

# Statistical Learning of Microstructure Characteristics in Design of Materials System

Graduate Student Fellows:  
**RUOQIAN LIU**  
**HONGYI XU**

Faculty Advisors:  
**WEI CHEN**  
**ALOK CHOUDHARY**

Academic Disciplines:  
**MECHANICAL ENGINEERING**  
**ELECTRICAL ENGINEERING & COMPUTER SCIENCE**

**PSED Cluster 2013-2014**

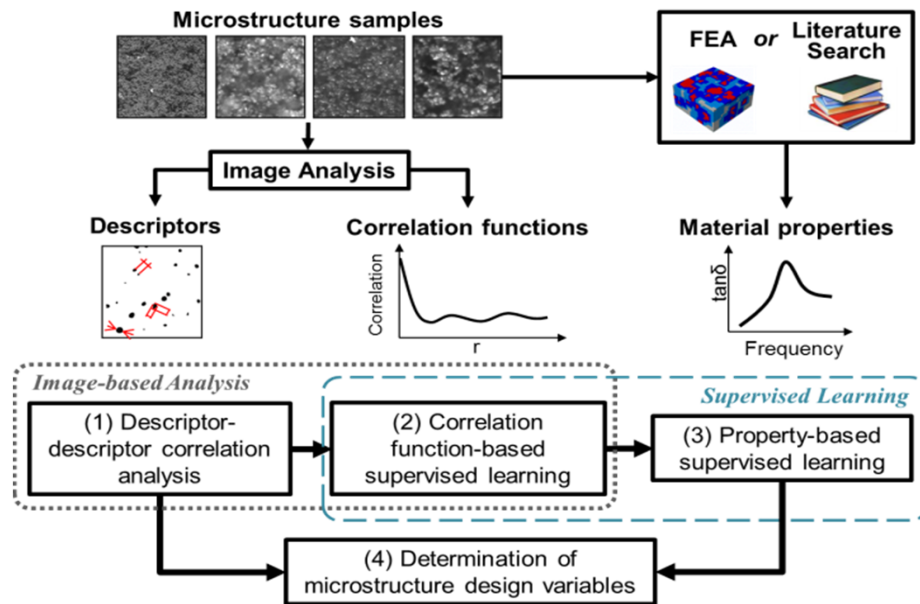
June 11, 2014

## RESEARCH OBJECTIVE

In designing microstructural materials systems, one of the key research questions is how to represent the microstructural design space quantitatively using a descriptor set that is sufficient yet small enough to be tractable. We propose a machine learning-based method for identifying the key microstructure descriptors from vast candidates as potential microstructural design variables. Not only redundant microstructure descriptors are eliminated via image analyses, key microstructure descriptors are also identified based on structure-property data, and microstructure design variables are determined. The objective is to effectively reduce the infinite dimension of the microstructure design space to a small set of descriptors without a significant information loss.

## PROBLEMS & CHALLENGES

- Traditional trial-and-error based material design is time-consuming and resource intensive
- Microstructure information, e.g. the morphology, is often not considered in the design process.
- In quantifying the morphology of microstructures,
  - Correlation functions are accurate but are of infinite dimension, and lack of physical meanings
  - Physical descriptors are of low dimension but require prior design.



A polymer nanocomposites design

Step (2) outcome

1. Filler area
2. Matrix area
3. VF
4. Local VF
5. Cluster num

Step (3) outcome

1. Matrix area
2. Filler area
3. Cluster num
4. VF
5. Local VF

Dispersion Composition

- Volume fraction (VF)
- Morisita's Index
- Nearest boundary dist
- Nearest center dist
- Local VF
- Cluster number
- Filler area
- Matrix area

Geometry

- Pore size
- Area
- Equivalent Radius
- Compactness
- Orientation
- Aspect ratio
- Roundness
- Eccentricity
- Elongation ratio
- Rectangularity
- Tortosity