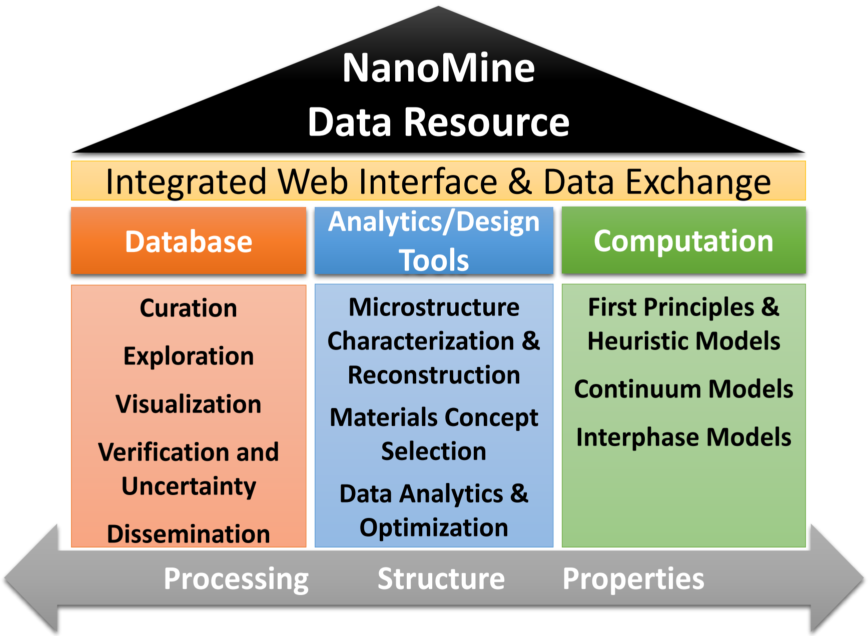
- ❑ Min L (Min wear)
- ❑ Max P (Max wet traction)
- ❑ Max H (Min rolling resistance)



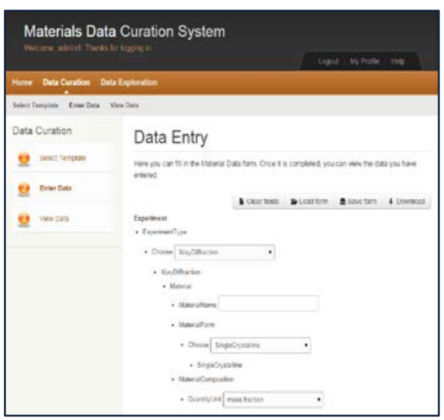


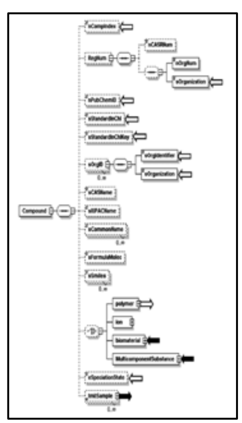
Xu, et al., JMD 2014.

NanoMine: Polymer Nanocomposite Data Resource



Using NIST Material Data Curator





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Nanomine.northwestern.edu

Database

- Curate and explore nanocomposite database with experimental and computation data
- Material Data Curator (NIST) with data template tailored for nanocomposites

Analysis/Design Tools

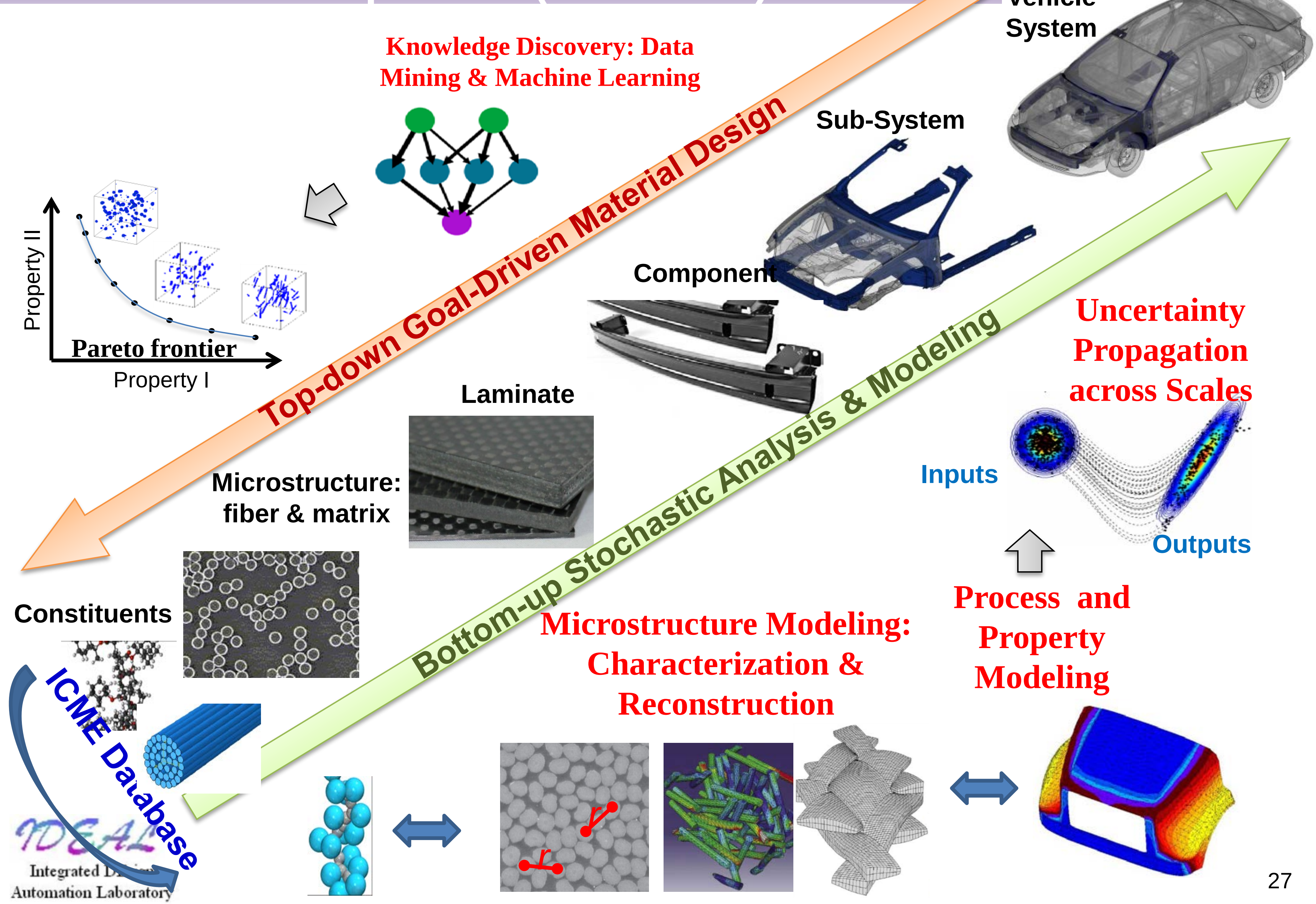
- MCR toolkit to calculate physical descriptors and reconstruct 2D/3D microstructure
- Data mining tools for processing, structure and property correlation and material design

Computation

- Heuristic and DFT models for polymer and surface chemistry
- Finite element modeling on thermomechanical and dielectric properties

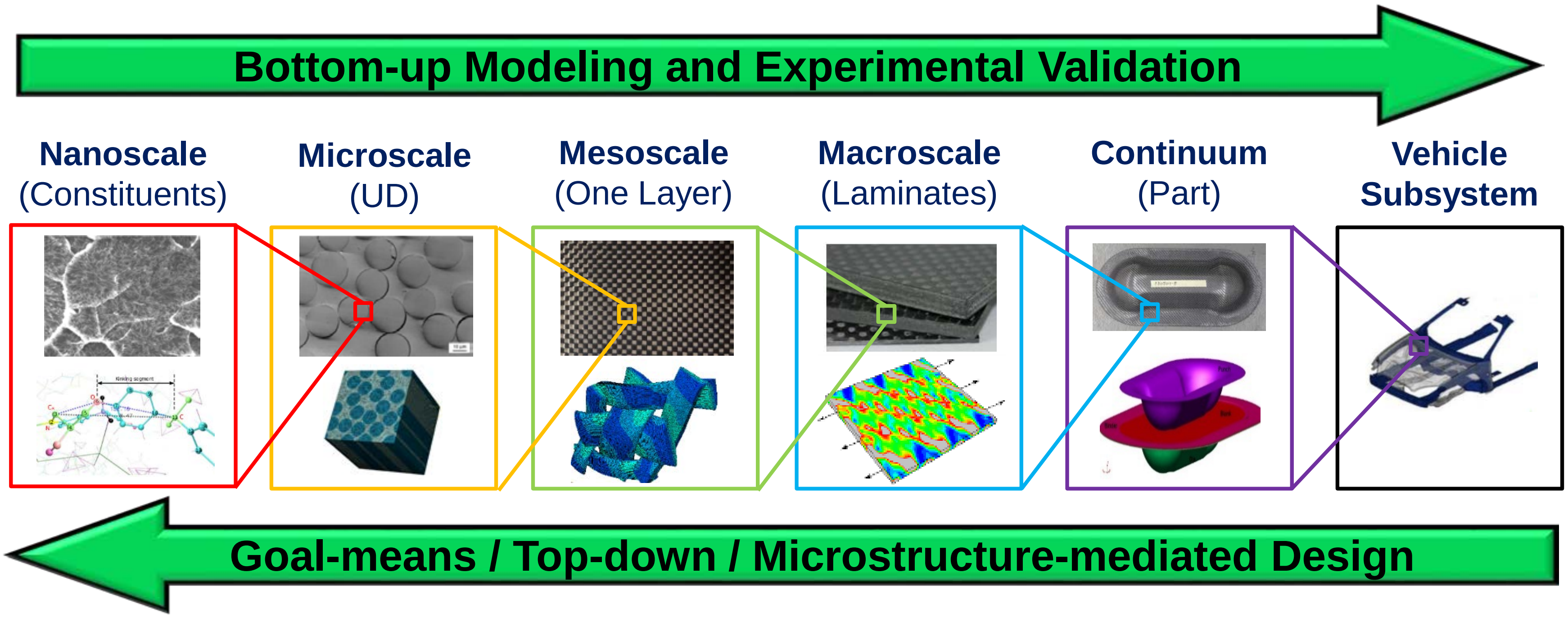
Zhao, et al., APL Materials, 2016,

Multiscale Design of Lightweight Carbon Fiber Composites (DOE/Ford)



Stochastic Multiscale Analysis and Design

GOAL: Multiscale Design of Material Systems with Targeted Properties



Challenges:

- The bottom-up approach is not tailored for material design and requires much time and effort.
- Coupling the computational models in the top-down approach is not trivial - what information needs to be passed up from fine to coarse scales?

Accounting Local Microstructural Variations and Defects

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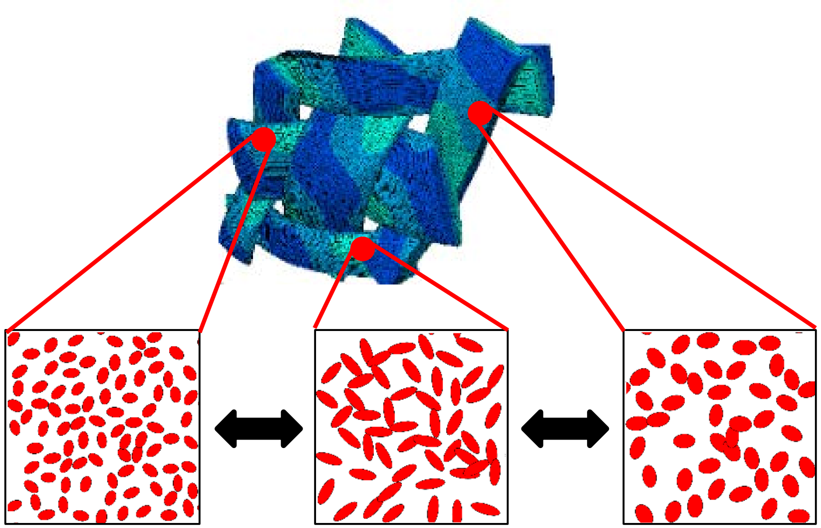
Spatial Microstructural Correlation



$\boldsymbol{S} = f_1(\boldsymbol{\varepsilon}, \boldsymbol{m_1}, \boldsymbol{P_1})$ $\boldsymbol{S} = f_2(\boldsymbol{\varepsilon}, \boldsymbol{m_2}, \boldsymbol{P_2})$ $\boldsymbol{S} = f_3(\boldsymbol{\varepsilon}, \boldsymbol{m_3}, \boldsymbol{P_3})$

Realizations

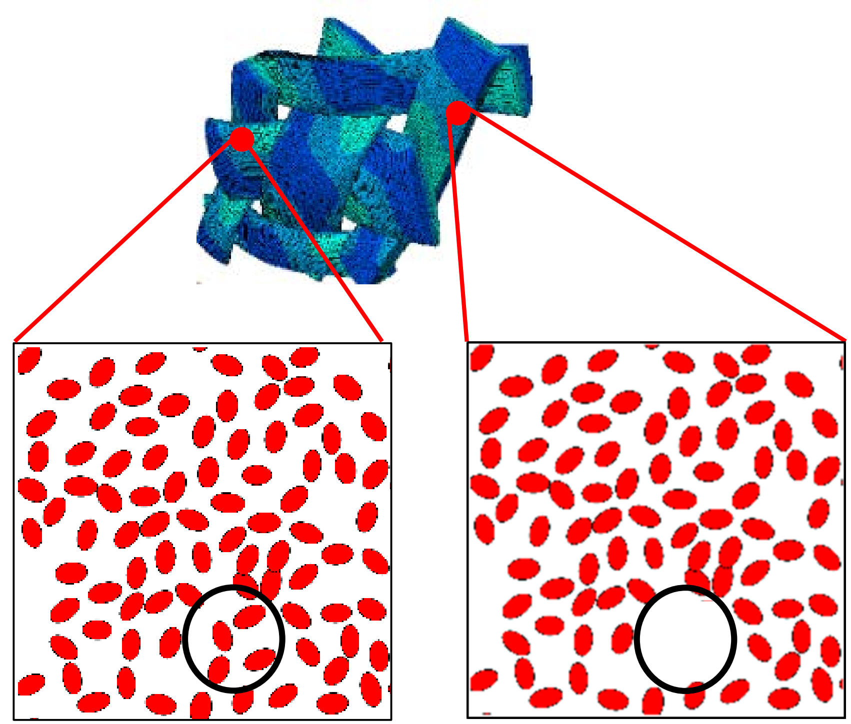
Underlying Random Field for the General Constitutive Law : $\boldsymbol{S} = \mathcal{F}(\boldsymbol{\varepsilon}, \boldsymbol{m}, \boldsymbol{P})$

$\boldsymbol{\varepsilon}$: Boundary Condition

$\boldsymbol{P}$: Constituents Properties

$\boldsymbol{m}$: Microstructural Descriptors

Defects and Anomalies



- Local morphological changes (such as volume fraction) can drastically affect the material performance.
- Monitoring local and global changes are essential to quality control.

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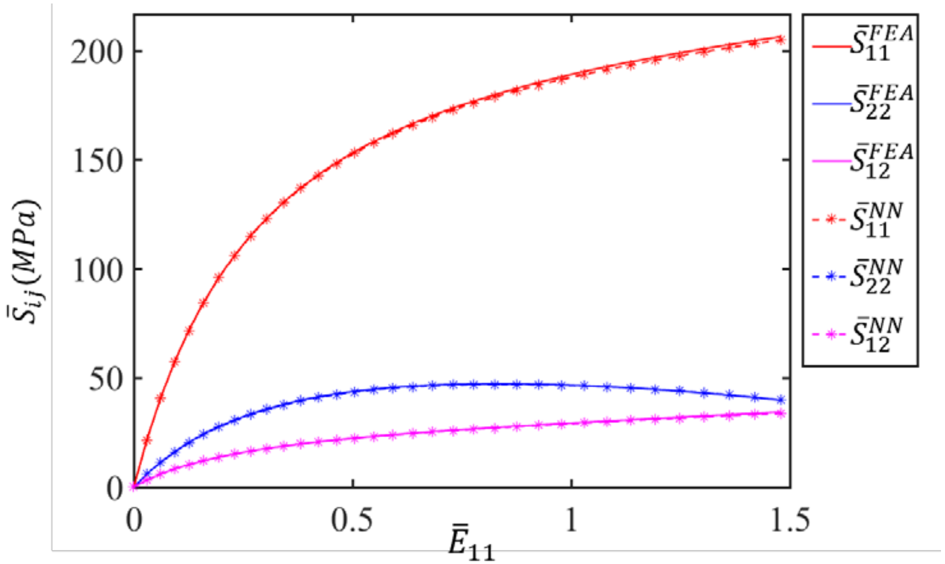
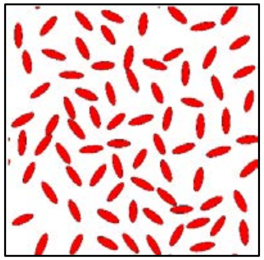
Response Surface of Constitutive Relations for Hyperelasticity

GOAL: Learn the macroscopic constitutive law of a **class** of microstructures, i.e., find f in $W = f(\bar{\boldsymbol{E}}, \boldsymbol{m})$.

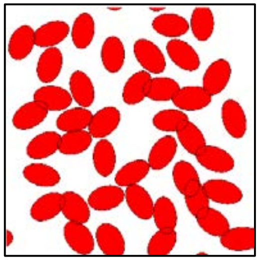
Descriptors	
VF	$[2, 45]\%$
μ_{nn}	$[0.3, 0.5]mm$
e	$[1, 5]$
N	$[40, 100]$
$\bar{E}_{11}$	$[-10, 150]\%$
$\bar{E}_{22}$	$[-10, 150]\%$
$\bar{E}_{12}$	$[-40, 40]\%$



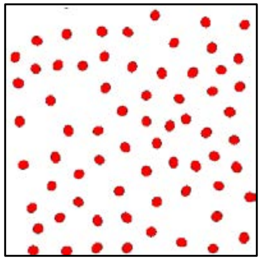
RVE 1



RVE 2



RVE 3



RVE 4

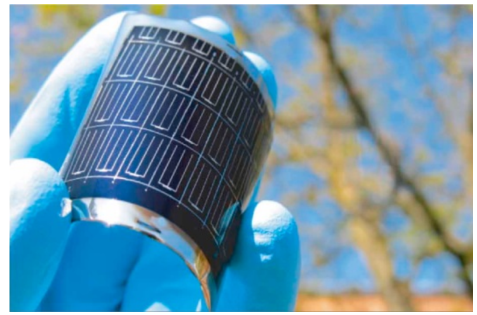
Metamaterial Design: Light-trapping for thin-film solar cell

Conventional bulk solar cell

Wikipedia

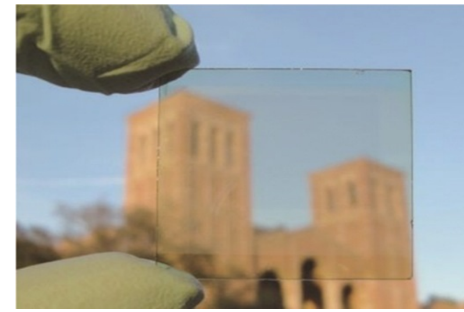
Thin-film solar cell

Flexible

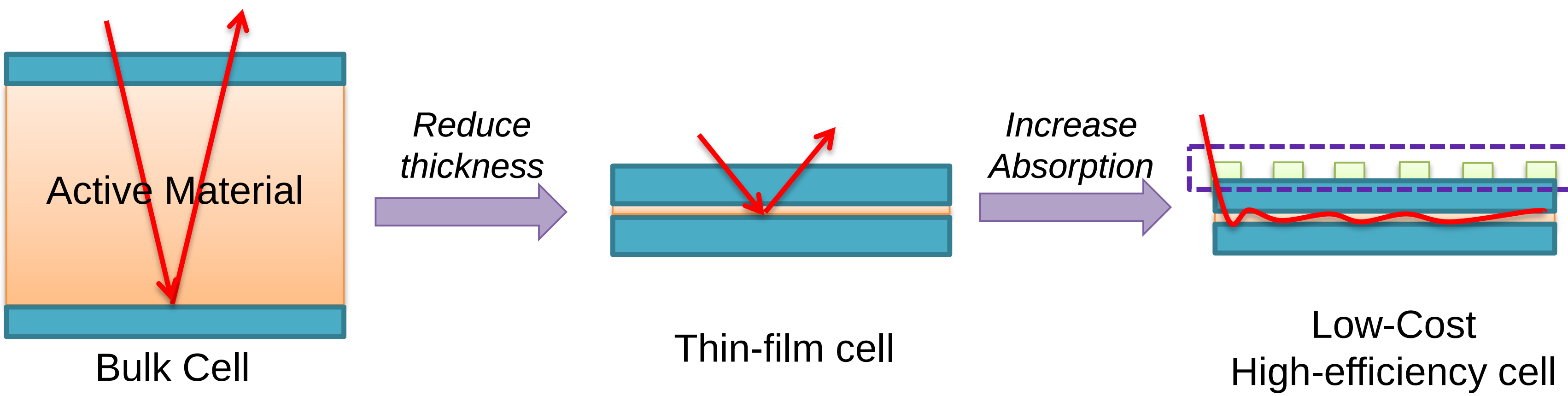


C. Adrian et. al,
Nature Materials, 2011

Transparent



C.C. Chen et. al.,
ACS Nano, 2012



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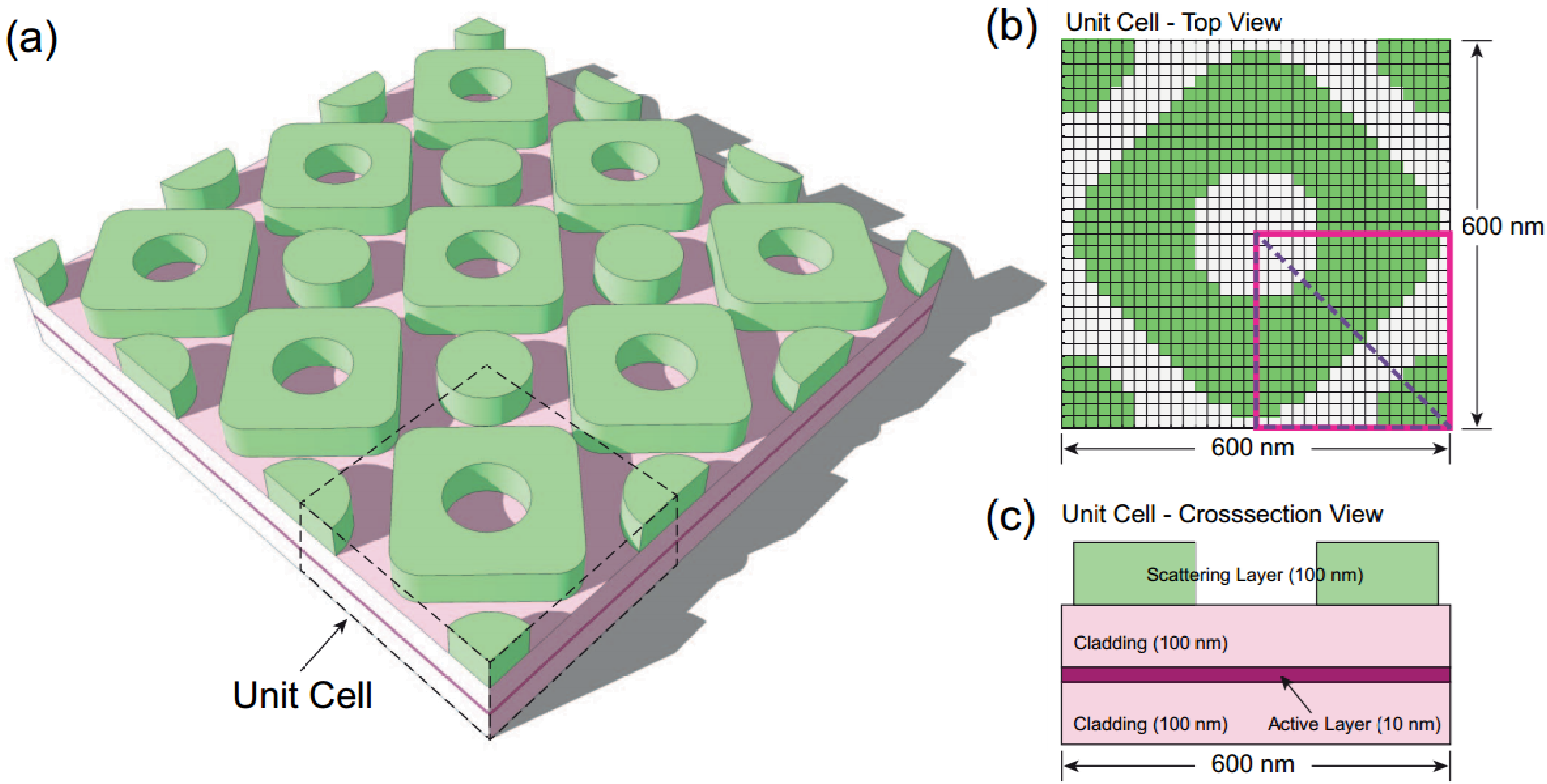
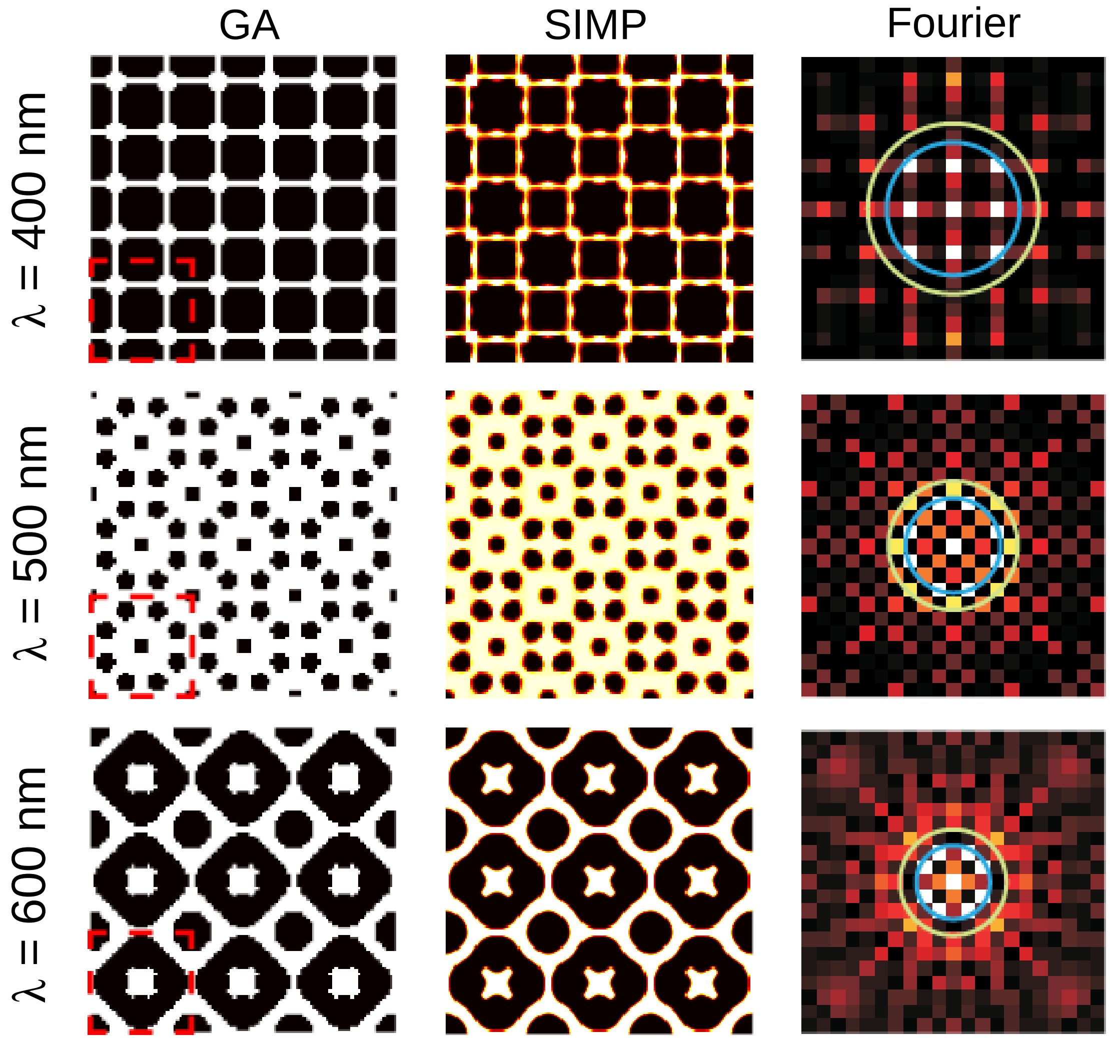
Topology optimization for highly-efficient nanophotonic light-trapping structure for thin-film solar cells

Optimizing the material distribution in elementised design space with periodicity constraint



C. Wang, S. Yu, W. Chen, C. Sun, Scientific Report, 2013
S. Yu, C. Wang, C. Sun, W. Chen, Struct. Multidisc. Optim., 2014

GA and SIMP based Topology Optimization of the Periodic Light-Trapping Structures



C. Wang, S. Yu, W. Chen, C. Sun, Sci. Rep., 2013
S. Yu, C. Wang, C. Sun, W. Chen, Struct. Multidisc. Optim., 2014

Topology optimization of the light-trapping structure at single incident wavelength using GA and SIMP

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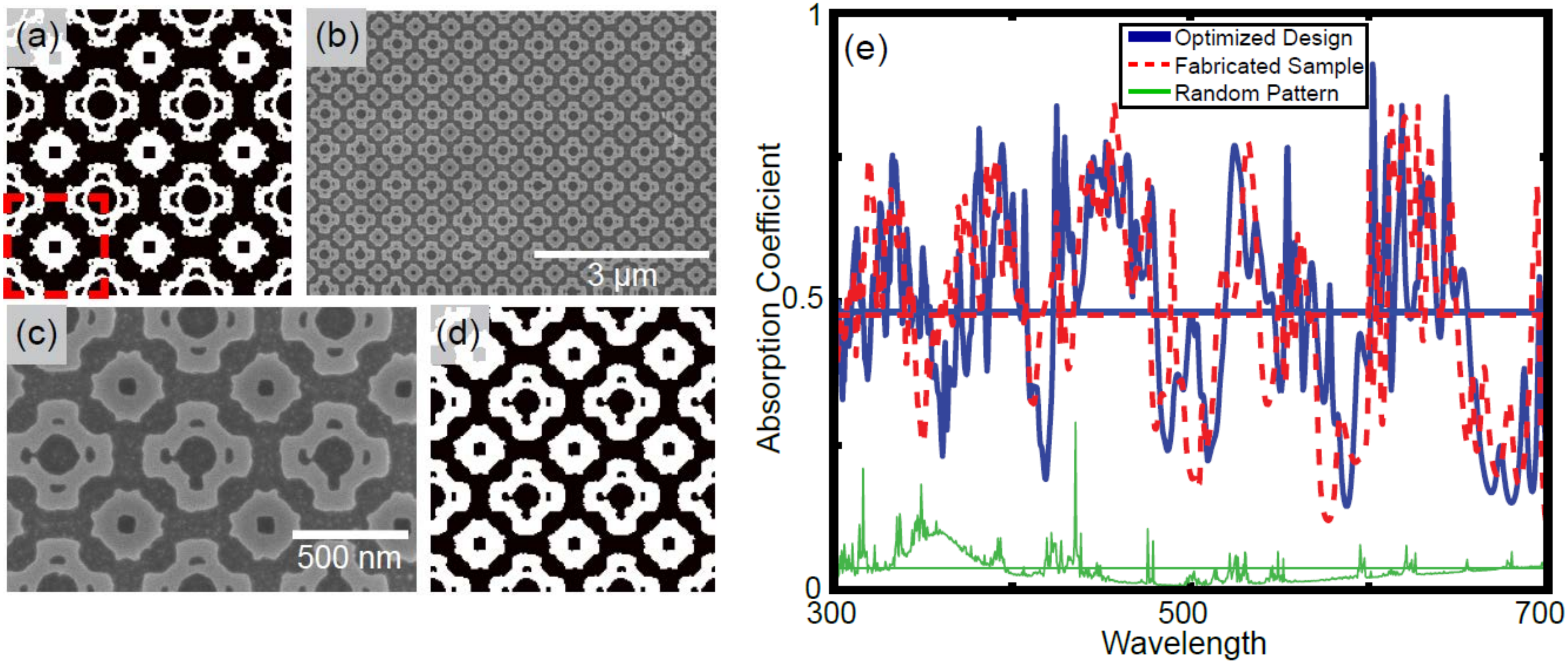
Validation of cost-effective, high-performance nanophotonic structures for efficient light control

Significant enhancement in light absorption efficiency has been achieved in the optimized nanophotonic light-trapping structure



More than **a week to pattern** the optimal design on a **4 inch wafer** using the state-of-the-art e-beam lithography (EBL), costs **thousands of dollar** by accounting for the total cost of ownership (TCO)

C. Wang, S. Yu, W. Chen, C. Sun, Sci. Rep., 2013
S. Yu, C. Wang, C. Sun, W. Chen, Struct. Multidisc. Optim., 2014

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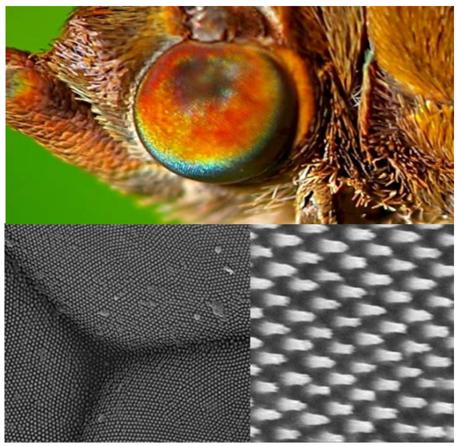
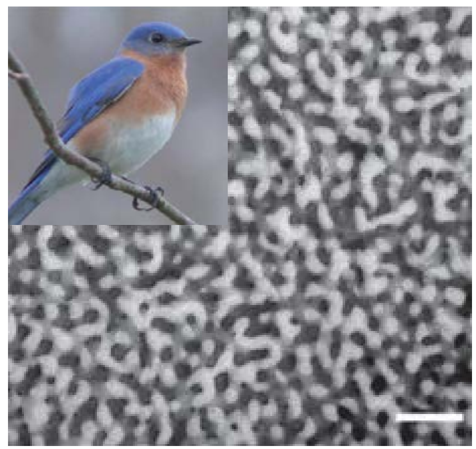
Quasi-random Structures in Nature

Nanophotonic structures in nature

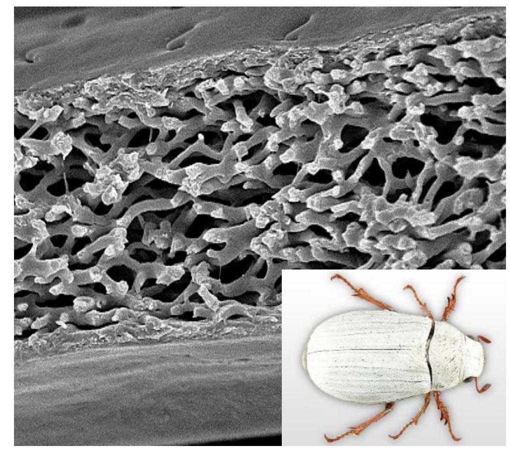
Moth-eye



Blue-bird feather barbs



Ultra-white beetle scale



Periodic —— **Quasi-random** ——→ **Random**

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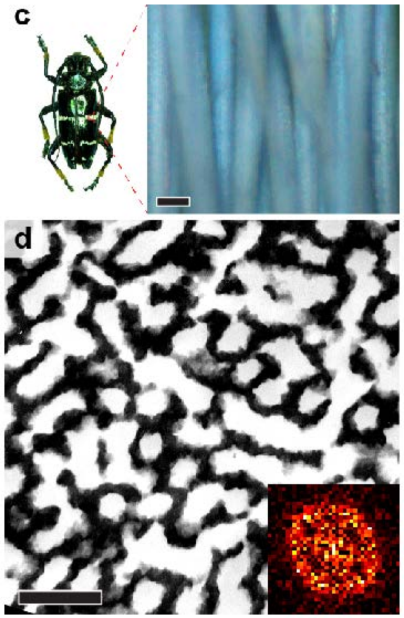
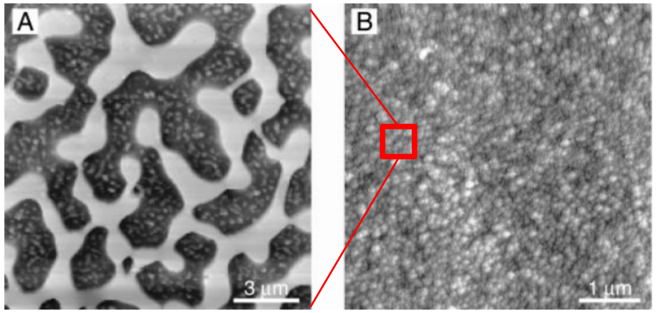
Cost-Effective Bottom-up Fabrications

Biological quasi-random nanostructures from **self-assembly** of biological medium



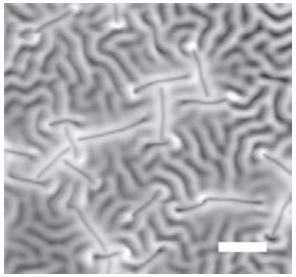
S. Yu, C. Wang, B. Dong, Z. Jiang, J. Zi, W. Chen, C. Sun, Submitted, 2015

Functional quasi-random nanostructures from **bottom-up processes**:



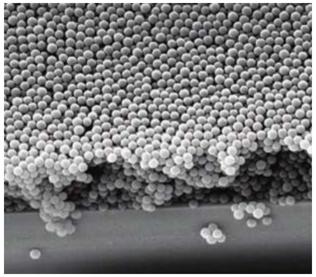
S. Walheim, et al, Science, 1999

Polymer phase-separated anti-reflection coating



W. H. Koo, et. al., Nat. Pho., 2011

Nano-wrinkled LED



J. D. Forster, et al, Adv. Mat., 2010

Particle assembling structural color

Spectral density function (SDF)

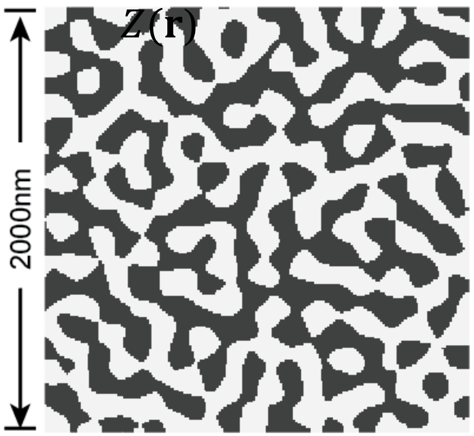
Fourier transformation of structure $Z(\mathbf{r})$

$$F\{Z(\mathbf{r})\} = A_{\mathbf{k}} \cdot e^{i\phi_{\mathbf{k}}},$$

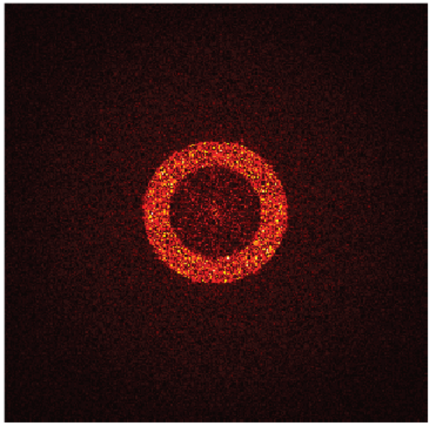
Spectral density function SDF calculation

$$f(k) = \left(A_k \cdot e^{i\phi_k}\right) \cdot \left(A_k \cdot e^{-i\phi_k}\right)/C$$

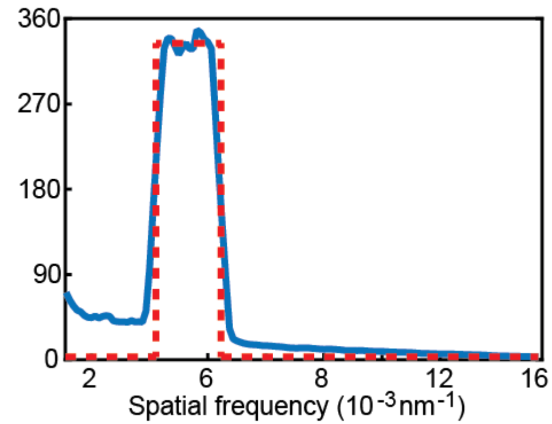
Structure $Z(\mathbf{r})$



Fourier spectrum $|F\{Z(\mathbf{r})\}|$



SDF $f(k)$



SDF describe the structure spatial correlation in frequency domain

Best Paper Award, 42th ASME Design Automation Conference, for paper Yu et al. “Characterization and Design of Functional Quasi-Random Nanostructured Materials using Spectral Density Function”

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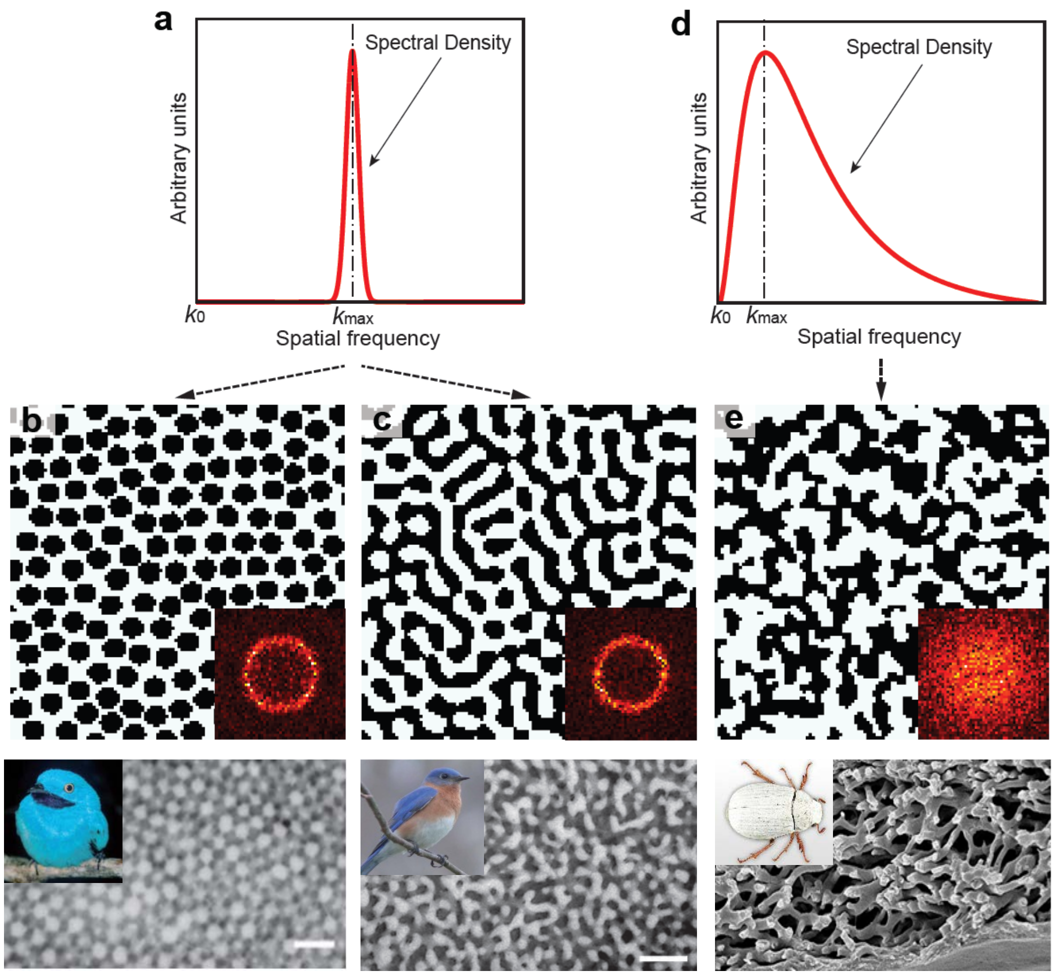
Spectral Density Function for Non-deterministic Quasi-Random Structure Representation

Spectral density function (SDF):

1D function of Fourier components distribution over spatial frequency



5: *Dufresne E. R. et al, Soft Matter, 2009*

6: *Vukusic P. et al, Science, 2007*

SDF

Statistical reconstruction:
Random sphere packing (b)
Gaussian random field (c, e)

Quasi-random structure

7: *Teubner, M., Europhys Lett, 1991*

Yu, et al. IDETC, 2016

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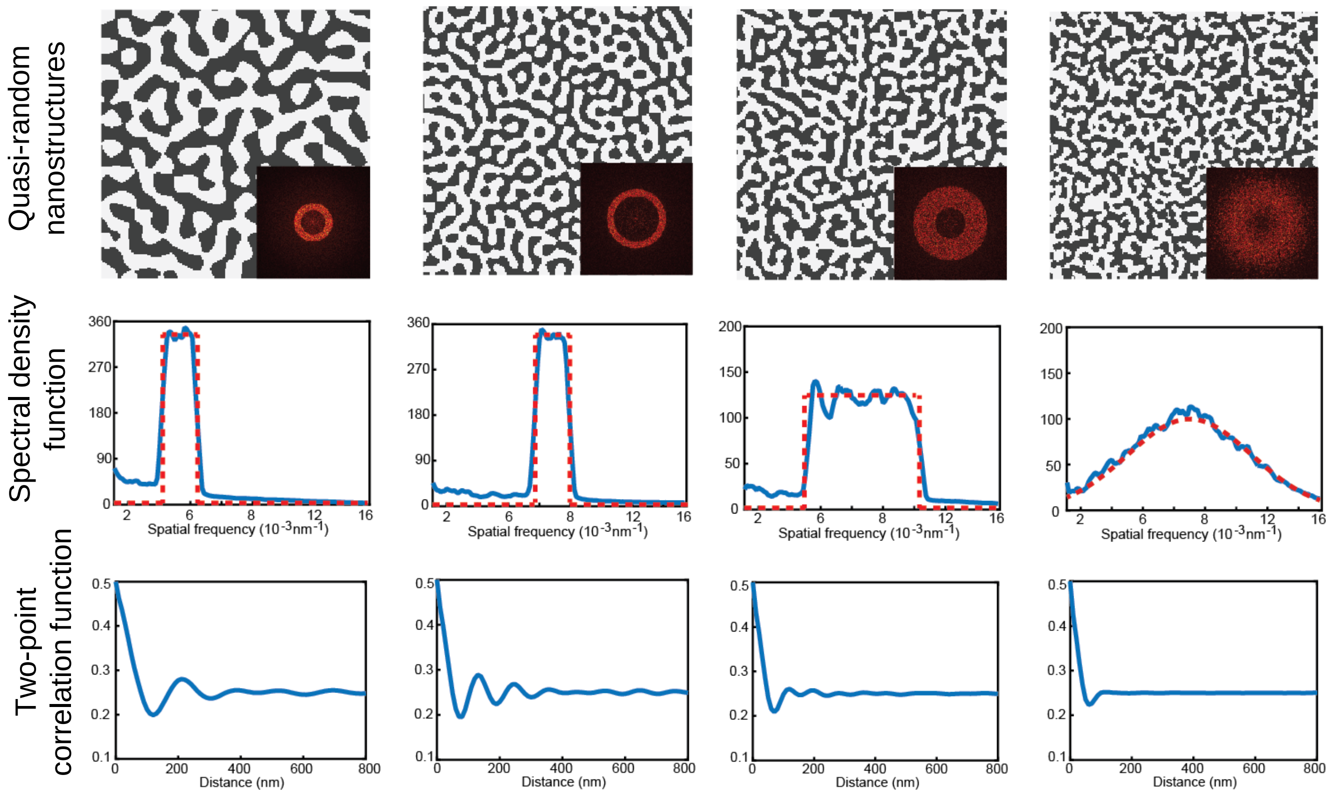
Spectral Density Function vs Correlation Function



- SDF captures the differences between structures more clearly than the conventional 2-point correlation function.
- Smaller number of parameters and fast reconstruction enable rapid explorations of optimal fabricable nanostructures

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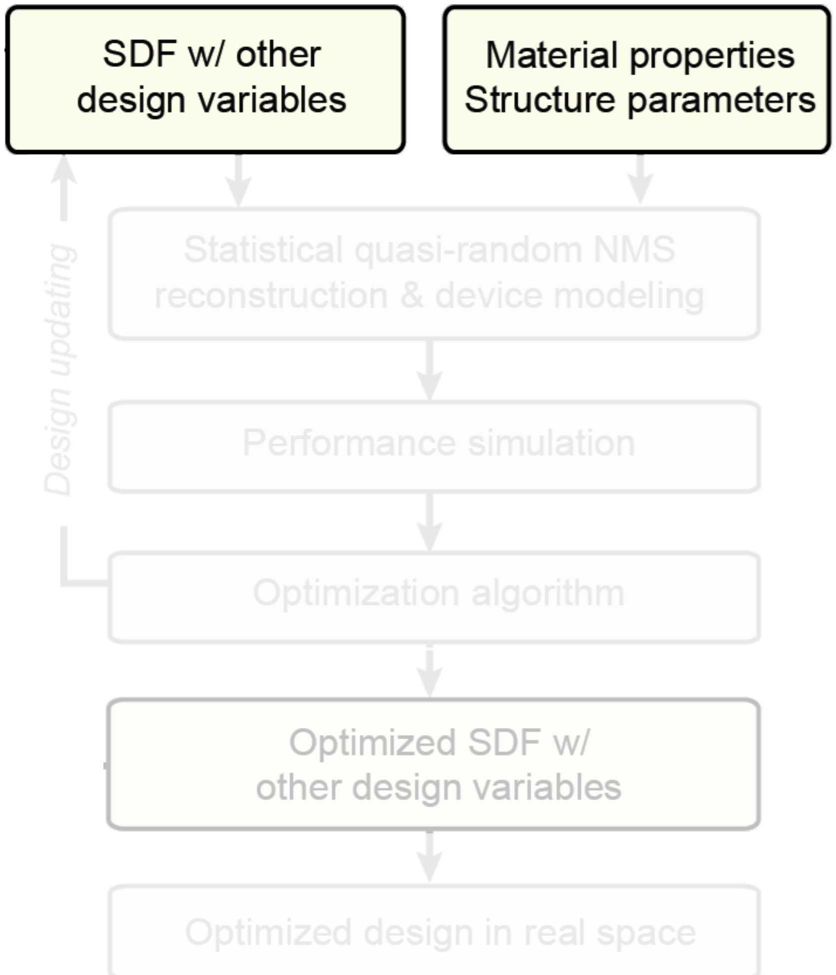
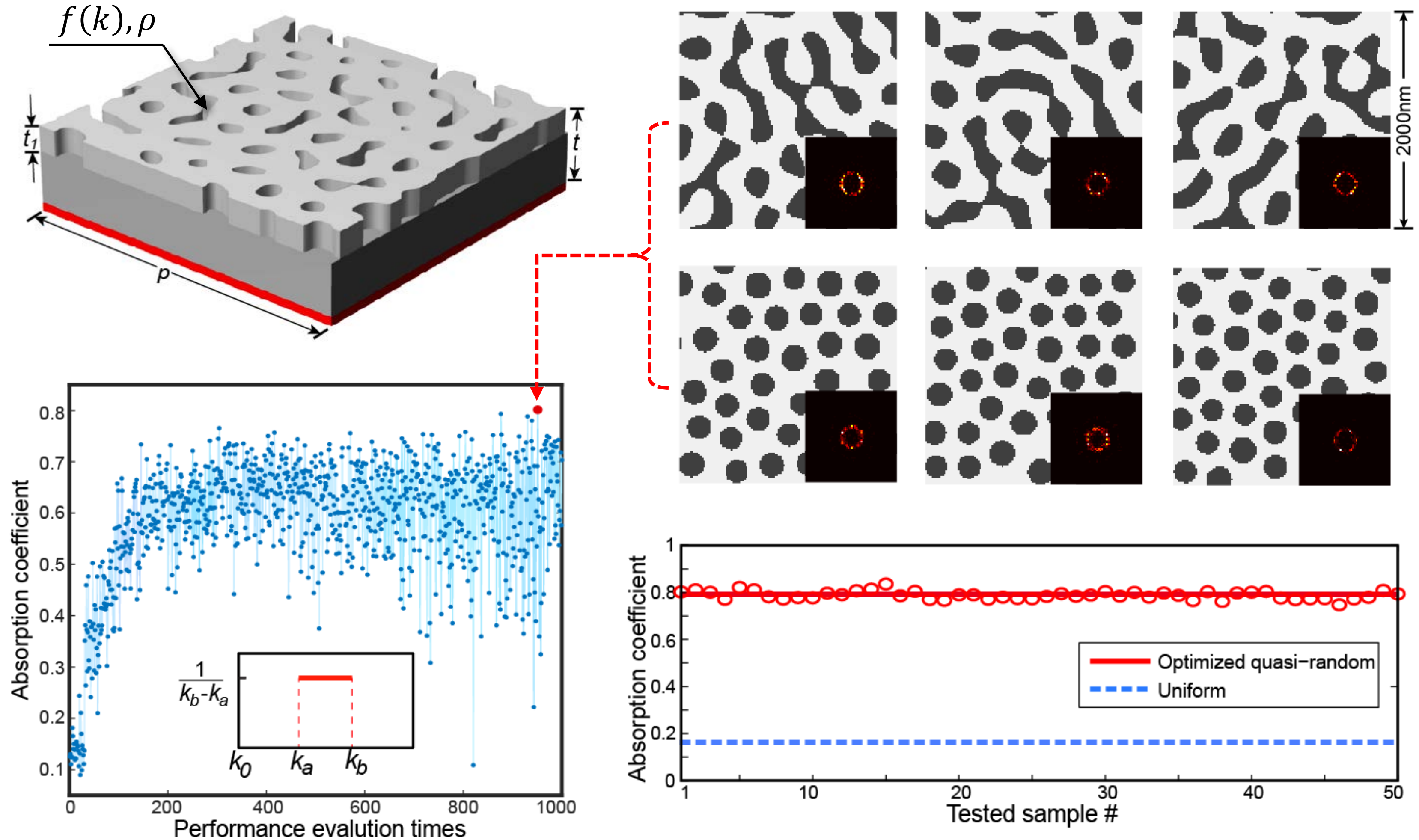
SDF based computational design methodology of quasi-random nanostructure materials



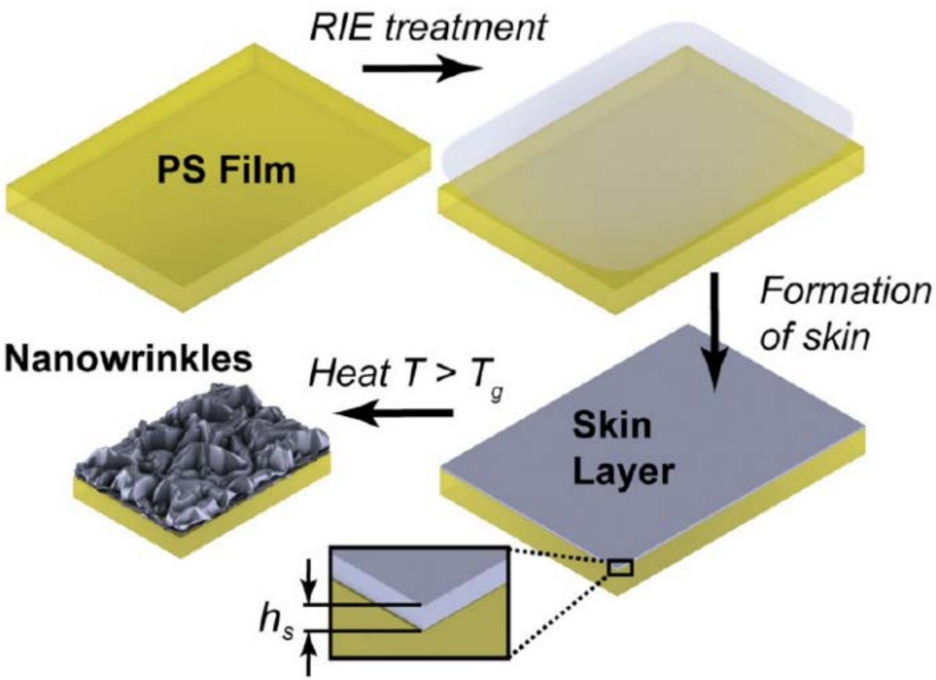
Designing quasi-random light-trapping nanostructure assuming a step SDF (single-wavelength)



$k_a^* = 0.0029\text{nm}^{-1}$, $k_b^* = 0.0030\text{nm}^{-1}$, $\rho^* = 62\%$, $t_1^* = 75\text{nm}$

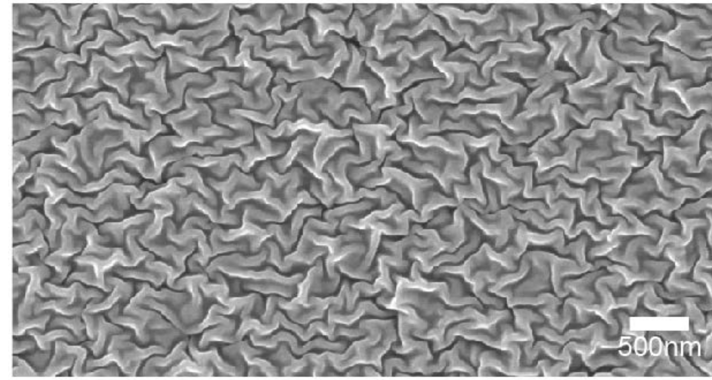
Scalable fabrication of quasi-random nanostructure using wrinkle lithography and the corresponding SDF

Thin-film wrinkling

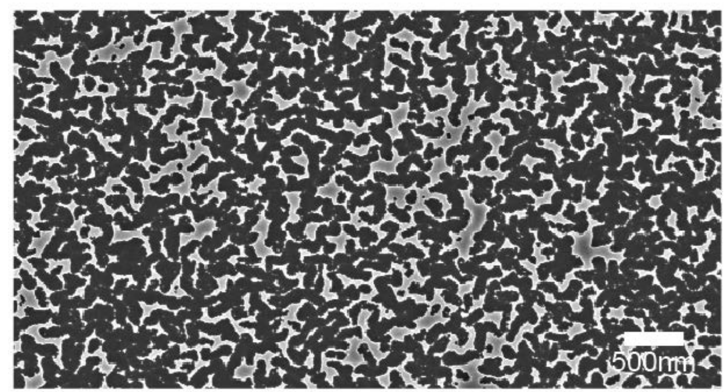


Prof. Teri W. Odom Group

Control wrinkle wavelength λ_w



Wrinkle patterning



Control filling ratio ρ and depth t_1

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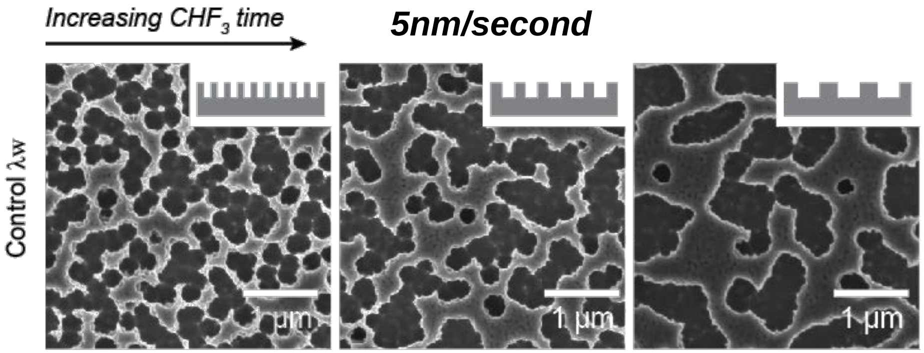
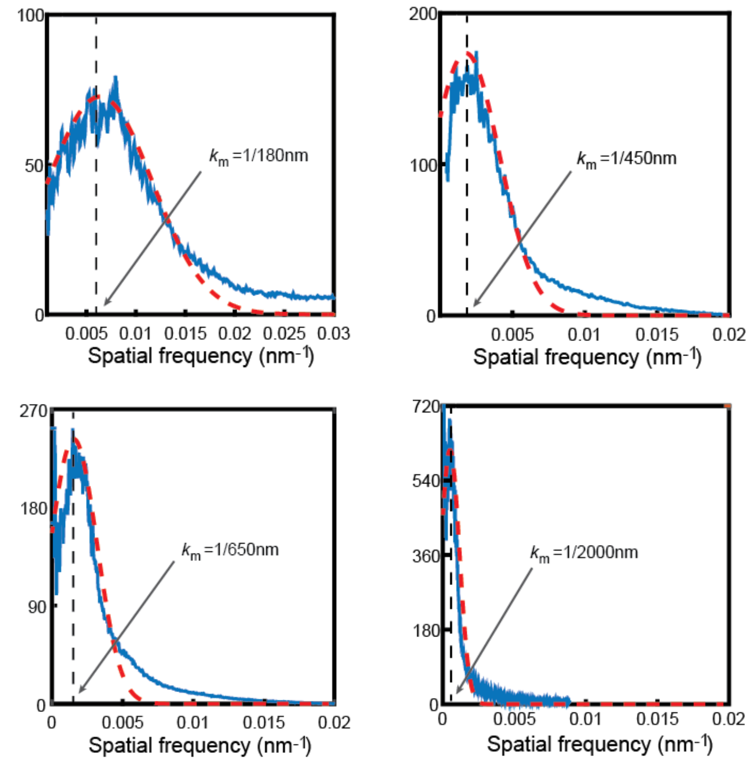
Processing-structure mapping and SDF derivation for wrinkle pattern

5nm/second



SDF derivation for wrinkle pattern



SDF~$N(\mu,\sigma)$;

$\mu = k_m = 1/\lambda_w$, $\sigma = 0.958/\lambda + 0.00017$

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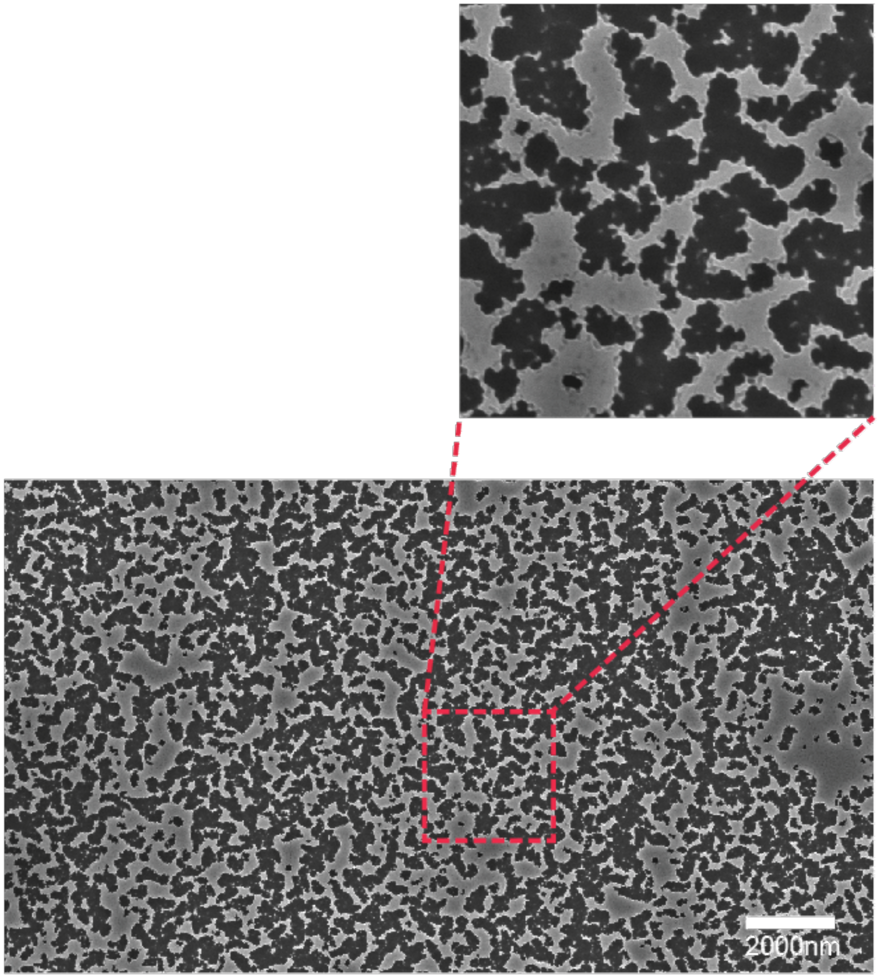
Concurrent design of quasi-random light-trapping nanostructure fabricated by wrinkle lithography



$\max_{Z}: A(Z(k_m, \rho, t_1), t, \lambda)$; $k_m^* = 0.0018\text{nm}^{-1}$, $\rho^* = 52\%$, and $t_1^* = 210\text{nm}$

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Closure

- Materials system is a complex engineered system that can benefit from state-of-the-art computational design methods.
- Stochasticity plays a critical role in material behavior prediction.
- Design and manufacturability are highly coupled in materials design.
- Big data and lack of data co-exist in materials informatics.

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