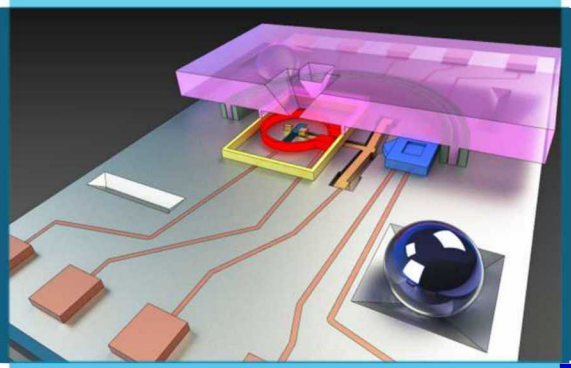
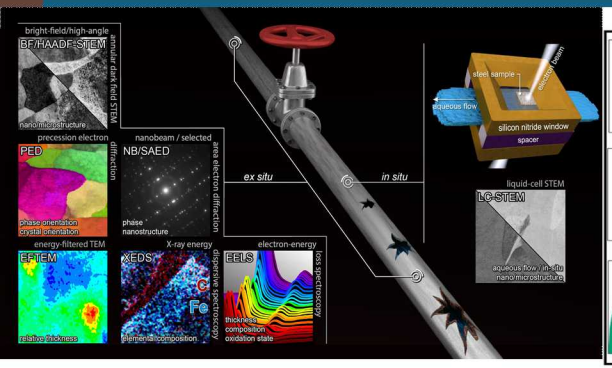
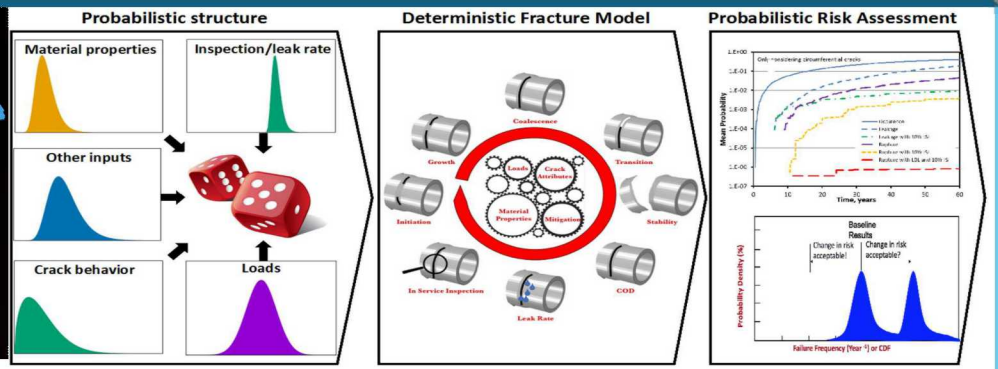
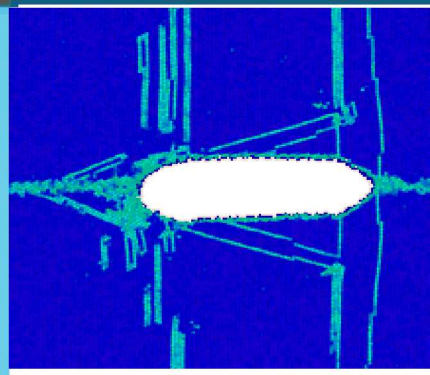
SAND2018-9475PE

Predictive Modeling and Experimental Characterization for Investigating Materials Degradation









PRESENTED BY

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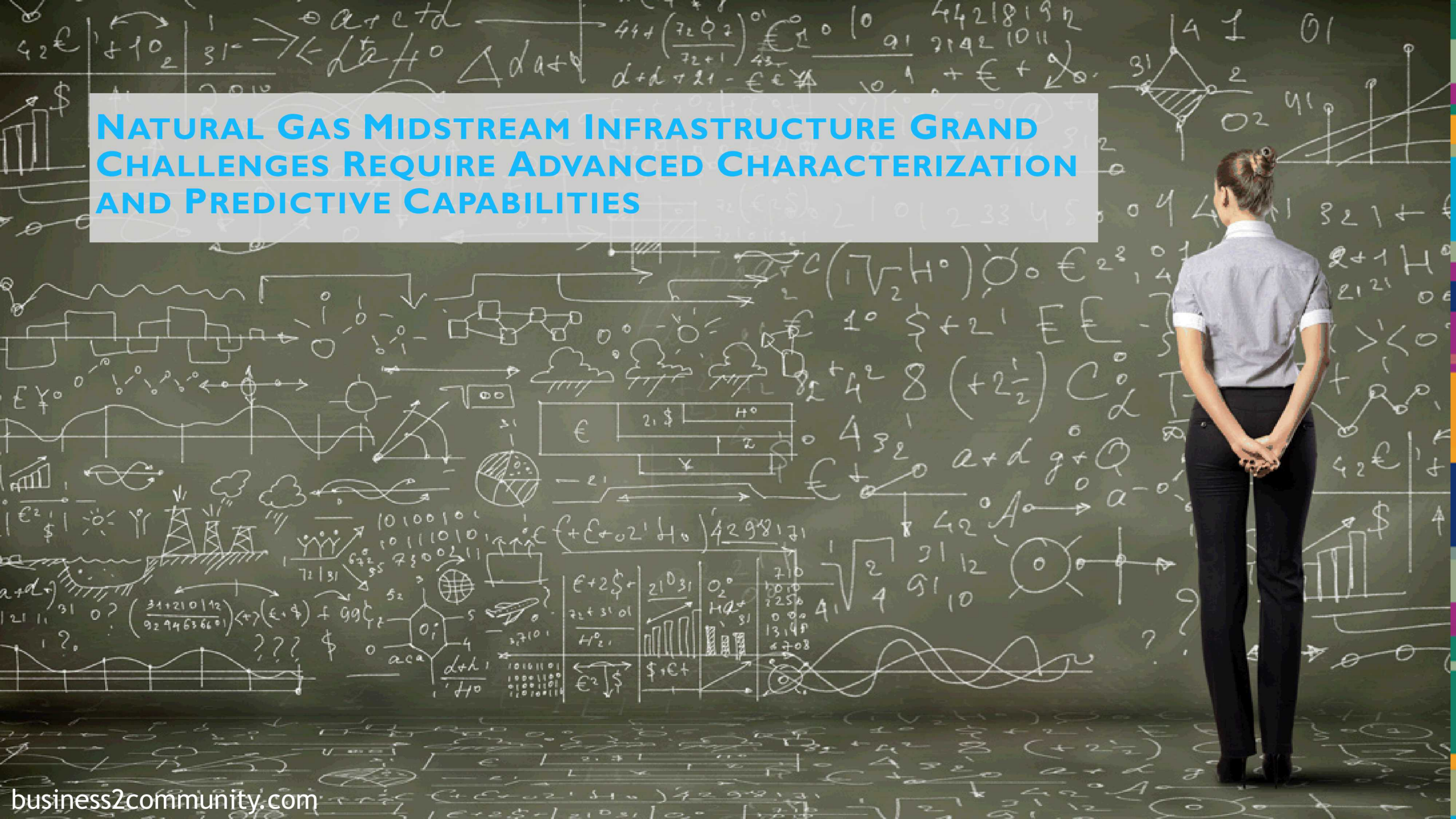
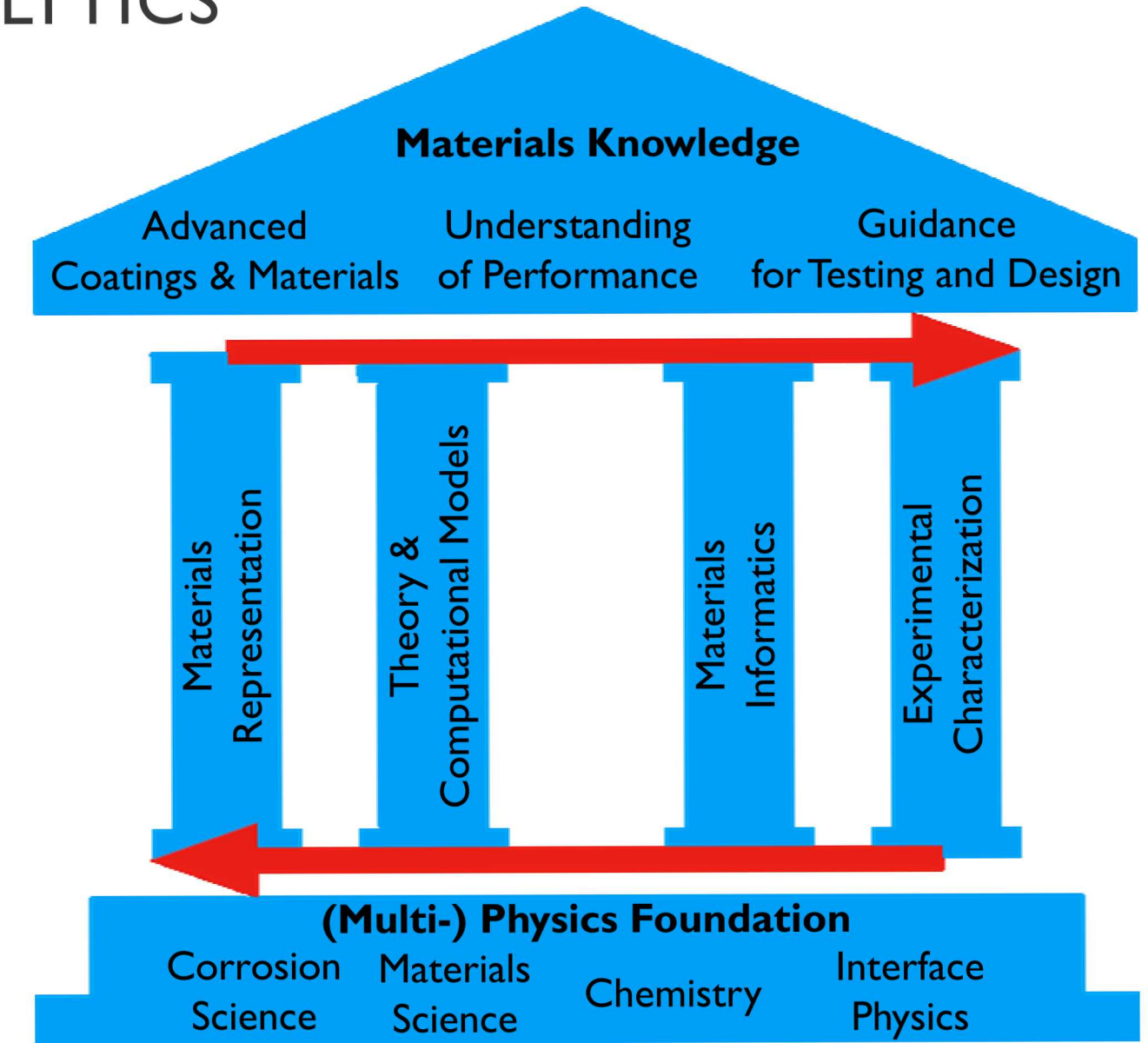
Natural Gas Midstream Infrastructure Grand Challenges Require Advanced Characterization and Predictive Capabilities

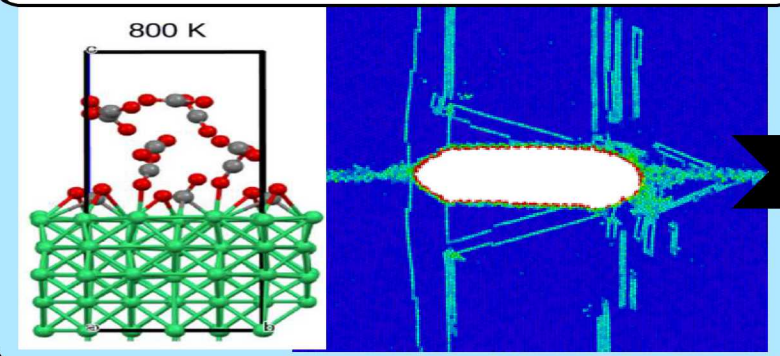


At the Intersection of Computational Materials Science, Experimental Characterization and Data Analytics

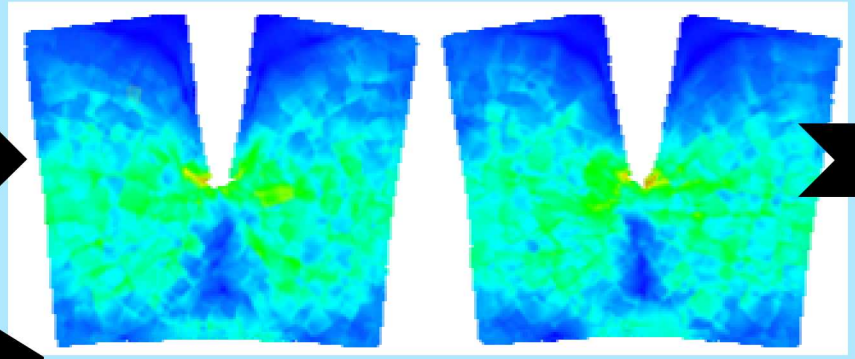


Predictive Modeling and Simulation

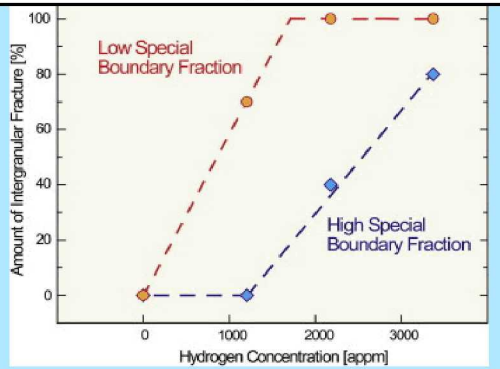
Atomistic simulations
Reactive pathways,
nanoscale mechanisms

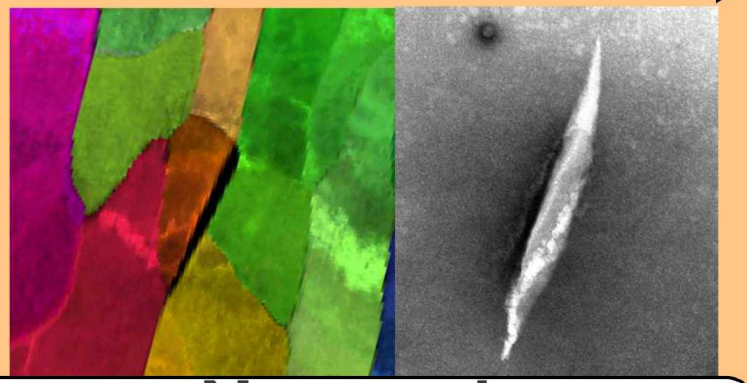


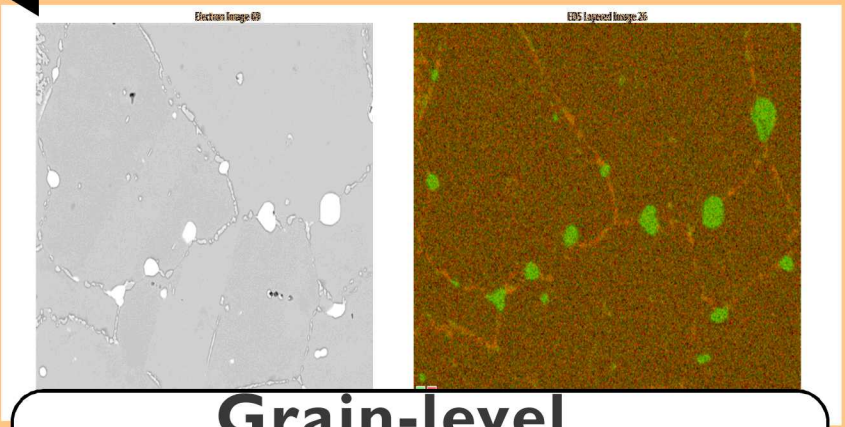
Grain-level framework
Localized
fracture corrosion processes

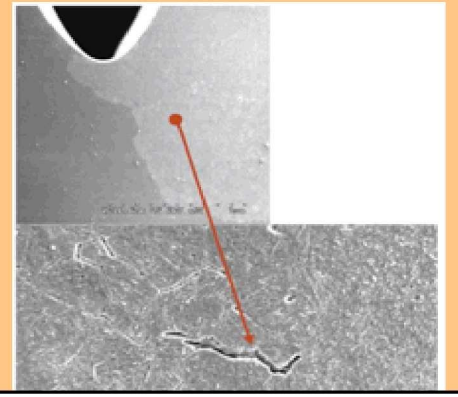


Fracture model
Environmental
fracture performance









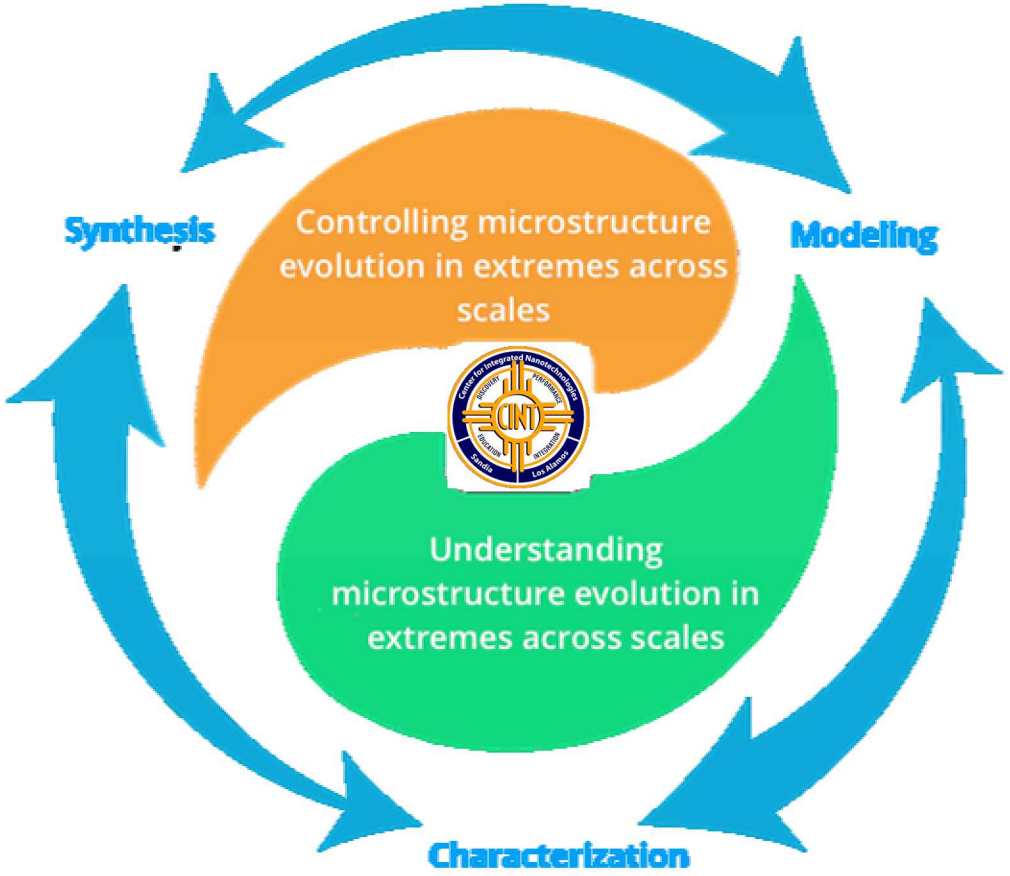
Nanoscale characterization & testing

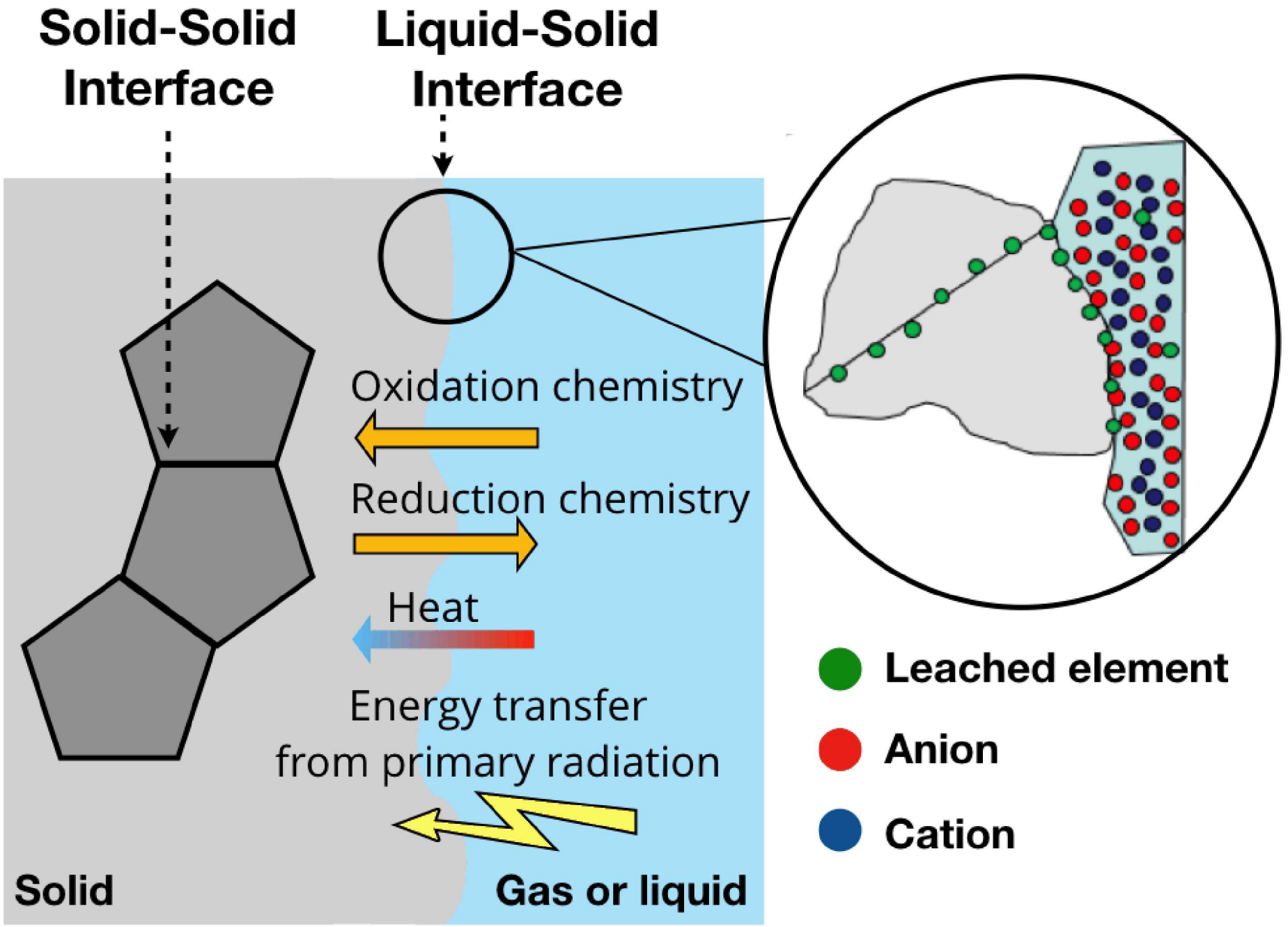
Grain-level characterization & testing

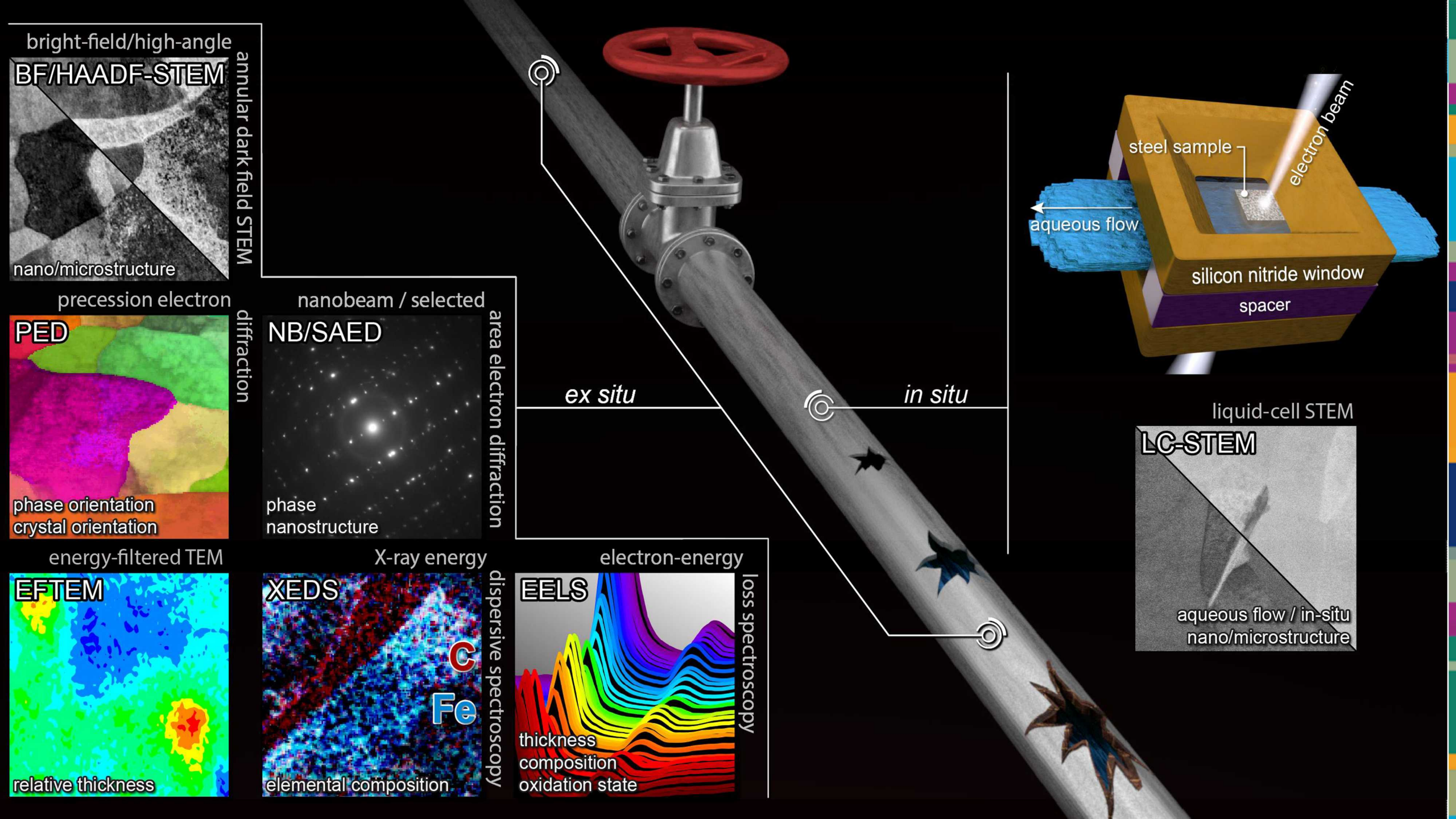
Macroscale testing

Experimental Discovery and Validation

EXAMPLES FROM PAST AND CURRENT R&D PROGRAMS




Solid-Solid Interface
Liquid-Solid Interface
Oxidation chemistry
Reduction chemistry
Heat
Energy transfer from primary radiation
Solid
Gas or liquid
Leached element
Anion
Cation


bright-field/high-angle
annular dark field STEM
BF/HAADF-STEM
nano/microstructure
precession electron
diffraction
PED
phase orientation
crystal orientation
nanobeam / selected
area electron diffraction
NB/SAED
phase
nanostructure
energy-filtered TEM
EFTEM
relative thickness
X-ray energy
dispersive spectroscopy
XEDS
C
Fe
elemental composition
electron-energy
loss spectroscopy
EELS
thickness
composition
oxidation state
ex situ
in situ
steel sample
electron beam
aqueous flow
silicon nitride window
spacer
liquid-cell STEM
LC-STEM
aqueous flow / in-situ
nano/microstructure

200 nm

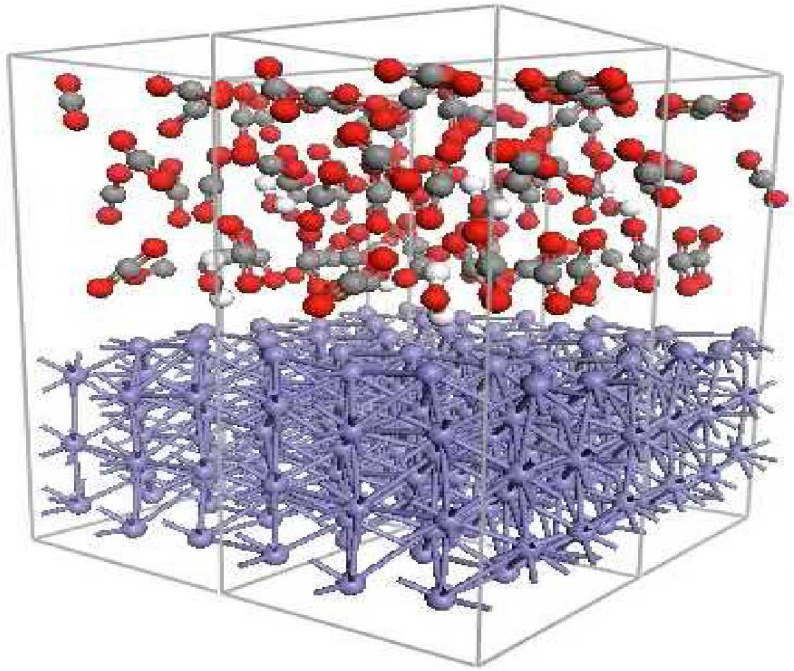
Real time in-situ TEM observation of the dissolution of PLD Cu thin films on a SiN substrate during the flow of brine

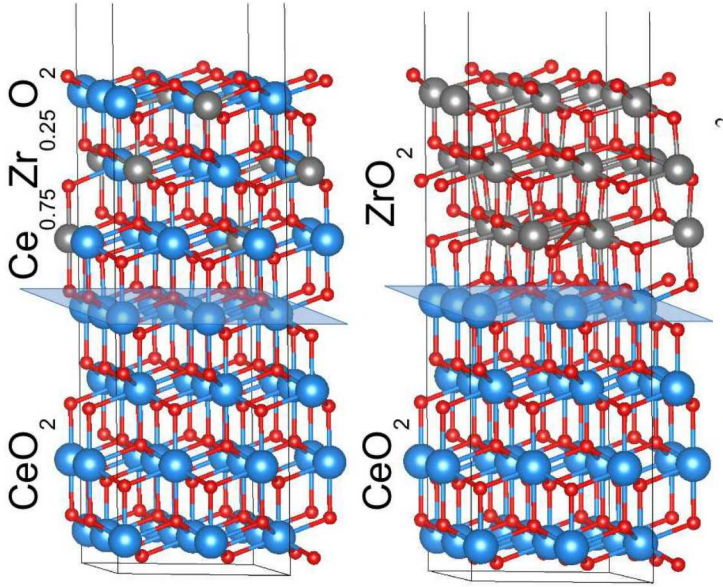
Bright field image sequence obtained using JEOL 2100 LaB6 TEM with a high contrast polepiece and Protochips Poseidon 210 Holder

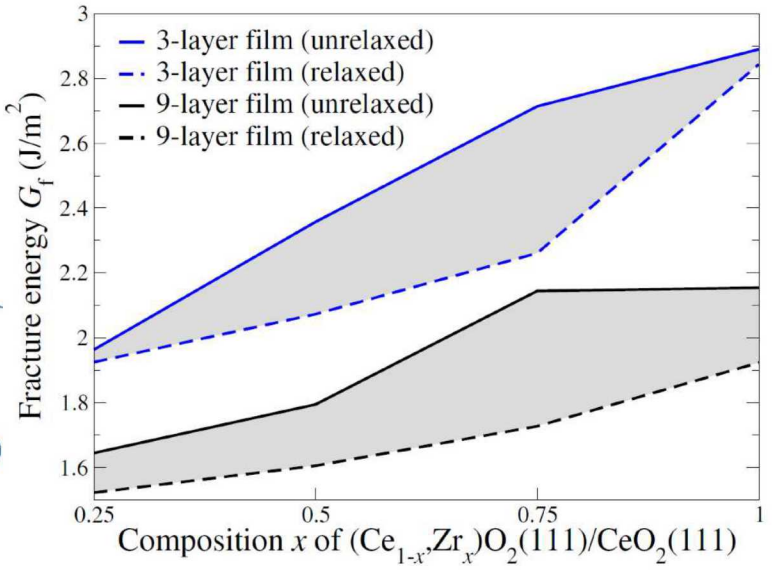
This work was partially funded by the US DOE, Office of BES, Division of Materials Science and Engineering. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

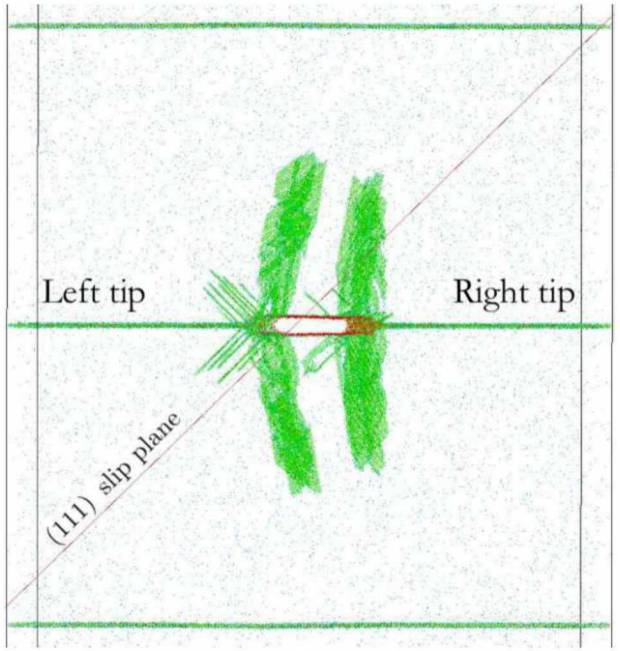
[Chee et al., Chemical Communications, 2015]

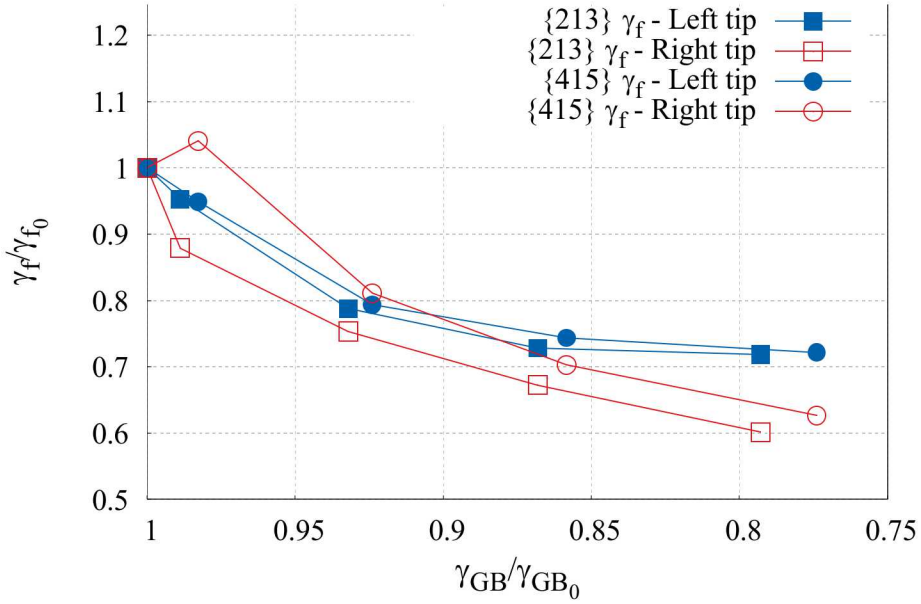
DEGRADATION MECHANISMS AT THE NANANOSCALE







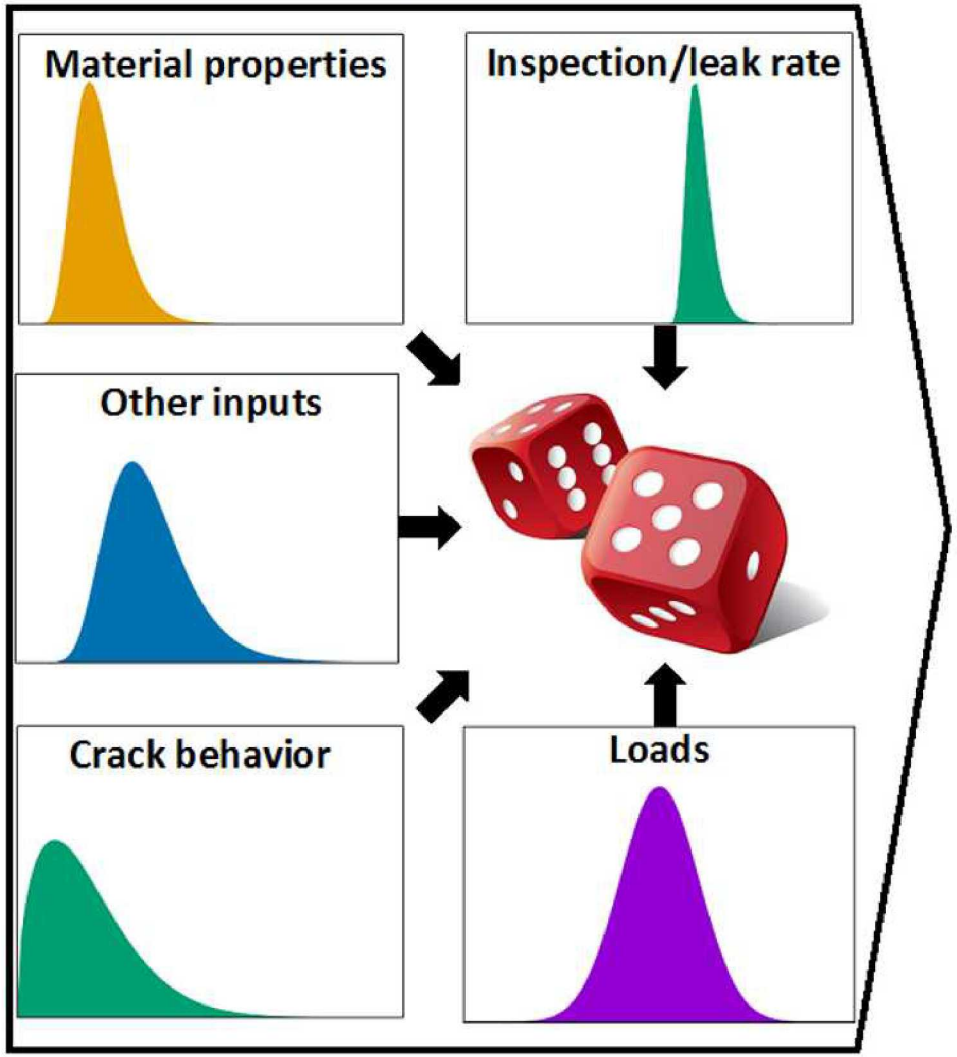




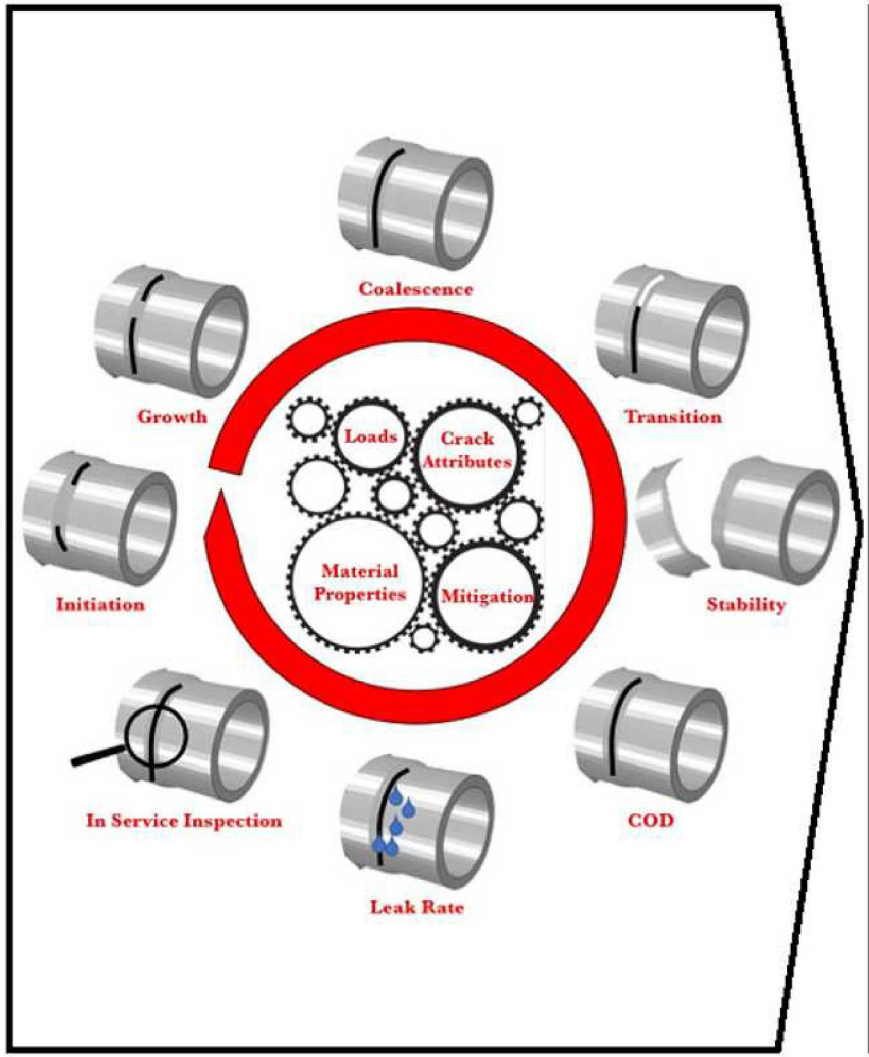
(a) Interfacial work of separation

HOLISTIC STRESS CORROSION CRACKING CAPABILITY FOR ASSESSMENT OF STRUCTURAL INTEGRITY OF PIPING SYSTEMS

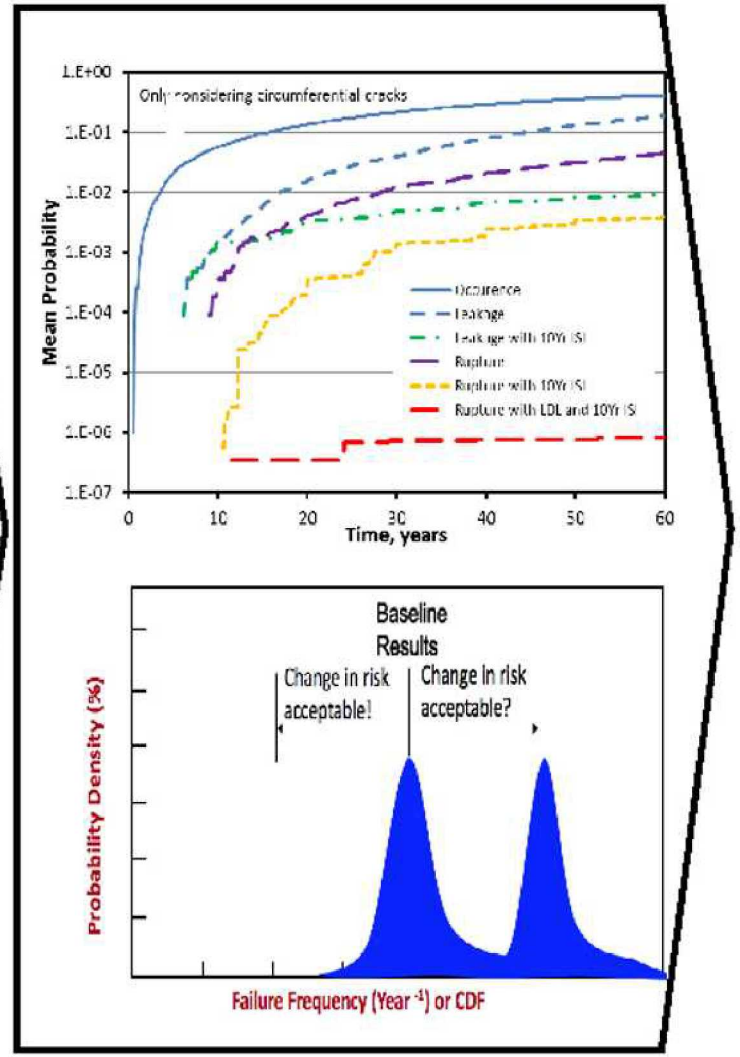
Probabilistic structure



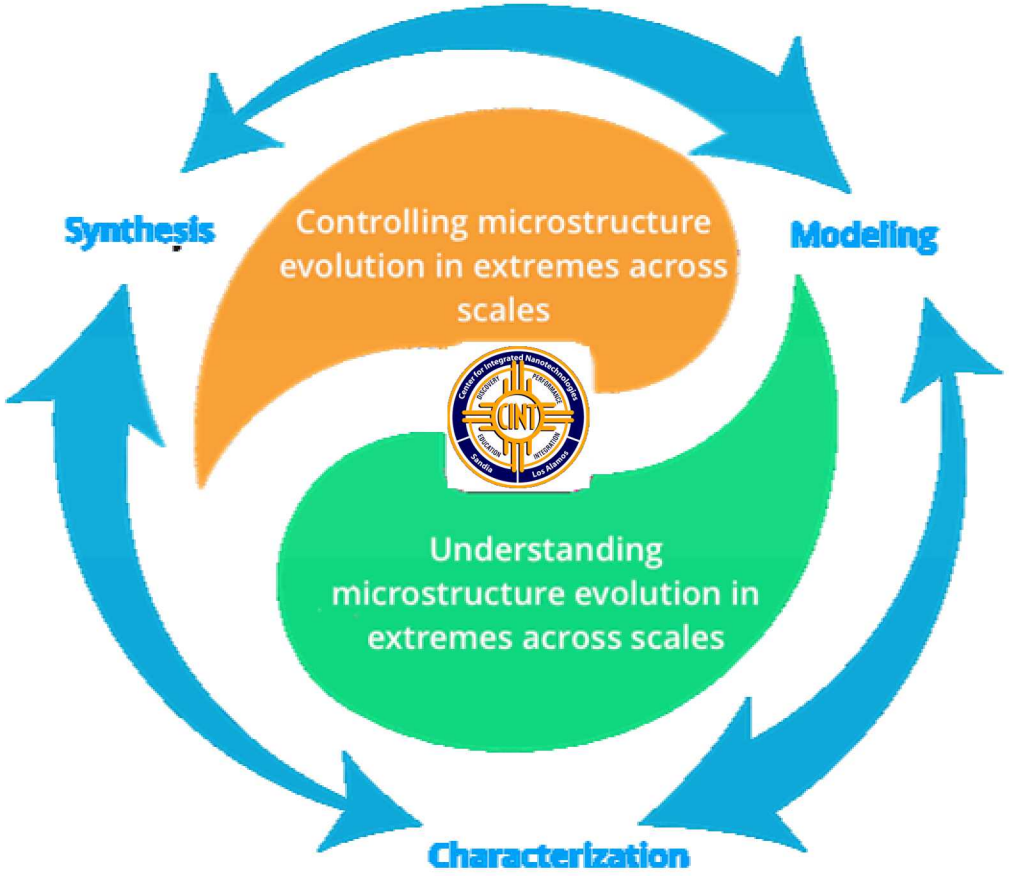
Deterministic Fracture Model



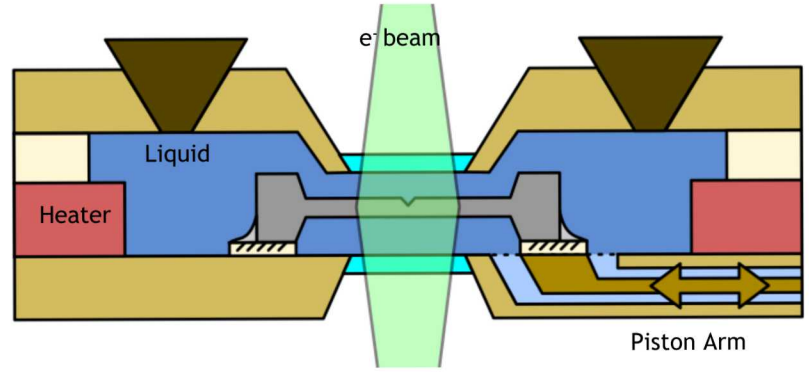
Probabilistic Risk Assessment

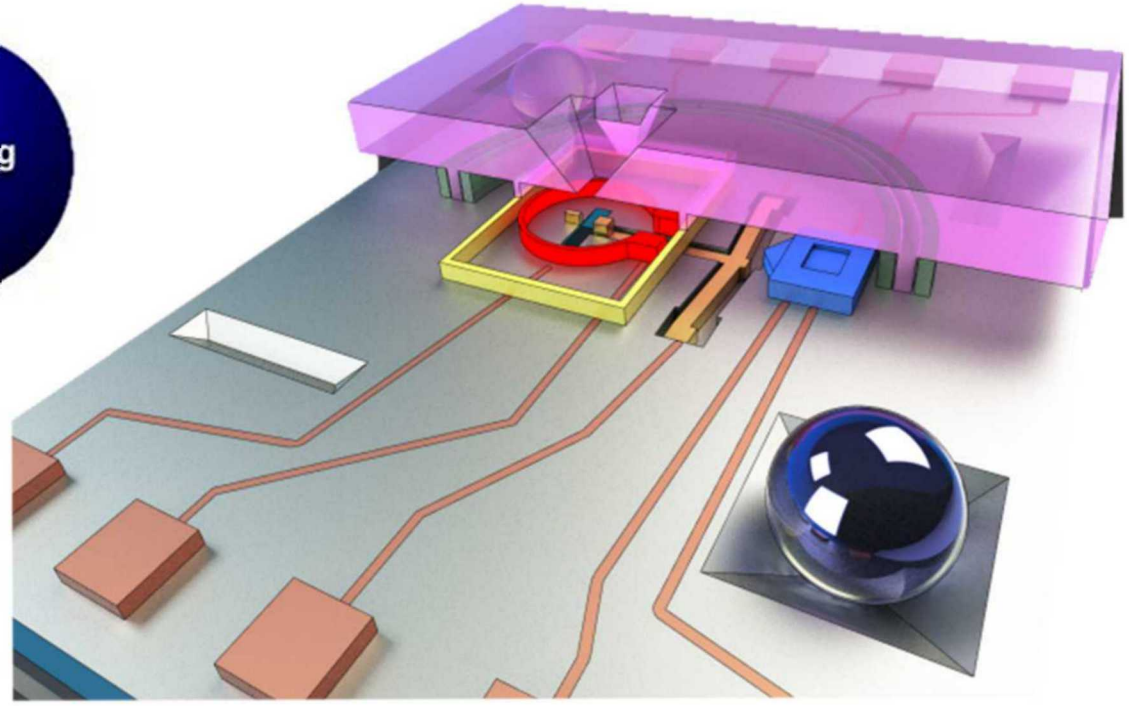


Upcoming Advancements of Capabilities and Functionalities

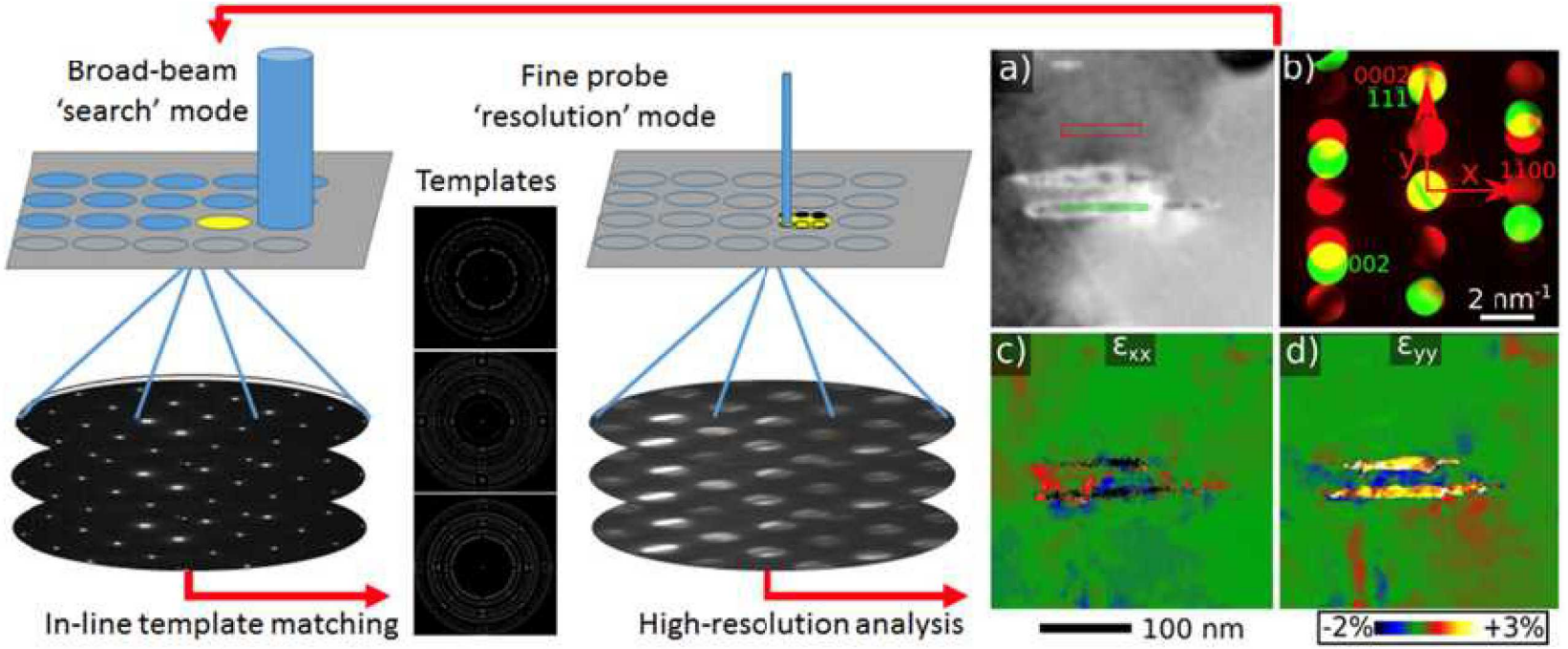


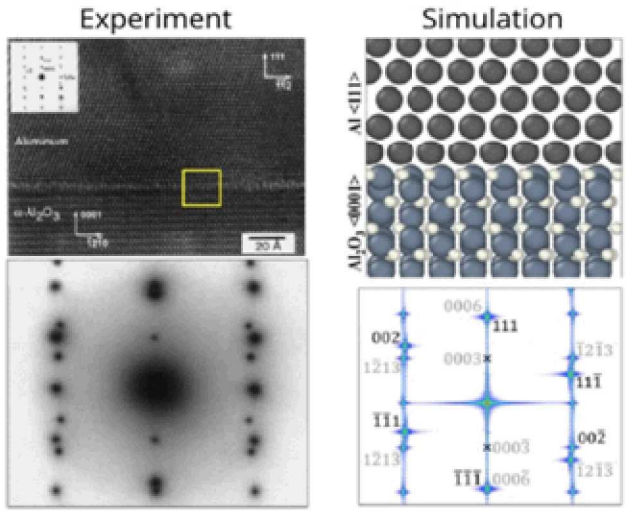
MECHANICAL-ENVIRONMENTAL-THERMAL DISCOVERY PLATFORM

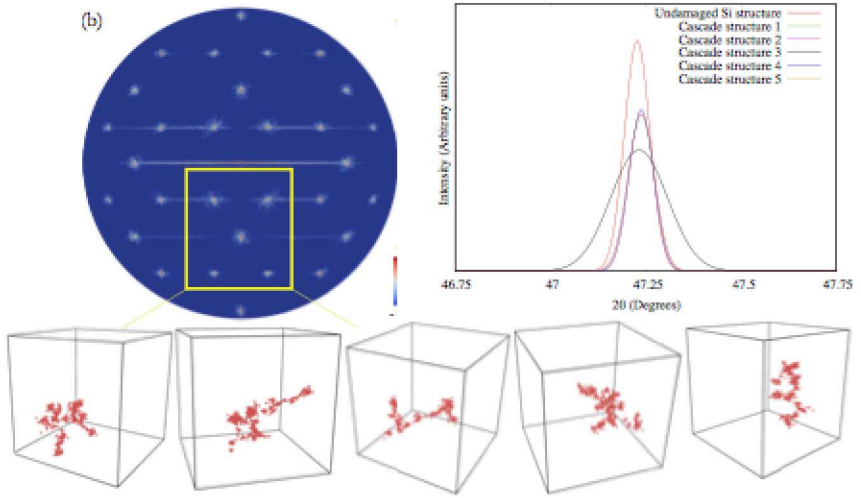




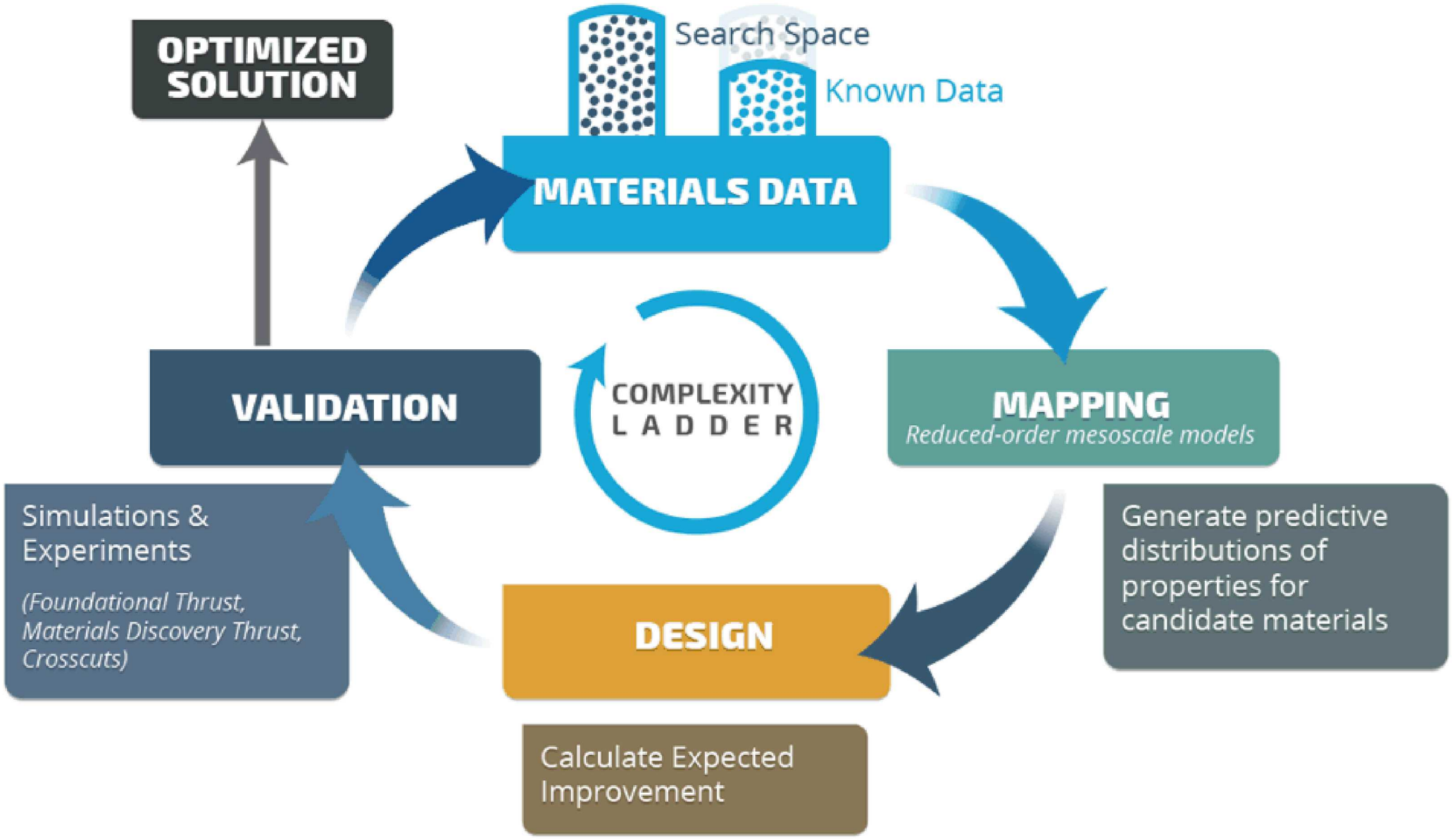
"Intelligent" Materials Characterization Capability







Integration of Modeling with High-Throughput Calculations and Combinatorial Experiments



Most Promising Opportunities are at the Crossroads of Modeling, Structure and Property Characterization, Chemistry, Data analytics

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