Integrated Computational Materials Engineering (ICME): An Industrial Perspective

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June 23, 2010

UMC Workshop on (Integrated?) Computational Materials Engineering

Research and Advanced Engineering

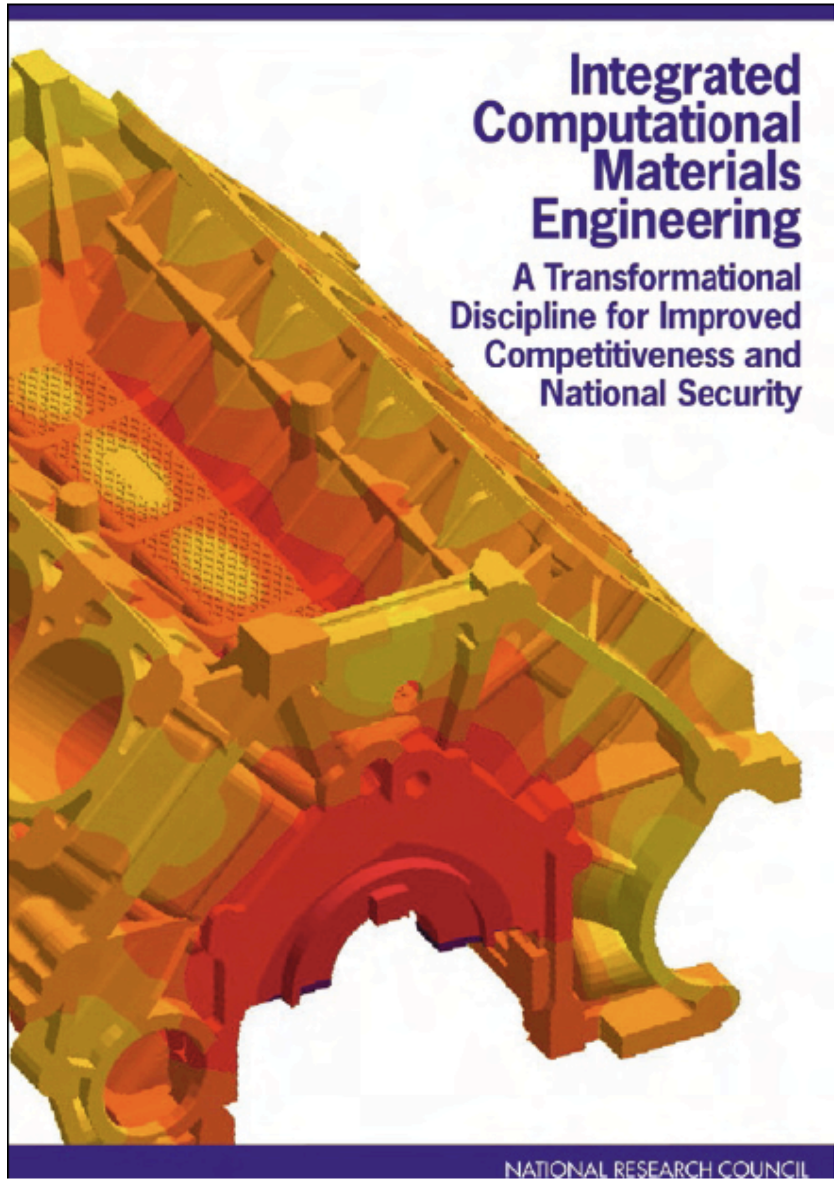
Outline

- Integrated Computational Materials Engineering (ICME) – What it is and why it's important
- Virtual Aluminum Castings – An ICME Case Study at Ford
- ICME – Prognosis and Encouraging Indicators

NMAB Committee on Integrated Computational Materials Engineering

Tresa Pollock, Chair
John Allison, Vice Chair

July 2008



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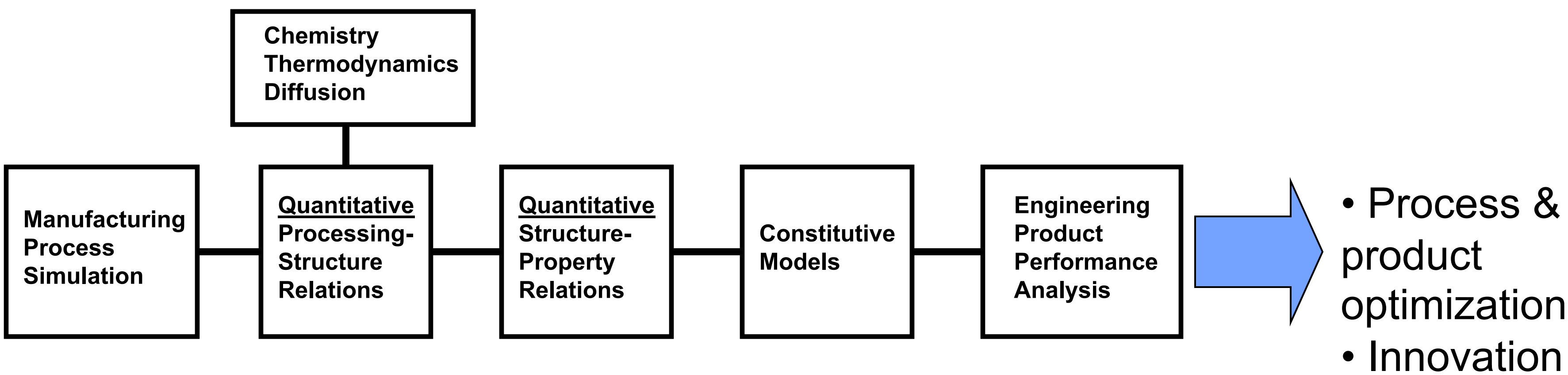
*http://books.nap.edu/catalog.php?record_id=12199

What is ICME?

Integrated Computational Materials Engineering (ICME) is the integration of materials information, captured in computational tools, with engineering product performance analysis and manufacturing-process simulation.*



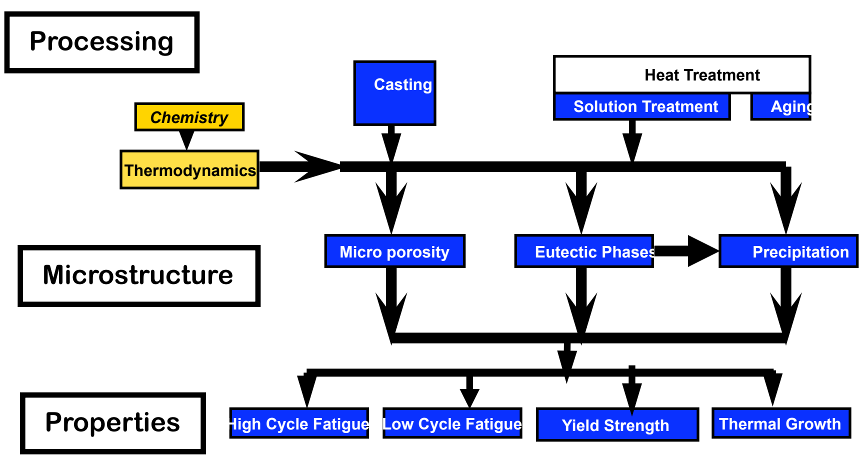
* NAE ICME Report, 2008

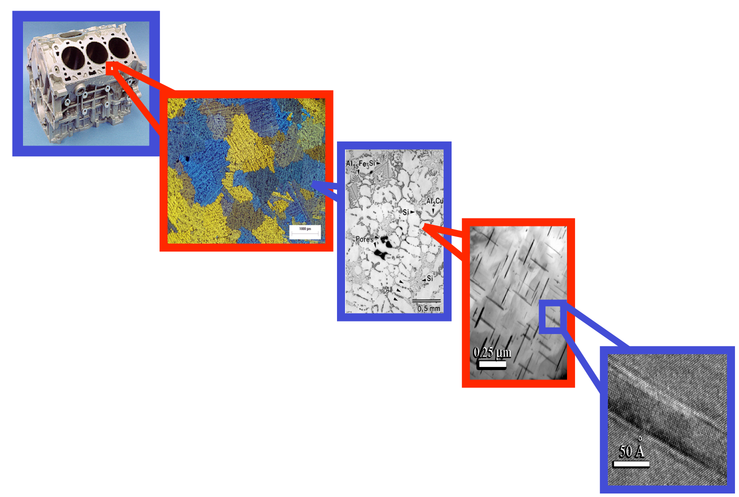
Why this is important

- Innovations in materials and tight coupling of component design, materials and manufacturing have been key sources of US competitiveness and security advantage
- These innovations and tight coupling are threatened by advances in computational capability in design and manufacturing that have "left materials field in the dust".
- The global economy requires efficient engineering (and R&D)

Materials represents a different class of computational problem

- Materials response and behavior involve a multitude of physical phenomena with no single overaching modeling approach.
- Capturing the essence of a material requires integration of a wide range of modeling approaches dealing with separate and often competing mechanisms and a wider range of length and time scales.





Integration of knowledge domains is the key to ICME

ICME "Case Studies" have demonstrated the promise

- Early ICME implementations have successfully integrated:
  - Materials, Component Design and Manufacturing Processes
  - Materials and Prognosis
  - Materials Modeling and Manufacturing Process Development

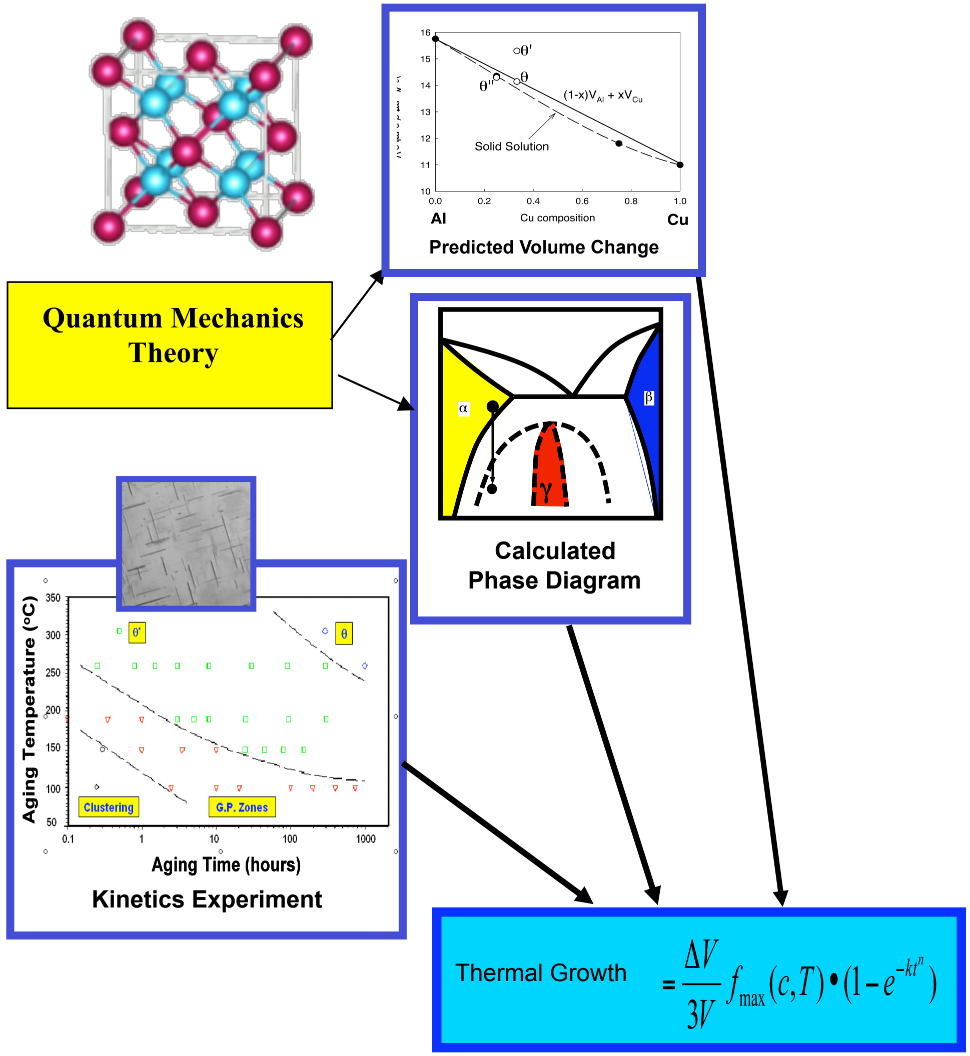
- The case studies described in the report demonstrated that application of an ICME capability, even if limited in capability, can result in a significant return on investment.*

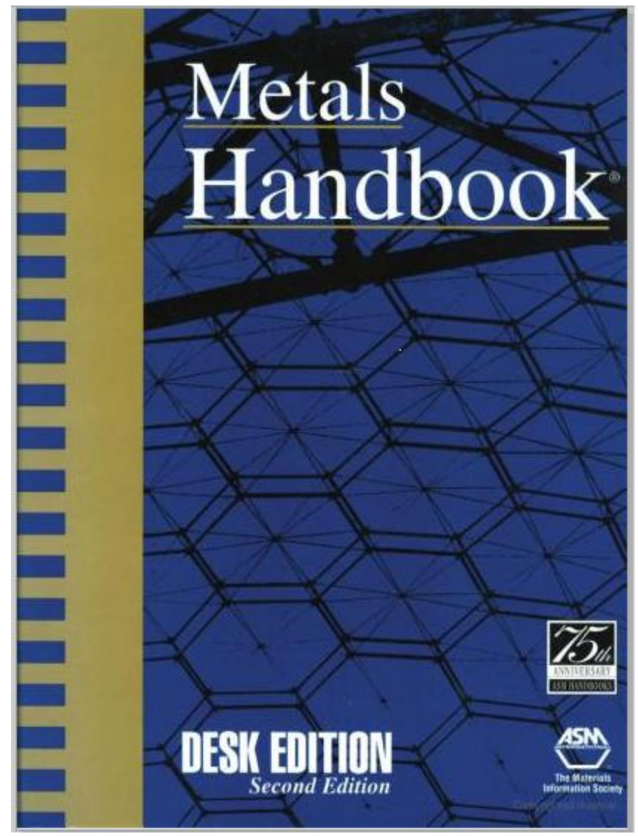
- A ROI in the range of 3:1 to 9:1 can be realized.

- Typical investments were in the $5-20M range.

* Note: Most of these case studies involved structural metals

The Divide Separating
Materials Science and Materials Engineering





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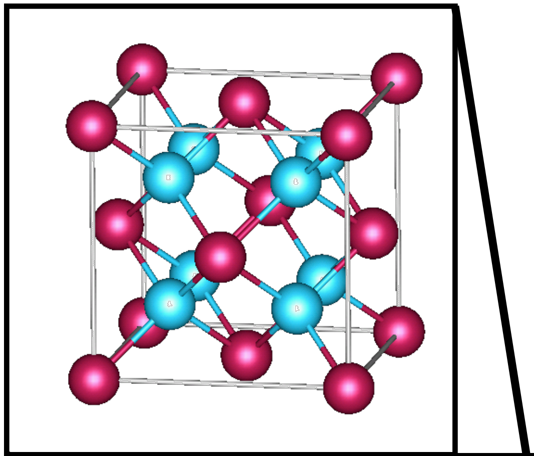
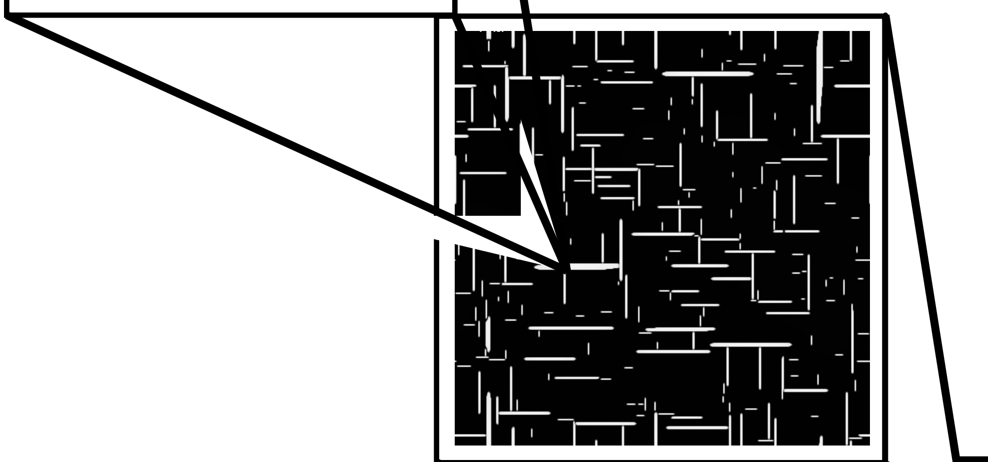
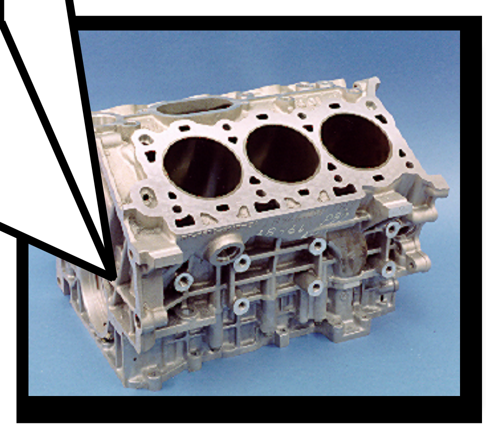
NMAB Committee Selected Findings

- ICME is an emerging and potentially transformational discipline, but in its infancy.
- Experiments are essential to development of ICME tools
- Curated knowledge bases are essential for capturing, archiving and disseminating information
- Development of ICME requires cross-functional teams focused on a common goal or "foundational engineering problem".
- Less than a 100% solution may be good enough.
- ICME requires a cultural shift.
- For ICME to succeed, it must be embraced as a discipline by the materials science and engineering community

Ford Virtual Aluminum Castings



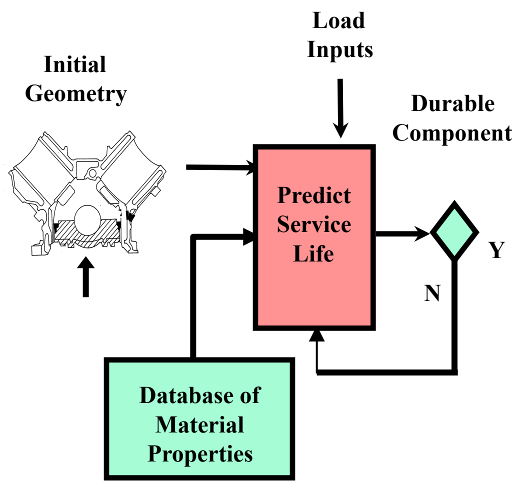


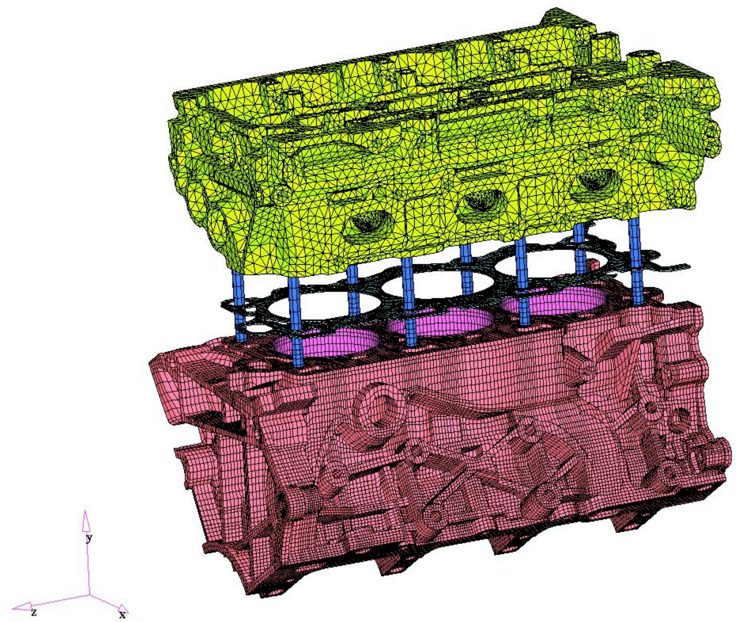


Research and Advanced Engineering

Traditional Durability Analysis

ABAQUS

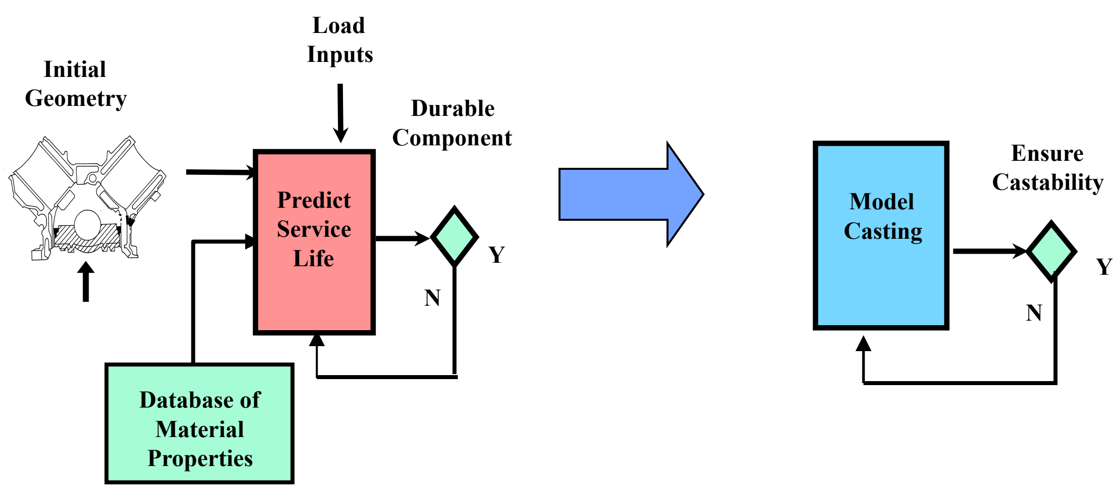




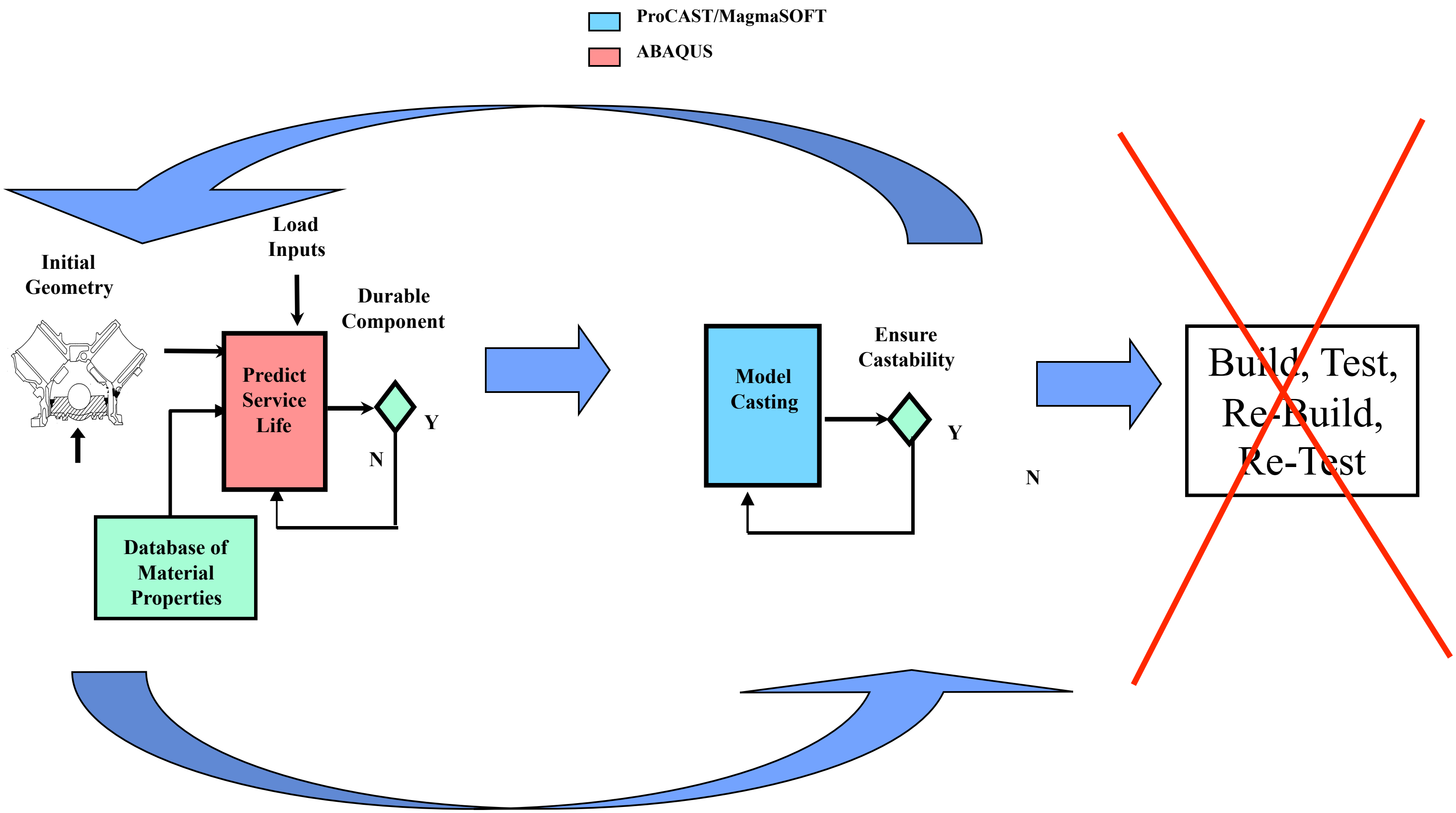
Traditional Durability & Manufacturing Analysis

MagmaSOFT/ ProCast

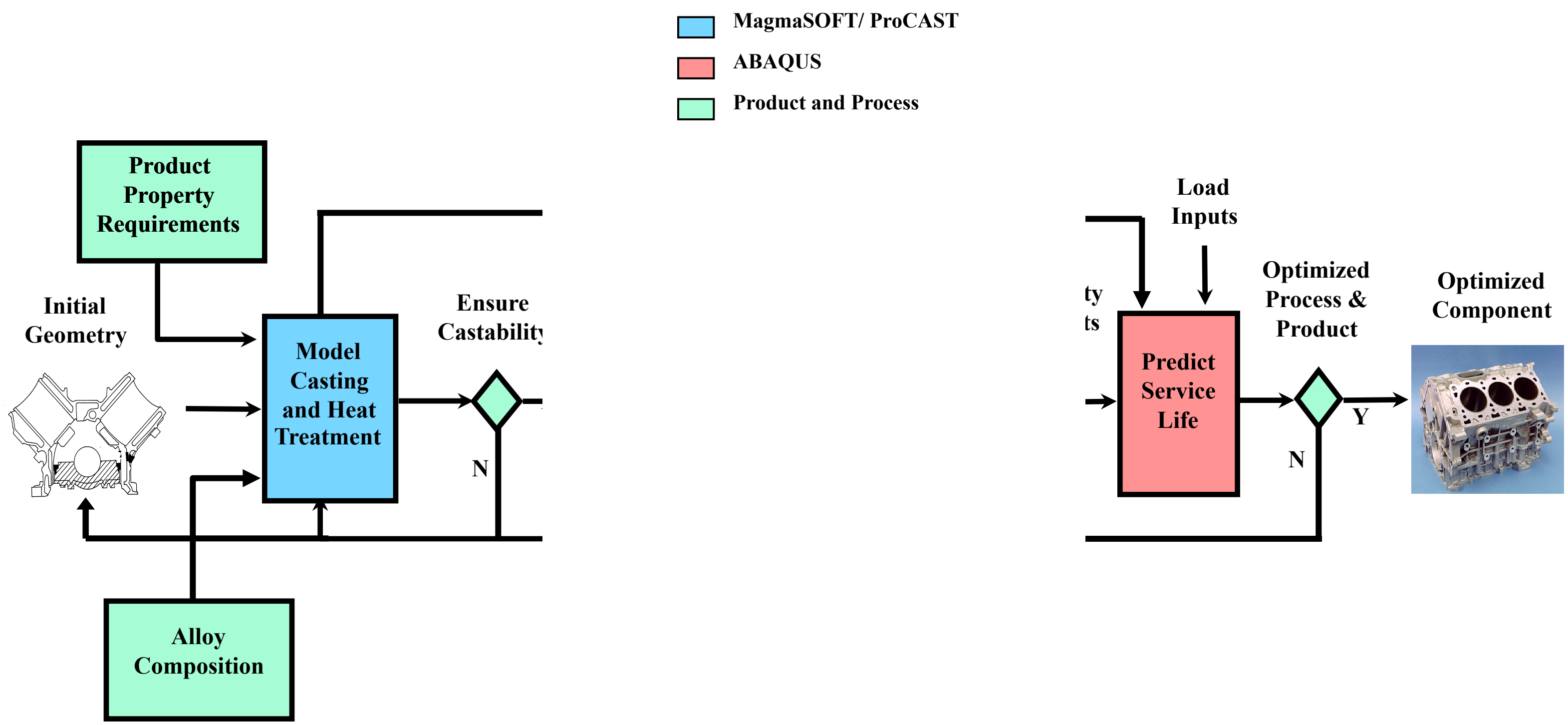
ABAQUS



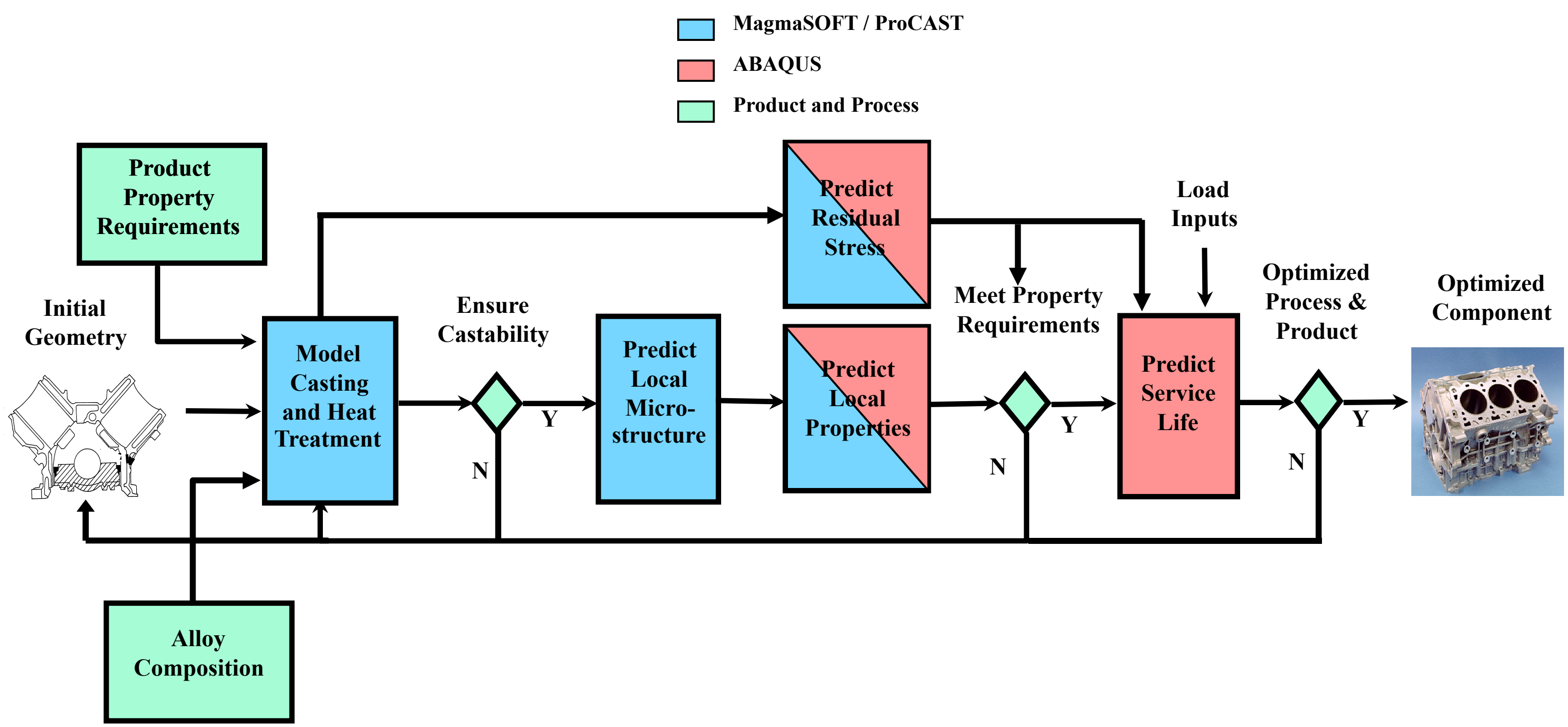
Traditional Product Development Process



Virtual Aluminum Castings

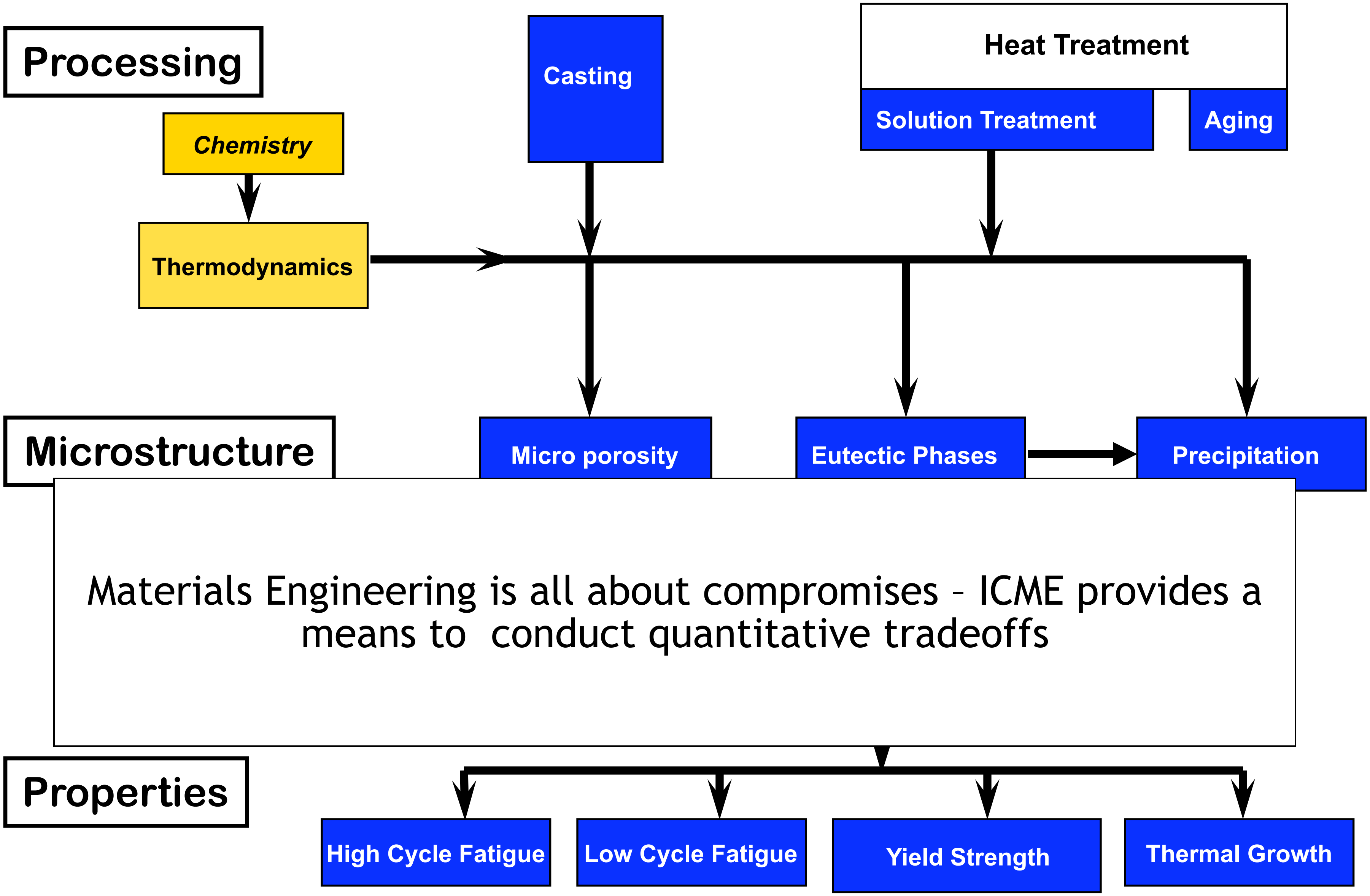


Virtual Aluminum Castings
The Ford Experiment in ICME



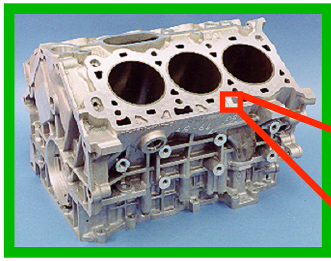
Research and Advanced Engineering

Cast Aluminum Processing-Structure-Property Linkages

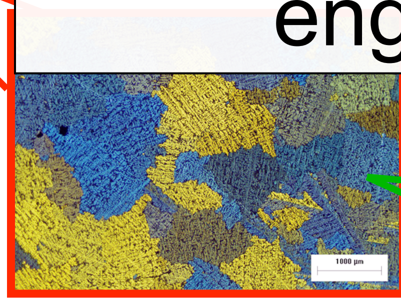


Materials Engineering is all about compromises – ICME provides a means to conduct quantitative tradeoffs

Need to determine which lengths scales are essential for the particular engineering requirement



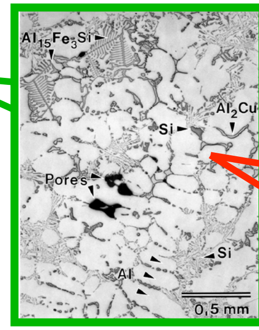
1 m
Engine Block



1 – 10 mm

Macrostructure
- Grains
- Macroporosity

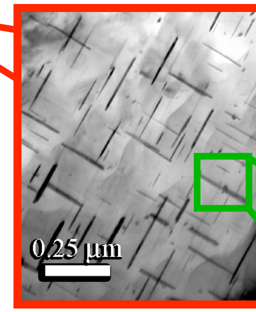
Properties
- High cycle fatigue
- Ductility



10 – 500um

Microstructure
- Eutectic Phases
- Dendrites
- Microporosity
- Intermetallics

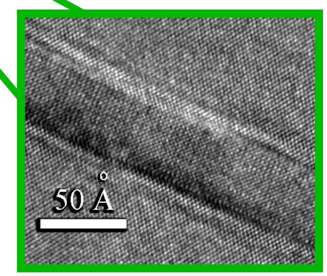
Properties
- Yield strength
- Tensile strength
- High cycle fatigue
- Low cycle fatigue
- Thermal Growth
- Ductility



1-100 nm

Nanostructure
- Precipitates

Properties
- Yield strength
- Thermal Growth
- Tensile strength
- Low cycle fatigue
- Ductility

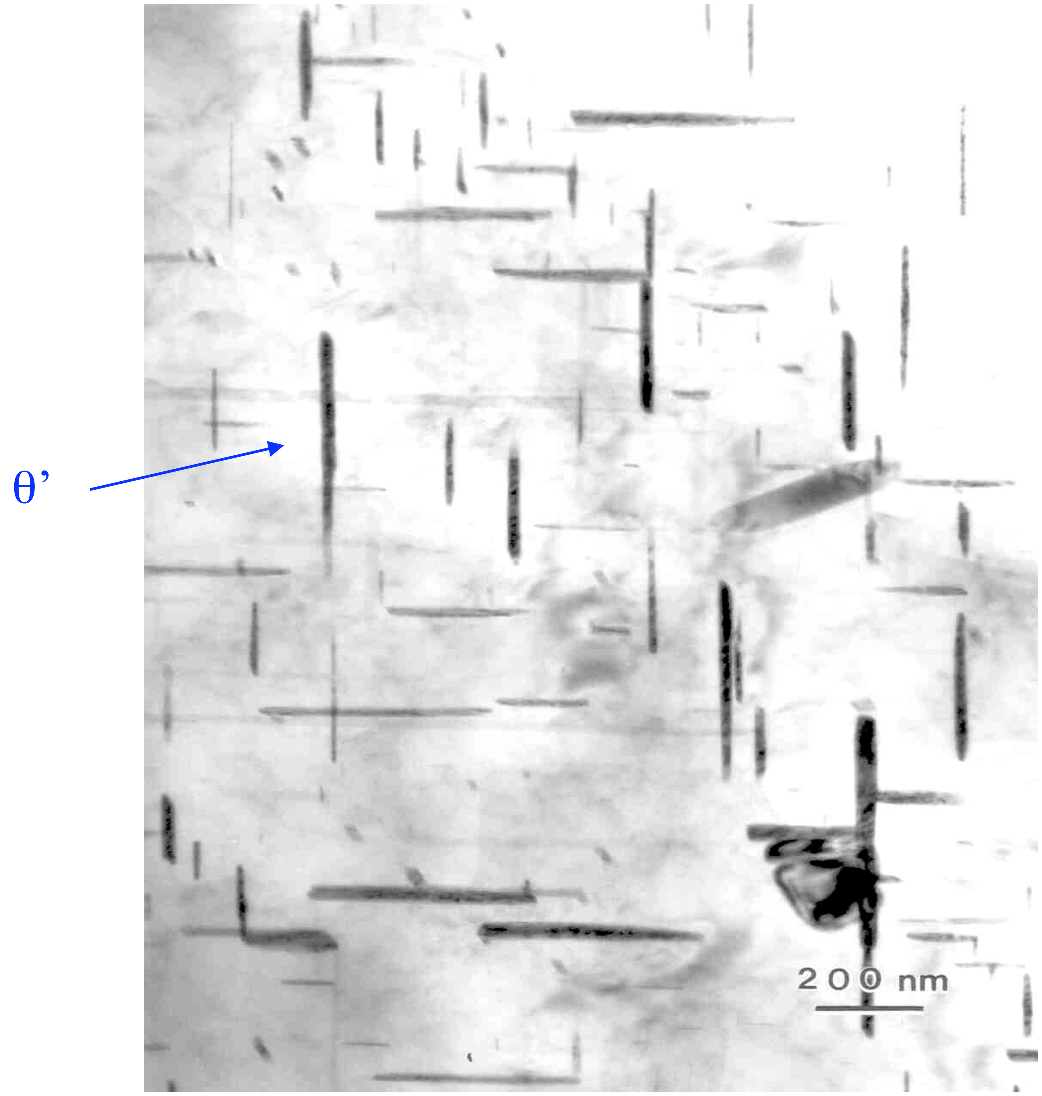


0.1-1 nm

Atomic Structure
- Crystal Structure
- Interface Structure

Properties
- Thermal Growth
- Yield Strength

Precipitate structures in W319 Aluminum are one of the critical scales for yield strength



Physics Based Models – Yield Strength

Yield strength (σ_Y) is the sum of an intrinsic strength (σ_i), a precipitation hardening strength (σ_{ppt}), and a solid solution strength (σ_{ss}):

$$\sigma_Y(T,t,c) = \sigma_{ppt}(T,t,c) + \sigma_{GP/ss}(T,t,c) + \sigma_i$$

$$\sigma_{ppt}(T,t,c) = M(0.13\left\{\frac{Gb}{\sqrt{dw}}\right\}\left\{\sqrt{f} + 0.75\sqrt{\frac{d}{w}f} + 0.14\frac{d}{w}f^{3/2}\right\}\left\{\ln\frac{0.87\sqrt{dw}}{r_o}\right\})$$

Zhu & Starke, 1999

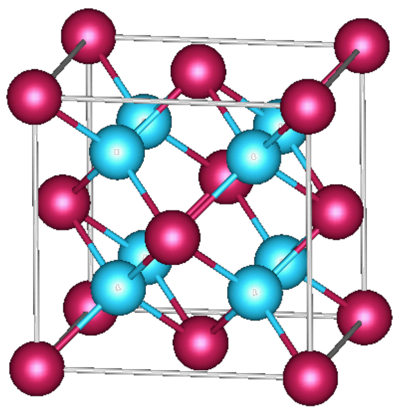
$$\sigma_{GP/ss}(T,t,c) = A\left(c_o - \frac{f}{3}\right)^{2/3}$$

$$\sigma_i = 70MPa$$

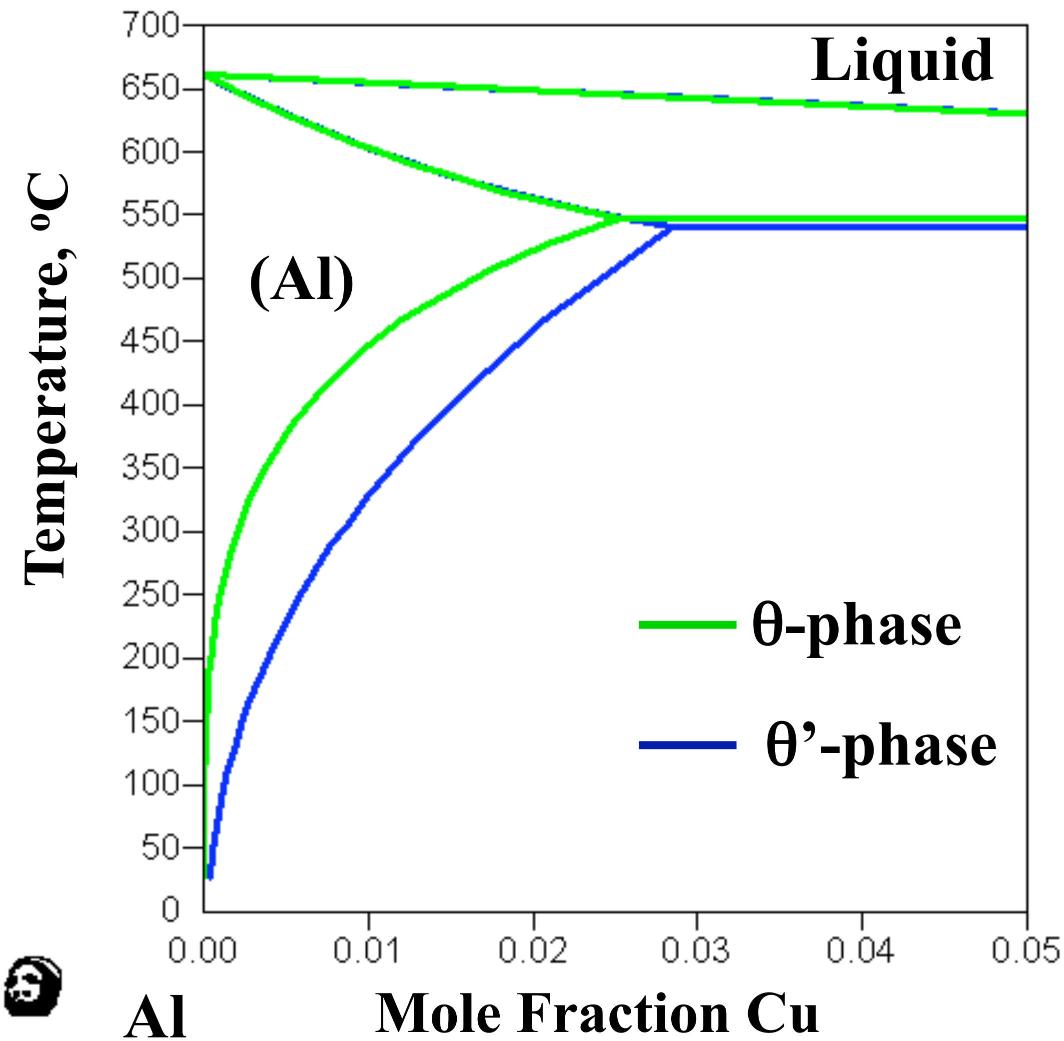
f = volume fraction of theta'

d = diameter of theta' platelet
w= thickness of theta' platelet

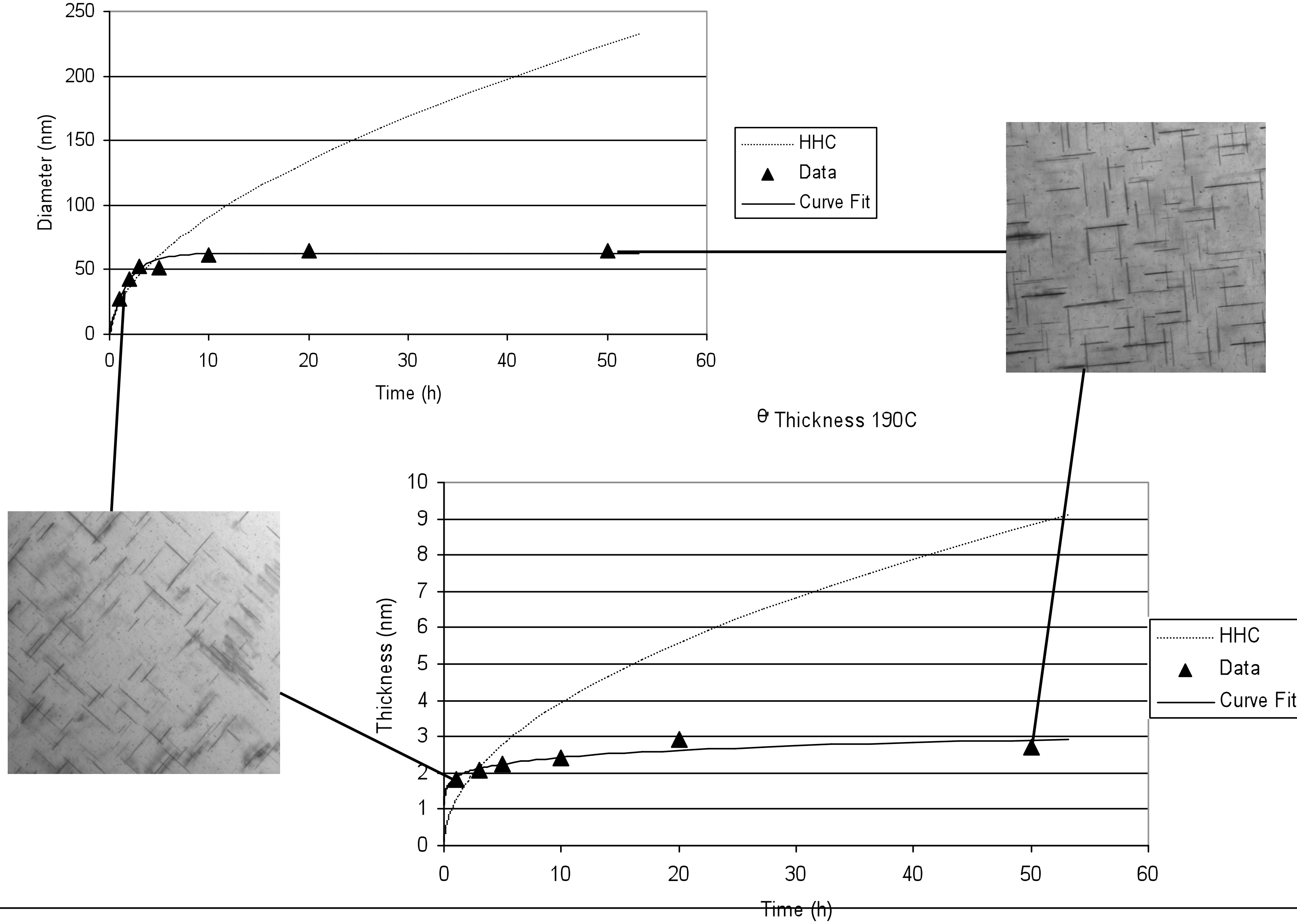
First-Principles Modification of Al-Cu Phase Diagram Incorporating Metastable θ'-phase



Metastable states just as easy to calculate as stable states

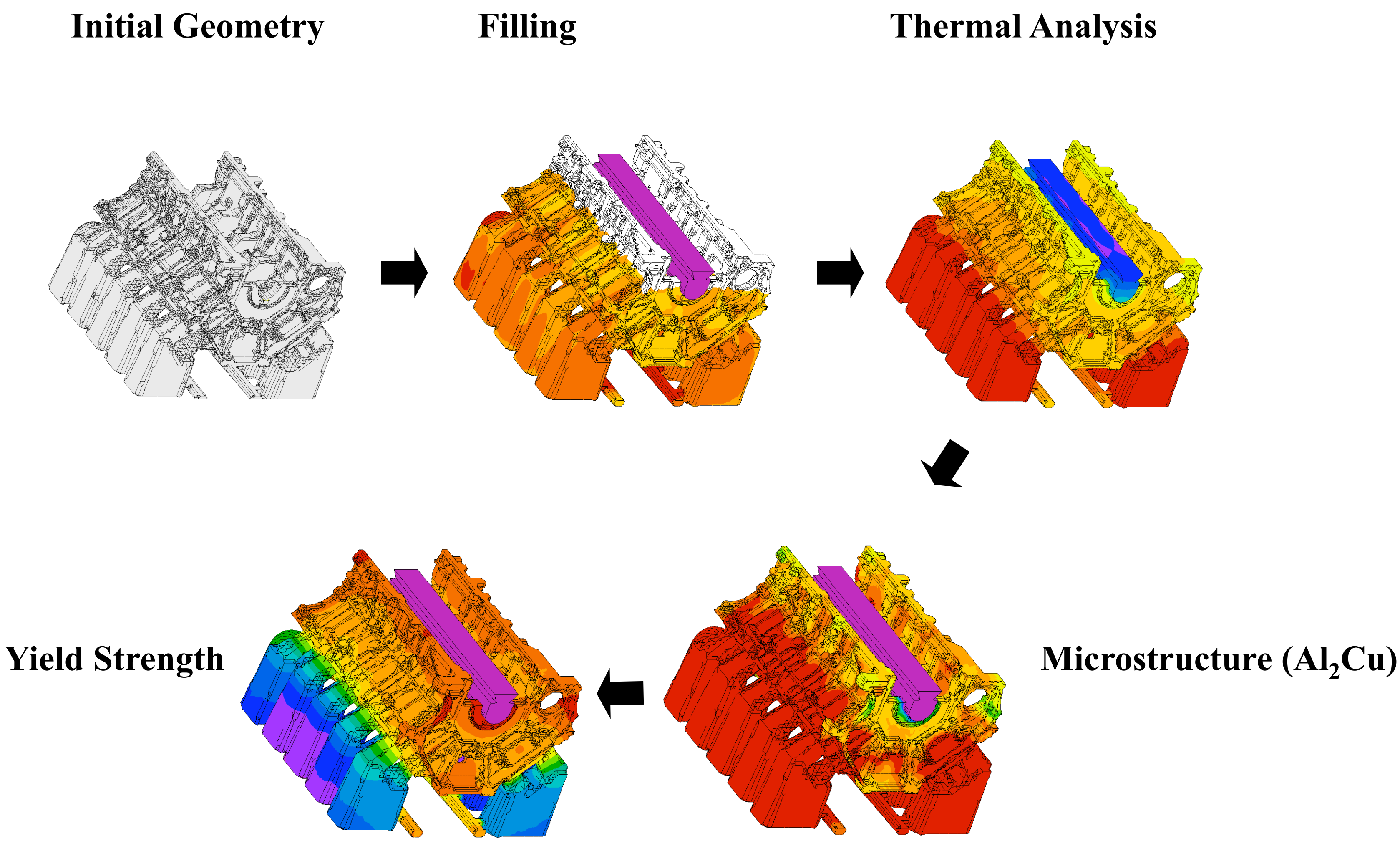


VAC models capture experimental understanding where robust physics-based models are not available

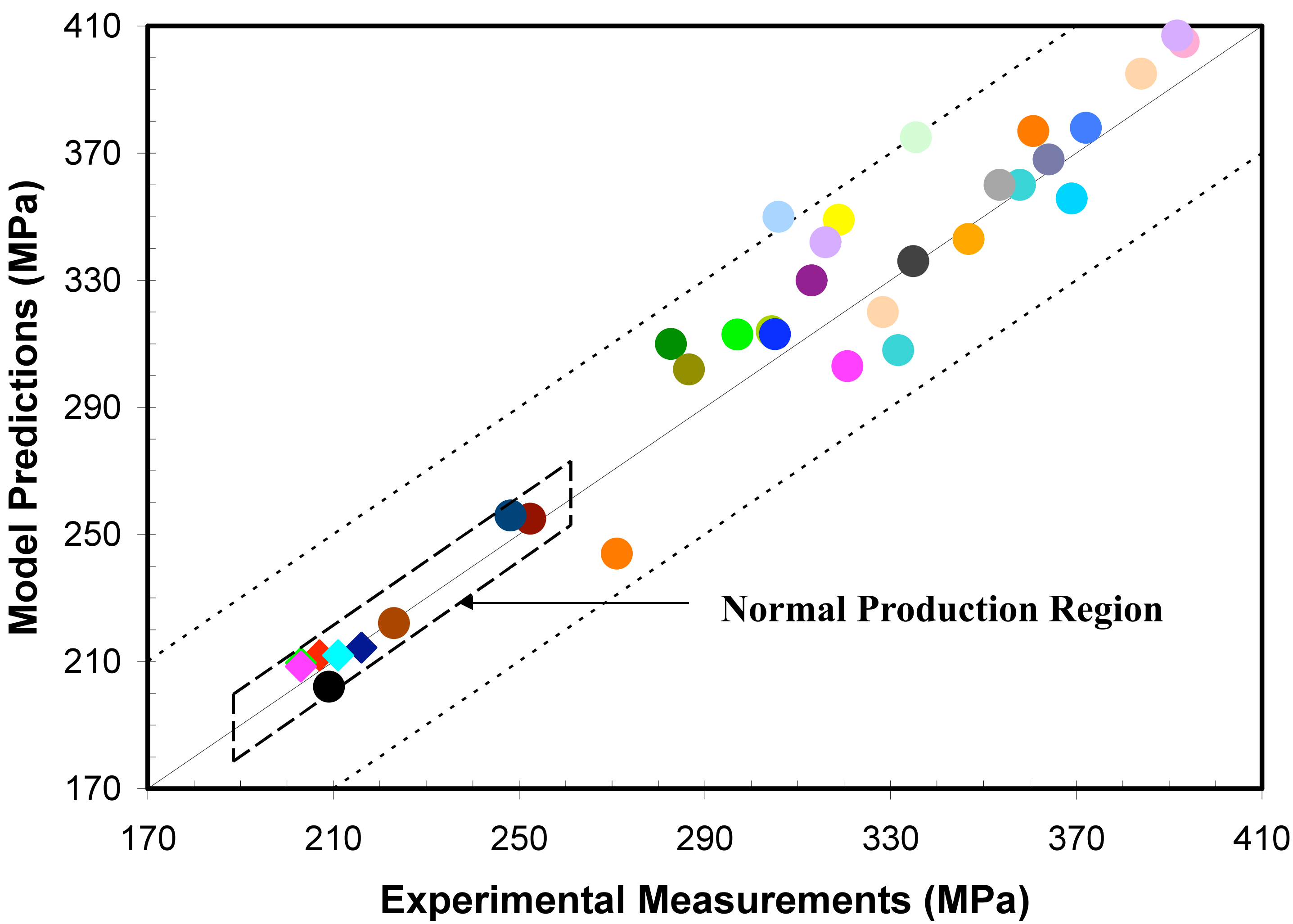


TEM Characterization of Precipitate Morphology vs Aging Time
(319 Al alloy with 3, 3.5 and 4%Cu)

Virtual Aluminum Castings Process Flow
Local Yield Strength

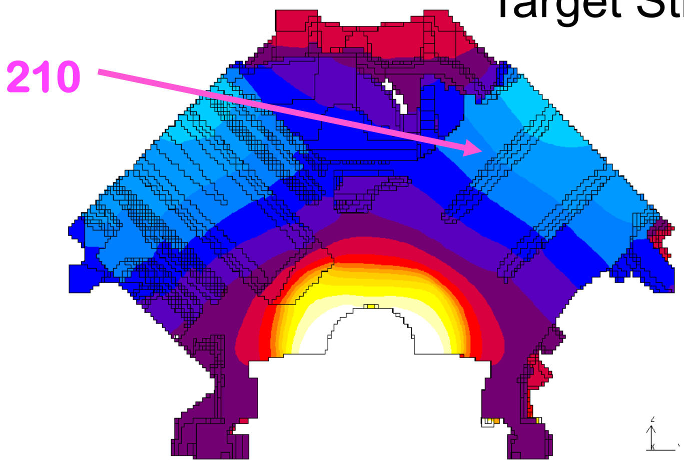


Model Validation & Accuracy



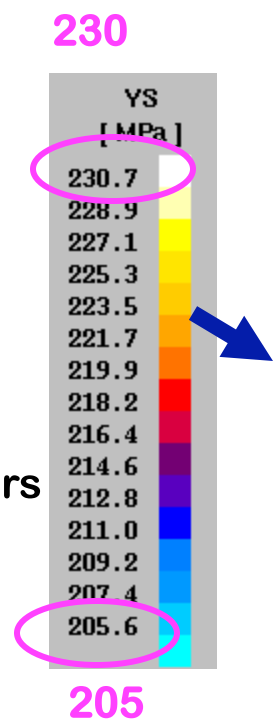
Using Virtual Aluminum Castings in Product and Process Optimization

Target Strength = 220 MPa

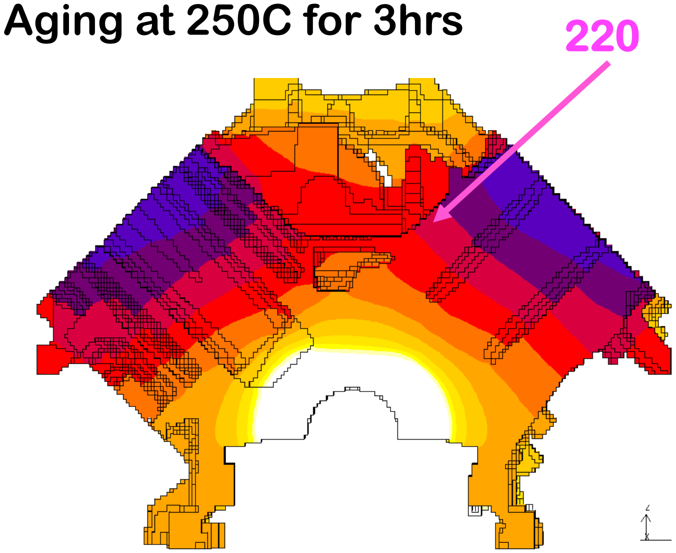


Aging temperature 240C for 5hrs

Initial Heat Treatment Process



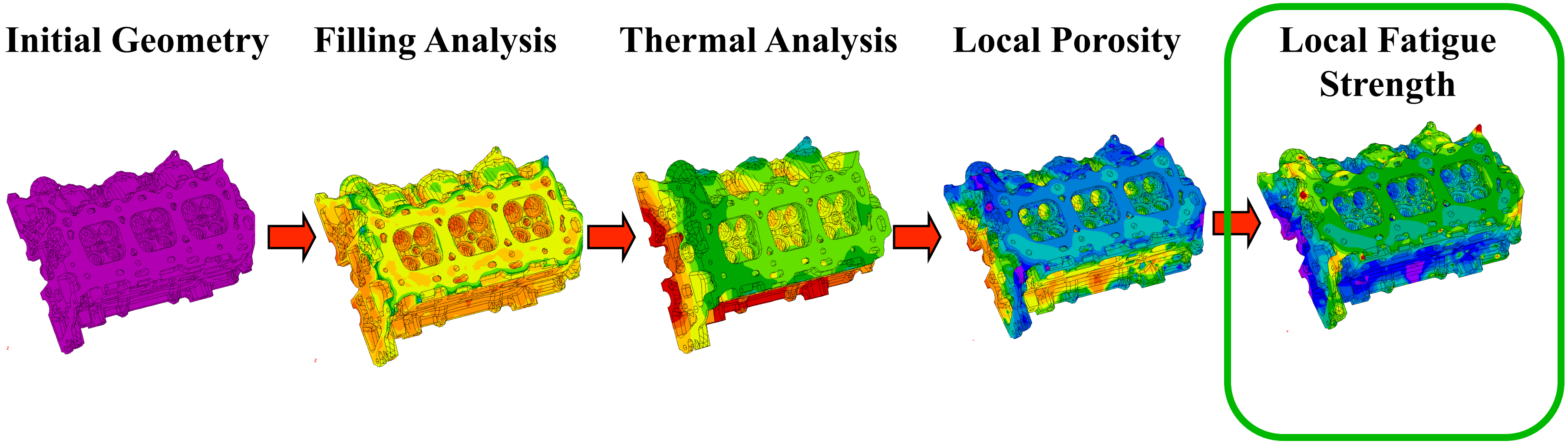
Aging at 250C for 3hrs



Optimized Heat Treatment Process

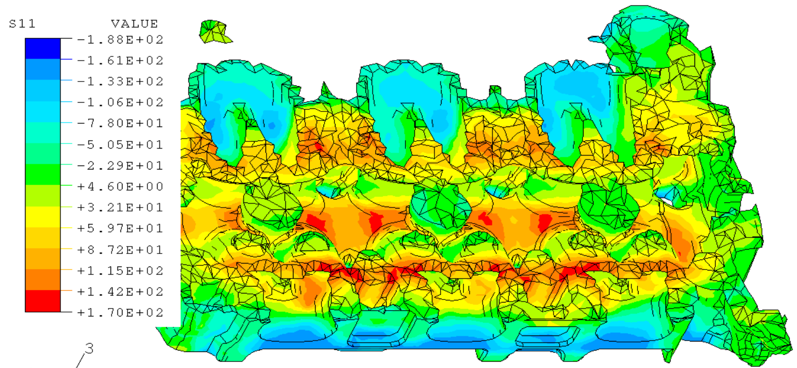
Faster and Stronger !!

Local Fatigue Strength Prediction & Component Durability Simulation

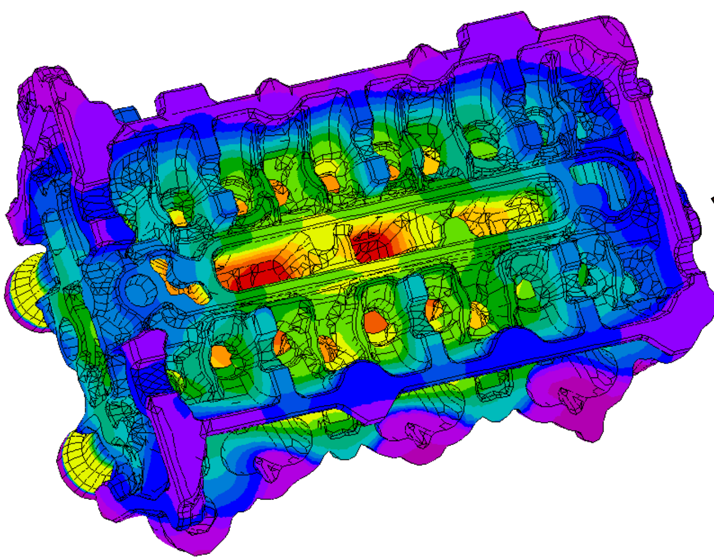


Virtual Aluminum Castings

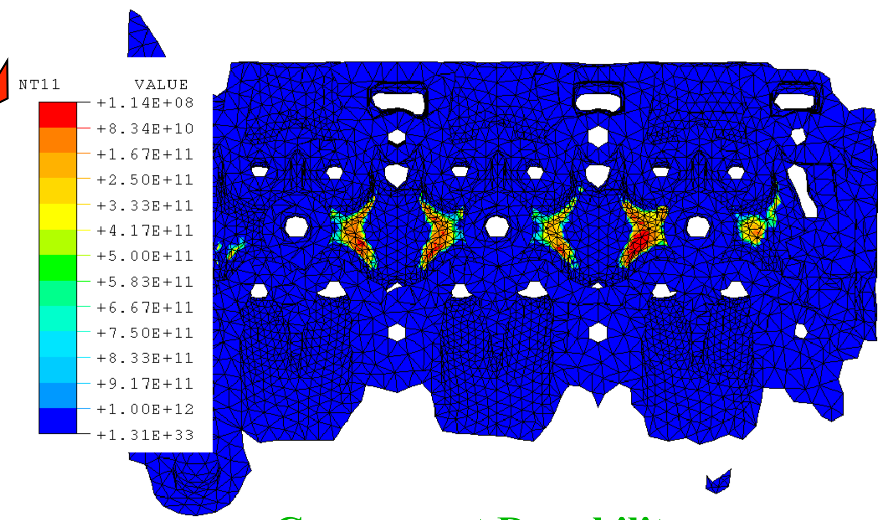
Linking Manufacturing, Materials and Design



Local Residual Stresses



Local Fatigue Properties



Component Durability

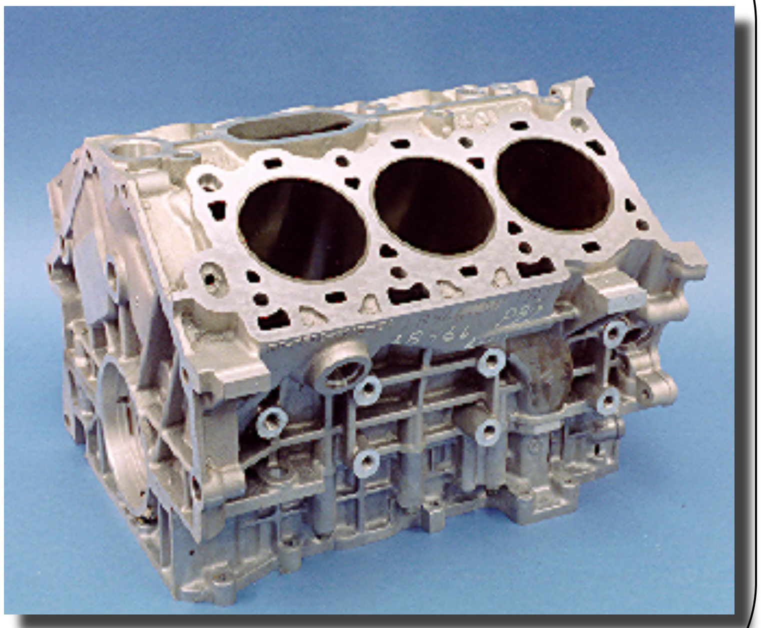
Ford Fusion Hybrid Engine

2011 Ford Super Duty 6.7L Diesel Engine

The VAC Business Case

Targets

- IMPROVE TIMING: Reduce product and process development time 15-25%
- IMPROVE QUALITY:
  - Improve launch quality /reduce scrap
  - Eliminate failures during product development
  - Ensure high mileage durability
- IMPROVE PERFORMANCE:
  - Enable high performance heads & blocks
  - Reduce weight of components
- REDUCE COST:
  - Reduce costs by $10-20M per year



GLOBAL ENGINEERING USERS

- North American Powertrain Operations
- (Volvo, Jaguar, Land Rover)
- Mazda
- European Powertrain Ops
- Ford of Australia

Ford Virtual Aluminum Castings Estimated Resources and ROI

Resources

- $15M over 5 years (over 50% experimental work)
- Approximately 25 people involved (15 internal + research at 7 universities)

Return on Investment:

- Over $100M in cost avoidance or cost save (7/1 ROI)
- 15-25% reduction in product development time
- Capability for upgrading and extending at significantly lower cost

Current Ford ICME Activities

• Virtual Alumnum Castings
• Sheet Steel – Stamping to Crash

• Virtual Mg Castings
• Exhaust Manifolds
• Gear Heat Treatment
• Wrought Al (Paint bake response & spot welds)
• Advanced Mg (USAMP/DOE ICME Program)
• Injection molded plastics

ICME: Prognosis

- The concept is fundamental and has potential to have a pervasive impact.
- The growing need for improved efficiencies in product development are clear and ICME can help
- The well developed fundamental knowledge base required of ICME is generally available for many structural materials
- Increased computational horsepower (hardware and software) indicate that this won’t be a limitation

Encouraging Indicators

- Growing recognition that ICME is feasible and important
  - **North America: ICME**
  - **Europe: Through-Process Modeling**
  - **China:** 集成计算材料工程
- Government interest and potential funding
- Industrial interest (USAMP ICME Consortia on Mg)
- Professional Society interest: TMS, ASM
- 2009 Physical Metallurgy Gordon Conference – Record attendance
- Academic Interest:
  - University Materials Council – Workshop on ICME!!
  - Three university ICME centers in the proposal stages (China, UK, US)

First World Congress on ICME

July 10-14, 2011 – Seven Springs, Pennsylvania

- **Have established an International Advisory Committee representing more than 15 countries**
- **Will involve leading modelers and experimentalists in the field**
- **Gordon Conference type setting and schedule:**
- **Sessions on:**
  - **Modeling Processing-Structure Relationships**
  - **Modeling Structure-Property Relationships**
  - **ICME in Education**
  - **Information Infrastructure**
  - **Success Stories**
- **Save the date: July 10-14, 2011**

Recommendations (continued)

<u>Recommendation 8:</u> The **University Materials Council (UMC**), with support from materials professional societies and the National Science Foundation, should develop a model for incorporating ICME modules into a broad spectrum of materials science and engineering courses. The effectiveness of these additions to the undergraduate curriculum should be assessed using ABET criteria.

Integrating ICME into MSE Curricula

- Develop awareness that ICME is possible and valuable
- Use ICME tools as a means to enhance the learning experience within the current curricula (but they're not available yet…)
- Curated knowledge repositories –
  - Use in research and education
  - Culture of sharing
- Focus on:
  - ICME as an <u>Engineering</u> tool
  - <u>Quantitative & predictive</u> understanding
  - <u>Computational</u> methods
  - <u>Linkages</u> between specialty areas
  - <u>Linkages</u> between science and engineering

SUMMARY

- Integrated Computational Materials Engineering (ICME) offers a means to link:
  - Manufacturing, materials and product development
  - Engineering and scientific disciplines
  - Information across knowledge domains
- Early case studies demonstrate that although ICME is in its infancy there is a significant Return-On-Investment
- Virtual Aluminum Castings is an example
  - integrated, comprehensive suite of CAE tools that capture extensive expertise in cast aluminum processing, metallurgy & design and provides it to a global engineering workforce.
- Encourging indicators that ICME may be the "Next Big Thing"
- Academia has a critically important role to play

Recommendations (continued)

Recommendation 3: The **National Science Foundation** through its Office of Cyberinfrastructure, Directorate of Engineering, and the Division of Materials Research should

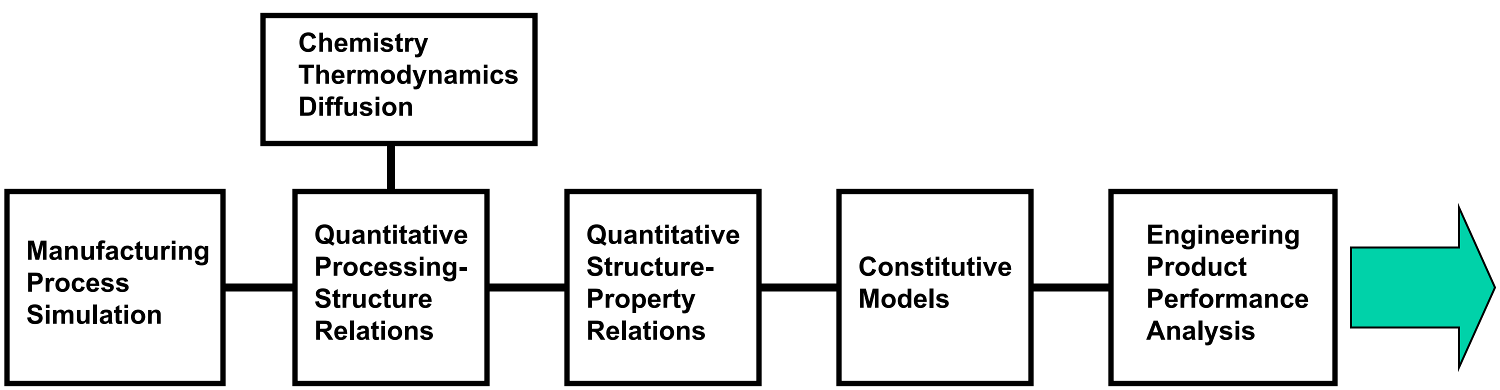
- Fund cross-disciplinary research and engineering partnerships to develop the taxonomy, knowledge base and cyberinfrastructure required for ICME.
- Establish incentives and requirements for materials researchers to place their materials information in open-access infrastructures, together with procedures to ensure the information and models can be used effectively.
- Develop engineering talent for ICME by supporting innovative curricula and student internship programs.

Integrating ICME Tool Development and MSE Curricula

- Graduate Education & Research:
  - Focus on developing contributors to and expert users of integrated tools and development of tools and cyberinfrastructure
  - Consider specializations in ICME:
    - Quantitative processing-structure-property relationships
    - Materials informatics / Web 2.0
    - Integration skills (code-writing and conceptual)
    - Computational & Simulation (DFT, Calphad, Phase Field, CFD, FEA etc)
    - Math skills
    - Mechanics of materials
    - Ability to make "engineering" approximations
    - Validation
    - Cross-functional teaming

Foundational Engineering Problems

Includes a manufacturing process(es), a materials system and an application or set of applications that define the critical set of materials properties and geometries



- Process & product optimization
- Innovation

Foundational Engineering Problems

Includes a manufacturing process(es), a materials system and an application or set of applications that define the critical set of materials properties and geometries

$10-40M per FEP (3-5 year funding)

- High dielectric materials and processes for improving the performance of microelectronic devices,
- Low-cost organics for robotics sensors,
- Thermal protection materials for hypersonic vehicle surfaces,
- Catalysts for optimizing the performance of hydrogen-fueled systems,
- Reliable and rapid recertification of aging structures
- Materials that allow ship hulls to survive a missile attack or large blast
- Thermoplastic injection molded materials for automotive structures
- Materials and electrochemical processes for advanced batteries,
- Nanoparticles for magnetic storage devices
- Composite or advanced metallic materials for aeroengine components

Cyberinfrastructure for ICME

To fully reach its potential, ICME requires new advances in networking, computing, and software:

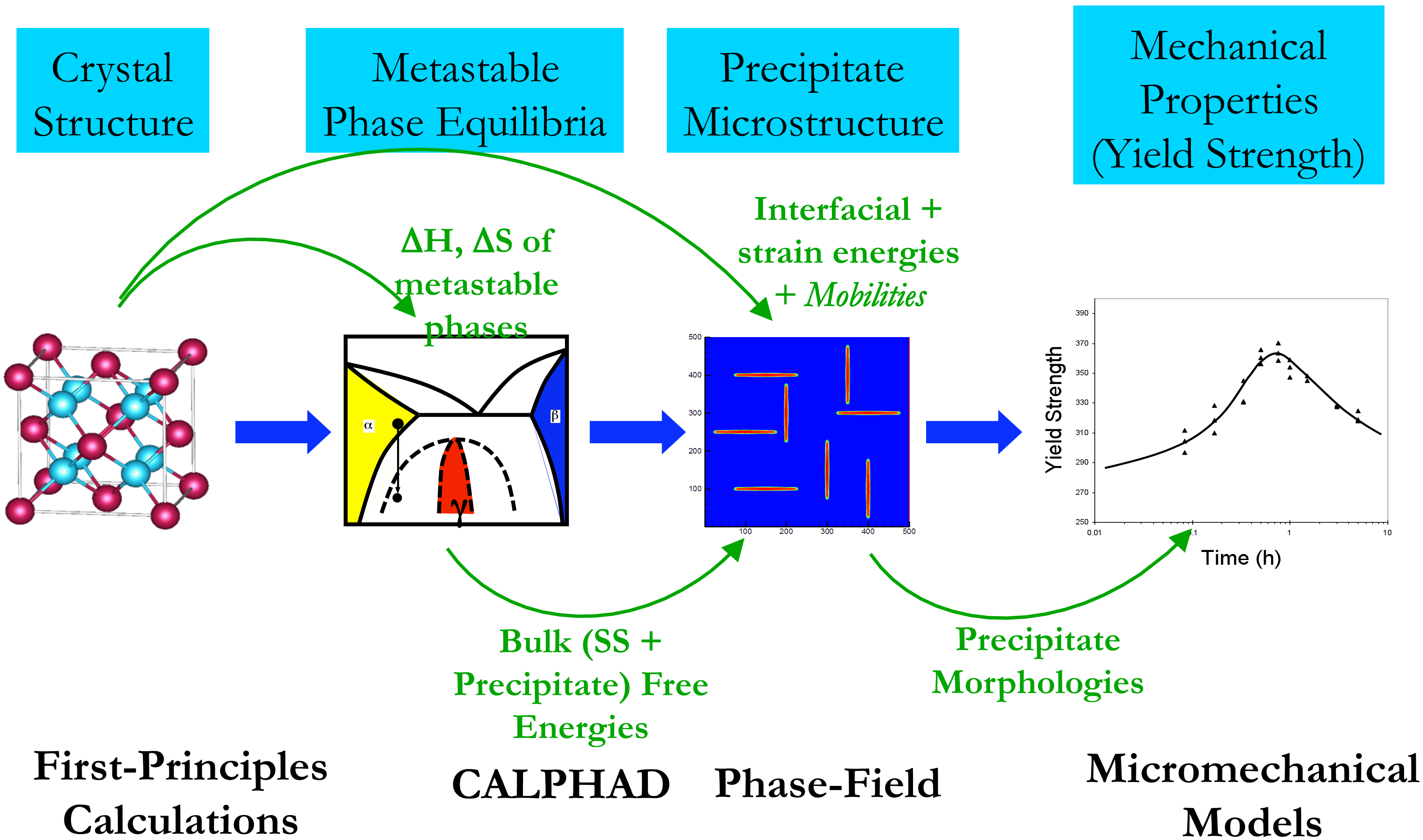
- Curated, repositories for data and material models and simulation tools
- Linkage of application codes with diverse materials modeling tools
- Geographically dispersed collaborative research
- Dispersed computational resources (Grid computing)

Integrating ICME Tool Development and MSE Curricula

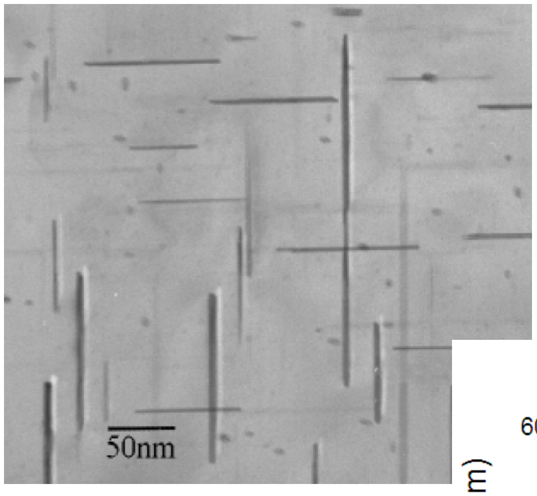
- Undergraduate Education:
  - Capstone courses using integrated tools
  - Courses with quantitative case studies to demonstrate scientific principles and relevance to engineering
  - Move from materials engineers who are proficient in the use of ASM handbook to proficiency in use of computational-based tools: stand alone and cyberinfrastructure tools (but these currently don't exist…)

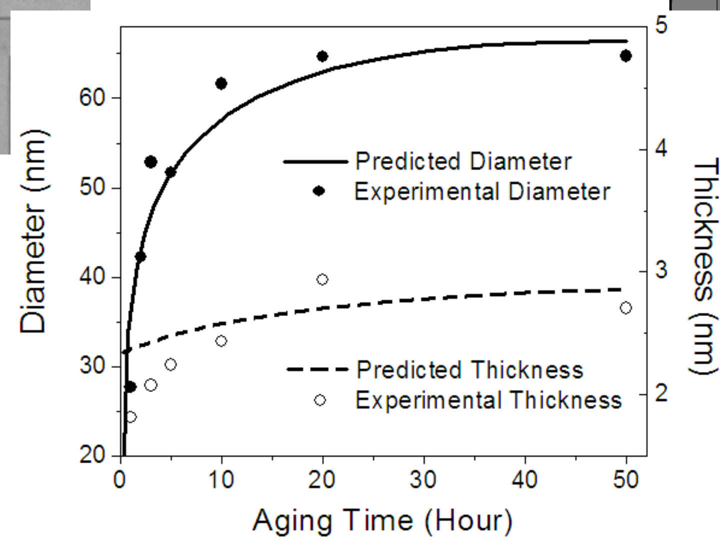
Extending VAC using advanced Computational Materials Science tools

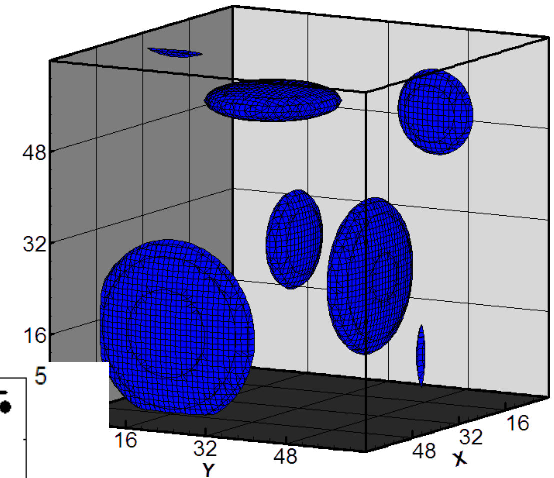
- **Reduce need for costly and time consuming experiments**
- **Alloy design**



Hybrid - Phase Field, First Principles Experimental Approach to Model θ' Evolution

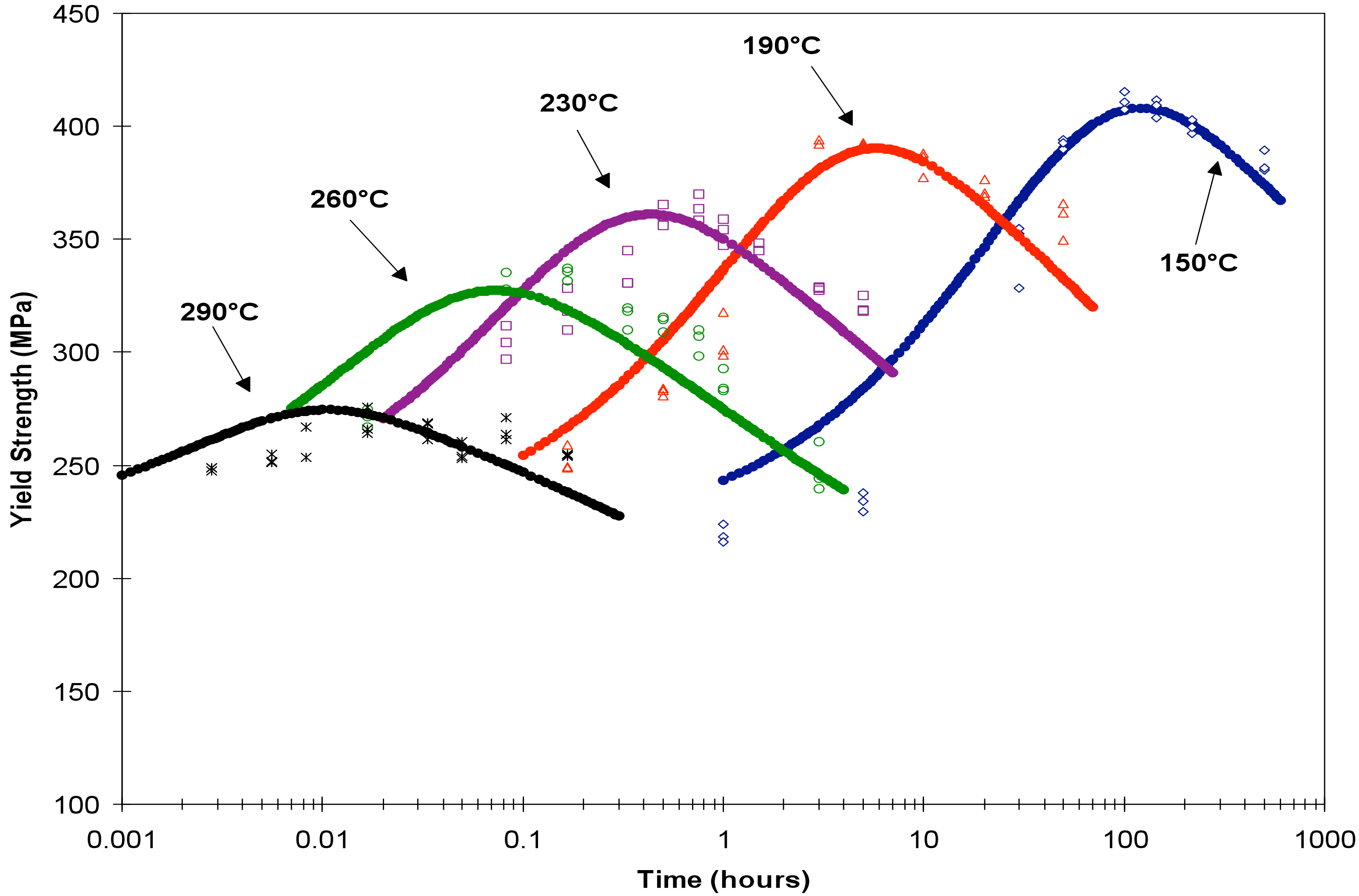




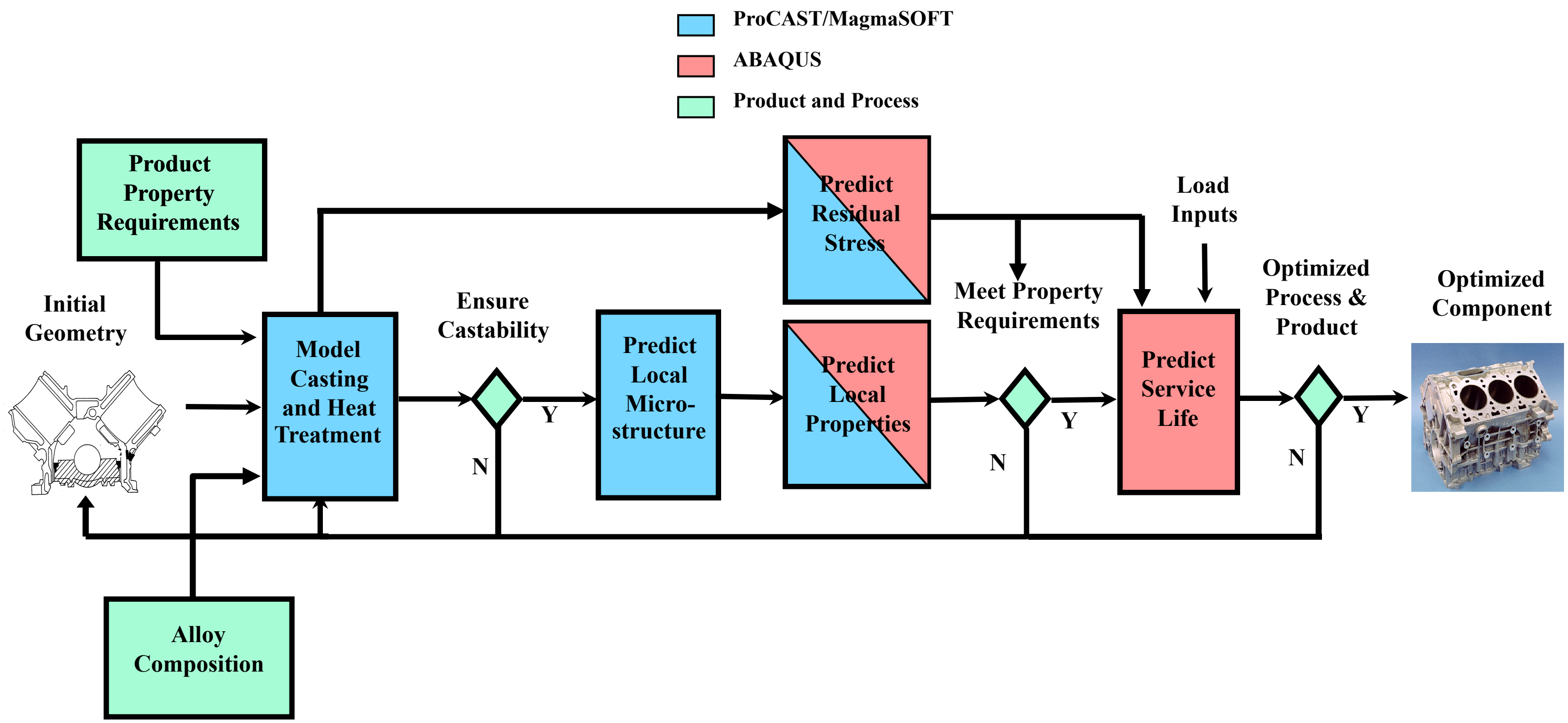


Nucleation rate and interface mobility coefficients are fitting parameters!

Aging Response of 319 Aluminum
Prediction vs. Experimental



Virtual Aluminum Castings



Recommendations (continued)

Recommendation 4: To promote U.S. innovation and industrial competitiveness, **NIST** should develop and curate precompetitive materials informatics databases and develop automated tools for updating, integrating, and accessing ICME resources.

Recommendation 5: Federal agencies should direct **SBIR and STTR** funding to support new ICME-based small businesses.

Recommendation 6: In pursuit of the promise of ICME to increase U.S. competitiveness and support national security, the **Office of Science and Technology Policy** should establish an interagency working group under the NITRD to set forth a strategy for ICME interagency coordination, including promoting access to data and tools from federally funded research.