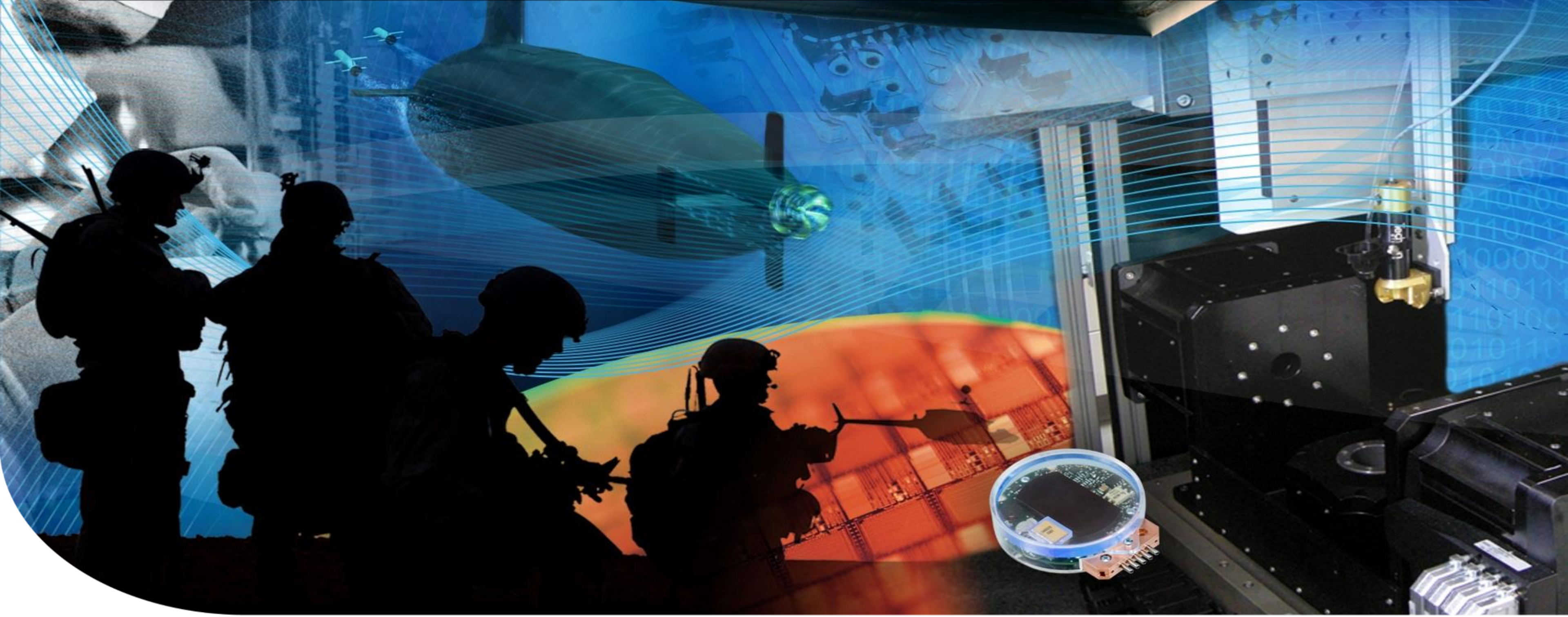
MULTISCALE APPROACH AND WORKFLOW DEVELOPMENT FOR ENHANCED UNDERSTANDING OF MANUFACTURING MATERIALS



08.01.2018
NCCoE Building

Ryan Thomas

NNSA

Honeywell

National Security Campus Operated by Honeywell

-60 Years of Continuous Service to Dept. of Energy

-Associates ~ 2500

-Area ~1.5 million sq. ft.

-Kansas City, Missouri

ELECTRICAL/ ELECTRONIC

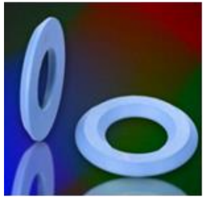
- Microelectronics
- Arming, Fusing and Firing Systems
- Embedded Software
- Fiber Optics
- Fire sets / Initiators
- Optics and Initiators
- Radars
- Secure Electronics
- Sensors
- RF / Antenna Design
- Telemetry
- RF / Microwave
- Film Deposition
- Systems Integrator

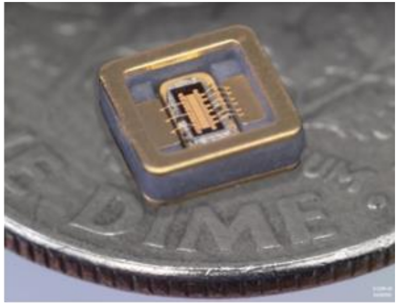
MECHANICAL

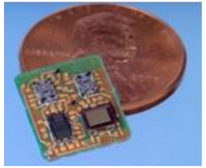
- Containers
- Mechanisms
- Machining
- Solid Modeling
- Prototyping
- Special Materials and Processes
- Welding Technologies

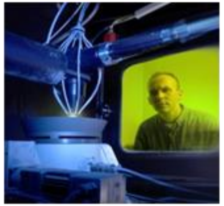
ENGINEERED MATERIALS

- **Ceramics**
- **Polymer Develop. and Production**
- **Materials Engineering**
- **Organic / Inorganic / Metallurgy**
- **Gas Transfer Systems**

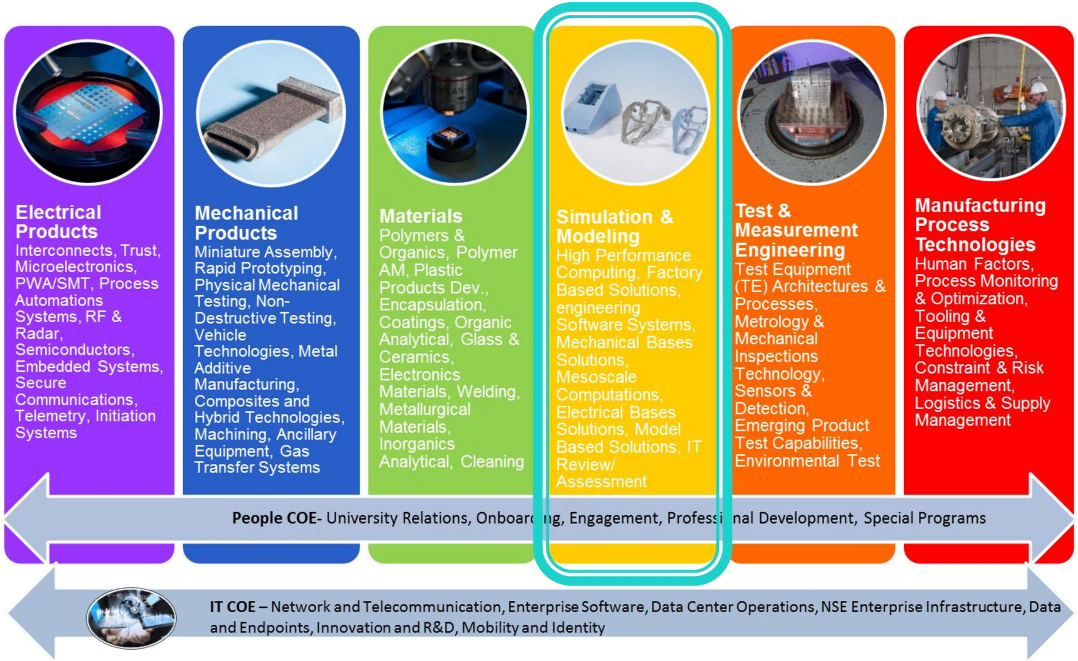






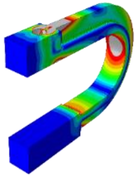


Centers of Excellence



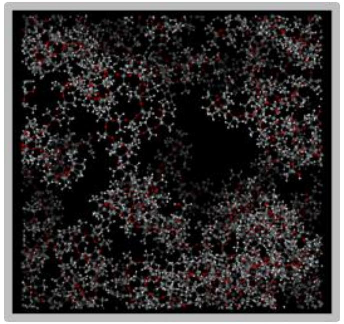
Simulation Technology History at KCNSC

- Have used Finite Element Analysis (FEA) to troubleshoot mechanical issues since 1979
  - 1979 – 1985: NASTRAN
  - 1985 – 2015: Abaqus



- Honeywell's simulation group, AESA, has grown from a few individuals to ~28 FTEs and conducts 150-200 projects per year

- **First molecular dynamics simulation in 2014**



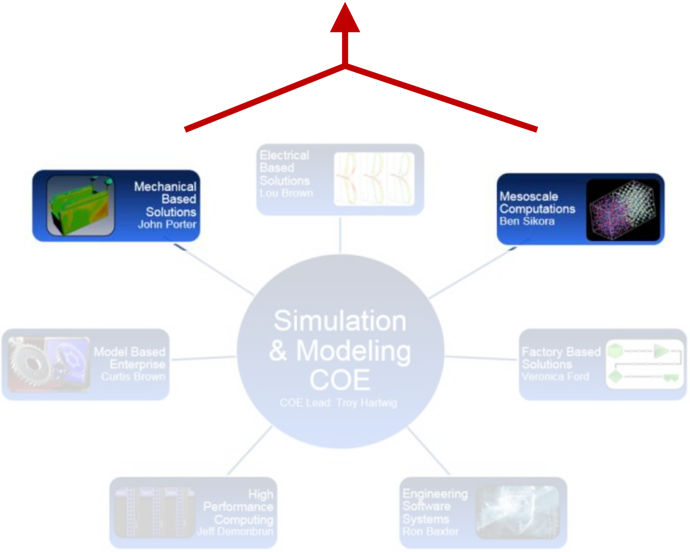
- **First *ab initio* simulation in 2015**

- **Computational Materials Group Started 2017**

Who is AESA?

- Advanced Engineering Simulations & Analysis
- A group focused on creative problem solving
  - Simulations – Virtual components/materials + manufacturing processes
  - Data analytics and visualizations
  - Innovative technology solutions
- Strong team of 28 mechanical engineers, a chemical engineer, and a physicist

ADVANCED ENGINEERING SIMULATIONS & ANALYSIS



AESA VISION:

To develop the technology and deploy simulation based solutions that serve as KCNSC engineers' first stop for manufacturing process modeling, development cycle acceleration, and other science-based insight.

Simulation first!

Who are AESA's customers and collaborators?

- Within the NSE
  - PRTs
  - MC owners
  - Simulation analysts from labs and production sites
  - Anyone in the plant with a need for simulation support!
- External
  - Universities and technology companies on the cutting edge of innovative research and design

Simulation Technology at KCNSC

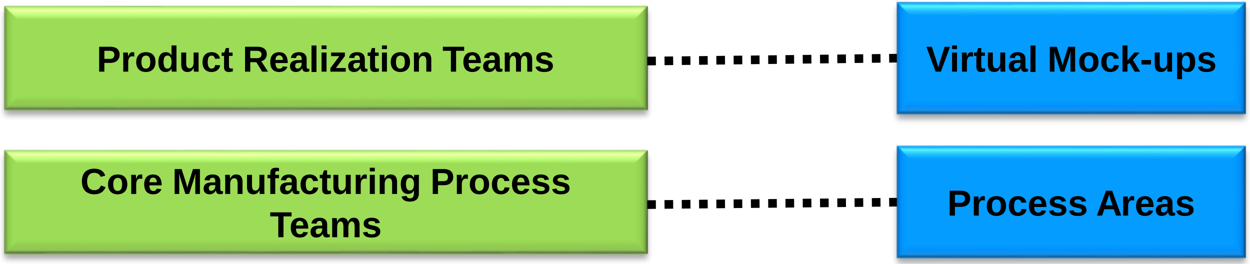
Value in Using Simulation Tools for Small Lot Production Environments

- Reduce or eliminate actual prototype builds.
- Reduce time to evaluate processes, designs, and/or fixturing.
- Allows for a more robust process, product or fixture.
- Uncover production problems before they occur.
- Allows for environmentally friendly ‘virtual’ evaluations.
- Aid if production failures do occur.

Simulations can make you agile and flexible to change for rapid response to needs and requirements.

Structure and Order to Technology Deployment

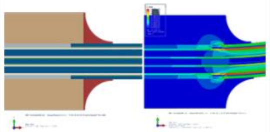
- Focus and use of simulation technology
  - Exploration of new, high risk production process areas and materials
  - Exploration of known challenge areas with respect to products and processes
- Close engagement with the engineering teams brings forward solutions that advance technology with greater understanding and surety.



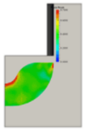
How Does AESA engage with Customers and Collaborators?

- vCons (virtual consultants) and other tools on the AESA website
  - Simple vetted simulation tools anyone in the plant can use whenever they need
- **Virtual Mock-ups**
  - A virtual twin of a component or assembly that evolves as the component passes through design iterations

Selection of AESA vCons

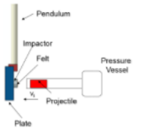


Flex Cable



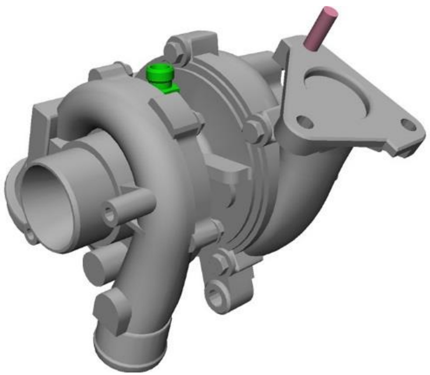
Forging

Axisymmetric forging simulation base on user defined geometry, material, temperature, and final d...



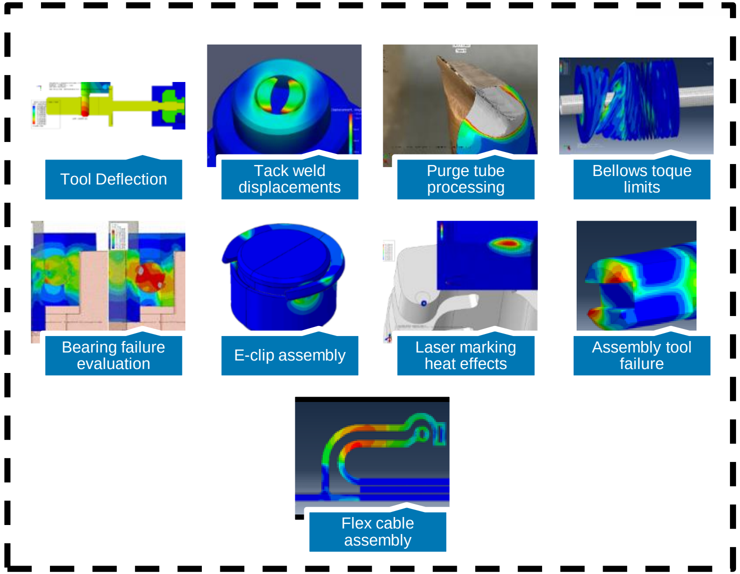
Resonant Plate

This simulation uses Sierra SM and SD to compute the natural frequencies, FRF, time domain respon...



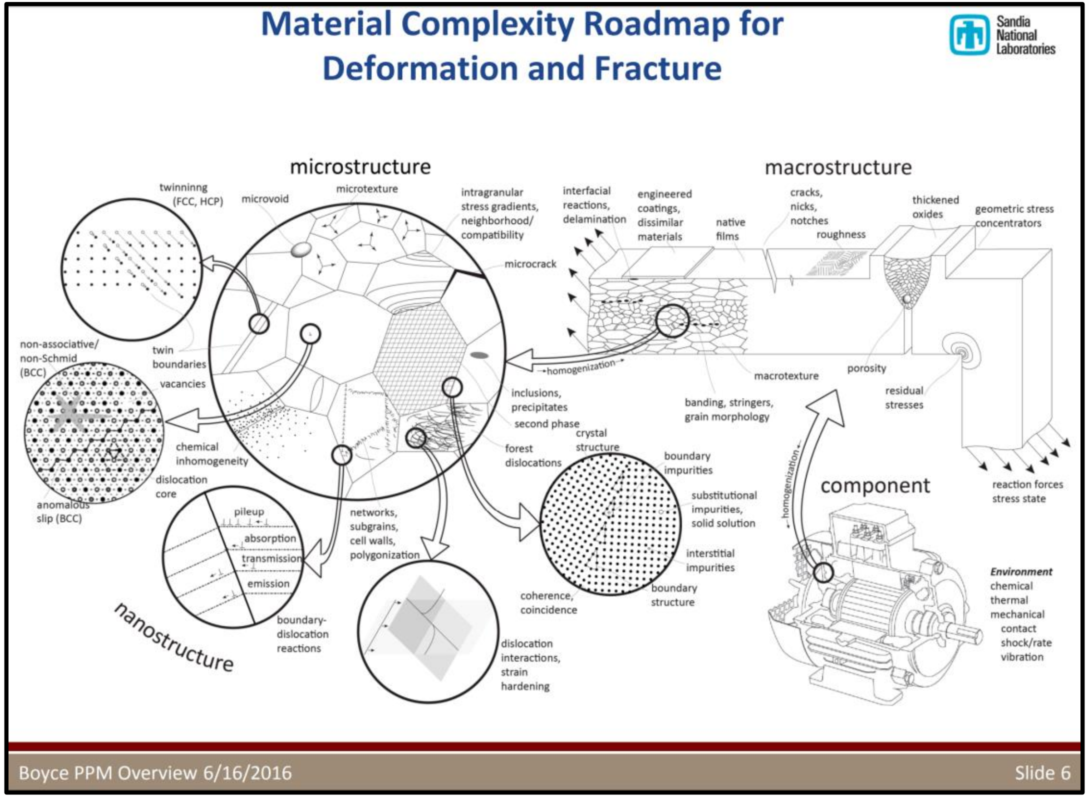
Virtual Mock-ups Philosophy

- AESA is a service organization
- Proactive engagement with PRTs
- "Simulate First"
  - Reduce or eliminate physical prototype iterations
  - Reduce time to evaluate processes, designs, and/or fixturing
  - Allows for more robust, optimized process, product, or fixture
  - Uncover production problems before they occur
  - Aid if production failures do occur



Understanding Manufacturing Materials

- How do we quickly address material issues?
- How do we begin to understand materials across a wide range of length scales?

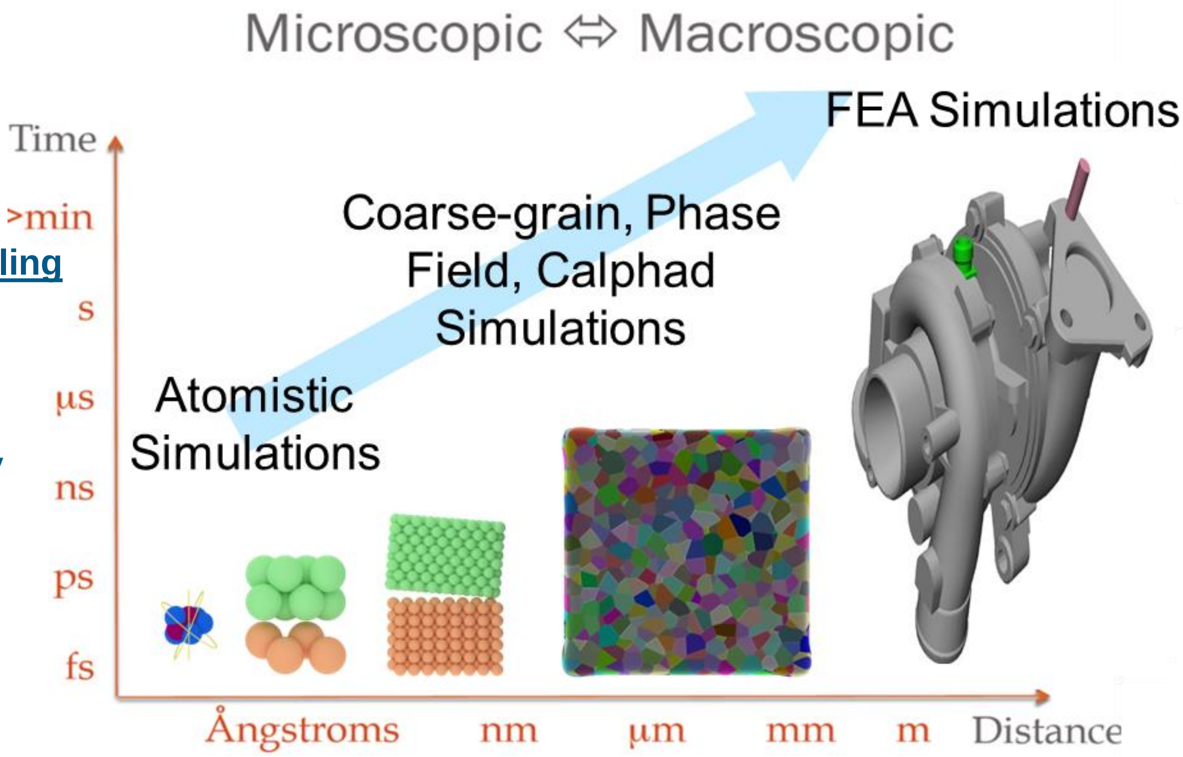


https://www.osti.gov/servlets/purl/1366804

Simulate First – Connecting the Length Scales

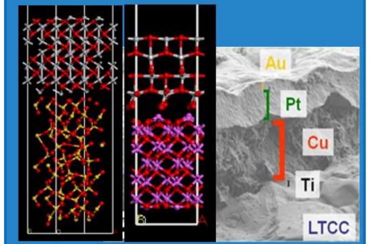
Molecular and Quantum Modeling

- Density
- Young's Modulus
- Shear Modulus
- Shear Yield Stress
- Heat Capacity
- Thermal Conductivity
- Thermal Expansion
- Mass Diffusion
- Transition Temps
- Cohesive Energy
- Surface Tension
- Molar Volume
- Solubility
- Gas Permeability

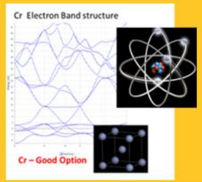


Continuum Modeling

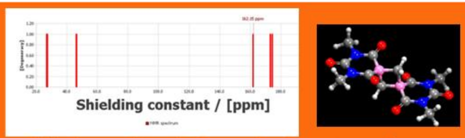
- Product Performance
- Energy Absorption
- Mechanical Response
- Thermal Conductivity



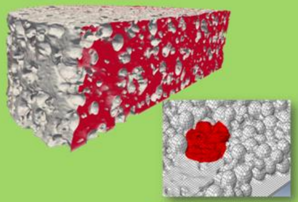
Interface Adhesion, Phase Formation and Reactivity



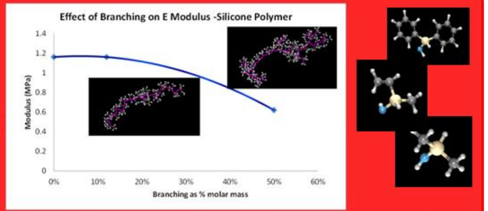
Thermal and Electrical Properties on Crystal Materials



Molecular Discriminator for XRD and NMR on Reverse Eng.

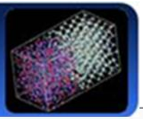


Large Scale Meshing



Polymer Composition and Morphology Architecture Effect

Mesoscale Computations



Technologies

- Mesoscale Computations
  - Meshing Capabilities
  - CAD Geometry Manipulation
  - Coarse-Grained
  - Molecular Dynamics
  - Quantum Mechanics
  - Correlation Tools
  - Kinetics
  - Thermodynamics

Services

- AM Metals
  - Phase formation/Oxidation
  - Elastic Constants
  - Thermal Aging and Diffusivity
- AM Polymers
  - Chemical Functionality
  - Viscoelasticity
  - Thermal Properties
  - Solubility and Diffusivity
- Reverse Engineering
  - NMR Spectrums
  - XRD Patterns
- Materials Information Management

Skills

- Chemical Engineering
- Physics
- Materials Engineering

Mesoscale Focus Area Thrusts

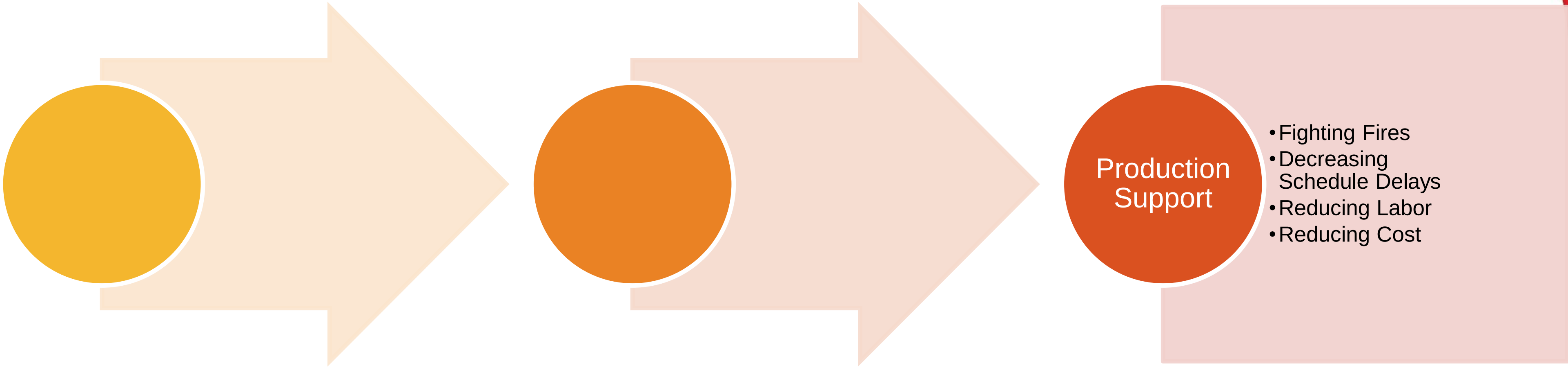
R&D
- Design
- Novel Material Development
- **ICME Methodology**
- New Simulation Tools
- **Workflows**

Advanced Development
- **Material Model Development**
- Refining & Developing Mesoscale Tools
- **Vmat Generation**
- **Workflows**

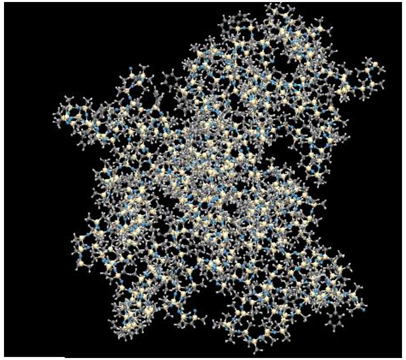
Production Support
- Fighting Fires
- Decreasing Schedule Delays
- Reducing Labor
- Reducing Cost

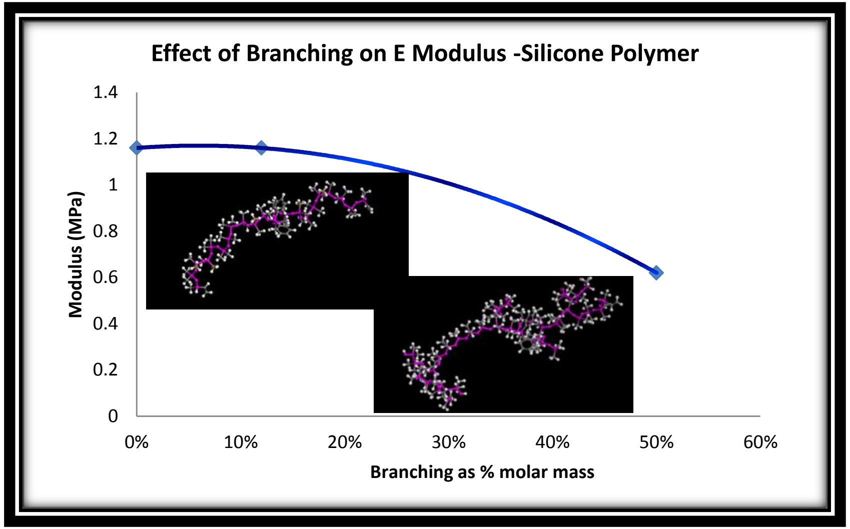
	R&D	Advanced Development	Production Support
FY18	High	Medium	Low
FY19	High	Medium	Low
FY20	Medium	Medium	Low
FY25	Low	Low	Medium
FY30	**Low**	**Low**	**High**

Mesoscale Focus Area Thrusts



Investigating Silicone Polymer Production

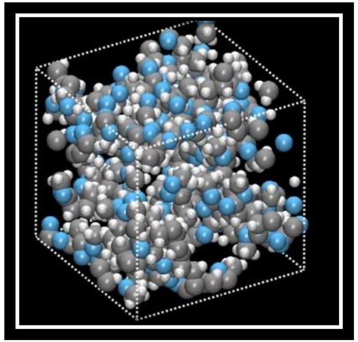




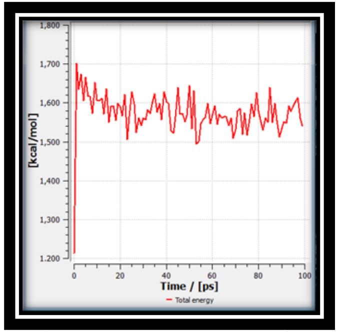
Allowable branching limits were determined using MD
This matched predictions derived from experiment.

Polymer Solubility and Compatibility

Polymer solubility can be calculated for any given chemical formulation



Polymethylacrylate (PMA)



$$\delta = \left(\frac{|\langle E_i \rangle|}{\langle V \rangle} \times 6947.28 \right)^{1/2}$$

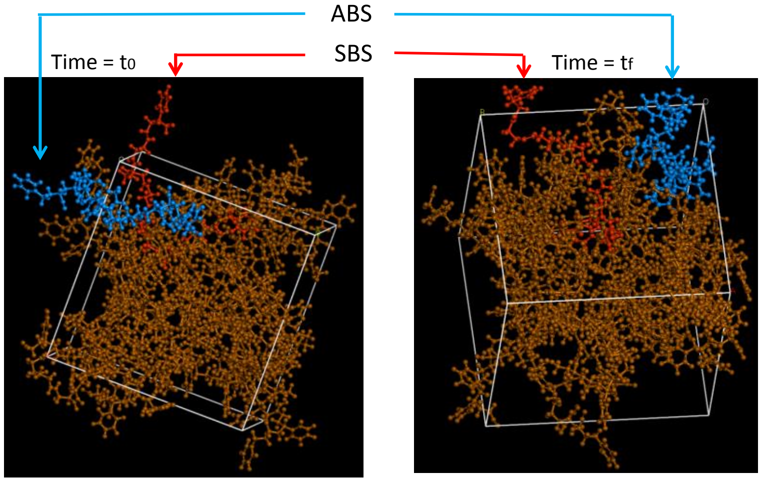
Solubility $(J/cm^3)^{1/2}$
Molecular Dynamics = 18.5
Experimental Value = 19.9

Total time to build, run and analyze simulation: **4 hours**

Mixing Polymers - Additive Manufacturing

- Great variety in polymers available for 3D printing
- Provide direction for choosing a blend that will yield improved properties for AM
  - Simulate polymer compatibility
  - Watch polymer movement during simulation
  - Compare solubility parameters

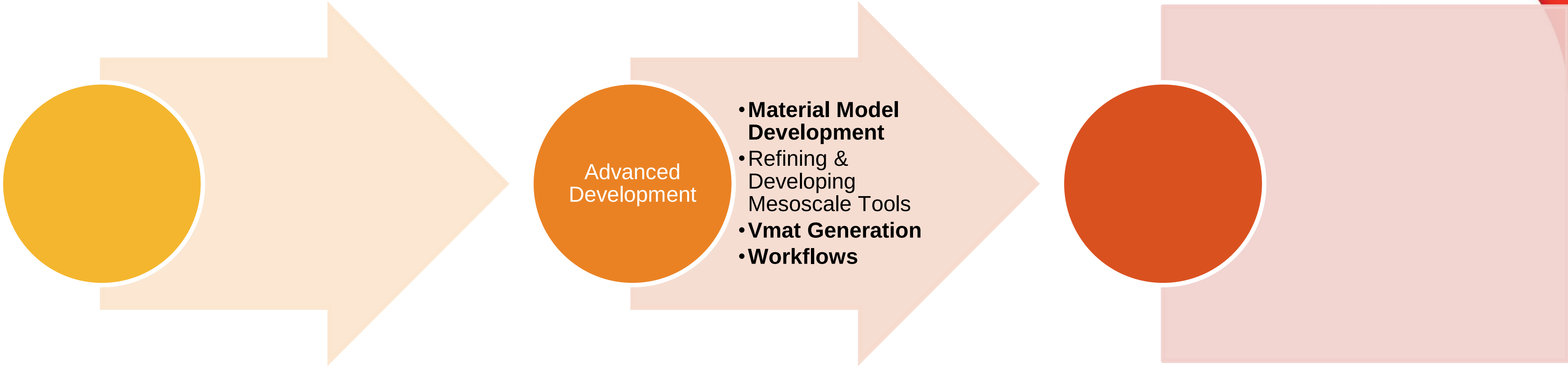
Molecular Dynamics – Amorphous Polymer Blend



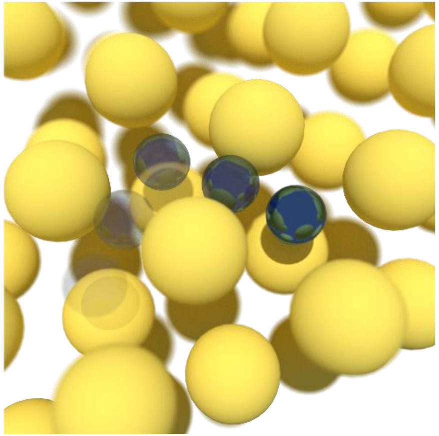
ABS and SBS chains at initial Energy

ABS and SBS chains at lowest Energy

Mesoscale Focus Area Thrusts



Advanced development



- Material model development legacy materials
  - Connecting the length scales with RTV
- New tools and capability Development
  - Multistage simulations
    - Hydrogen embrittlement
  - vCons for analytical lab support
  - CALPHAD Methods
    - Gold embrittlement

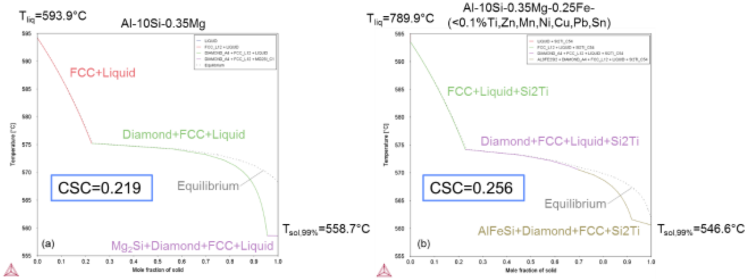
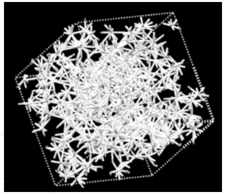
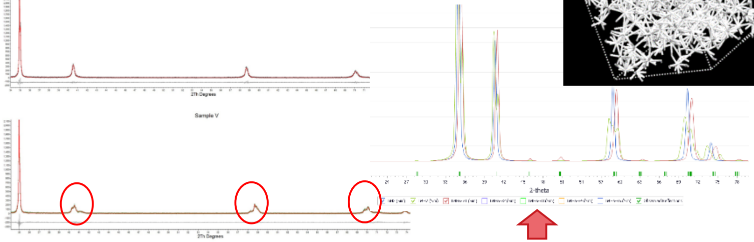


Figure 13 Scheil solidification step diagrams for (a) Al-Si-Mg and (b) Al-Si-Mg-(Fe,Ti,Zn,Mn,Ni,Cu,Pb,Sn) systems, with compositions selected to be within the Renishaw specifications for powder bed Al alloys





QM Model- CASTEP- Diffraction Pattern Prediction with crystals of Ti and different amount of Hydrogen content

Workflows

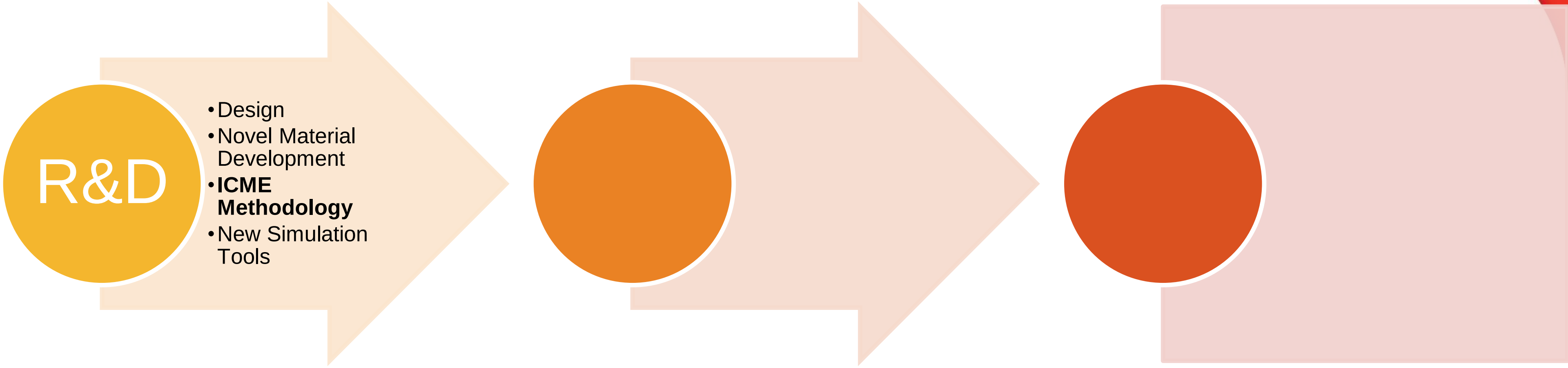
- Workflows at KCNSC: *A plug-and-play simulation process/tool that can be used to determine material properties in a seamless and straightforward manner*
  - *Diffusion of small molecules*
  - *Stress/strain curves*
  - *Moduli*
- What is important to us:
  - Plug-and-play of Materials and simulation types
  - Access to the workflow backbone to generate our own
  - High-throughput capabilities
  - Multi-scale/simulation linkages
  - Democratization of the tools for easy material property prediction
    - Rapidly and easily address problems within the manufacturing environment

Workflows (Not All Encompassing)

Software	Framework	Type	Workflows	Cost to us	Creating Workflows
Vendor A	Assumed C++, closed	Wrapper GUI	**Drag and drop**	$$	Easy, but limited capabilities
Vendor B	Python/C++, some open	Wrapper/Proprietary GUI	**~Python backbone**	$	Very hard as of now
Vendor C	Unknown	Proprietary GUI	Widget	$$$	N/A - Haven't tried
Vendor D	Unknown	Proprietary GUI	Drag and drop, stream lined	$$$$	Easy, but limited capabilities
Jupyter Notebooks	Python, open-source	Wrapper/User made	**User Made**	Free	Hard, extensive scripting

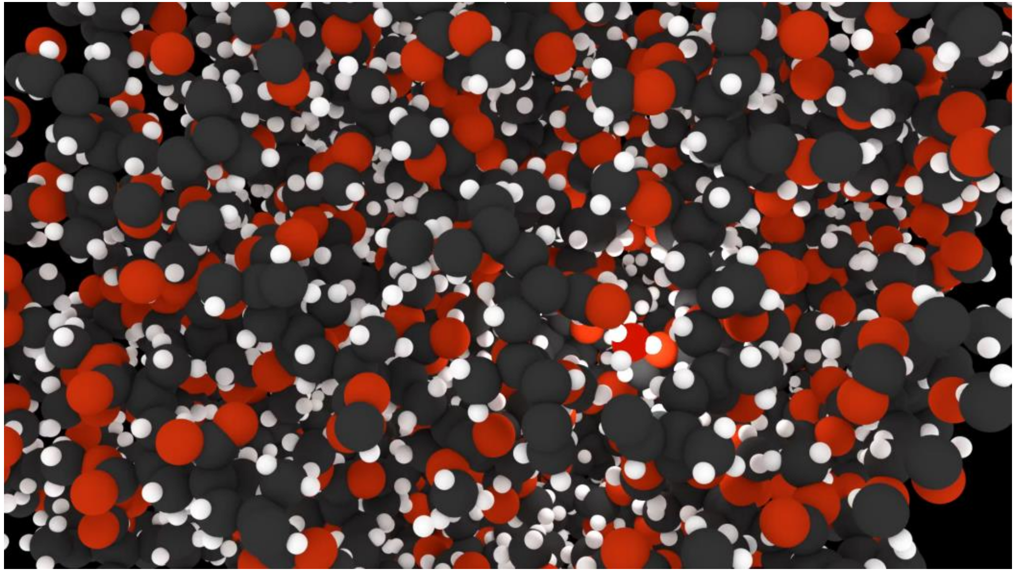
Current problem with commercial software is "**oversimplified**"
Closed software built for non-computational chemists, limits extendibility

Mesoscale Focus Area Thrusts



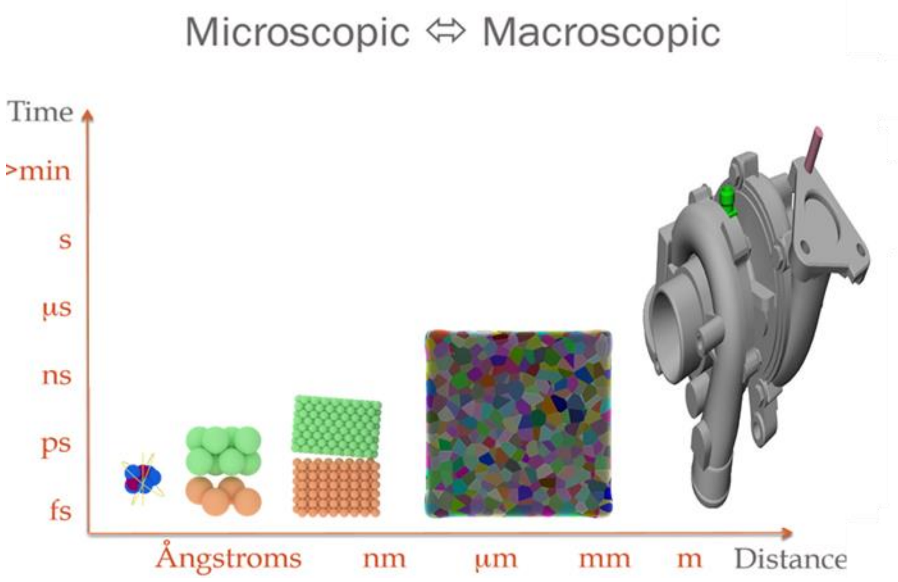
R&D Capability for Design

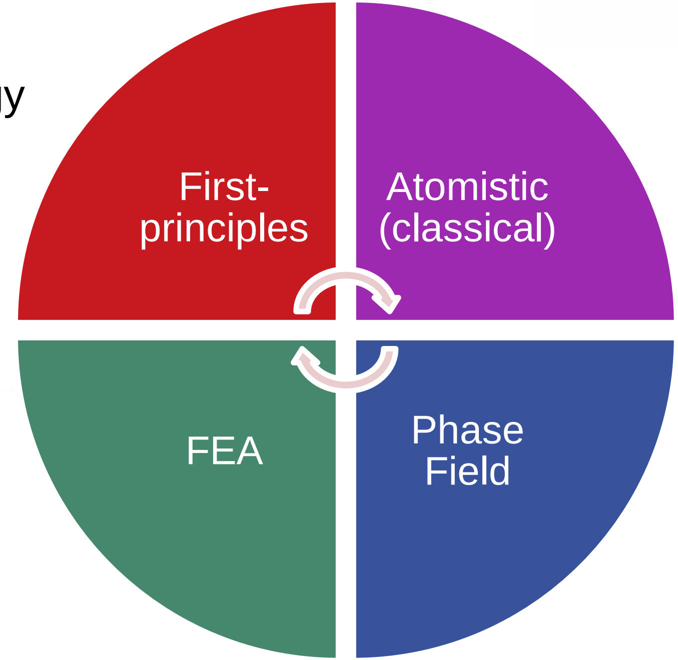
- Material model development for new materials
  - 3D printed materials
    - Siloxanes
    - Ti-6-4
    - Stainless steels
  - Aging of polymeric materials
- New tools to help drive "Simulate First" mentality
  - High-throughput analysis
  - Free energy methods
  - Machine learning to drive DOEs
  - "Big Data"/Data analytics



Multiscale Modeling

- Generation of high fidelity models at each length scale
  - "vMats" for use with plug-and-play workflows
  - Connecting length scales using an ICME methodology





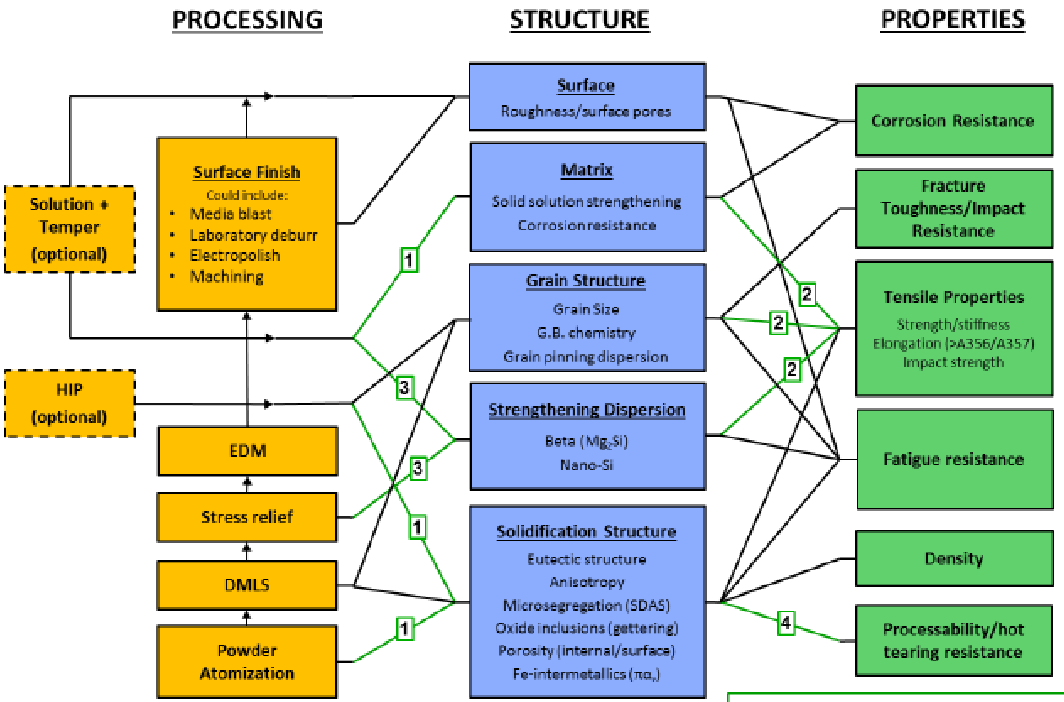
Integrated Computational Materials Engineering

What is ICME:

- **I**ntegrated –
  - Material model linkages at multiple length scales
  - Bringing computational modeling into the design cycle
- **C**omputational
  - Simulate first mentality, where we are trying to understand these materials using computational tools
  - Overarching framework built on material models, with variations analyzed computationally
- **M**aterials **E**ngineering – The **design** and **discovery** of new materials

What does the ICME Methodology mean to KCNSC

- ICME methodology is used to gain a holistic understanding of the materials we use within the complex

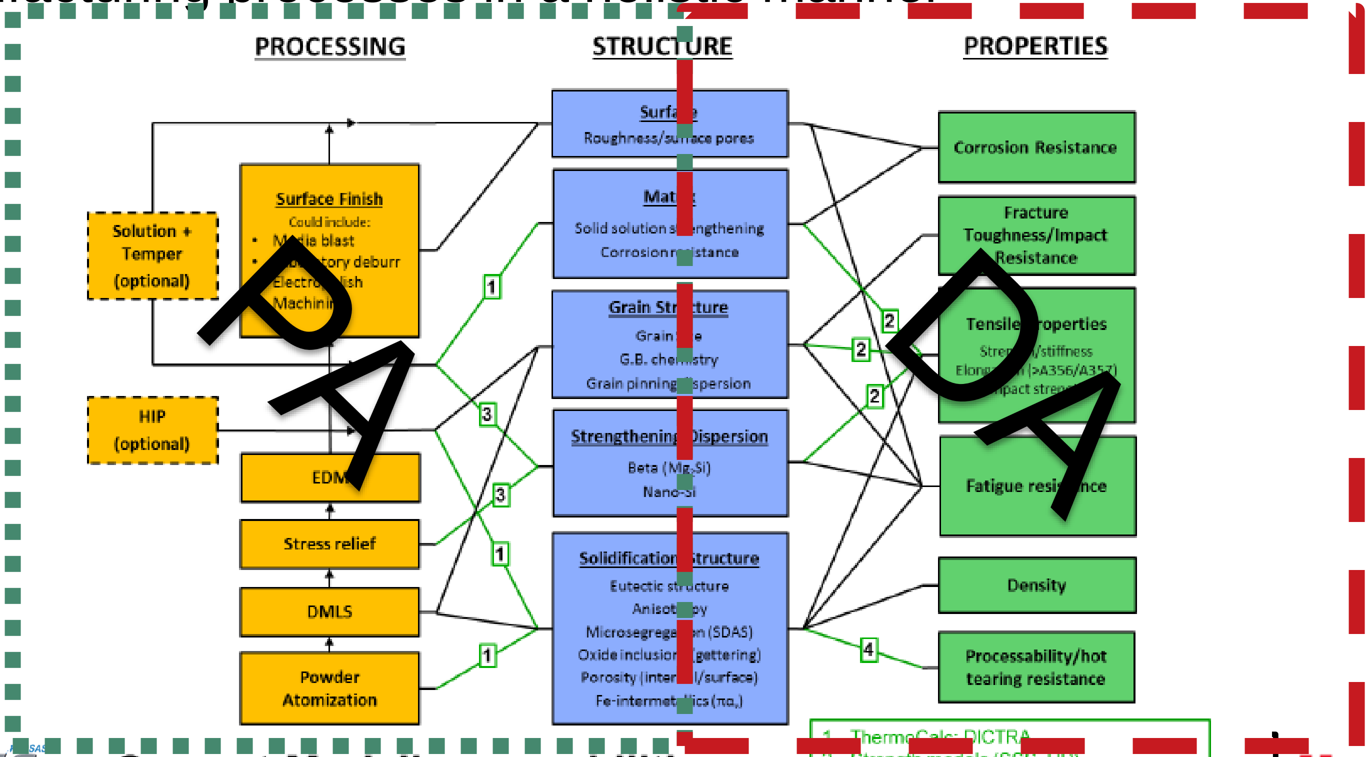


Current Modeling capabilities

1. ThermoCalc; DICTRA
2. Strength models (SSS, HP)
3. PrecipiCalc®/PRISMA
4. Cracking susceptibility (CSC) model

What does the ICME Methodology mean to NSC

- ICME methodology used to design new materials and manufacturing processes in a holistic manner



Current Modeling capabilities

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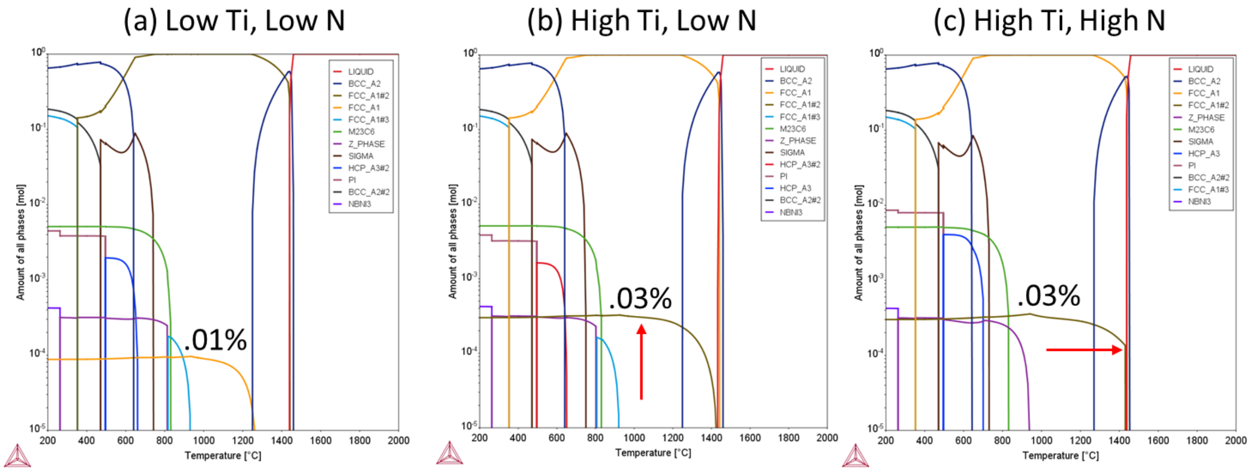
SS-304L: Thermodynamic-based process-structure modeling

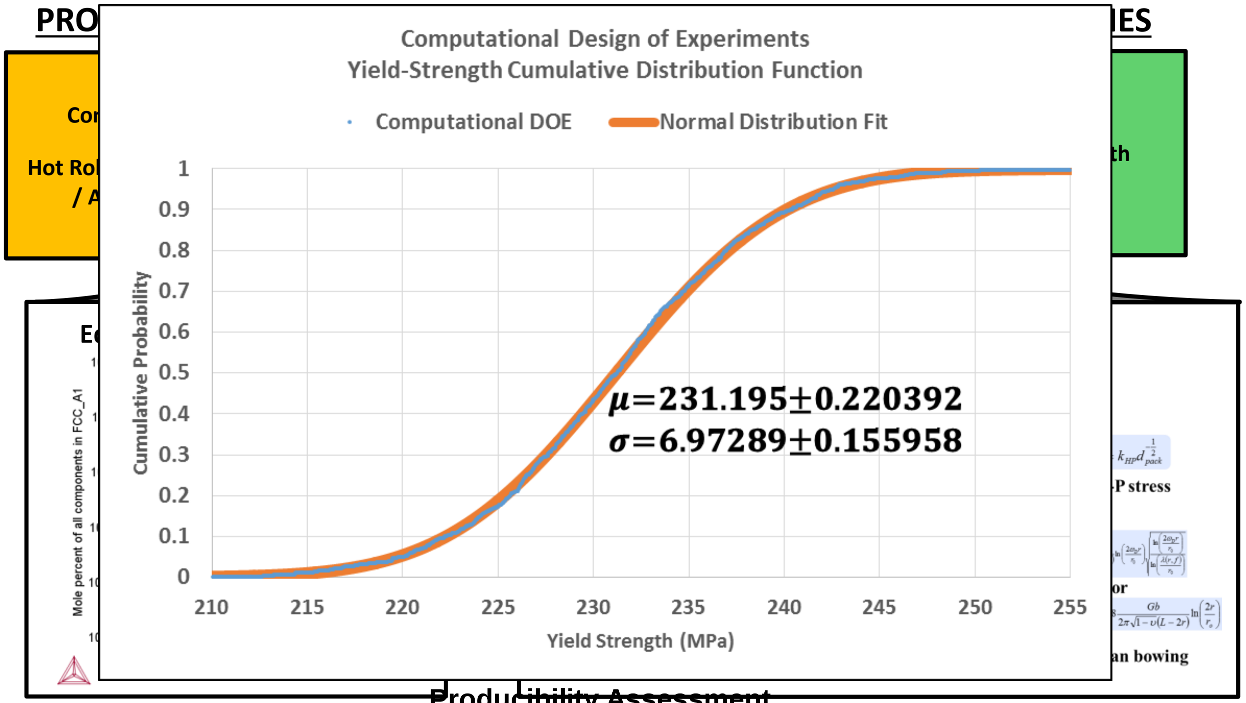


Computational experiments allow new engineers to gain knowledge without conducting expensive trial-and-error experiments.

When computational experiments are conducted within optimization frameworks, rapid solutions are possible

Thermodynamic modeling can inform processing windows, property models

SS304L: ICME-based Strength Model



Producibility Assessment

99.9% likelihood of producing steel part with yield strength of at least 210 MPa

SS304L: ICME-based Weldability

PROCESSING

Melt Composition

Solidification

Welding

STRUCTURE

Weld metal – Austenite, ferrite

Martensite (austenite stability)

Sigma phase

Grain size

PROPERTIES

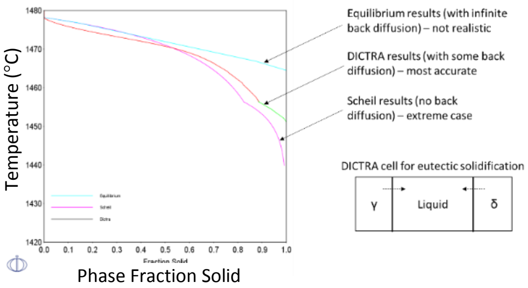
Hot cracking susceptibility

Toughness

Weldability criteria

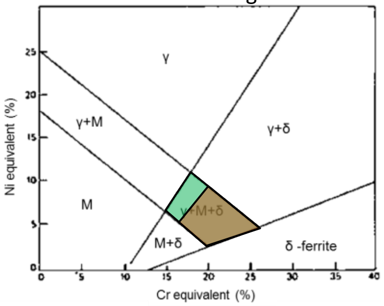
KCNSC Specification

Solidification Modeling



ICME-based Weldability Criteria

Schaeffler Diagram



Chemistry → Np(δ-ferrite) → HCS model → ASP model → Np(sigma) → Allow / Reject

Use existing models to develop an ICME-based universal welding criteria

Solidus Temperature Modeling

PROCESSING

- Composition
- Thermal history
  - -Sealing cycle
  - -Cooling/annealing

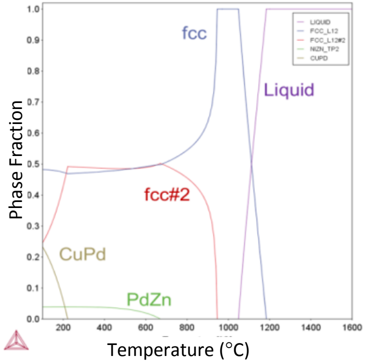
STRUCTURE

- Phase composition
- Site Fraction
- FCC phase separation (spinodal and/or cellular reaction)
- PdZn precipitates

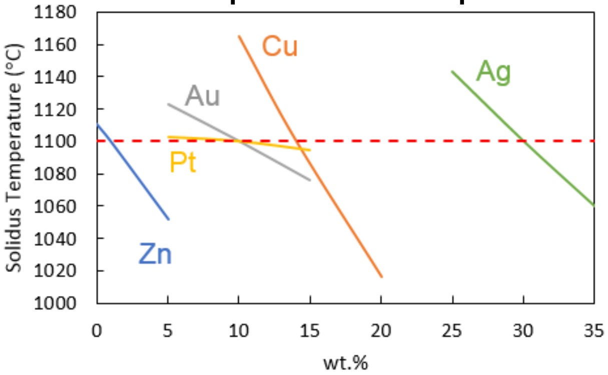
PROPERTIES

- Solidus temperature (Melting point)
- High temperature structural stability

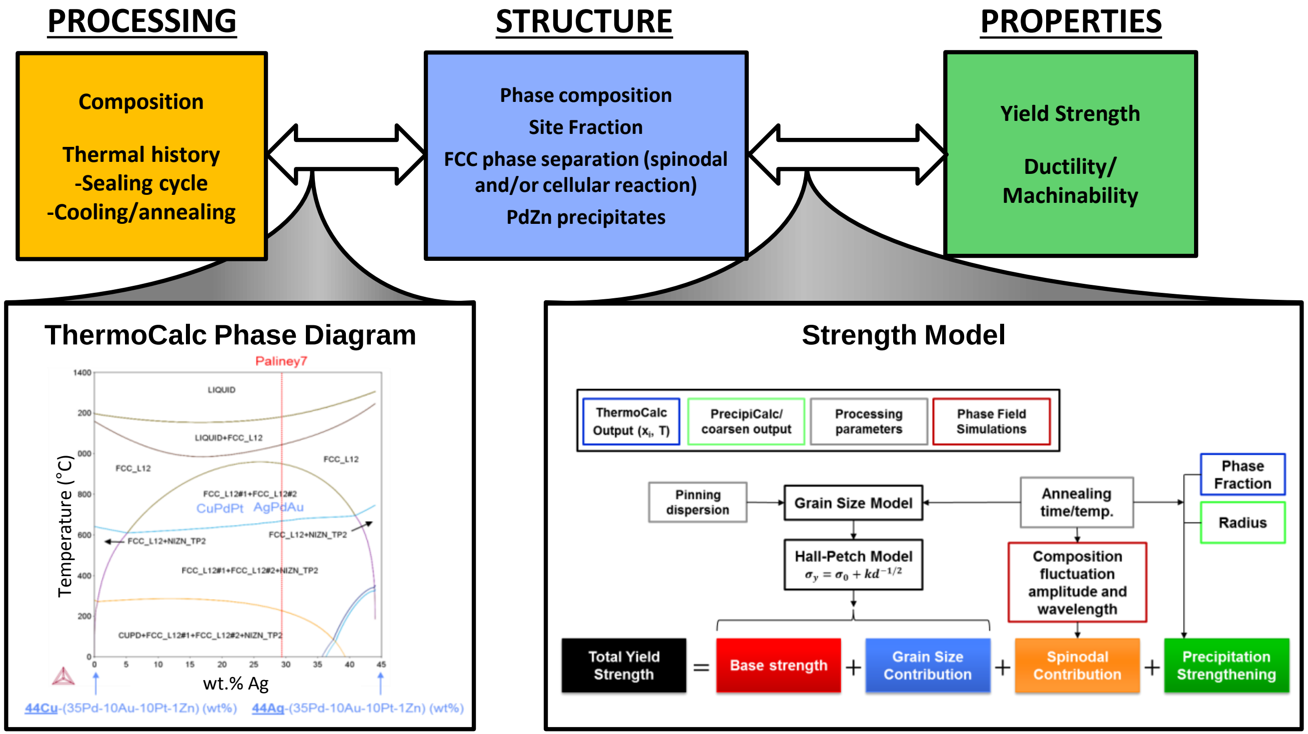
ThermoCalc Step Diagram



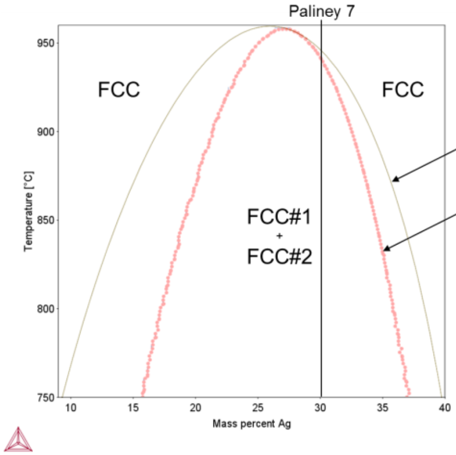
Solidus Temperature vs. Composition

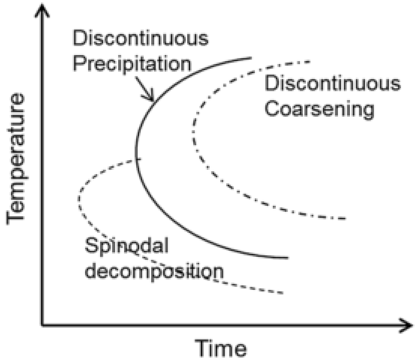


Strength Modeling

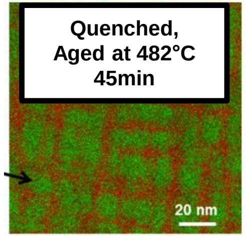


Spinodal decomposition in Paliney

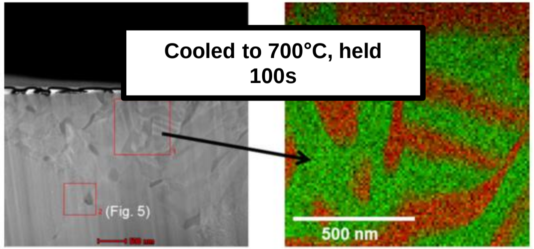




Complex phase separation mechanisms contribute to strengthening



SPINODAL

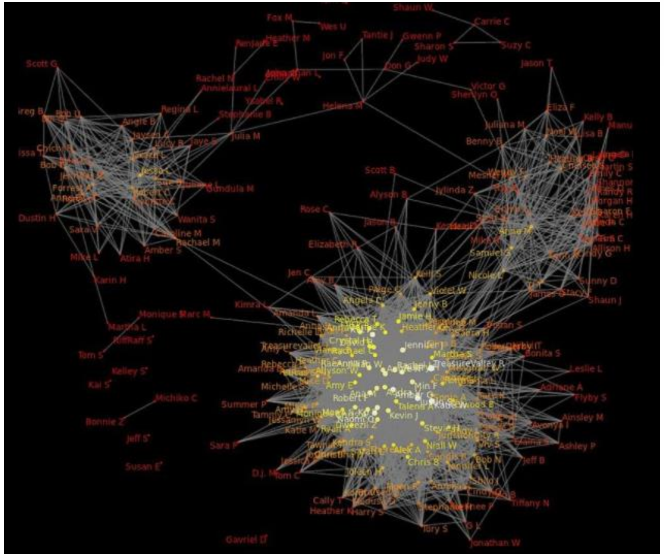


DISCONTINUOUS/CELLULAR PRECIP.

Susan, Donald F. et al. 2014. "Characterization of Continuous and Discontinuous Precipitation Phases in Pd-Rich Precious Metal Alloys." *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science* 45(9): 3755–66.

Mesoscale's Current Plan

- Modeling Infrastructure
  - Workflows/ELN – Jupyter notebooks
  - PSP builder
  - Linking the length scales
    - Close collaboration with FEA group (monolithic)
- Codes
  - MD/Quantum codes
  - CALPHAD
- Materials Data
  - GRANTA
  - Hyperthought
- People (Open to collaborative efforts)
  - Big Data and network analysis
- Deep dive on materials
  - Comprehensive understanding of our SS304L
  - Ti alloys (exploration of composition space)
  - AM polymers



Next Steps to Address

- Pain points and next steps
- Addressing “Big Data” and data science (e.g. social network graph to identify collaborative avenues in the complex)
- Linking the length scale codes – Multiscale modeling
  - Use of ICME to help identify easy paths
  - Using codes outside our traditional infrastructure (e.g. MOOSE out of INL)
  - Cross-industry ICME collaboration
    - Creating a collaborative ICME group for lower length scales
    - Shared data on commonly used manufacturing materials