

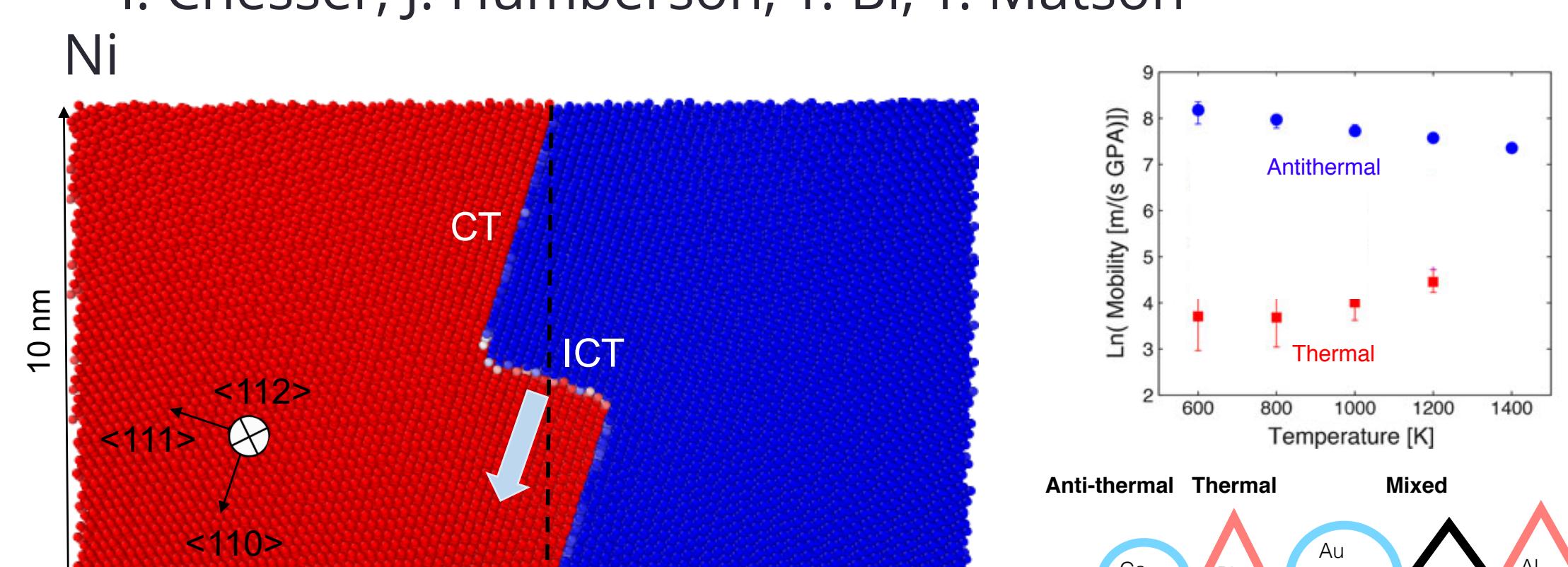
Computational Materials Research: Professor Elizabeth A. Holm

Carnegie Mellon University
Department of Materials Science and Engineering

PHYSICAL SIMULATION

ATOMISTIC SIMULATION OF GRAIN BOUNDARY MIGRATION

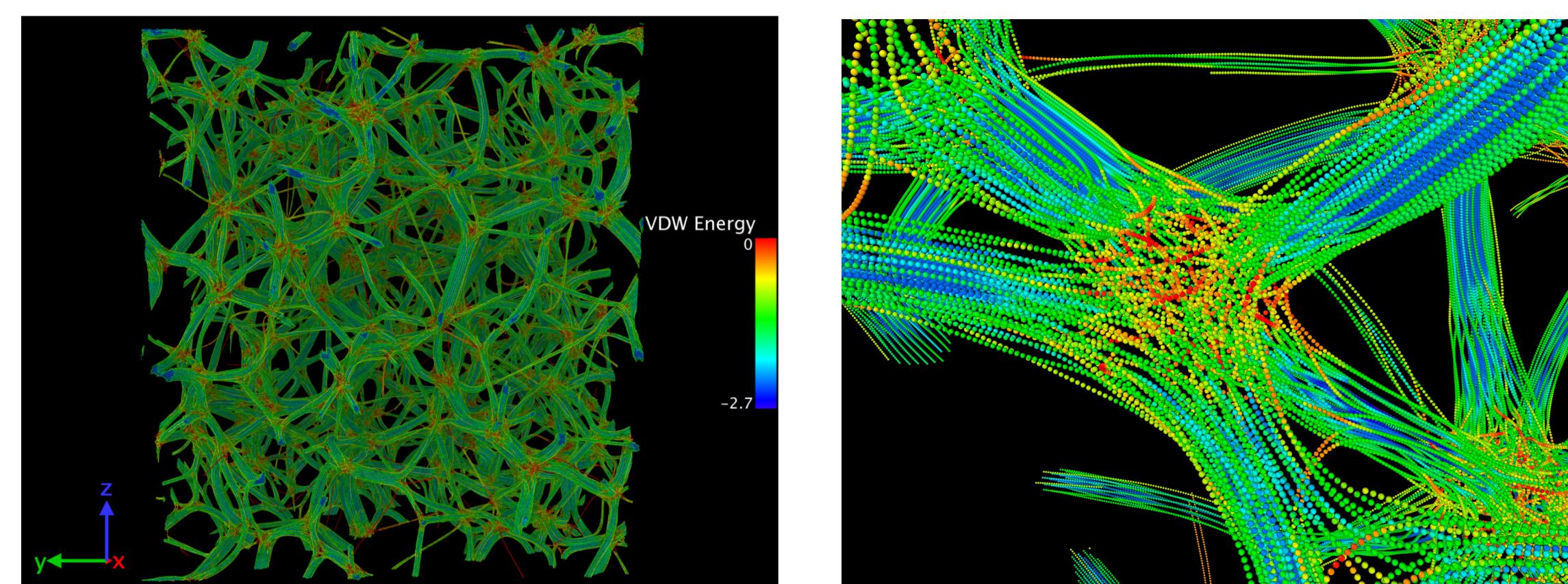
I. Chesser, J. Humberson, Y. Bi, T. Matson



- Identical crystallographically defined grain boundaries in different FCC metals can show distinct thermal behavior

CARBON NANOTUBE MODELING

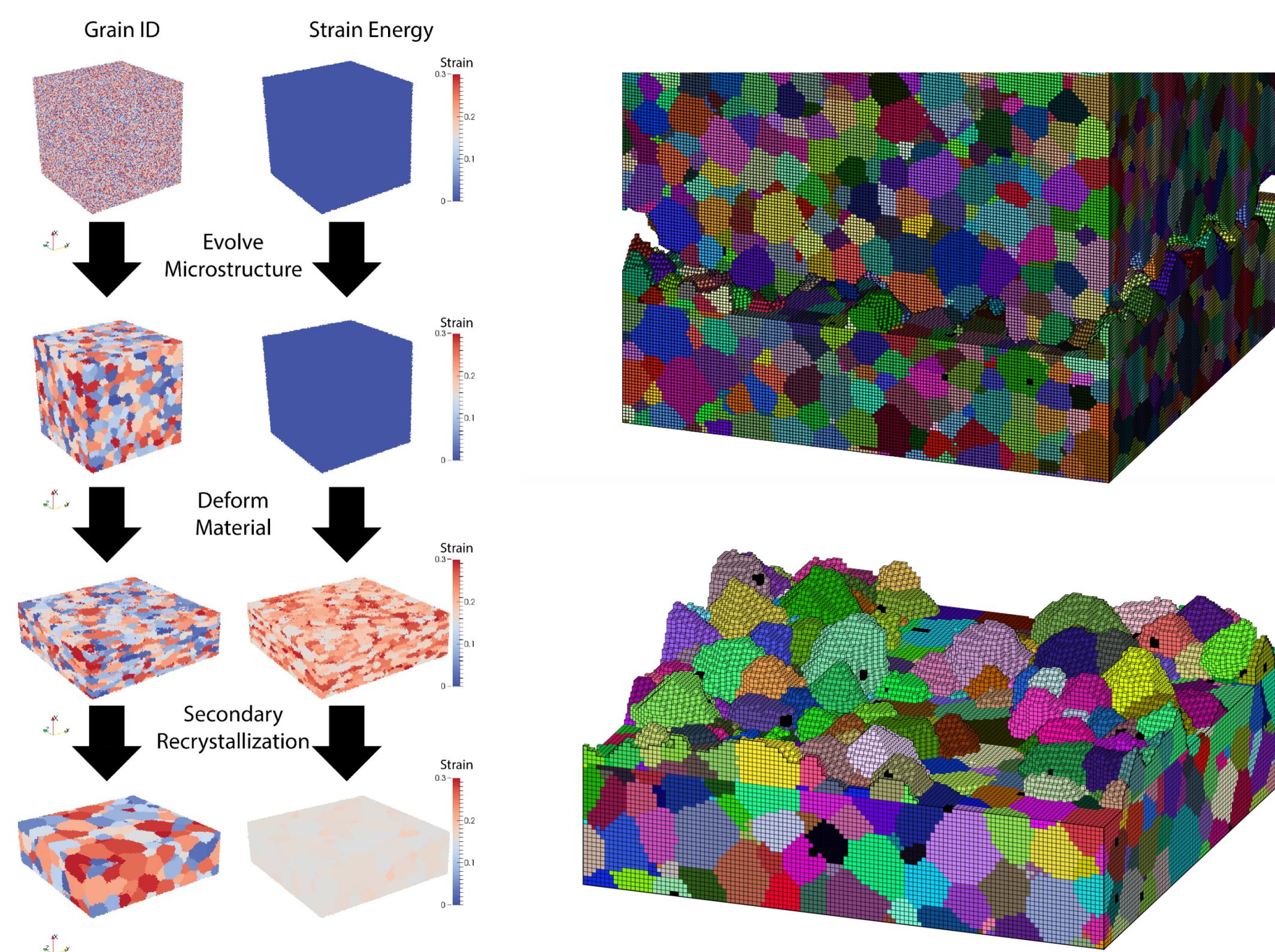
A. Gupta, A. Jiang



- Physical insight from CNT models complements experimental observations of nanotube bundling in aerogels

MULTIPHYSICS MICROSTRUCTURAL EVOLUTION MODELING

K. Kang, P. Goins, B. DeCost

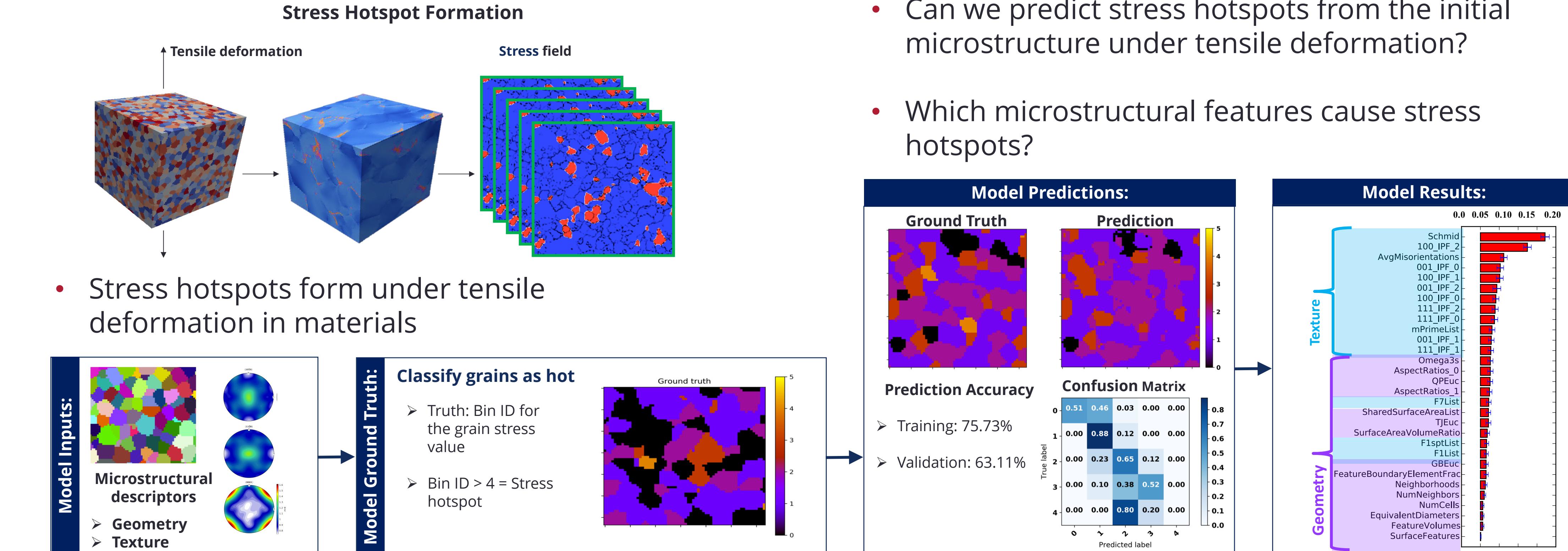


- 3D simulations of materials with multiphysics microstructural evolution models provide more realistic insight to material behavior

MATERIALS INFORMATICS

MACHINE LEARNING APPROACHES FOR MATERIALS DATA SCIENCE

A. Mangal, I. Chesser, T. Francis

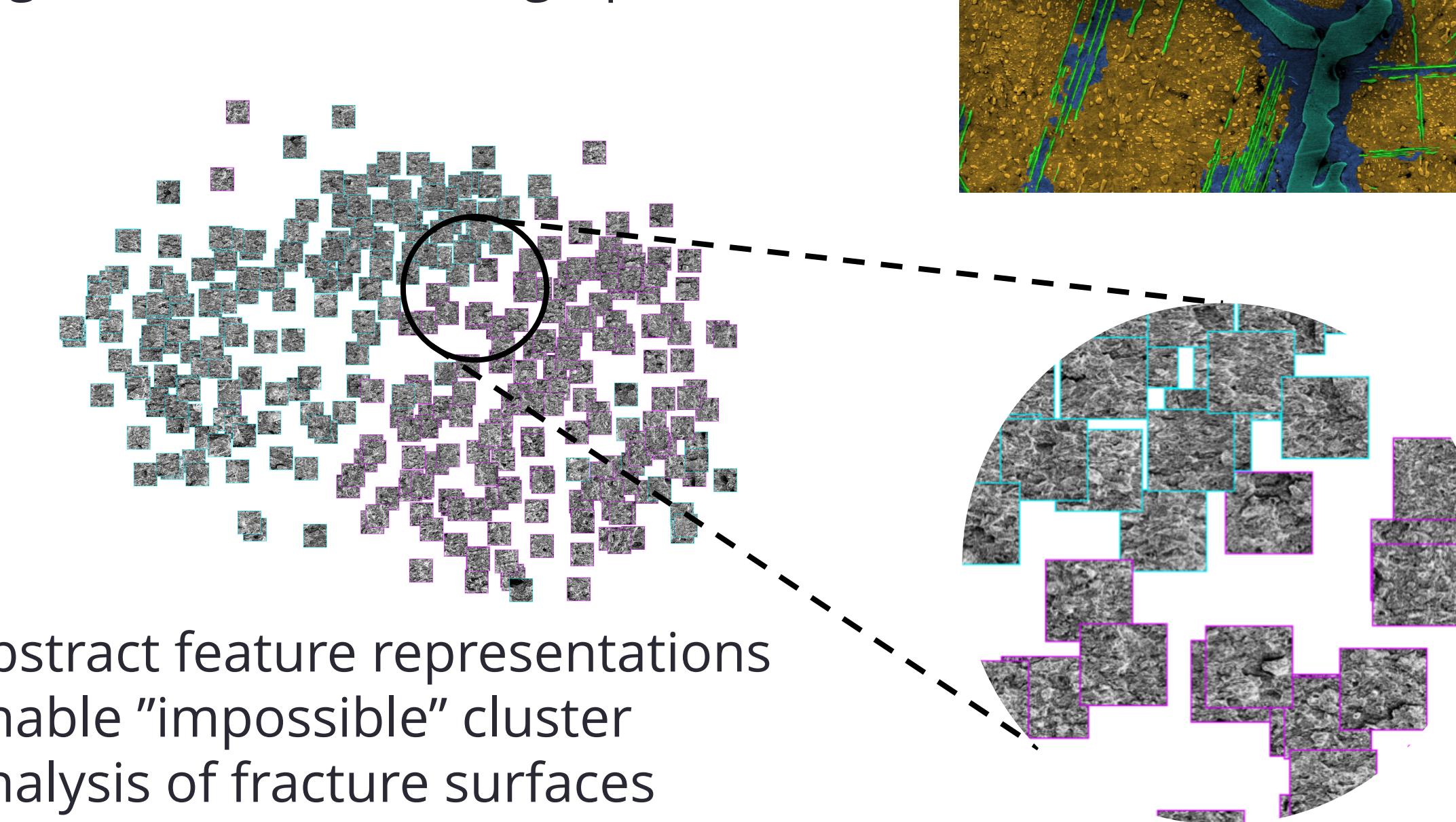


- Stress hotspots form under tensile deformation in materials

COMPUTER VISION FOR MICROSTRUCTURE SCIENCE

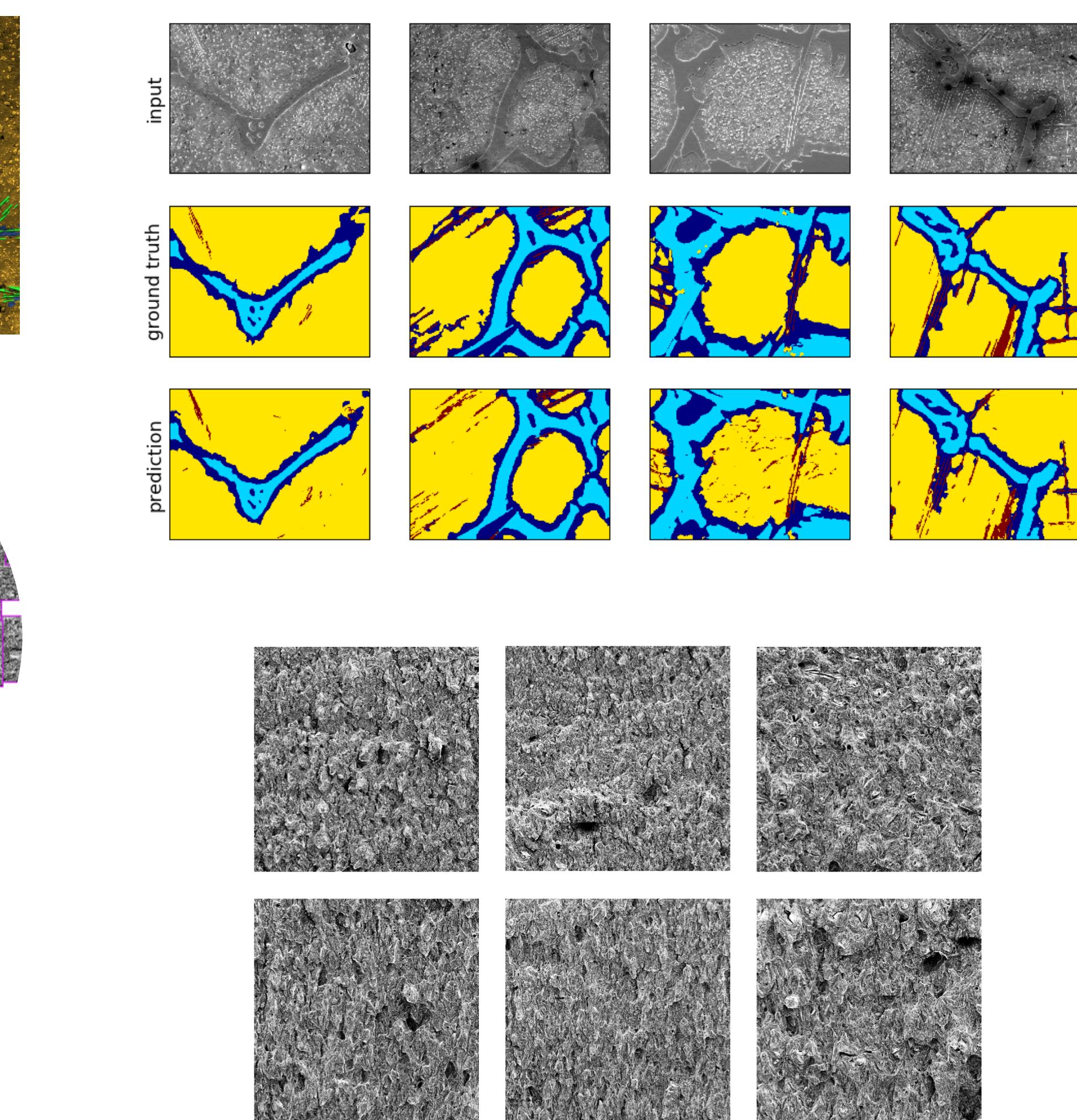
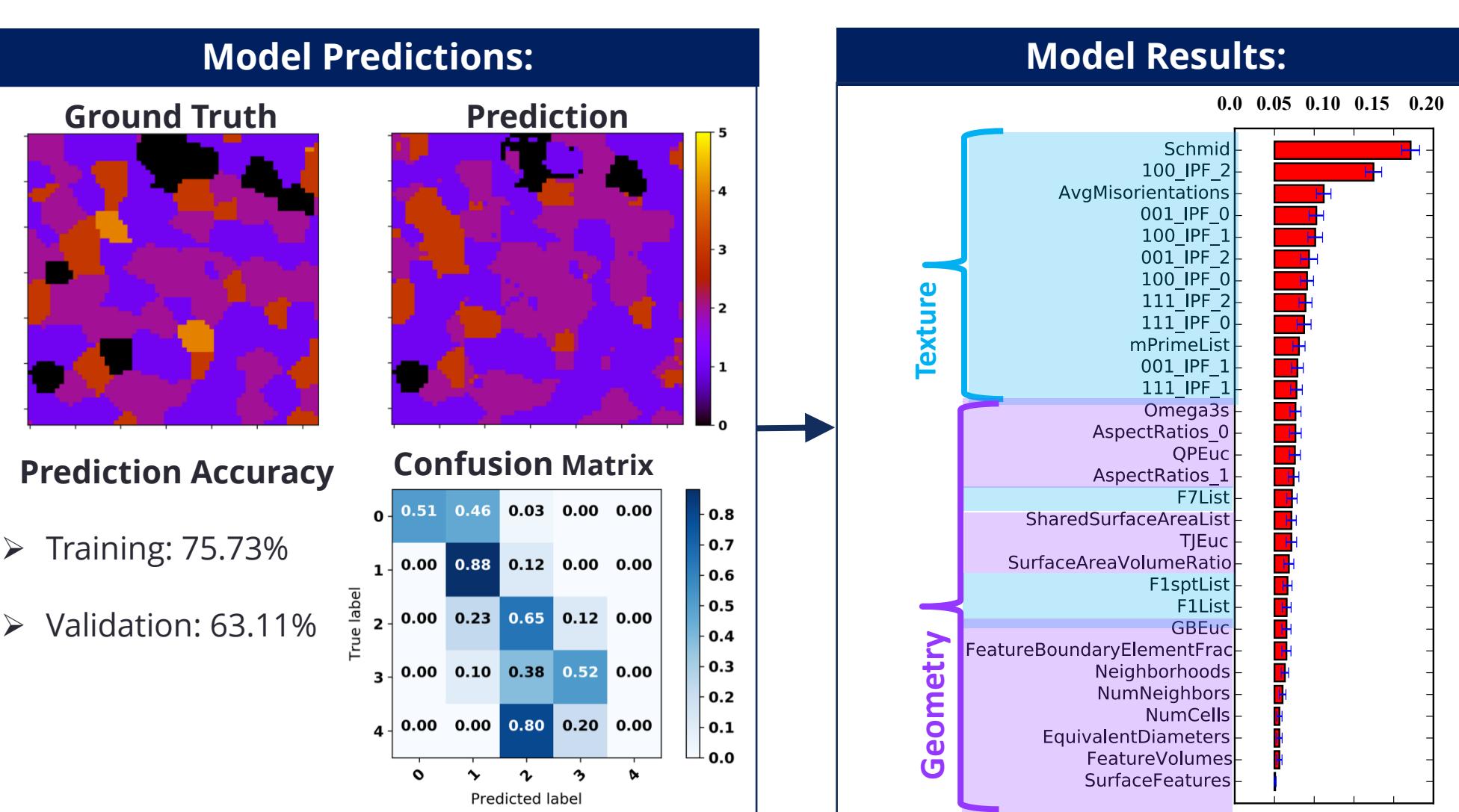
A. Kitahara, N. Gao, B. Lei, T. Francis, J. Huang, B. DeCost

- Computer vision and machine learning perform automatic segmentation of micrographs



- Abstract feature representations enable "impossible" cluster analysis of fracture surfaces

- Can we predict stress hotspots from the initial microstructure under tensile deformation?
- Which microstructural features cause stress hotspots?



Can you classify these six images into two categories?*

GROUP MEMBERS

Ph.D.

- Ankita Mangal
- Ian Chesser
- Andrew Kitahara
- Anna Smith
- Nan Gao

B.S.

- Toby Francis
- Yutong Bi
- Andy Jiang
- Thomas Matson

M.S.

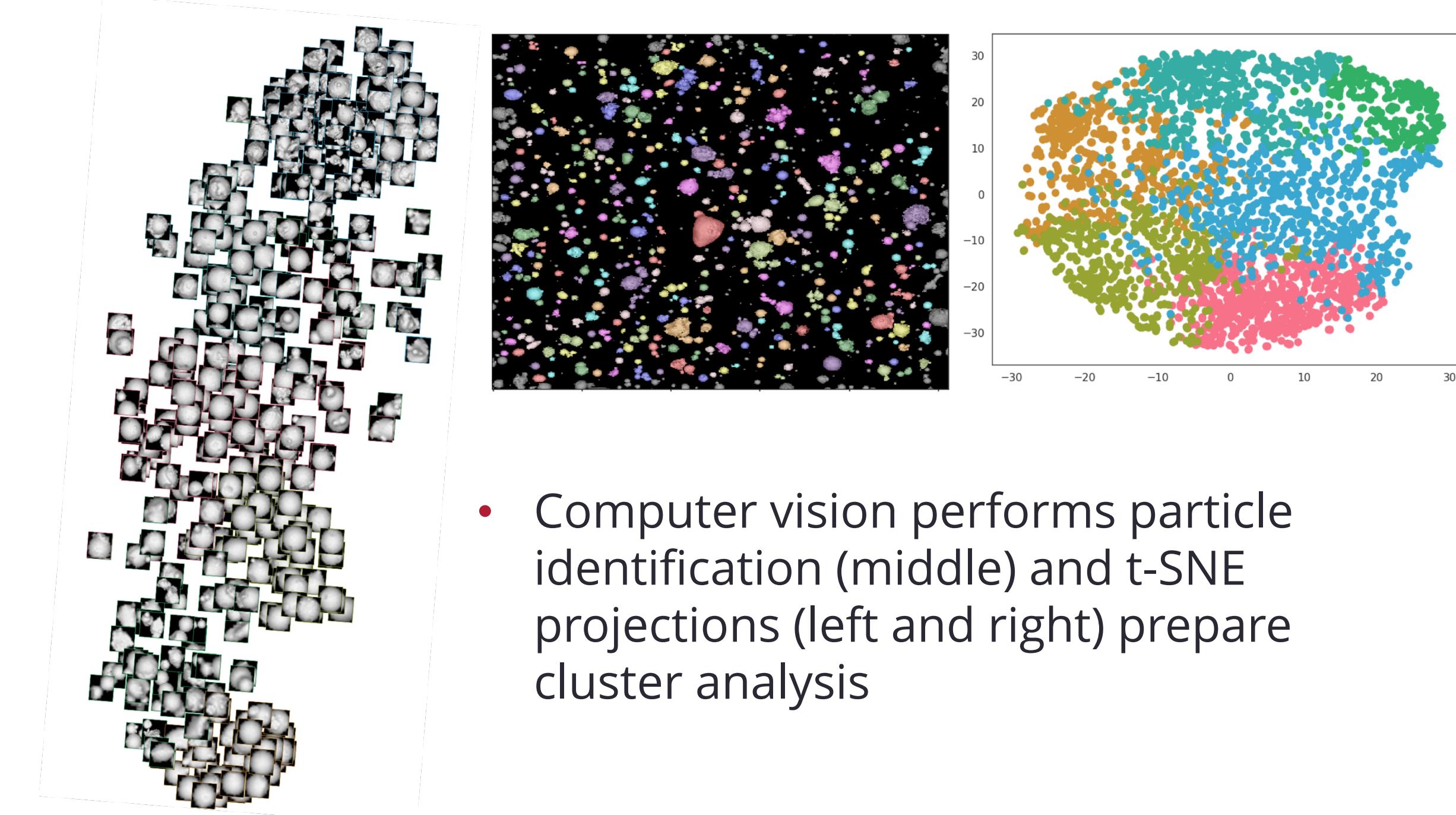
- Kai Kang
- Junrong Huang
- Bo Lei
- Srujana Rao Yarasi

Ph.D. Alumni

- Philip Goins
- Brian DeCost
- Jonathan Humberson
- Ankit Gupta

COMPUTER VISION FOR ADDITIVE MANUFACTURING CHARACTERIZATION

A. Kitahara, A. Smith, B. Lei, S. Yarasi, B. DeCost



- Computer vision performs particle identification (middle) and t-SNE projections (left and right) prepare cluster analysis