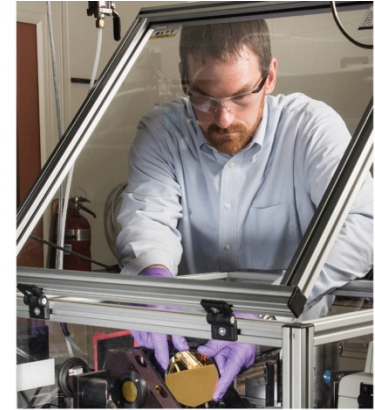


# AI and Materials

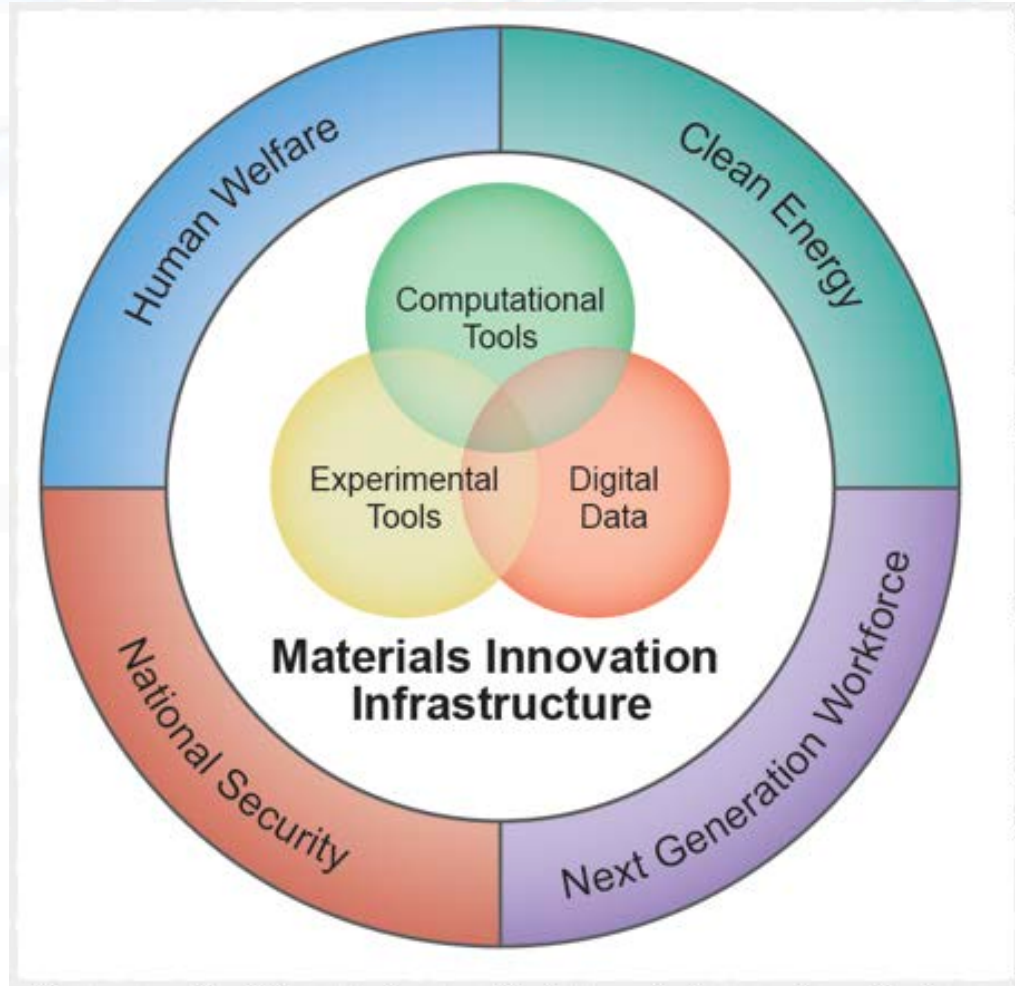


Eric K. Lin, Jim A. Warren

Director, Material Measurement Laboratory

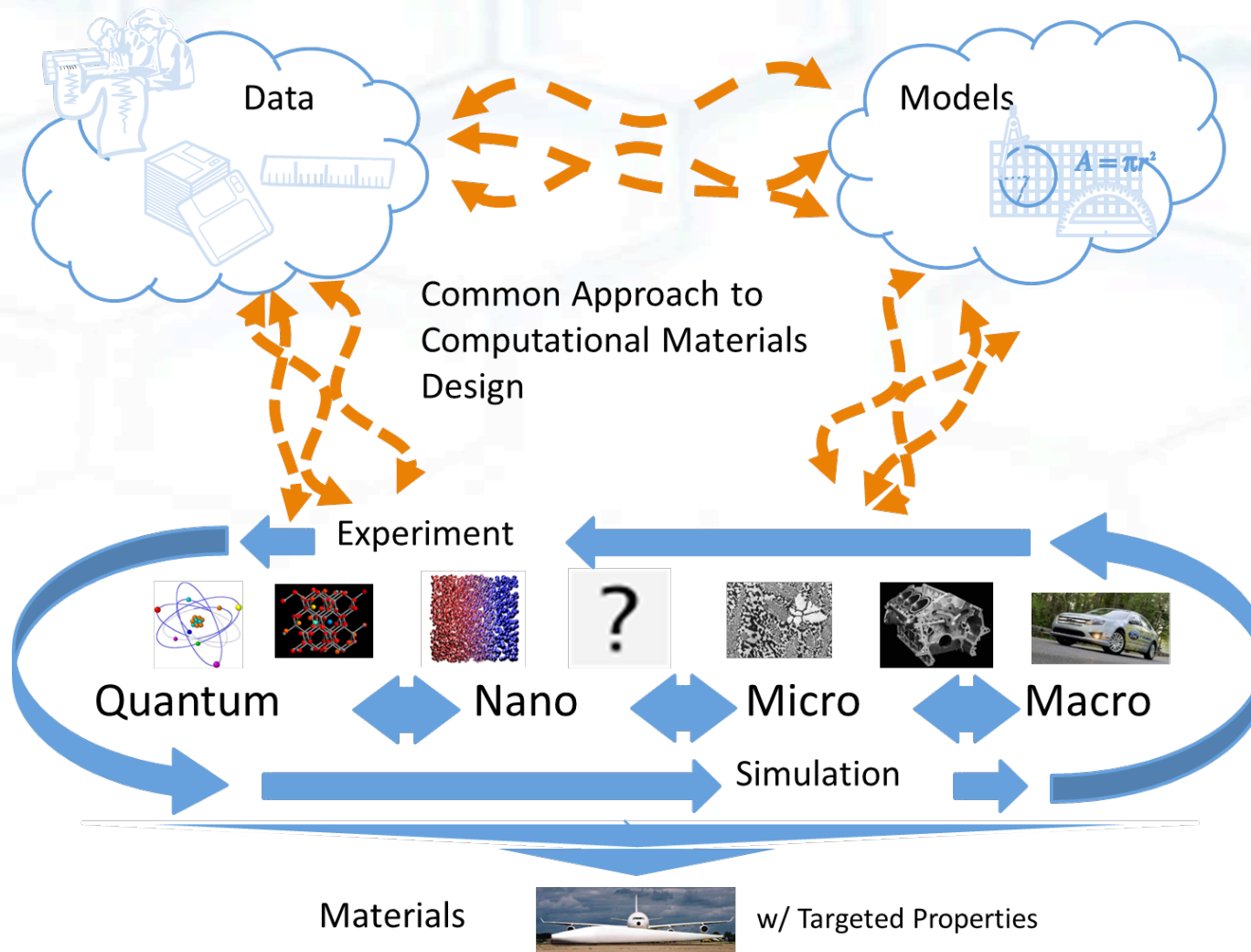
Director, Materials Genome Program

# Materials Genome Initiative (MGI) 1.0

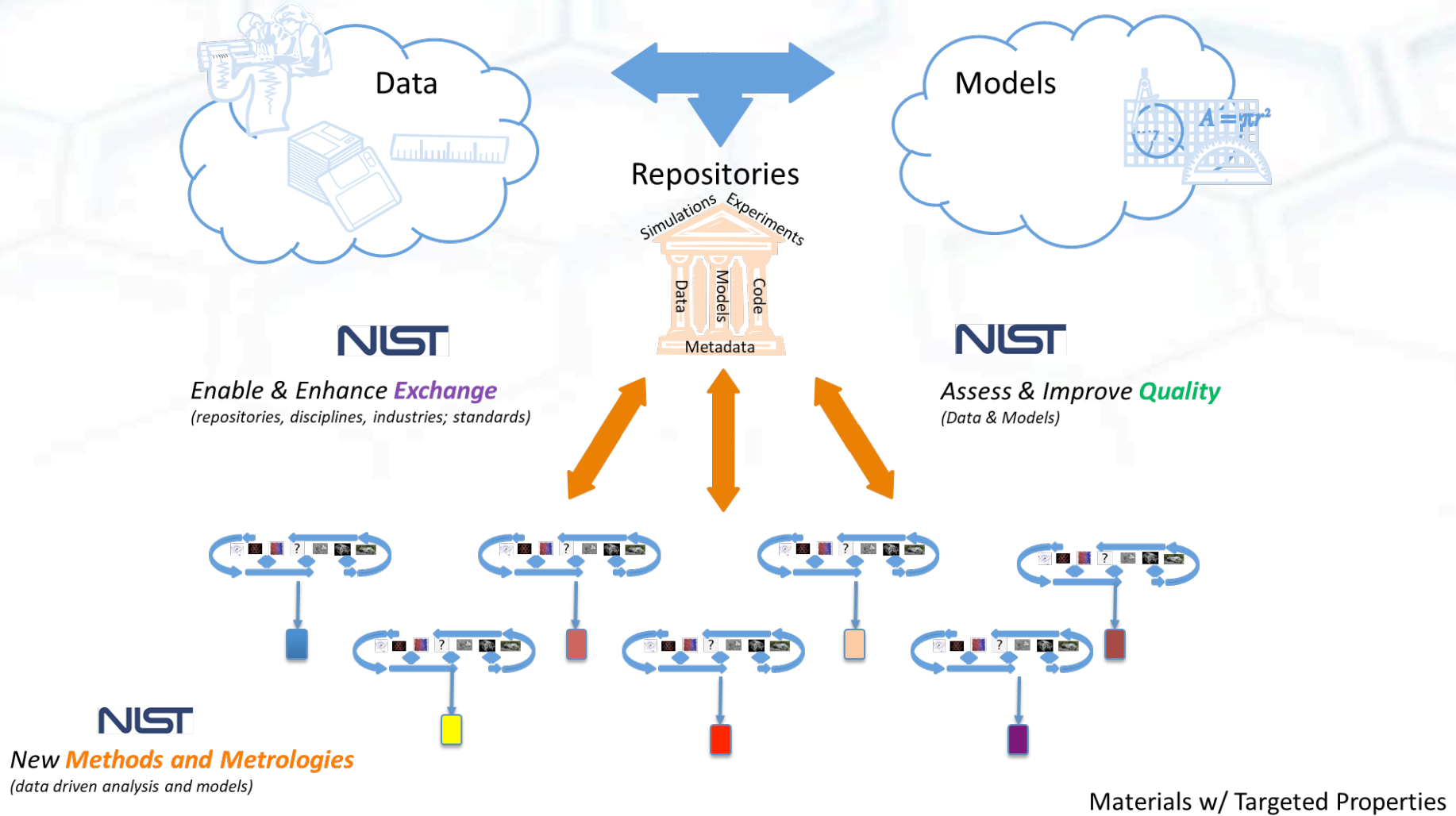


- Develop a Materials Innovation Infrastructure
- Achieve National goals in energy, security, and human welfare with advanced materials
- Equip the next generation materials workforce

# From Use-Case



# To an Ecosystem



# MGI Success

- Facilitating Data Science
  - Standards
  - Repositories
  - Enabling Data Discovery
- Trust in models
  - Force fields
  - Phase field methods
- New Materials
  - Superalloys
  - US Mint (Nickel)
  - Directed Self-Assembly

The screenshot shows the NIST Materials Genome Initiative Gateway website. The header includes the NIST logo and the text "NIST Materials Genome Initiative Gateway to Materials Genome Information". A navigation menu contains links for HOME, PROJECTS, ABOUT, MATERIAL RESOURCE CENTERS, FEDERAL MATERIALS GENOME INITIATIVE, ONLINE TOOLS, and CONTACT. The main content area features a large image of a BCARS composite image of a polyethylene blend, with the caption "BCARS of Polyethylene" and a sub-caption "Typical BCARS composite image of a polyethylene blend taken at NIST showing circular polarization". Below this, there are sections for "CHiMaD" (Center for Hierarchical Materials Design), "MGI Reports - What's New" (announcing the 2015 annual report), and "Welcome to Materials Genome Initiative (MGI) at NIST". A circular diagram titled "Materials Innovation Infrastructure" shows the integration of Human Ventures, Computational Tools, Experimental Tools, and Digital Data. A "Quick Navigation by Project Category" sidebar lists various project areas like High Throughput Materials Science, Data and Model Dissemination, and Software Tools. The "Recent Updates" section lists several recent publications and reports.

# NIST Center of Excellence: Advanced Materials



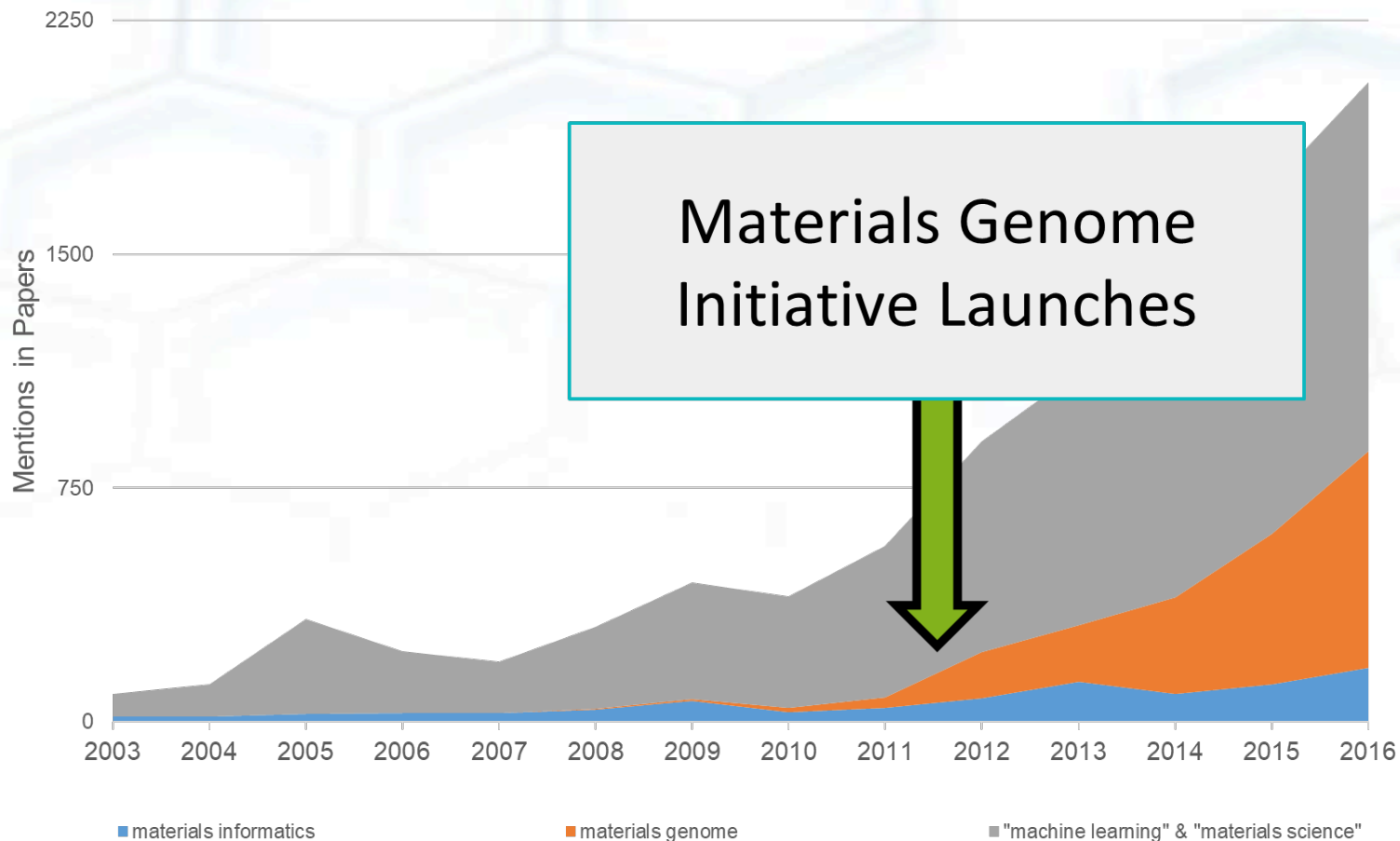
## CENTER FOR HIERARCHICAL MATERIALS DESIGN

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[chimad.northwestern.edu](http://chimad.northwestern.edu)

# Materials Informatics Growth



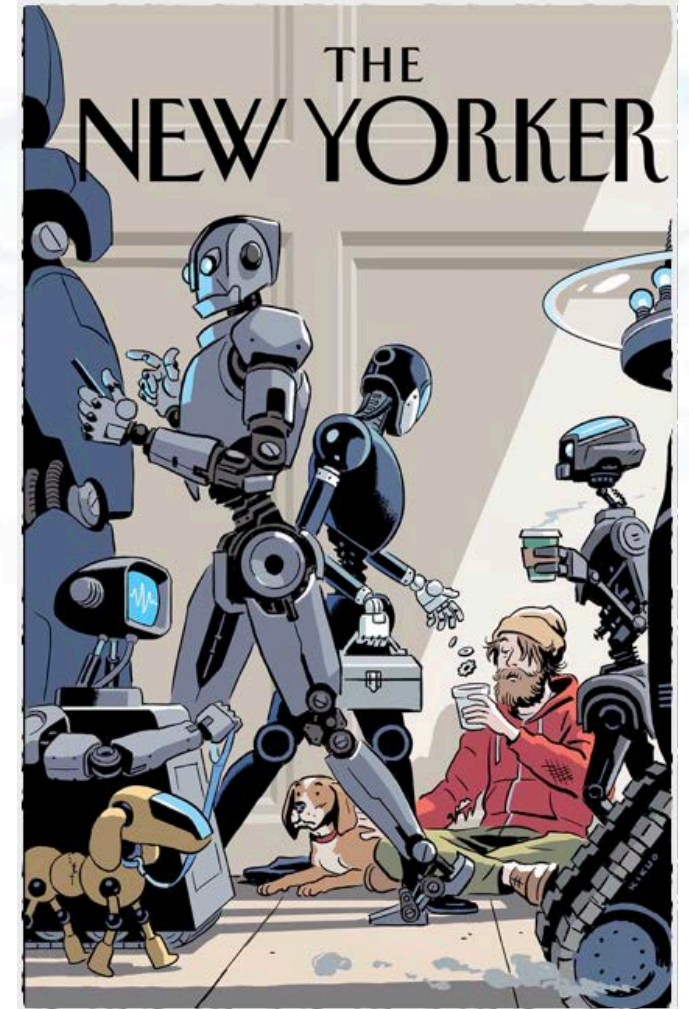
Bryce Meredig



Citrine Informatics

# MGI 2.0: Accelerate Progress

- MGI 1.0 provided a foundation for AI approaches
- Materials Design is full of opportunity
- Early Examples
  - Improve Materials Modeling: Force Fields
  - Classification of Microscopy Images
  - Efficient Phase Diagram Measurements
  - Enable New Materials Measurements: Strain Tensor

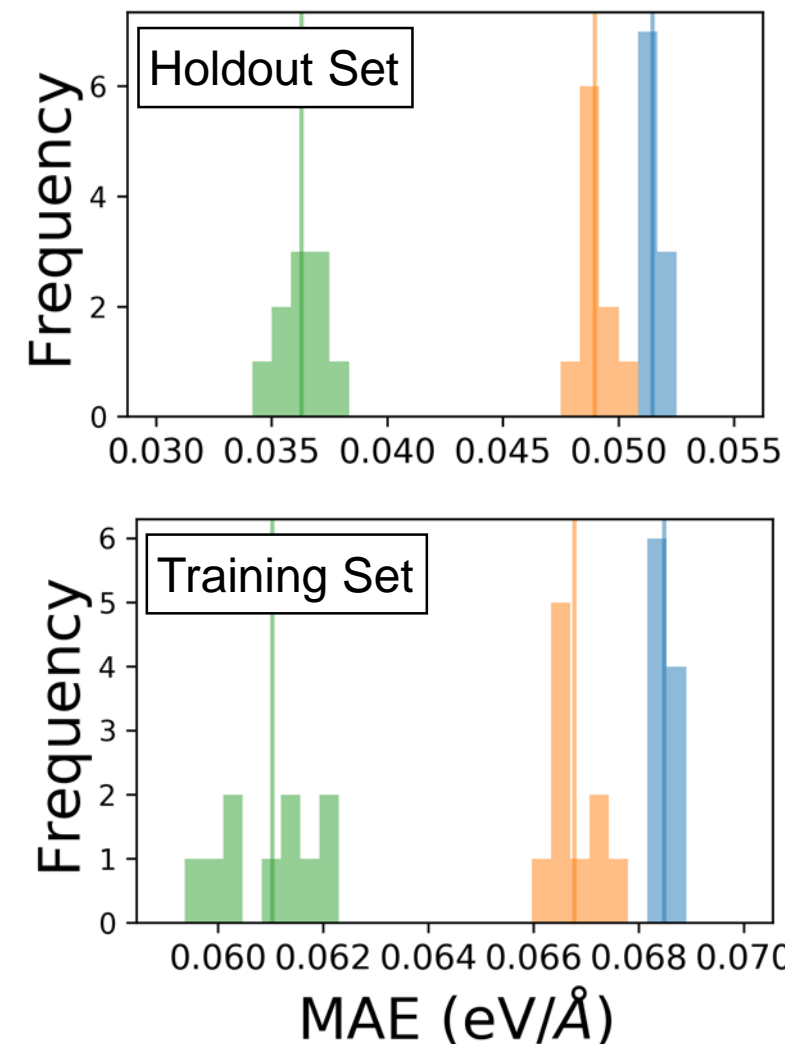
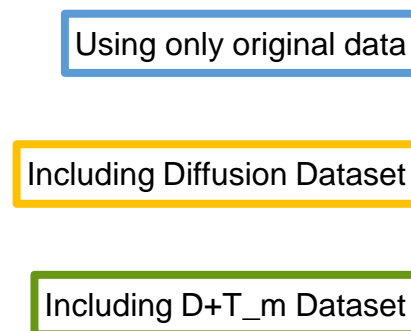




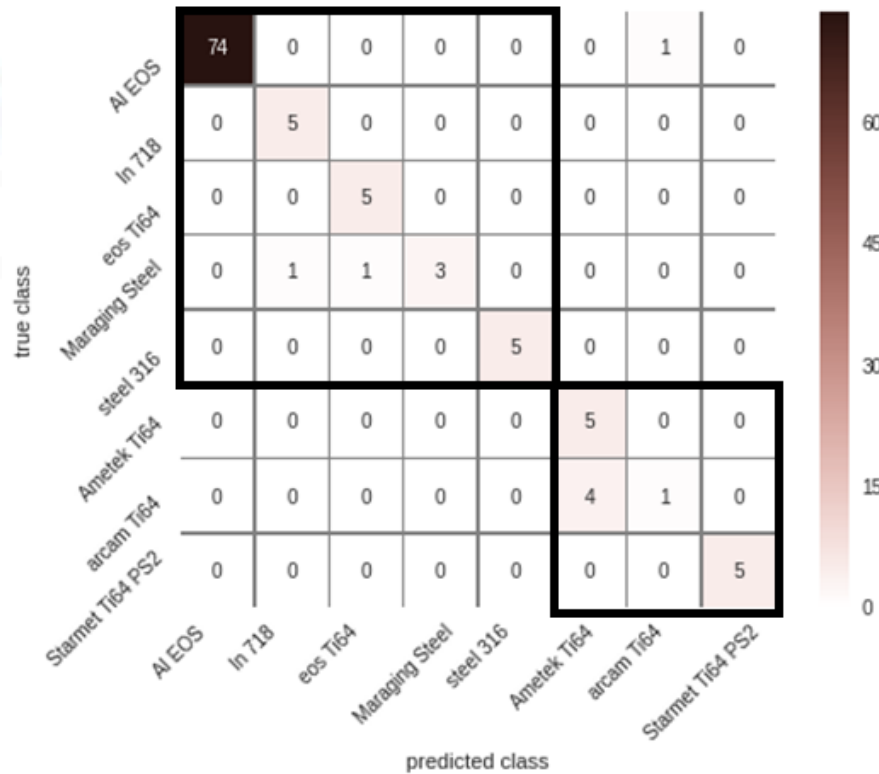
# Improve Modeling: Force Field Determination

- Quality of materials simulation is dependent on quality of governing equations: force field, interatomic potentials
- Up to 50% of research time spent on validation, verification of force fields
- Use ML with multiple data sets

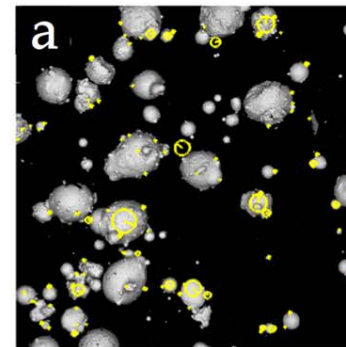
Better performance in original application:  
No new DFT calculations needed



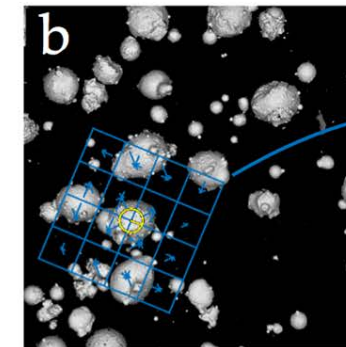
# Classification of Materials Microscopy Images



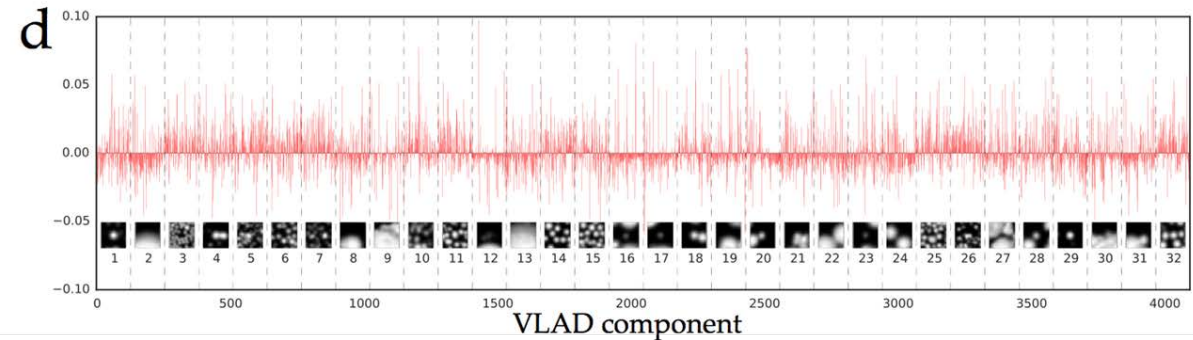
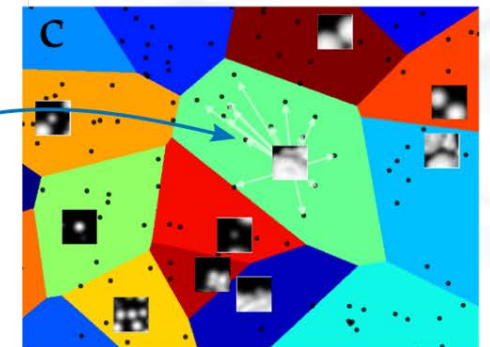
1: select image features



2: characterize image features



3: encode image features

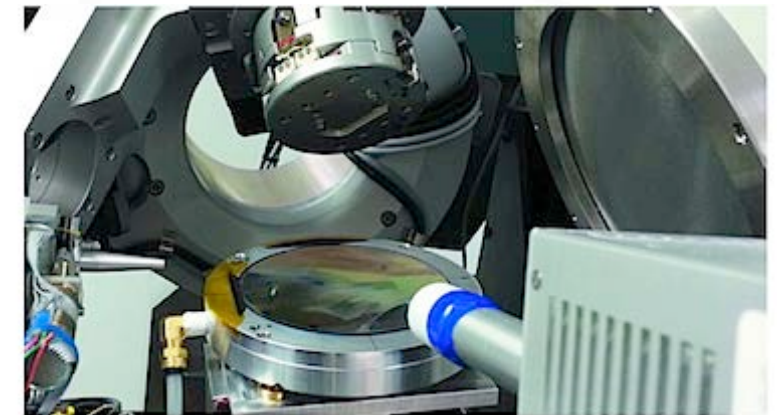
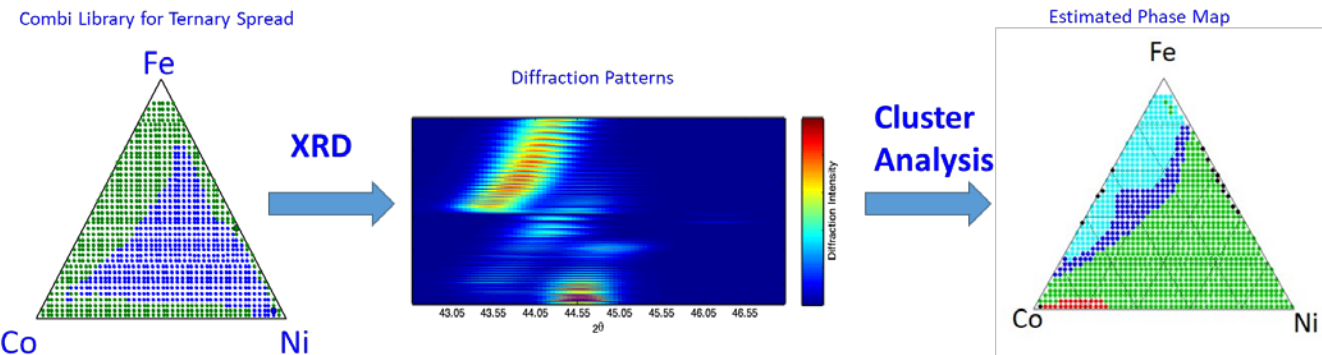
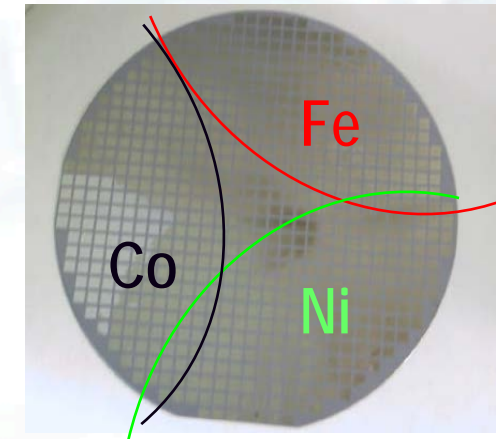


ML-derived and curated data sets

B. DeCost, H. Jain, A. Rollett, and E. Holm  
*JOM* (2016). doi:10.1007/s11837-016-2226-1

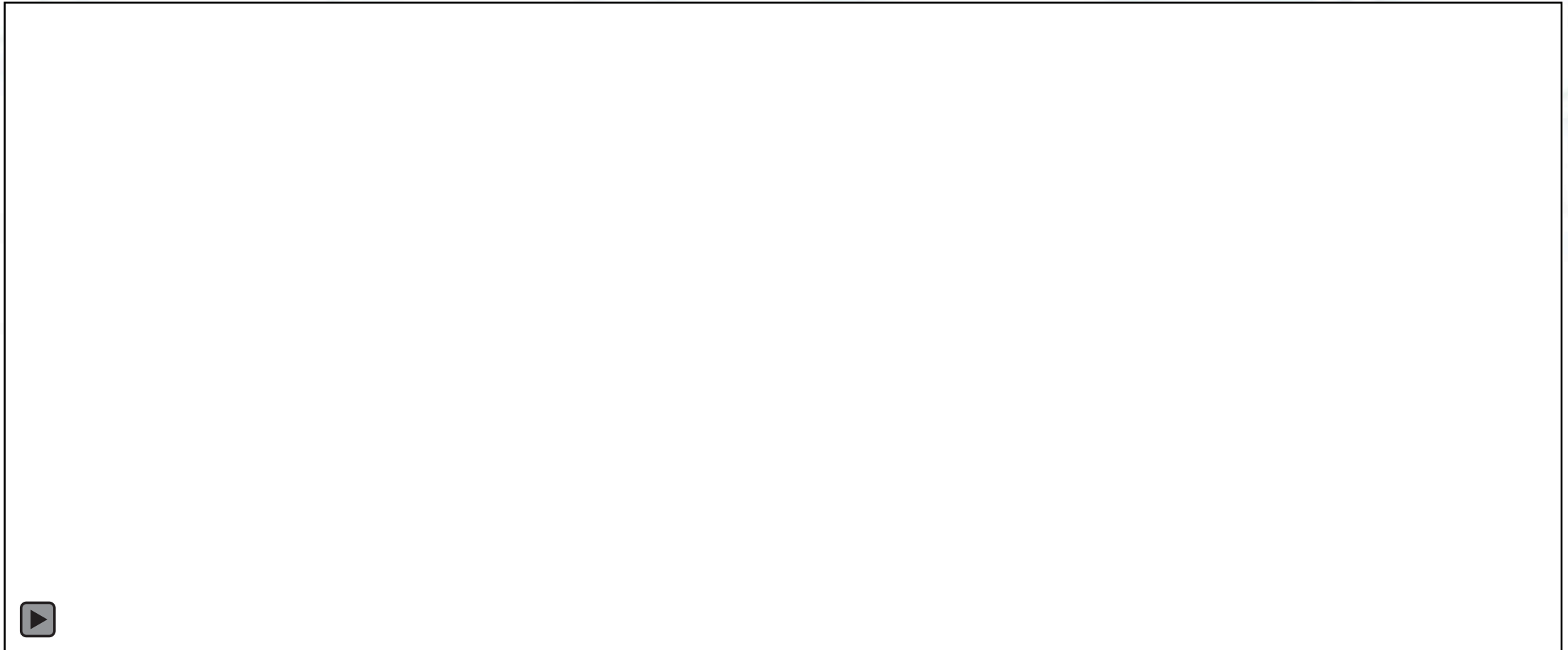
# Efficient Phase Diagram Measurement

- High-Throughput and Autonomous Materials Science
- Enabling Framework for AI
  - Access to Materials Databases
  - Access to Modeling Results and Programs
  - Underpinning Scientific 'Rules'
- Provide AI control over Experimental Systems

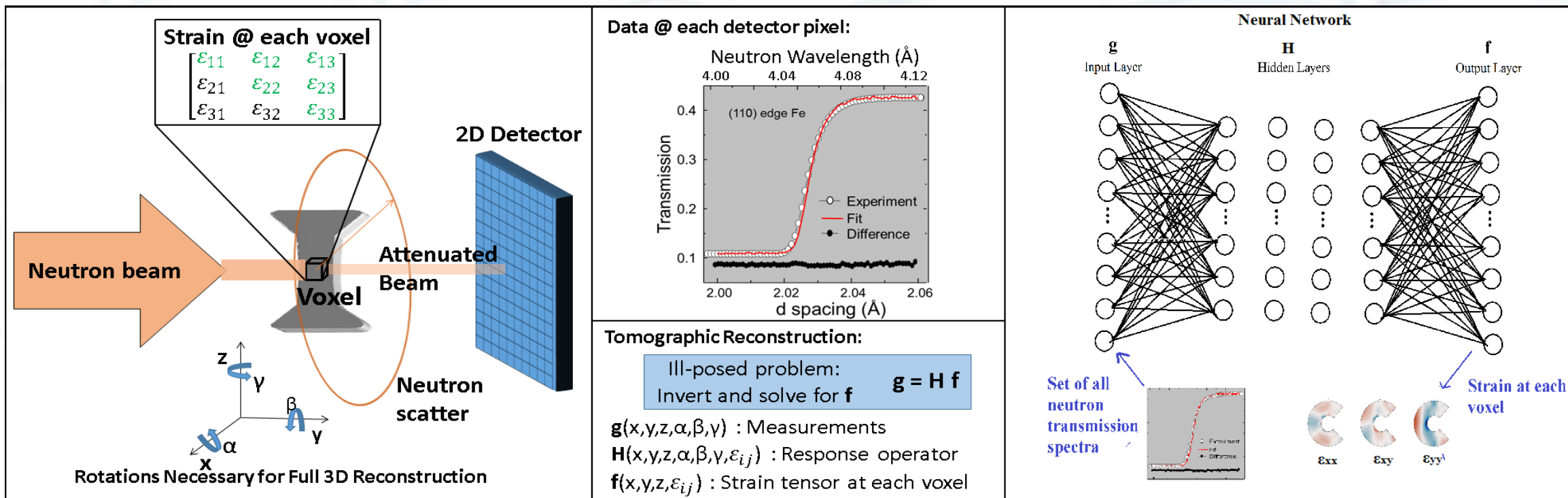


# Autonomous Phase Mapping (Fe-Ga-Pd)

A. Gilad Kusne and collaborators



# Strain Tensor Tomography



Strain tensor would be a ML-derived quantity

Matthew Connolly et al.

# Closing Thoughts



- ML and AI are powerful tools to enhance materials science and engineering
- New measurement questions, e.g. what is the uncertainty in a ML derived quantity?
- Opportunities with convergence with advances in synthetic control and additive manufacturing
- Need to invest in internal capabilities and expertise