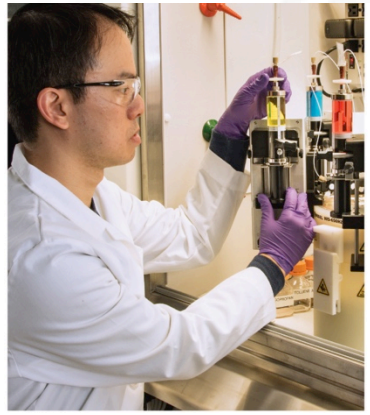
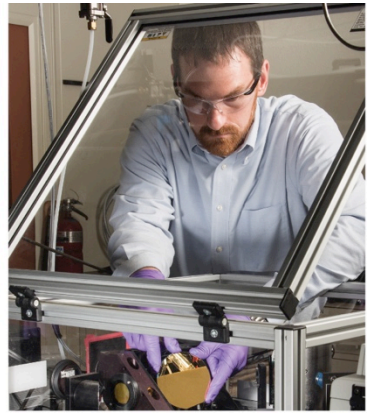
AI and Materials





Eric K. Lin, Jim A. Warren

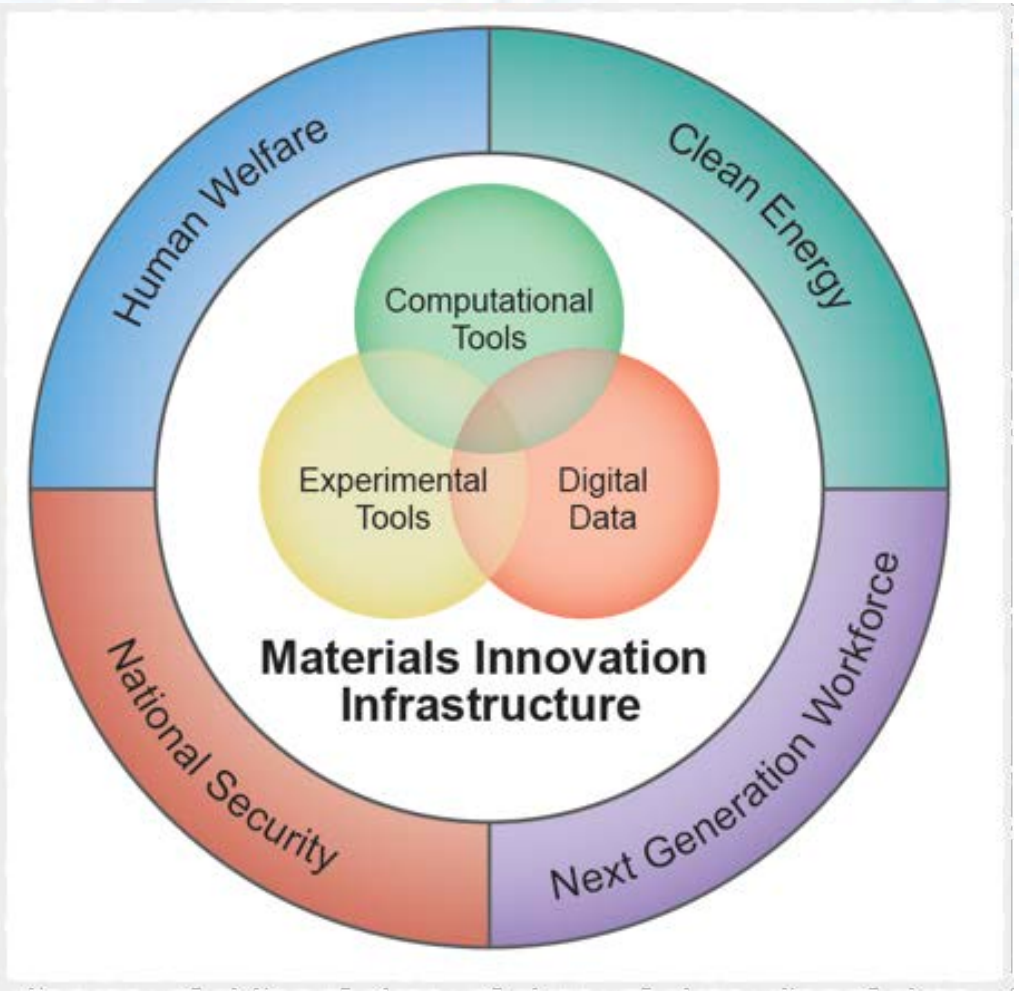
Director, Material Measurement Laboratory

Director, Materials Genome Program

NIST
National Institute of
Standards and Technology
U.S. Department of Commerce

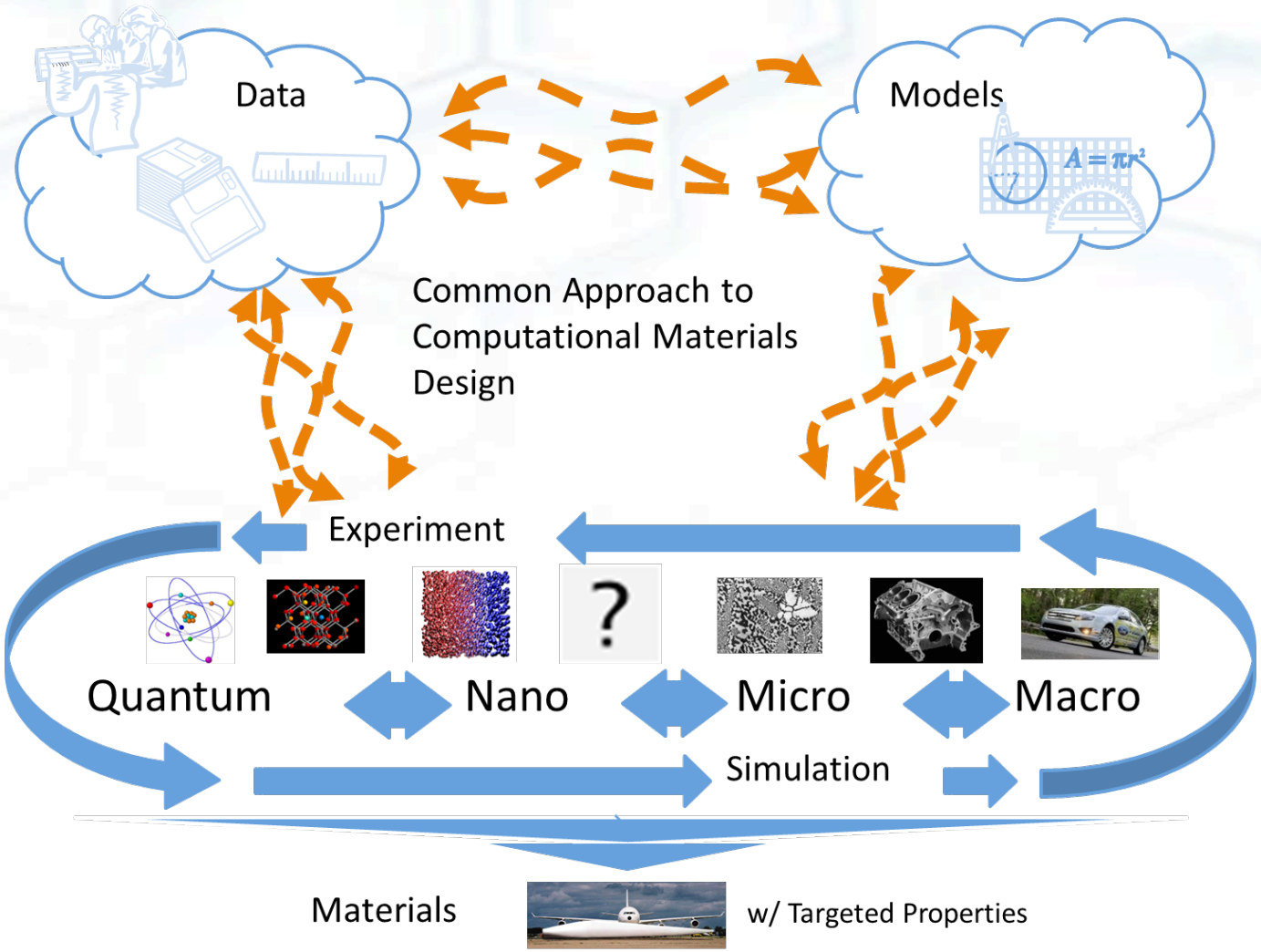
MATERIAL
MEASUREMENT
LABORATORY

Materials Genome Initiative (MGI) 1.0

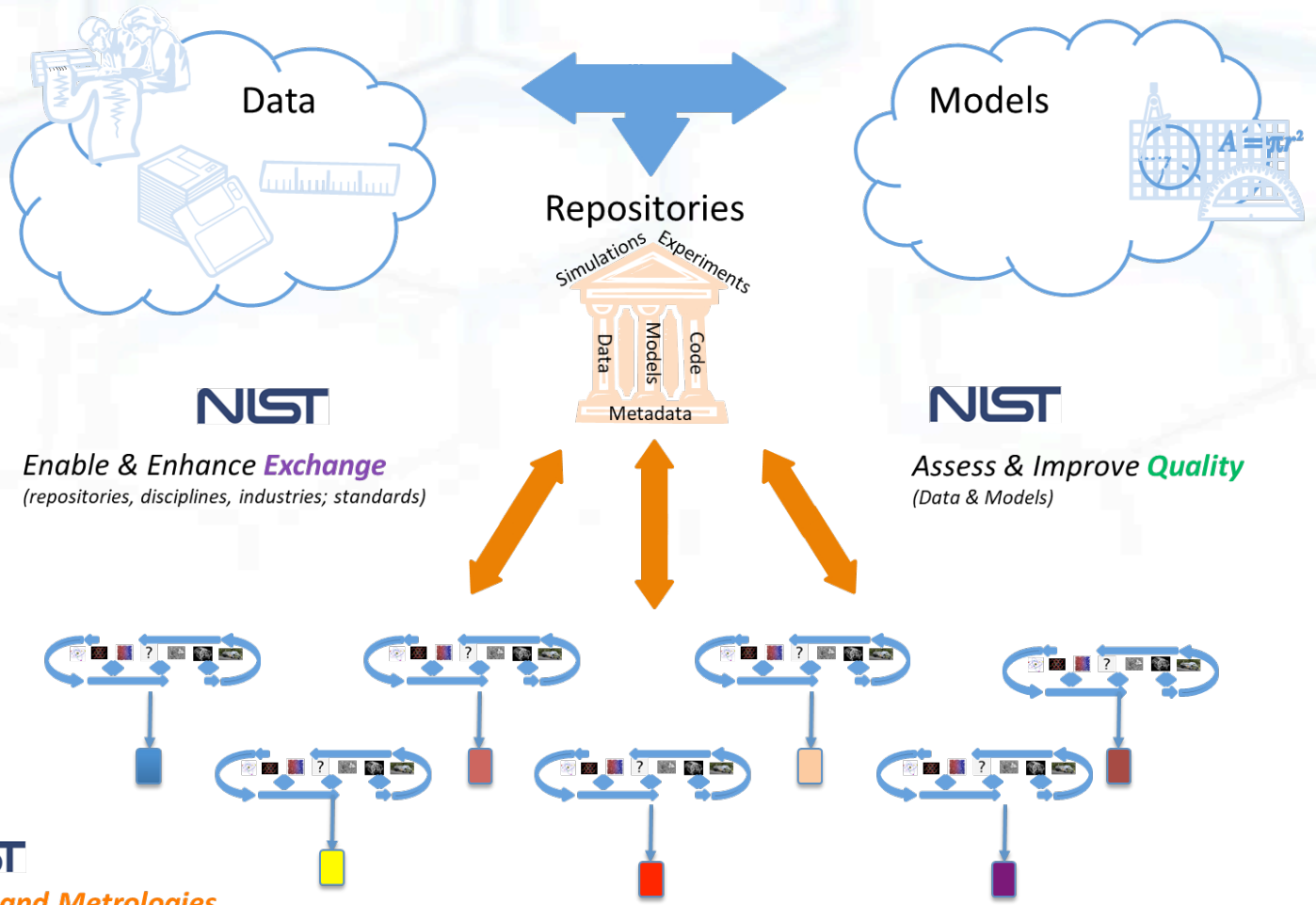


- Develop a Materials Innovation Infrastructure
- Achieve National goals in energy, security, and human welfare with advanced materials
- Equip the next generation materials workforce

From Use-Case

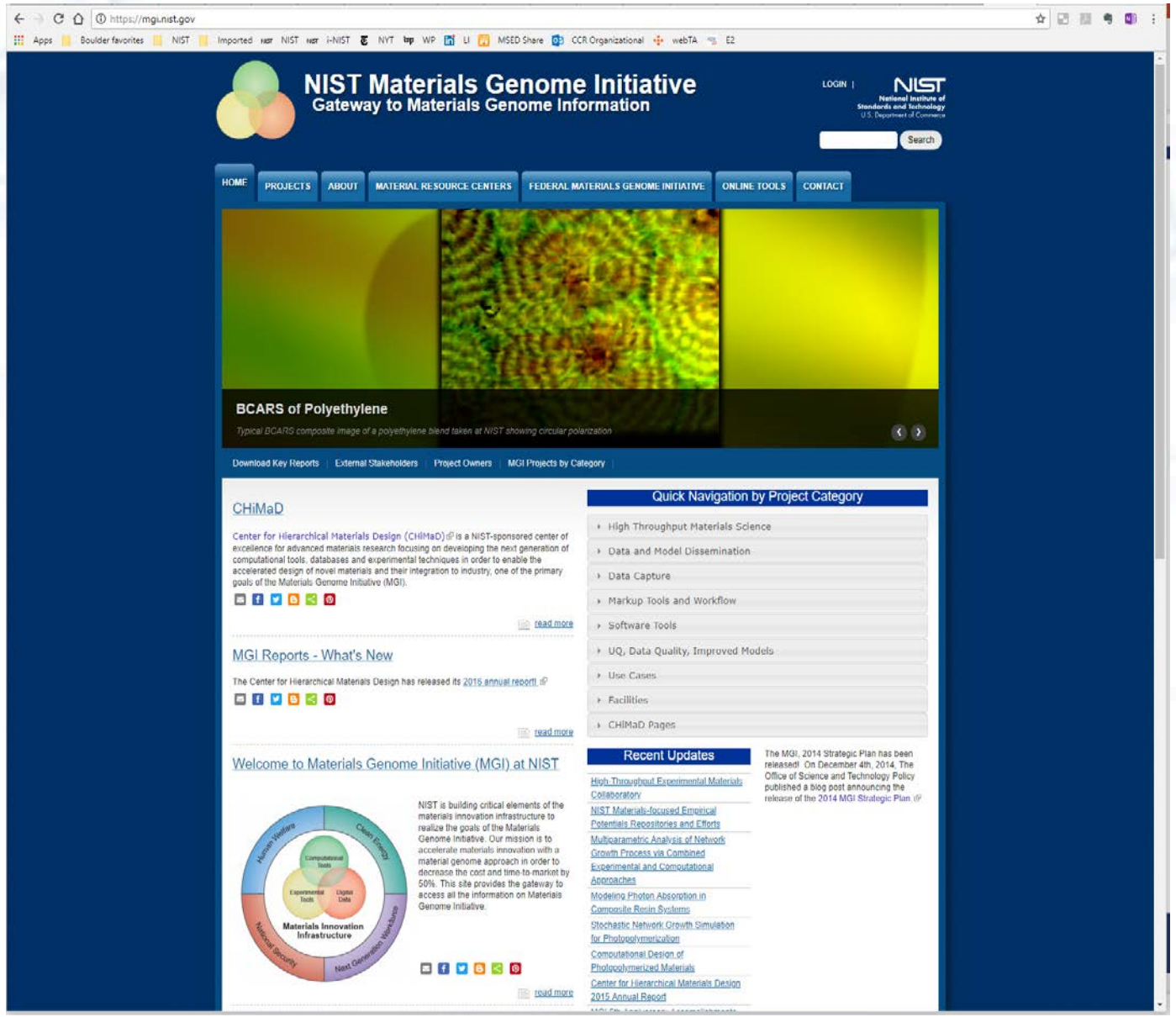


To an Ecosystem



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



NIST Center of Excellence: Advanced Materials

CHiMaD

CENTER FOR HIERARCHICAL MATERIALS DESIGN

THE UNIVERSITY OF CHICAGO

NORTHWESTERN UNIVERSITY

Argonne NATIONAL LABORATORY

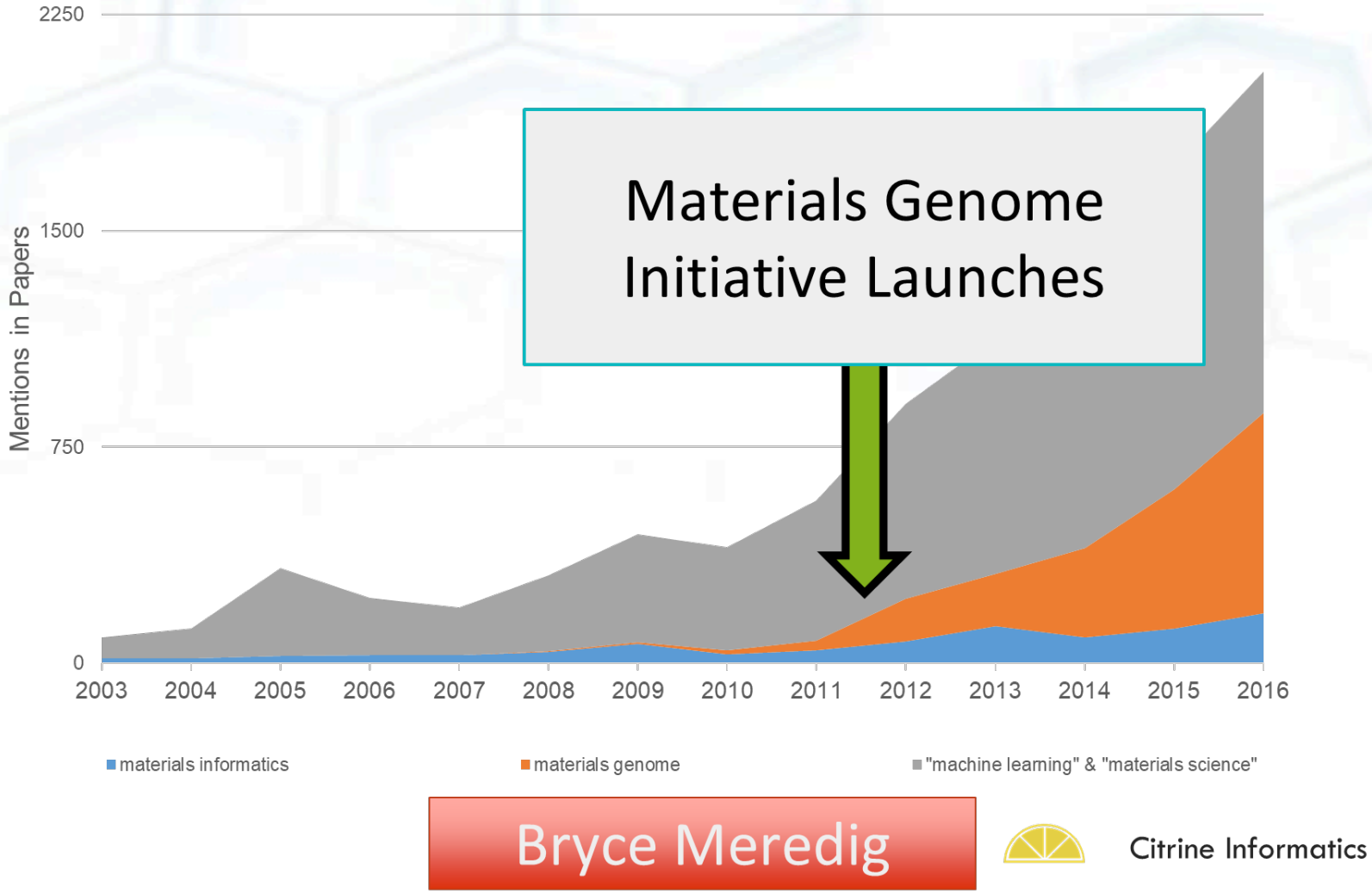
QUESTEK INNOVATIONS LLC

ASM INTERNATIONAL

FAYETTEVILLE STATE UNIVERSITY

chimad.northwestern.edu

Materials Informatics Growth

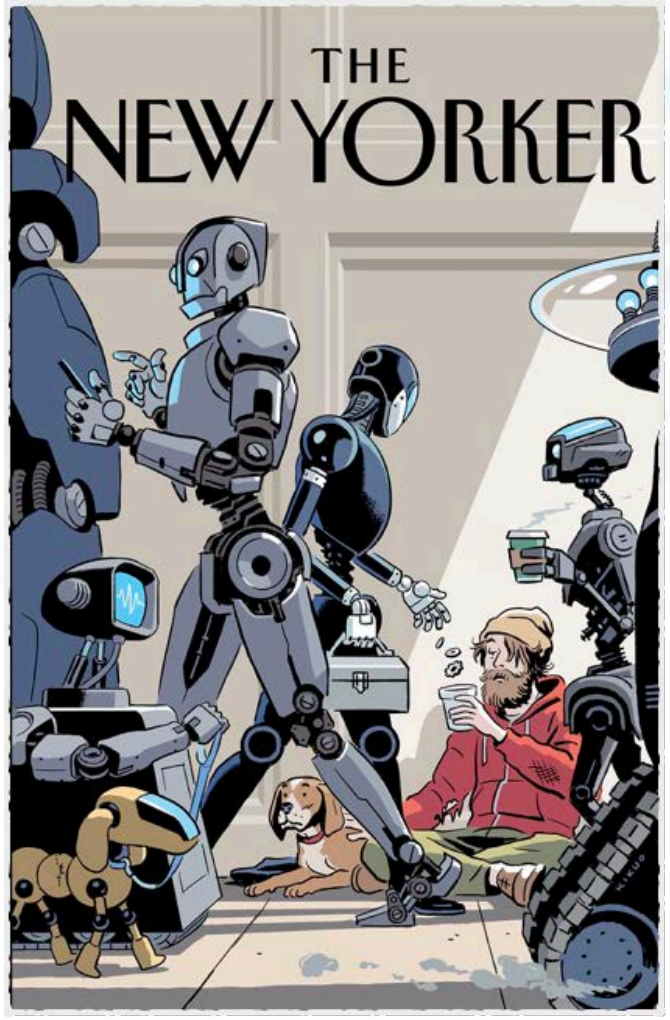


Bryce Meredig

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

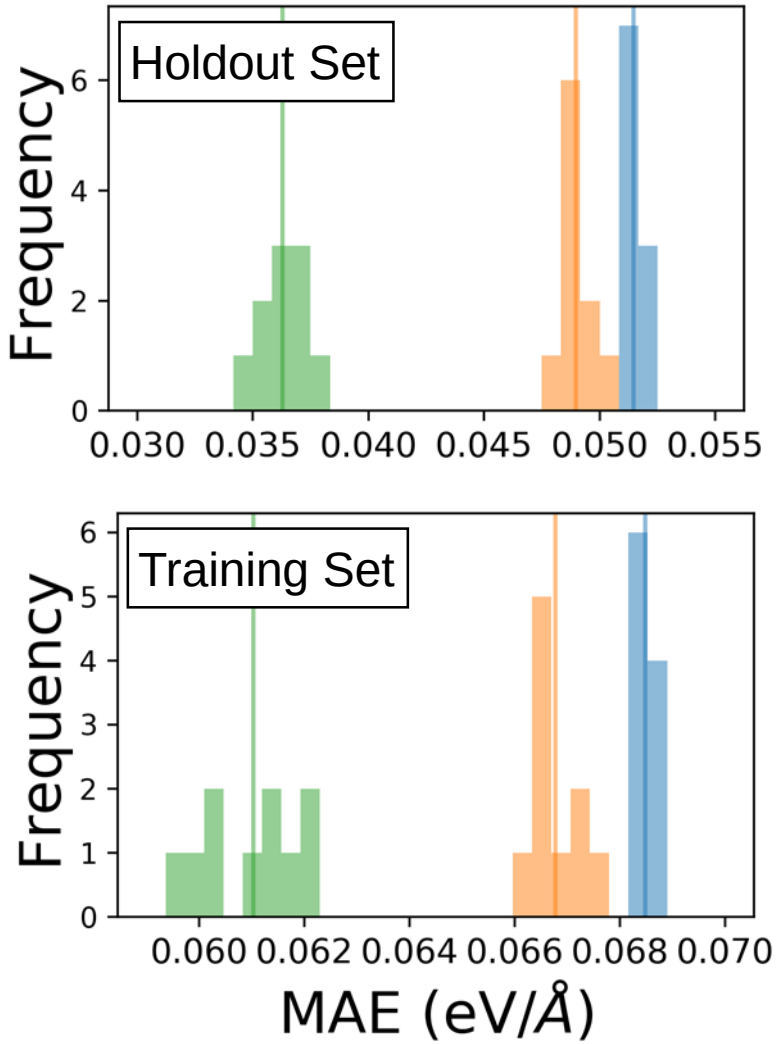
- Quality of materials simulation is dependent on quality of governing equations: force field, interatomic potentials
- Up to 50% of research time spent on validation, verification of force fields
- Use ML with multiple data sets

Better performance in original application:
No new DFT calculations needed

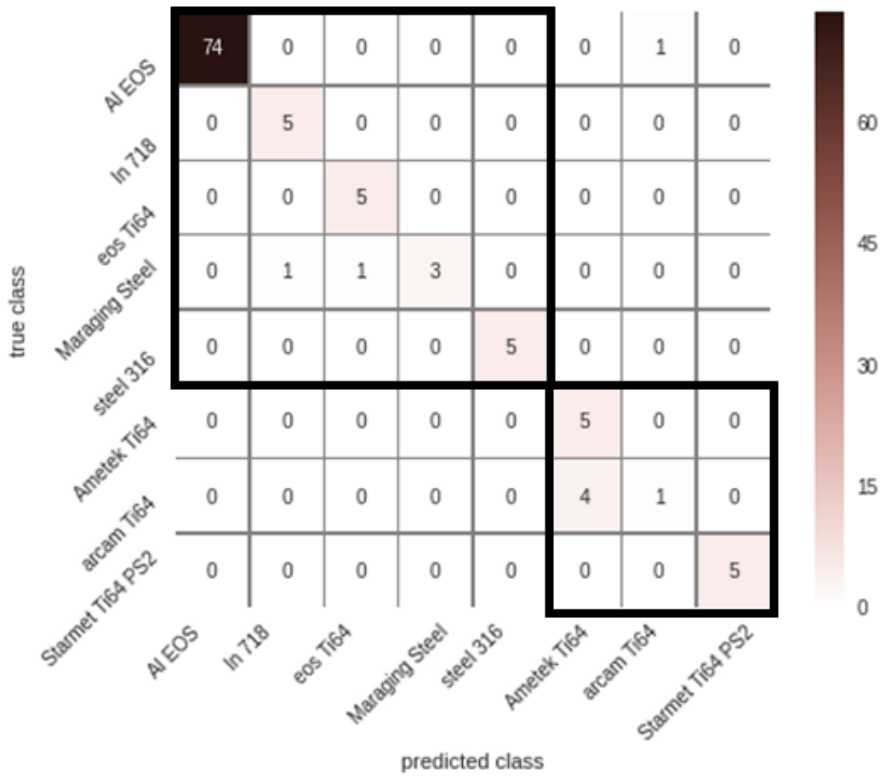
Using only original data

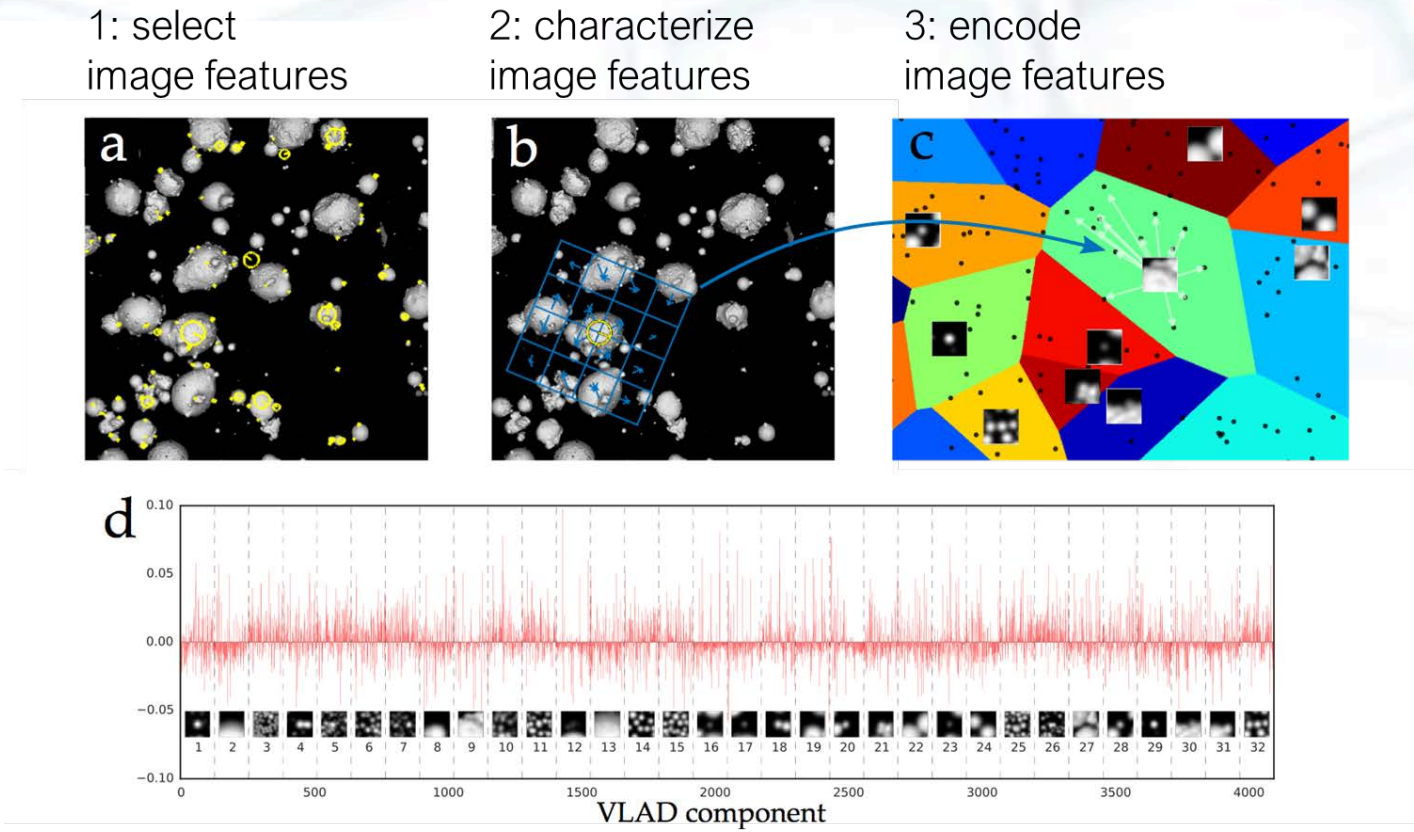
Including Diffusion Dataset

Including D+T_m Dataset



Classification of Materials Microscopy Images





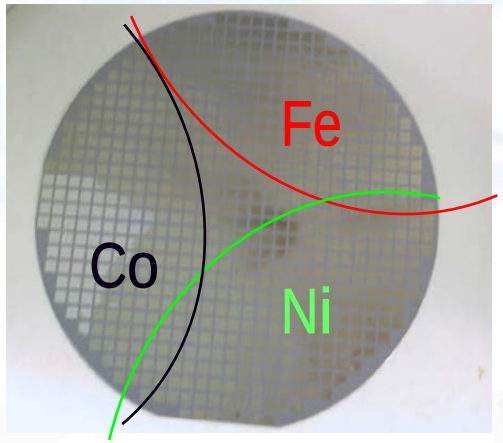
ML-derived and curated data sets

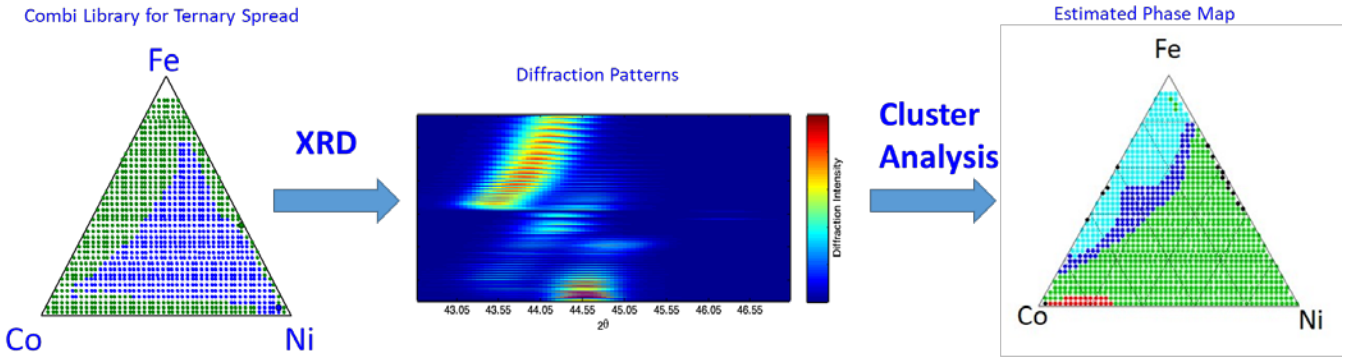
B. DeCost, H. Jain, A. Rollett, and E. Holm
JOM (2016). doi:10.1007/s11837-016-2226-1

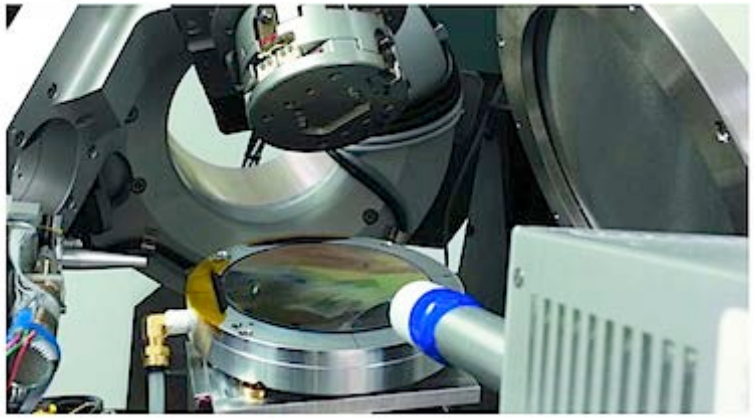
Efficient Phase Diagram Measurement

A. Gilad Kusne and collaborators

- 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

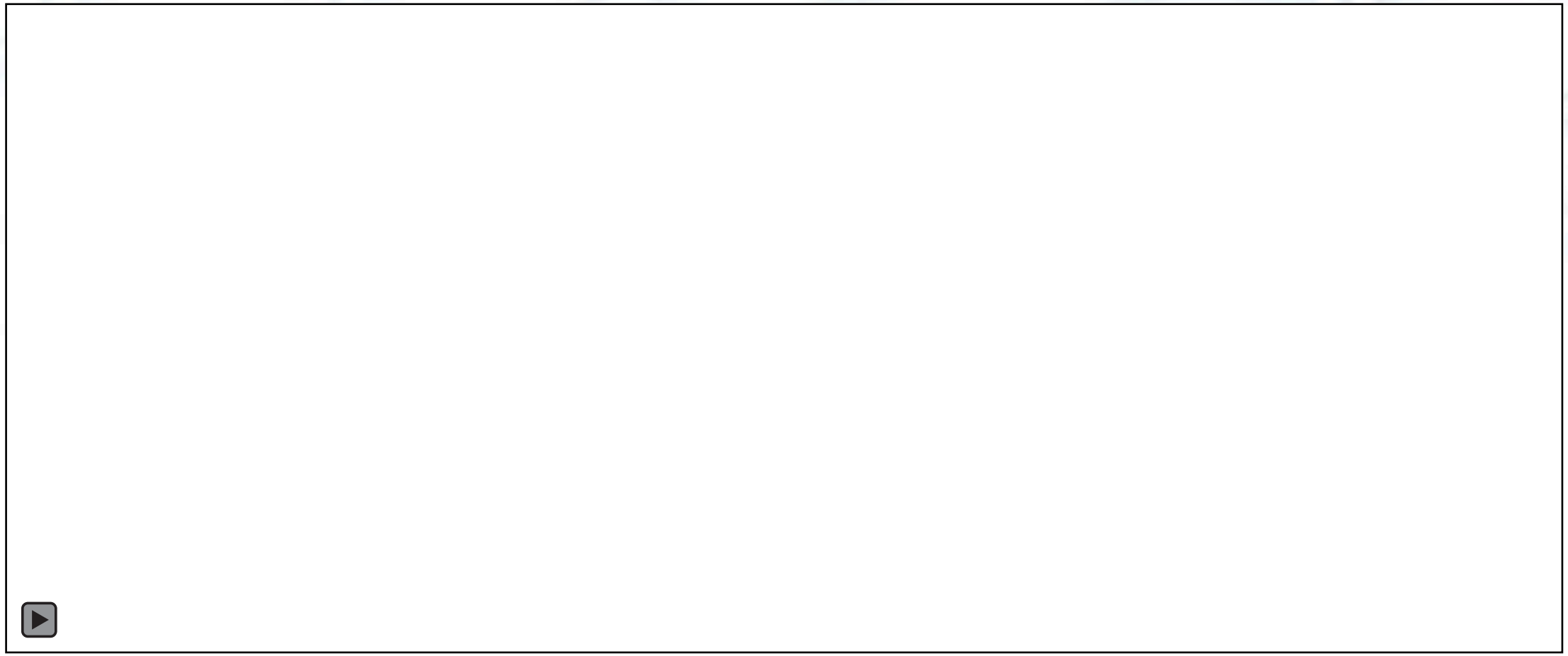




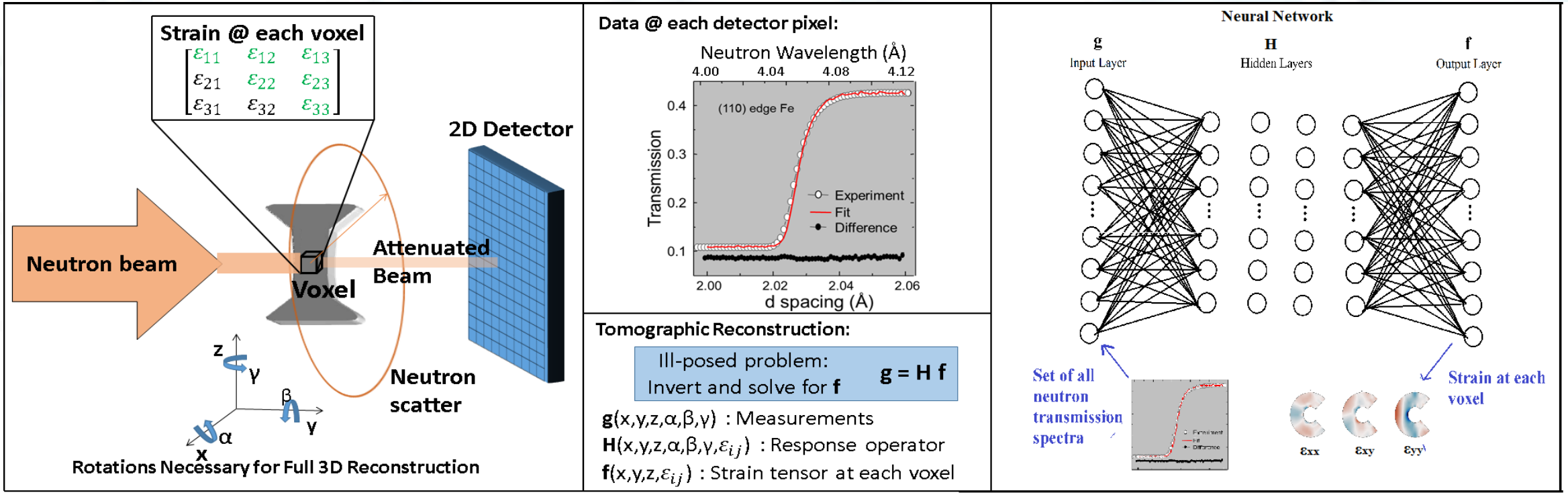


Autonomous Phase Mapping (Fe-Ga-Pd)

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