LA-UR-17-27063
Approved for public release; distribution is unlimited.

Title: Materials modeling efforts at LANL

Author(s): Kress, Joel David
Capolungo, Laurent

Intended for: Briefing

Issued: 2017-08-07

Materials modeling efforts at LANL

Joel Kress
Laurent Capolungo

Abstract

This briefing describes some the materials theory, modeling and simulation capability at Los Alamos National Laboratory.

Natures' idea of lightweight high toughness material

Damascus swords (the lost recipe)

Natures' scintillators (aka Butterflies)

Outline

Materials Design

- Philosophy
- Virtual materials processing and characterization
- Process-structure-property performance

Applications

- Civil nuclear energy
- Carbon capture technology
- Semi-conductor

Using 'defects' to improve materials performance

Metals

This image cannot currently be displayed.

EBSD map of 304 stainless steel deformed up to 30% strain

EBSD map of as-received 304 stainless steel

This image cannot currently be displayed.

Phase transformation from austenite to martensite allows tailoring the materials to reach an optimal strength/ductility compromise

Ceramics

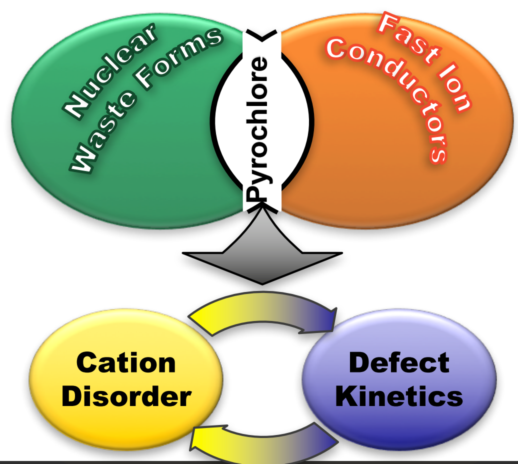
$TiO_2/SrTiO_3$

This image cannot currently be displayed.

$SrTiO_3/LaAlO_3$

This image cannot currently be displayed.

Phase structure can be used to control defect flow



Polymers

This image cannot currently be displayed.

This image cannot currently be displayed.

Adding functional chemical groups to polymers

Materials related issues

How does material chemistry affect microstructure and performance?

How does ion implantation, neutron irradiation affect microstructure in metals, semi-conductors, polymers?

How does thermo-mechanical loading affect microstructure evolutions

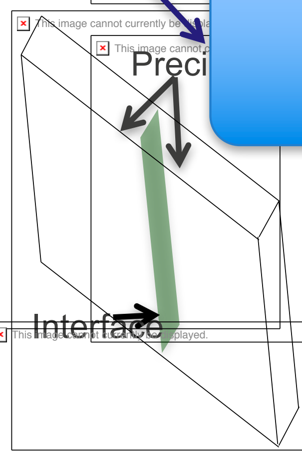
How does chemical environment affect lifetime

Virtual Characterization

Applications to

Gen II
Gen II
Gen IV
Fusion technology

MD Simulations:
Hg on top of a Al surface



Microstructure effects on thermal and electrical conductivity

Microstructure effects on mechanical performance, lifetime

Materials related issues

This image cannot currently be displayed.

How to tune thermo-mechanical loading to control microstructure?

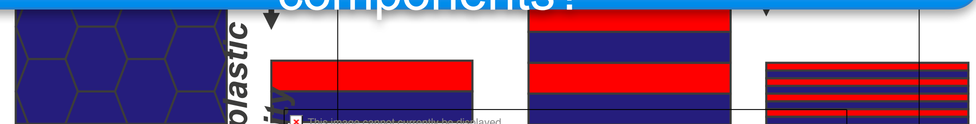
This image cannot currently be displayed. Section/stack

How to tune process parameters during Additive Manufacturing of metallic components?

polycrystalline sheet A

Virtual Processing

polycrystalline sheet B



This image cannot currently be displayed.

This image cannot currently be displayed.

This image cannot currently be displayed.

Cu

Nb

This image cannot currently be displayed.

This image cannot currently be displayed.

This image cannot currently be displayed.

This image cannot currently be displayed.

This image cannot currently be displayed.

Interface plastic stability

Normalized interface energy

Using advanced simulations of the manufacturing process LANL could define a figure of merit describing potential for processing industrially relevant materials

This image cannot currently be displayed.

This image cannot currently be displayed.

Computer modeling identified the ideal coil to maximize the efficiency of a heat exchanger. Computer-aided design mapped a component with the optimized coils. Los Alamos additively manufactured the complex shape that was impossible with traditional machining techniques.

Outline

Materials Design

- Philosophy
- Virtual materials processing and characterization
- Process-structure-property performance

Applications

- Civil nuclear energy
- Carbon capture technology
- Semi-conductor

Long-term vision: process aware modeling and simulations

Process Modeling ⟷ **Microstructure Modeling** ⟷ **Properties Modeling** ⟷ **Performance Modeling**

TRUCHAS code

Moving heat source

Direct numerical simulation of grain growth

Initial grain distribution (Nucleation site)

Final grain shape and composition

Polycrystal models to determine elastic/plastic/damage properties

Polycrystal and grain boundary properties

AM specific interface properties

Thermal - mechanical models to predict elastic/plastic/damage and failure processes

Mesoscale to macroscale prediction of performance

Liquid/solid phase change

Solid/solid phase transformation

This image cannot currently be displayed.

This image cannot currently be displayed.

This image cannot currently be displayed.

Outline

Materials Design

- Philosophy
- Virtual materials processing and characterization
- Process-structure-property performance

Applications

- Civil nuclear energy
- Carbon capture technology
- Semi-conductor

Multiscale modeling paradigm

FE-VPSC allows, e.g. prediction of gap opening in fuel rod assemblies

This image cannot currently be displayed.

This image cannot currently be displayed.

This image cannot currently be displayed.

This image cannot currently be displayed.

FE-VPSC: ABAQUS or MOOSE/BISON
Coupled FE-VPSC code gives dimensional changes & strength of grid assembly under complex conditions of dose, stress & temperature

VPSC Code
Polycrystal model of creep accounting for crystallo-graphic mechanisms, texture, processing conditions

Thermal creep
→ thermally activated obstacle overcoming by dislocations

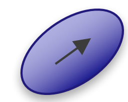
Irradiation creep and growth
→ nucleation and evolution of dislocation loops by climb

Radiation hardening
→ Dislocations interacting with loops, precipitates & other dislocations

Molecular Dynamics and Discrete Dislocation Dynamics
Interaction between dislocations and irradiation induced defects

VPSC accounts for grain orientation and interaction with neighbors

This image cannot currently be displayed.

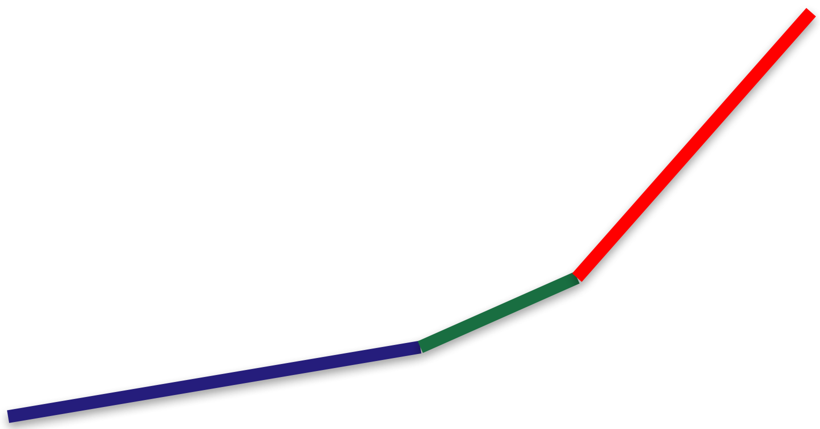


This image cannot currently be displayed.

e.g. creep and growth of P91, Zr4 etc.

This image cannot currently be displayed.

Experimental data

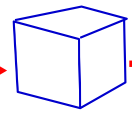


371^{o}C/122MPa

In the context of LOCA, one MUST capture the both stress and temperature effects on transient relaxation processes

Kombaiah and Murty, 2015, Morrow et al. 2014, Graff et al. 2008

Crystal plasticity model based on statistical distributions



Using DDD to probe and characterize low-scale with the purpose of passing statistical information to grain-size scale

Statistical effects of long-range interactions (stress fluctuations)

Statistical effects of short-range interactions (hardening)

Internal stress distribution

Cell formation

Local shear strain rate in grains

Effective shear strain rate in grains

H. Wang et al, IJP (2017)

High Throughput Microstructure Analysis

METIS is a software that analyzes EBSD maps on low symmetry materials and extracts statistical correlations between key markers of the microstructure (e.q. twins, grain size, grain boundary length). The data is used to guide materials design and test reduced order microstructure evolution models

This image cannot currently be displayed.

Processing EBSD image

This image cannot currently be displayed.

Microstructure metric quantification

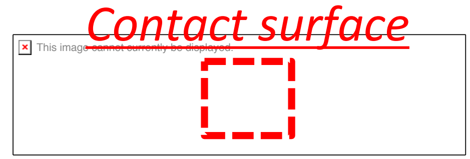
This image cannot currently be displayed.

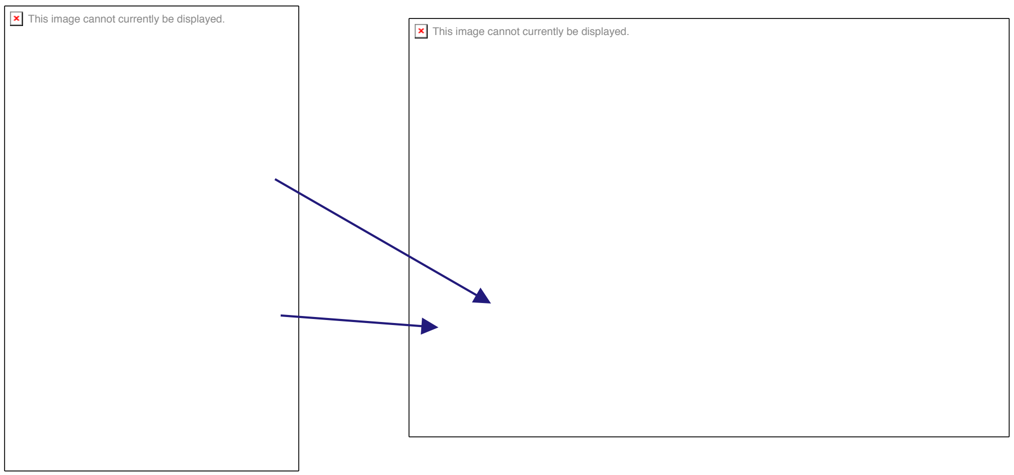
- Grain size
- GB length
- Twinning features
  - Twinning frequency
  - Twin area fraction
  - # of twins per twinned grain
  - Average twin thickness
  - Twin variant distribution
  - Twin thickness at GB
  - Crossing twin thickness at GB
  - Twin crossing frequency
- Grain orientation
- GB Misorientation

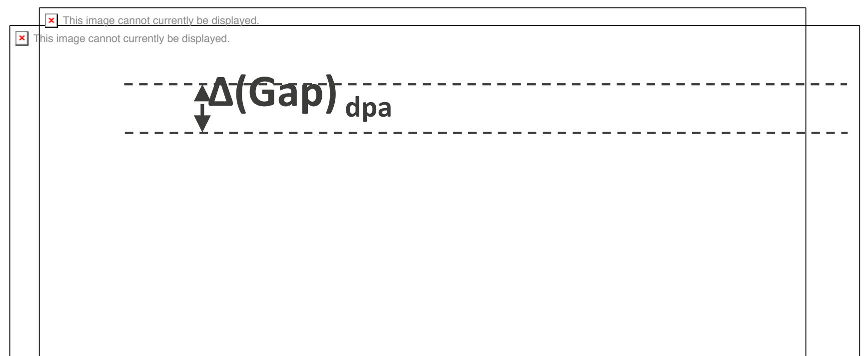
Zr EBSD analysis: Juan et al., Acta Mater (2015); Mg EBSD analysis: Beyerlein et al, Phil. Mag (2010)

Gap Opening between Clad and Spacer Grid

Characterize gap opening by keeping track of the distance between nearest nodes on spring/dimple and clad tube (Gap= Average over all nodes considered)







Leaking rods at the periphery of Westinghouse fuel rod assembly. Yan et al., Nucl. Engg. Design (2011)

- Analytical calculations (Billerey, IAEA-TECDOC-1454 (2005) 101): gap opening at end of life = 10 µm
- GTRF wear setups typically use displacement amplitudes 5 to 30 µm
- We predict from 15 to 30 µm at 20dpa

Carbon capture simulation initiative

Rapidly synthesize optimized processes to identify promising concepts → Better understand internal behavior to reduce time for troubleshooting → Quantify sources and effects of uncertainty to guide testing & reach larger scales faster → Stabilize the cost during commercial deployment

Industry

National Labs

Berkeley Lab

Pacific Northwest National Laboratory

NETL

Los Alamos National Laboratory EST. 1943

Lawrence Livermore National Laboratory

Polyamine/Microporous Silica CO_2 Adsorbents

This image cannot currently be displayed.

SEM (a), TEM (b), HRTEM (c) images and particle-size distribution histogram (d) of the S600-10 sample

This image cannot currently be displayed.

PEI structure

This image cannot currently be displayed.

Length scale: (1) macroporosity
(2) meso-porous particles
(3) Silica-PEI composite

Mass transport:

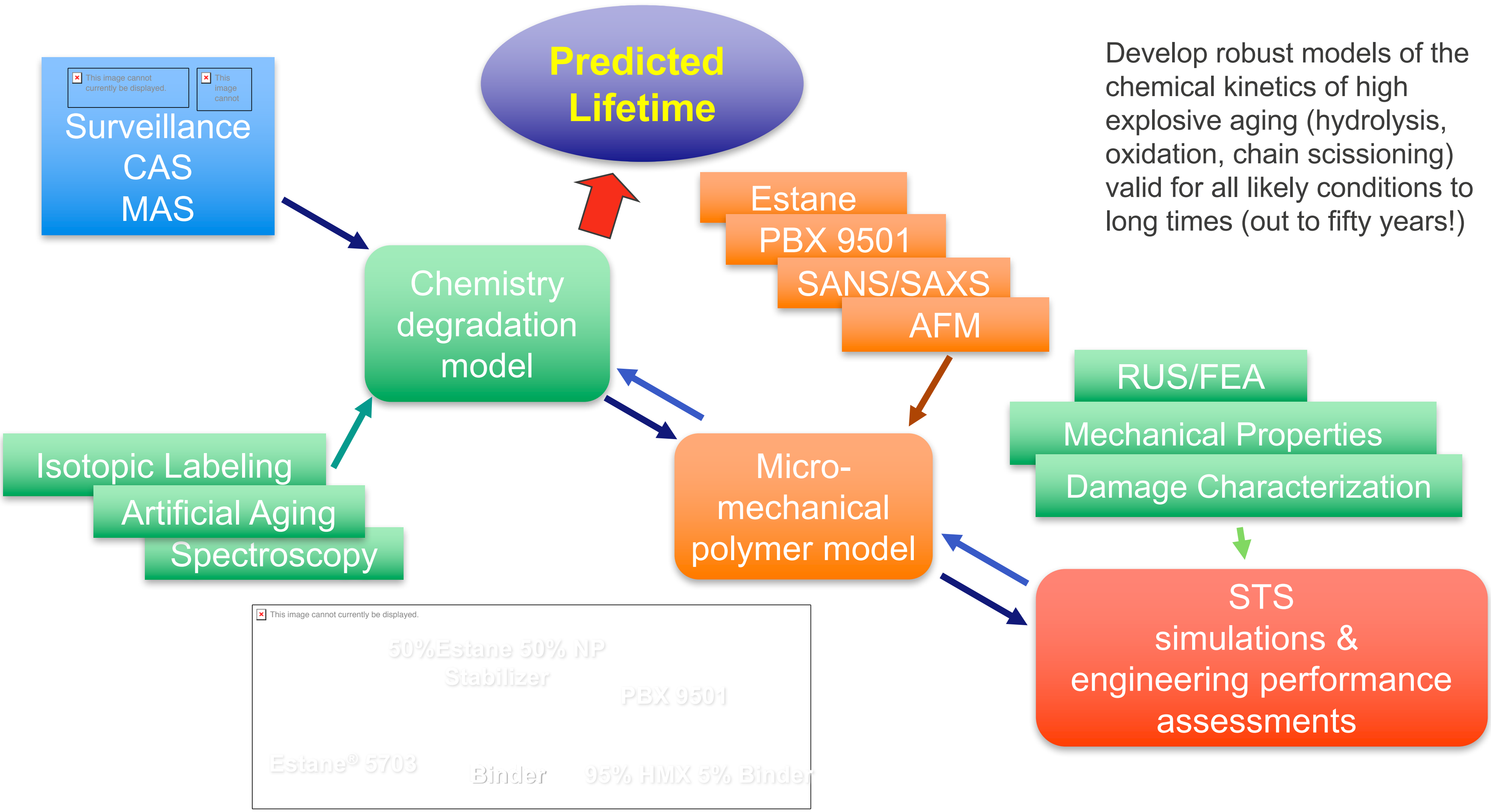
Gas phase diffusion in mesopores;

Solid state diffusion in silica-PEI composites.

Yao, L., et al., Journal of colloid and interface science 408 (2013): 173-180
Mebane, D.S., et al., The Journal of Physical Chemistry C 117.50 (2013): 26617-26627.

Polymer Lifetime Prediction for High Explosives

Develop robust models of the chemical kinetics of high explosive aging (hydrolysis, oxidation, chain scissioning) valid for all likely conditions to long times (out to fifty years!)



R ~ 3 nm
(SAXS, SANS)

Estane 5703: Block copolymer

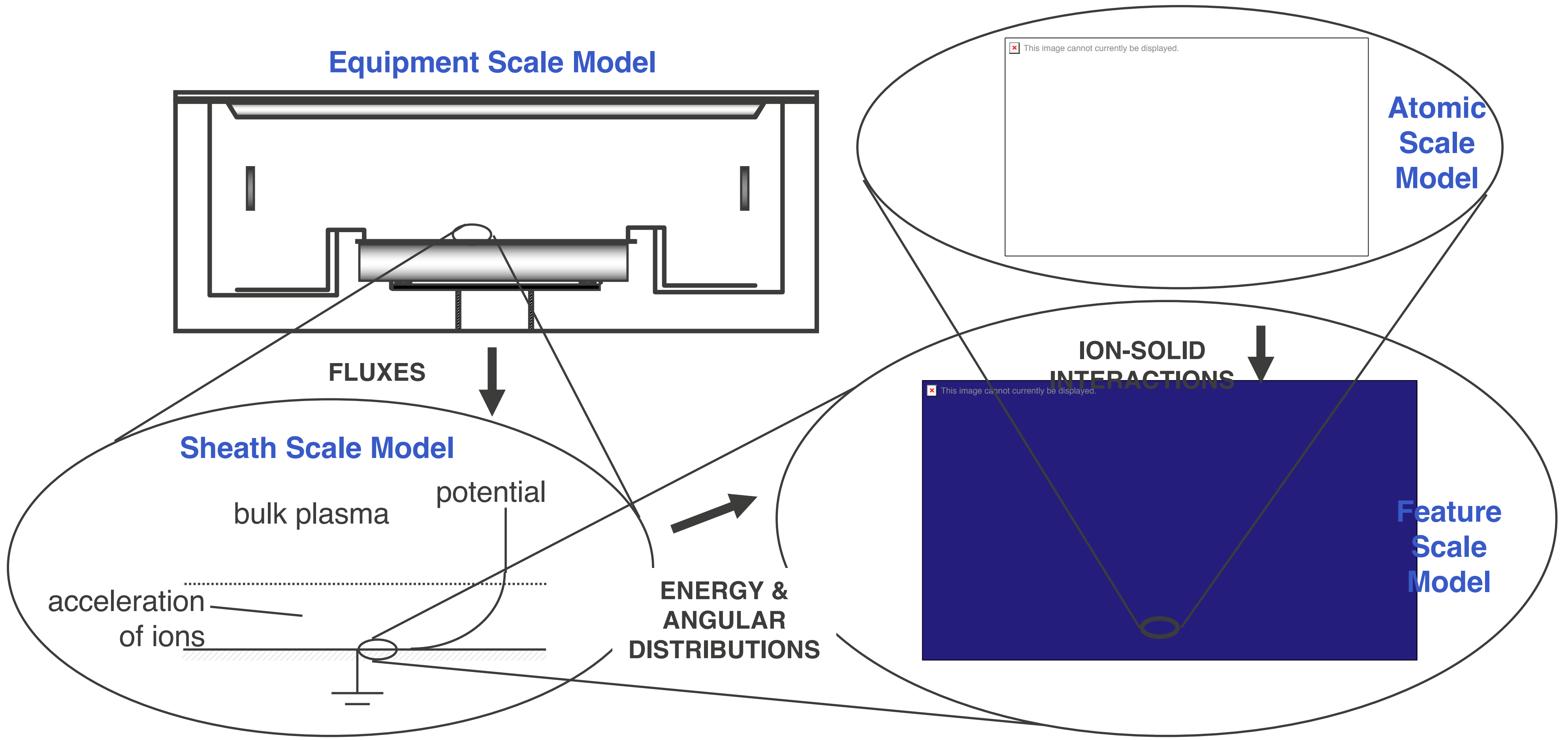
- Segmented poly(ester urethane)
- Phase separation of rigid aromatic hard segments and flexible soft segments
- Elasticity theory of molecular networks

This image cannot currently be displayed.

This image cannot currently be displayed.

This image cannot currently be displayed.

Multi-Scale Process Modeling



Ionized Physical Vapor Deposition

This image cannot currently be displayed.

Materials Design

- Philosophy
- Virtual materials processing and characterization
- Process-structure-property performance

Applications

This image cannot currently be displayed.

- Civil nuclear energy
- Carbon capture technology
- Semi-conductor