Integrated Computational Materials Engineering (ICME)

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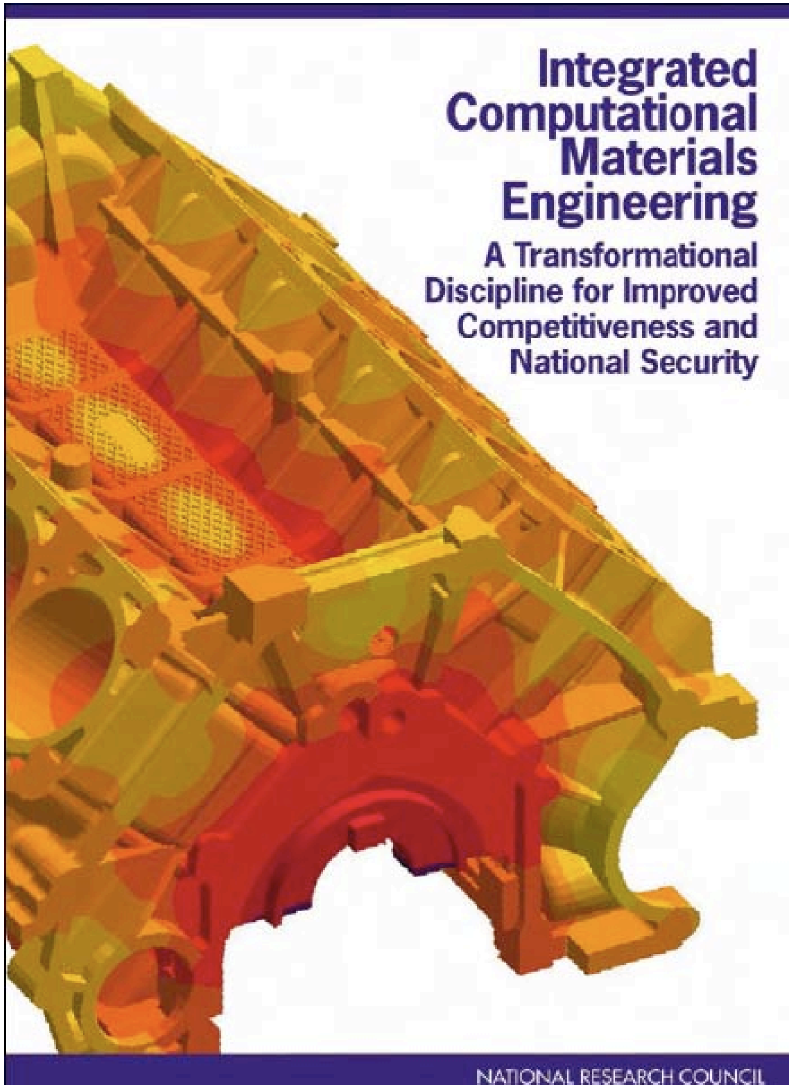
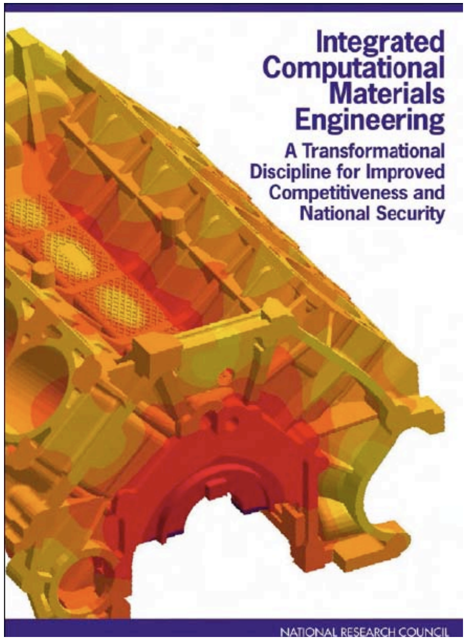


MichiganEngineering

Integrated Computational Materials Engineering (ICME)

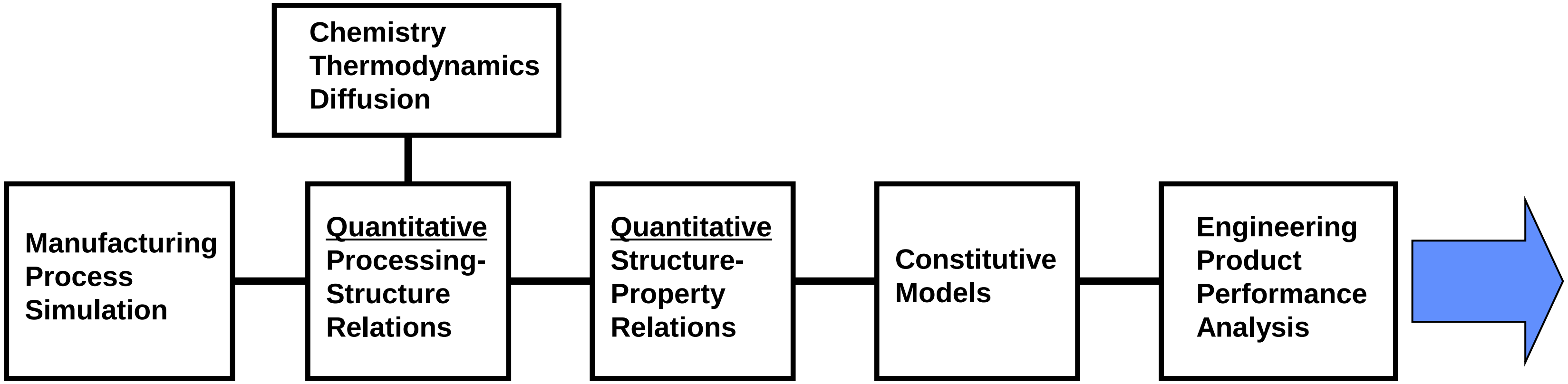
- What is ICME & Why It's Important?
- Case Studies & Findings
- A Path Forward



*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.*



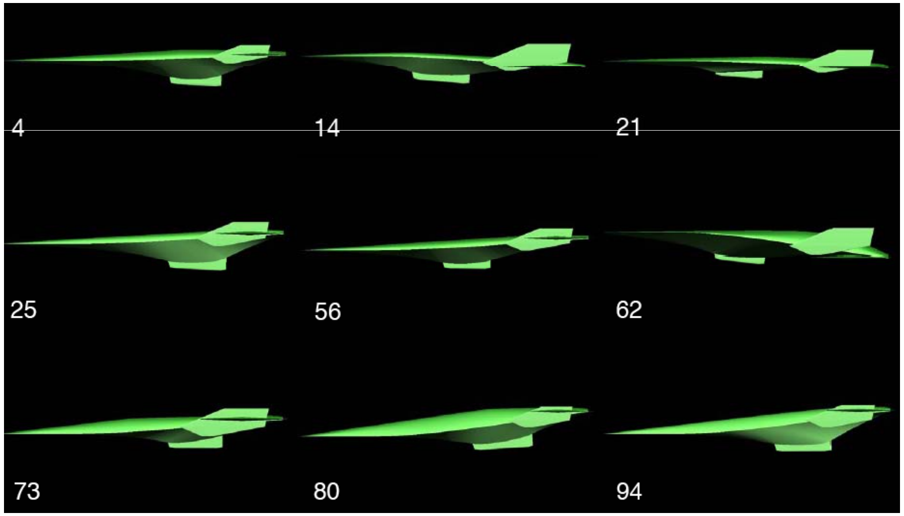
- Process & product optimization
- Innovation

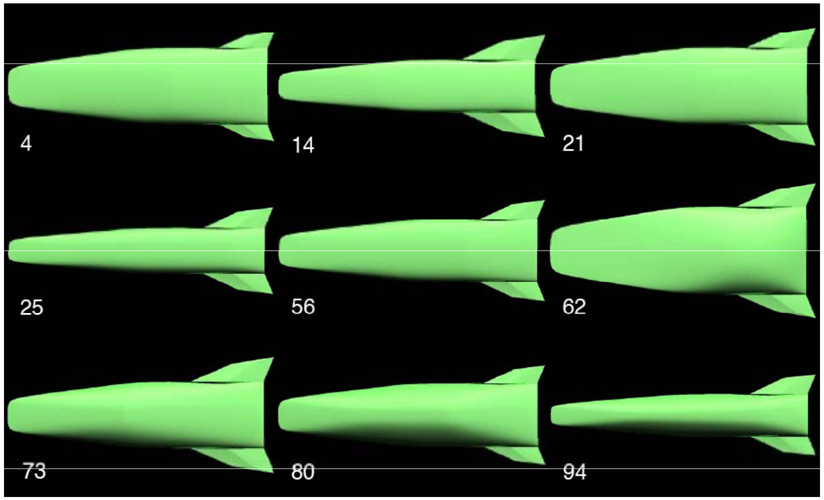
* NAE ICME Report, 2008

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 efficient R&D)

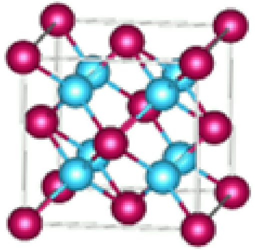
Using advanced computational techniques, designs can be studied and optimized in matters of hours or days. Optimization of new materials must be done experimentally and can take 10-20 years.

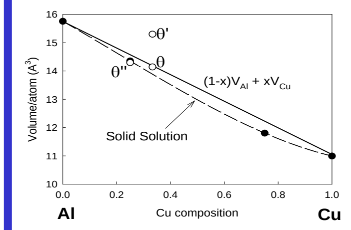




Shape optimization of hypersonic vehicles
Source: K. Bowcutt, Boeing

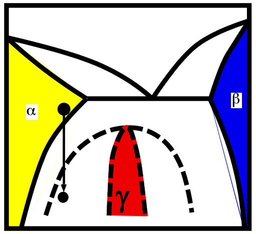
The Divide Separating
Materials Science and Materials Engineering



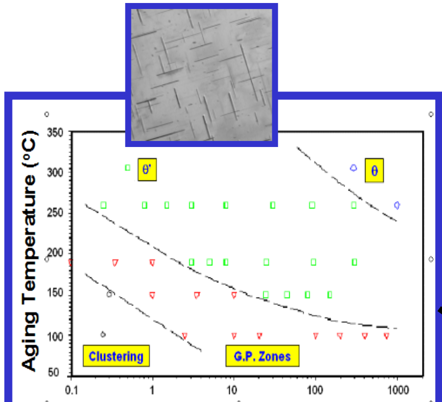


Predicted Volume Change

Quantum Mechanics Theory

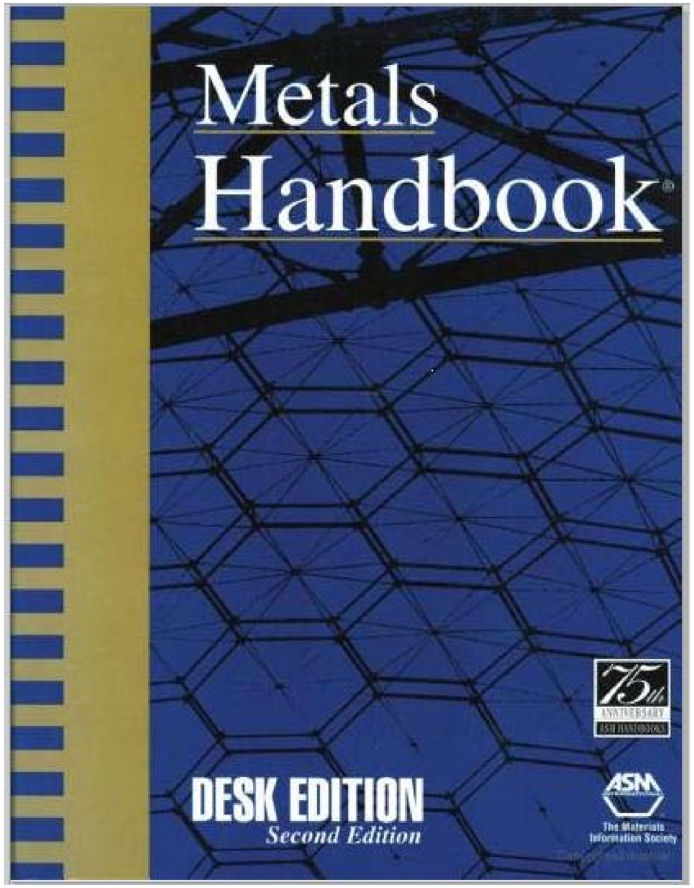


Calculated Phase Diagram



Kinetics Experiment

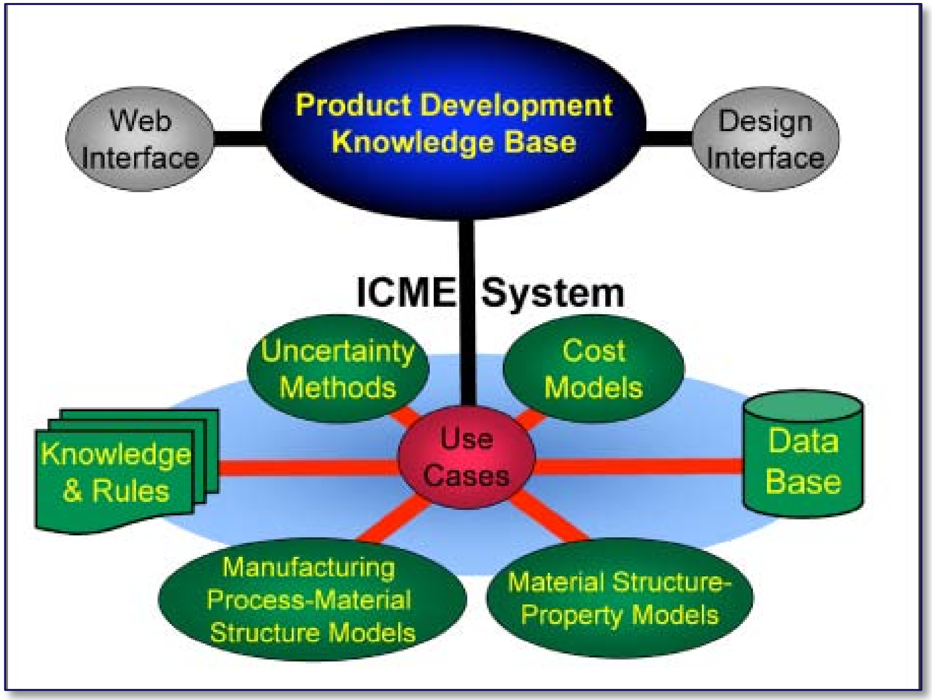
Thermal Growth $= \frac{\Delta V}{3V} f_{max}(c,T) \bullet (1 - e^{-kt^n})$



THE NATIONAL ACADEMIES
Advisers to the Nation on Science, Engineering, and Medicine

Integrated Computational Materials Engineering provides a means to link:

- Science and Engineering
- Manufacturing, Materials and Design
- Theory, Simulation and Experiments
- Information Across Disciplines



Case Studies

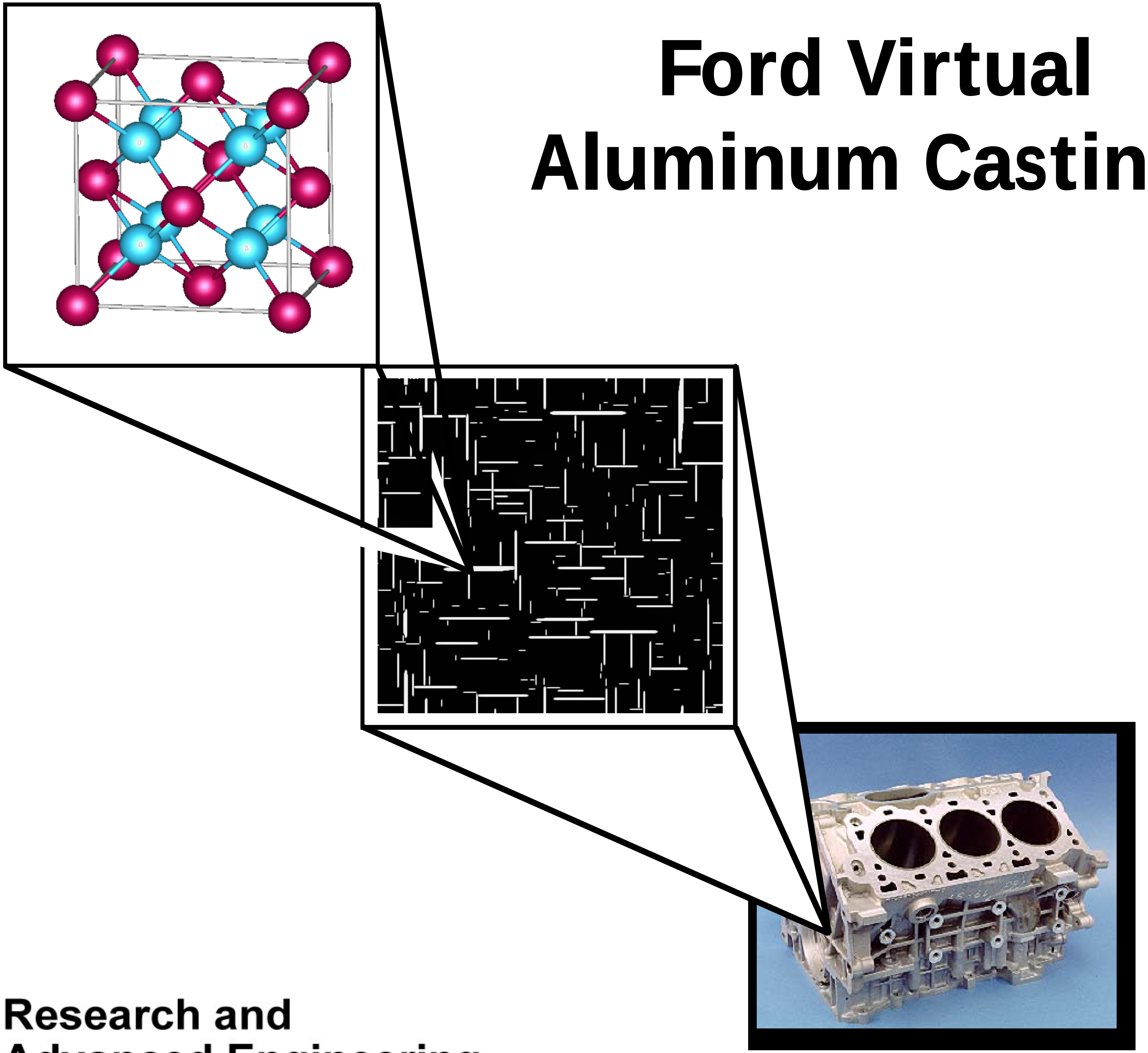
- Early ICME implementations have successfully integrated:
  - Materials, Component Design and Manufacturing Processes
  - Materials and Prognosis
  - Materials Modeling and Manufacturing Process Development

- The case studies described in the report demonstrates 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.

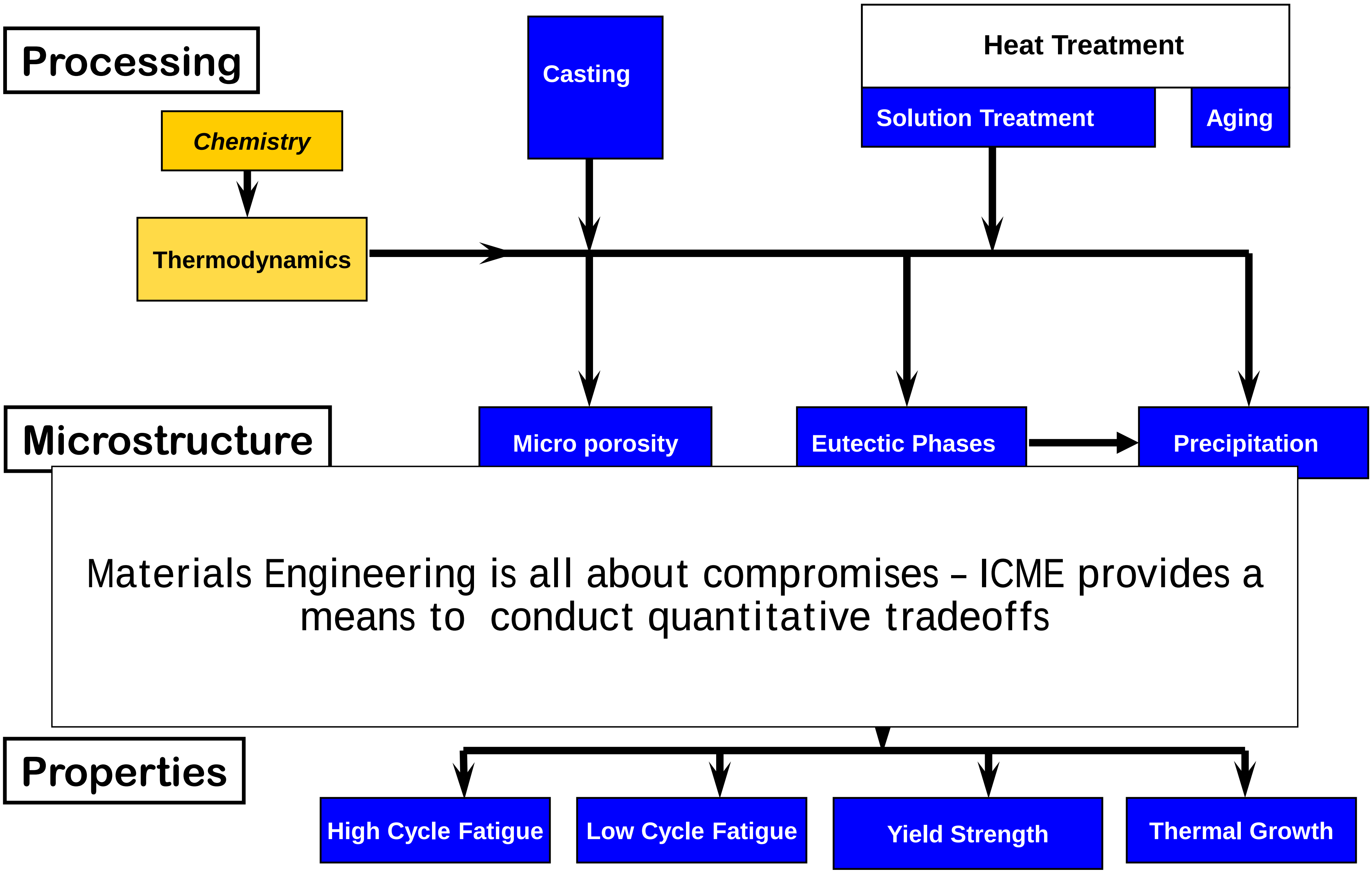
- Typical investments were in the $5-20M range.

Ford Virtual Aluminum Castings



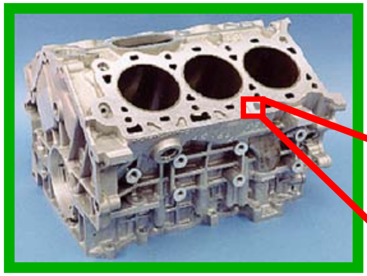
Research and
Advanced Engineering

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

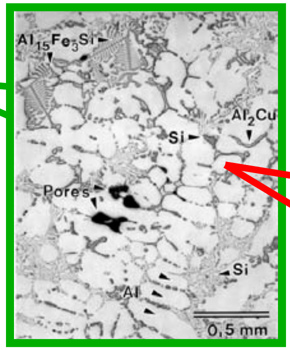


1 m
Engine Block

1 – 10 mm

Macrostructure
- Grains
- Macroporosity

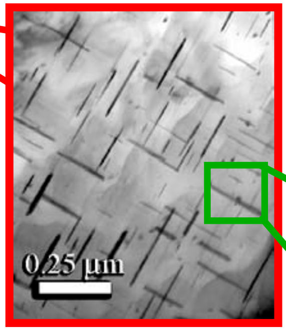
Properties
- High cycle fatigue
- Ductility



10 – 500um

Microstructure
- Eutectic Phases
- Dendrites
- Microporosity
- Intermetallics

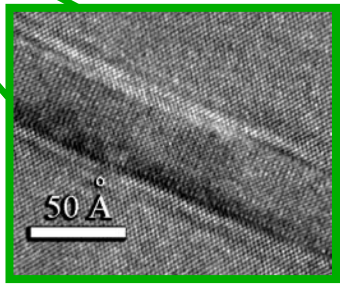
Properties
- Yield strength
- Tensile strength
- High cycle fatigue
- Low cycle fatigue
- Thermal Growth
- Ductility



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

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}):

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

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

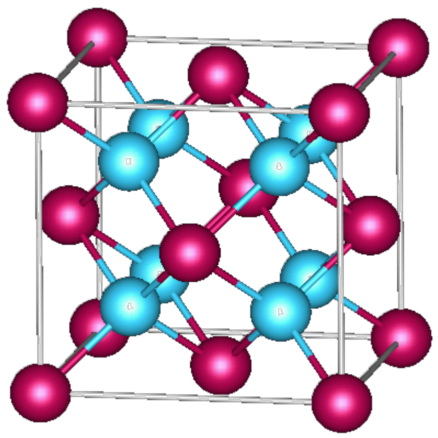
$$\sigma_{GP/ss}(T,t,c) = A\left(c_o - \frac{f}{3}\right)^{2/3}$$

$$\sigma_i = 70MPa$$

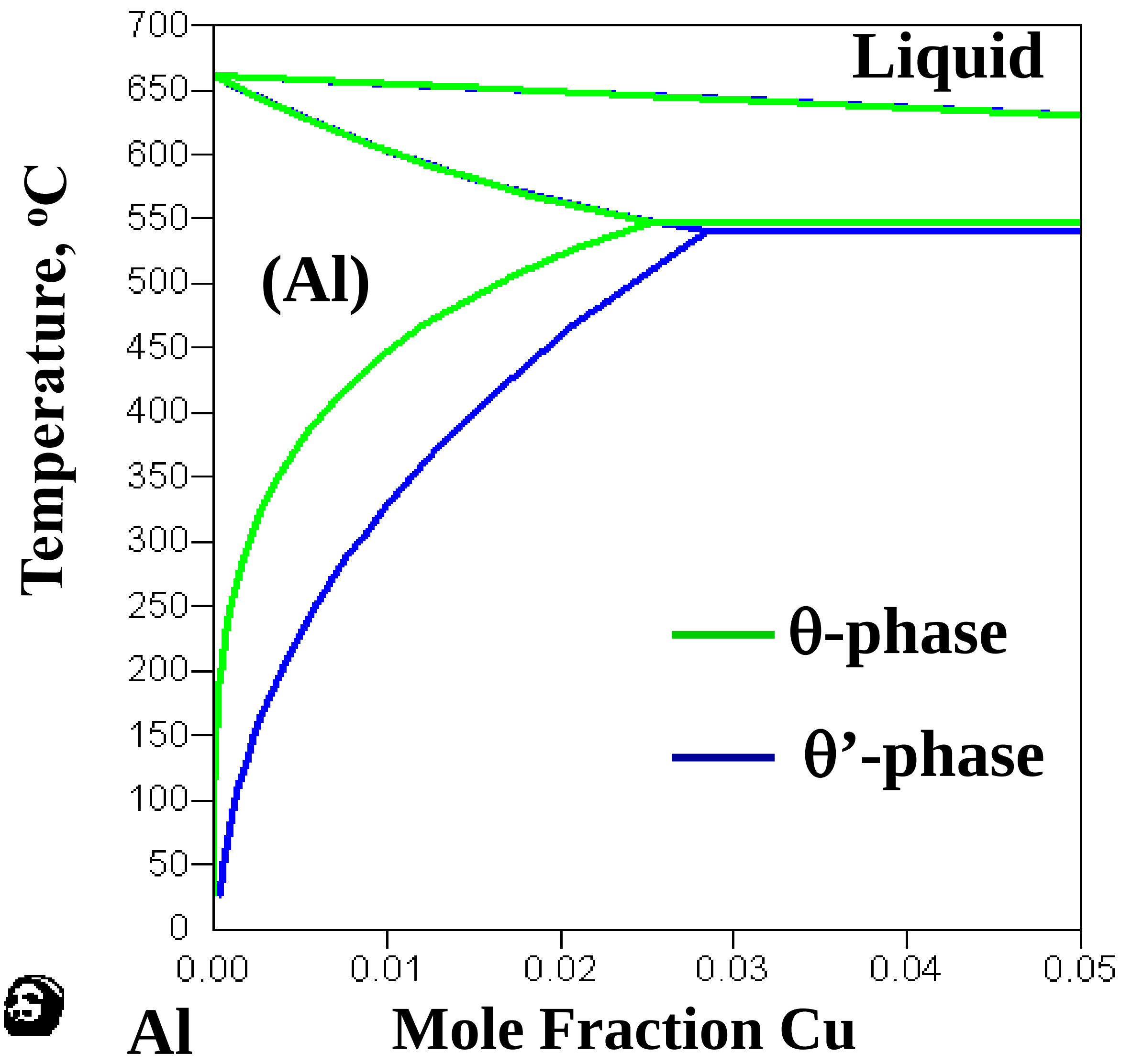
f = volume fraction of theta'

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

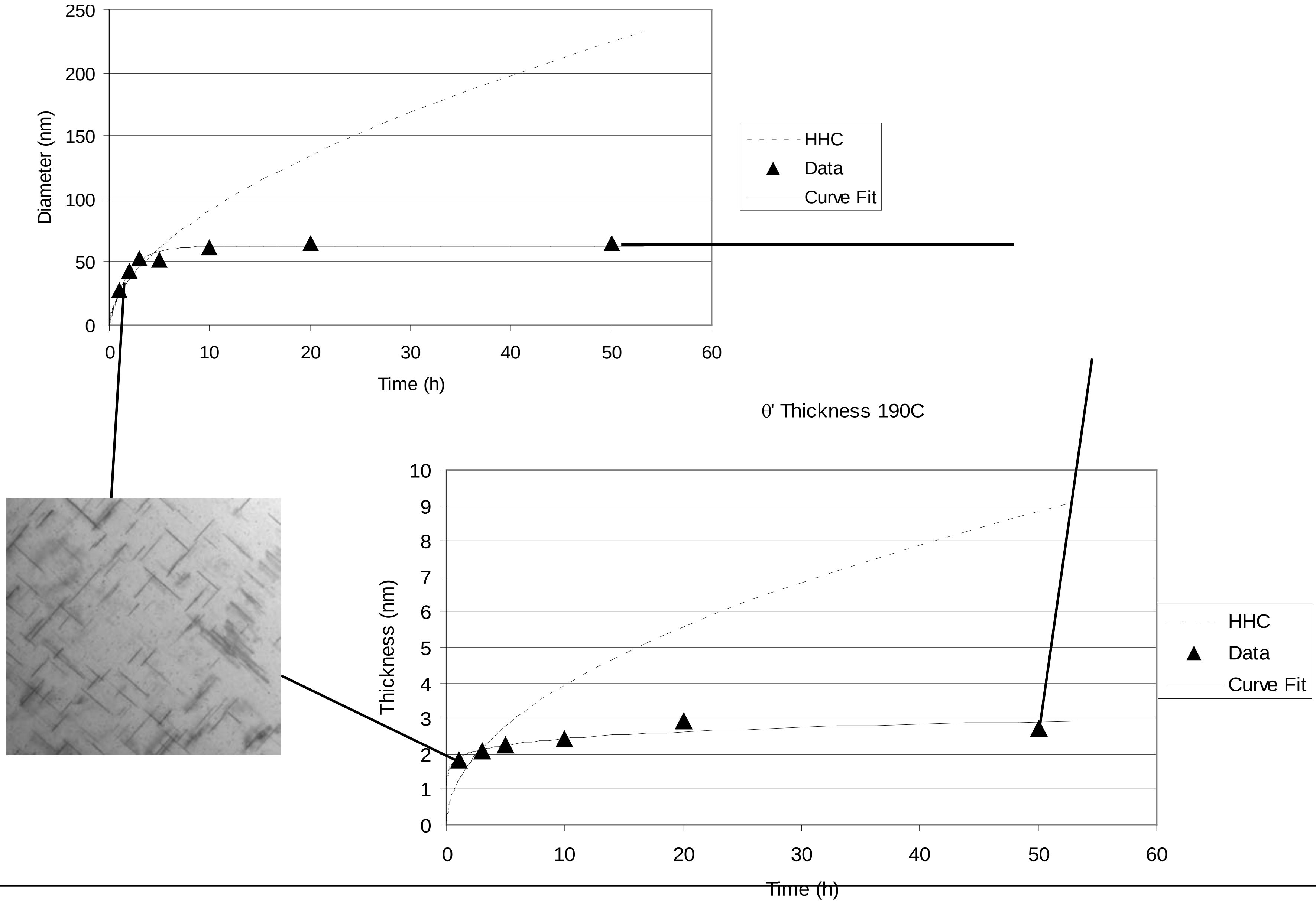
First-Principles Modification of Al-Cu Phase Diagram Incorporating Metastable θ'-phase



Metastable states just as easy to calculate as stable states

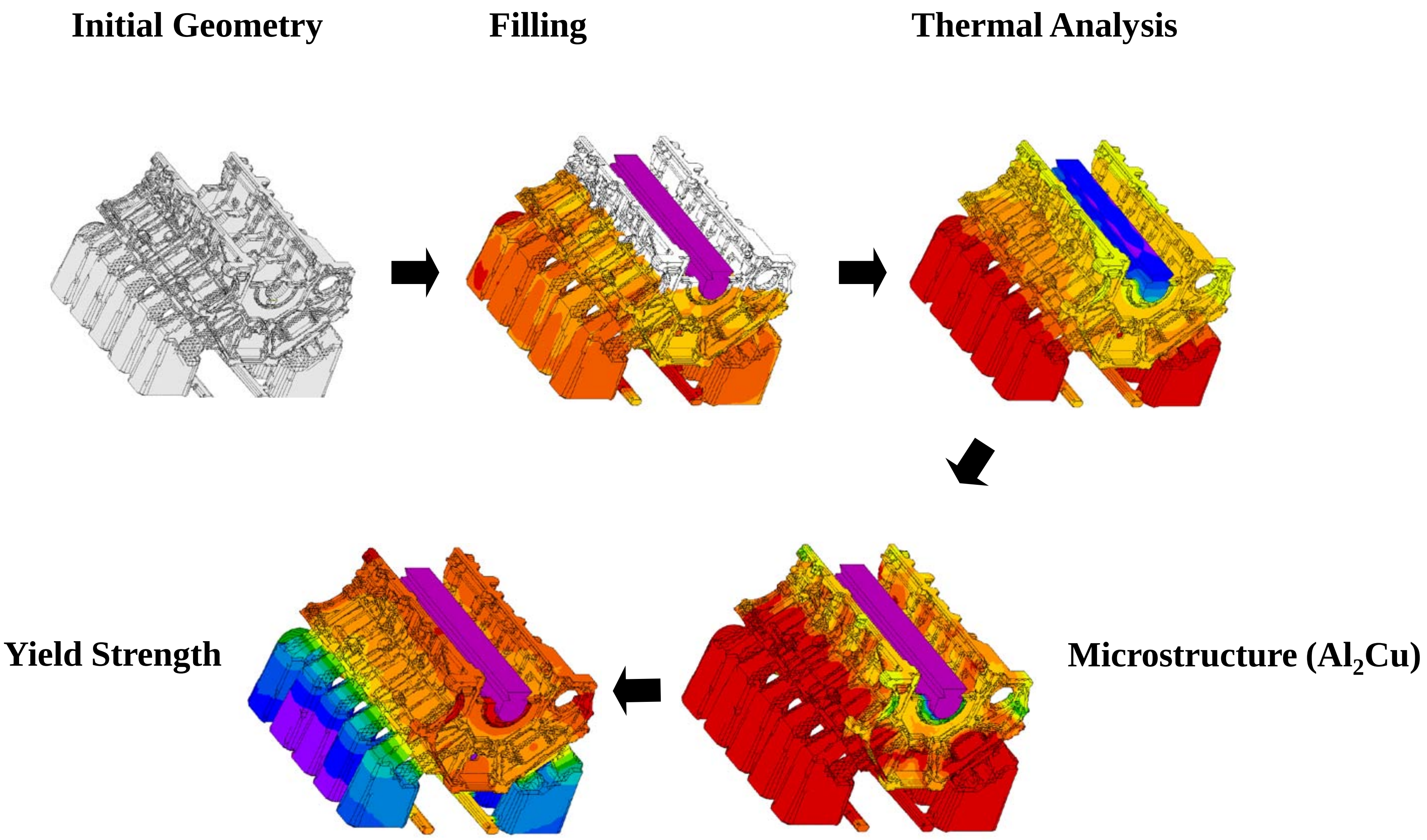


VAC models capture experimental understanding where robust physics-based models are not available

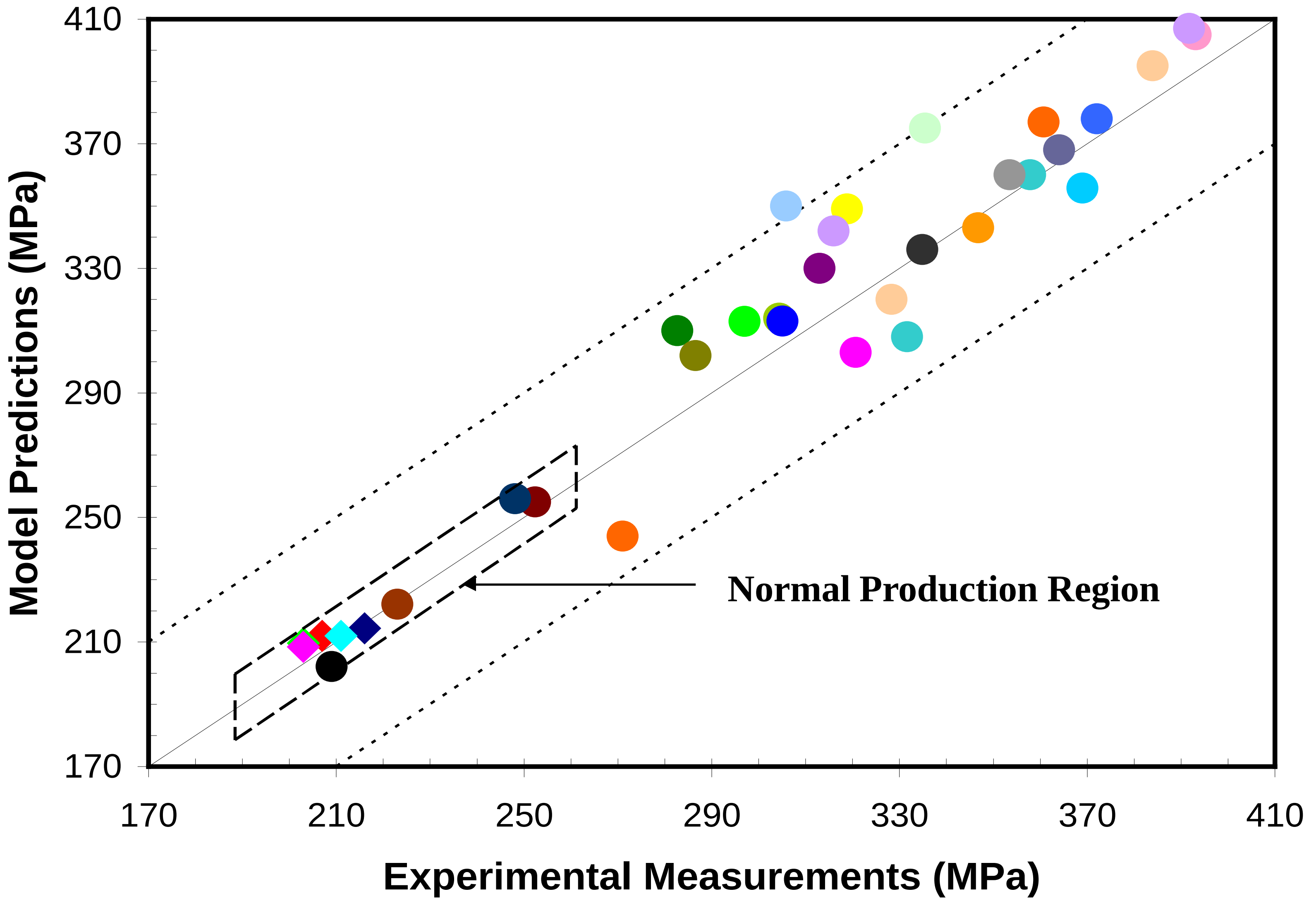


TEM Characterization of Precipitate Morphology vs Aging Time
(319 Al alloy with 3, 3.5 and 4%Cu)

Virtual Aluminum Castings Process Flow
Local Yield Strength

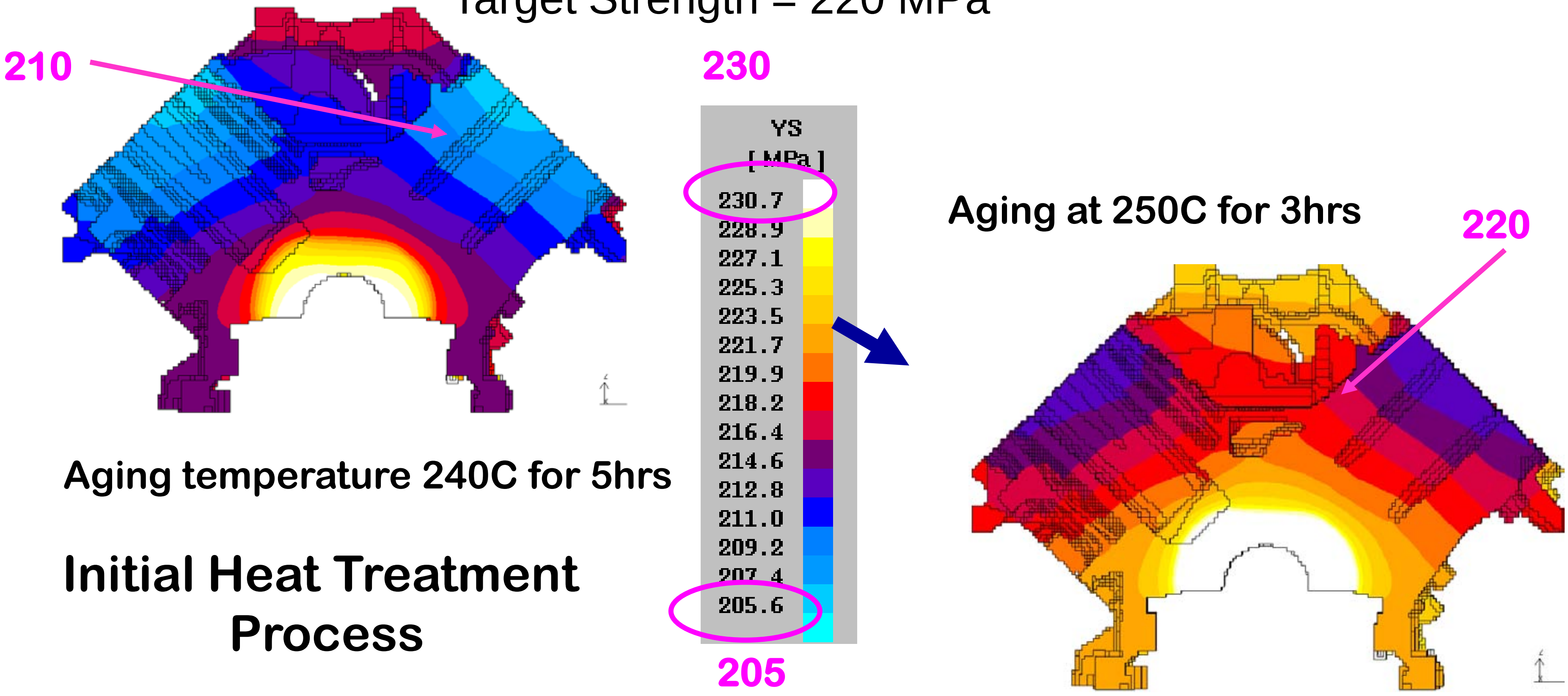


Model Validation



Using Virtual Aluminum Castings in Product and Process Optimization

Target Strength = 220 MPa



Optimized Heat Treatment Process

Faster and Stronger !!

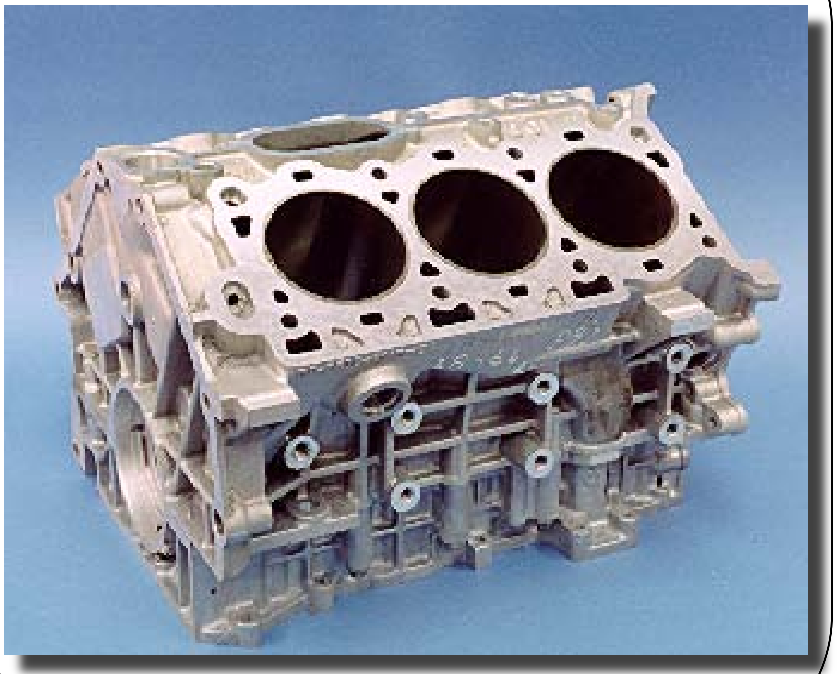
Ford Fusion Hybrid Engine

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 of India**

Ford Virtual Aluminum Castings Estimated Resources and ROI

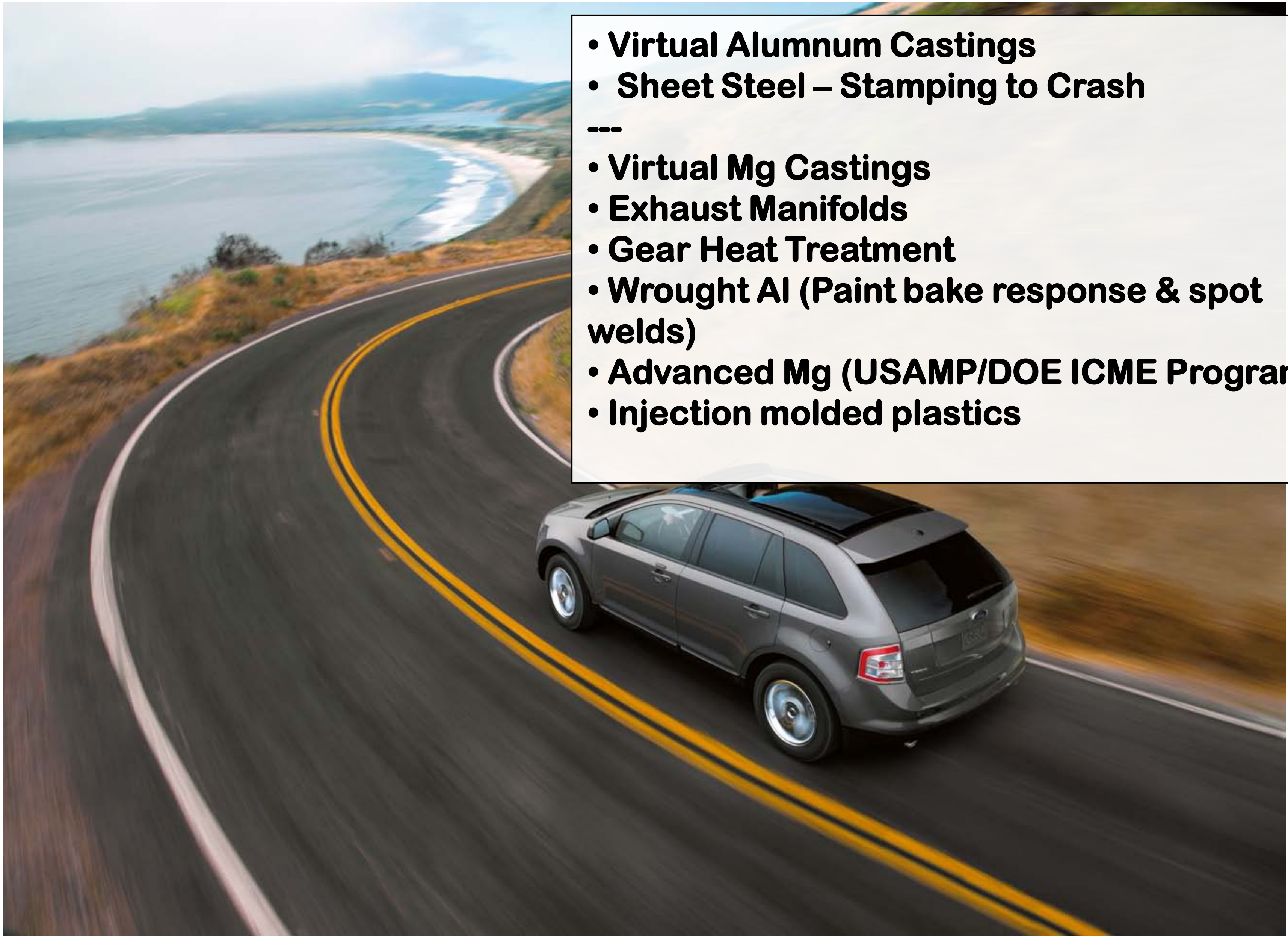
Resources

- $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

Case Studies - Lessons Learned

- *ICME is an emerging discipline, in its infancy.*
- *ICME can provide a significant positive return on investment.*
- *Achieving the full potential of ICME requires sustained investment.*
- *ICME requires a cultural shift.*
- *Successful model integration involves distilling information at each scale.*
- *Experiments are key to the success of ICME.*
- *"Knowledge-bases" are the key to capturing, curating, and archiving critical information required for development of ICME.*
- *ICME activities are enabled by open-access data and integration-friendly software.*
- *Less than a 100% solution may be good enough.*
- *Development of ICME requires cross-functional teams focused on a common goal or "foundational engineering problem".*

The Vision

Computationally-driven materials development is a core activity of materials professionals in the upcoming decades, uniting materials science with materials engineering and integrating materials more holistically and computationally with product development.

Recommendations

Nine recommendations for specific actions for the development, support and national co-ordination of ICME

DOD, DOE, OSTP, NIST, NSF, University Materials Council (UMC), Industry, Professional Materials Societies

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

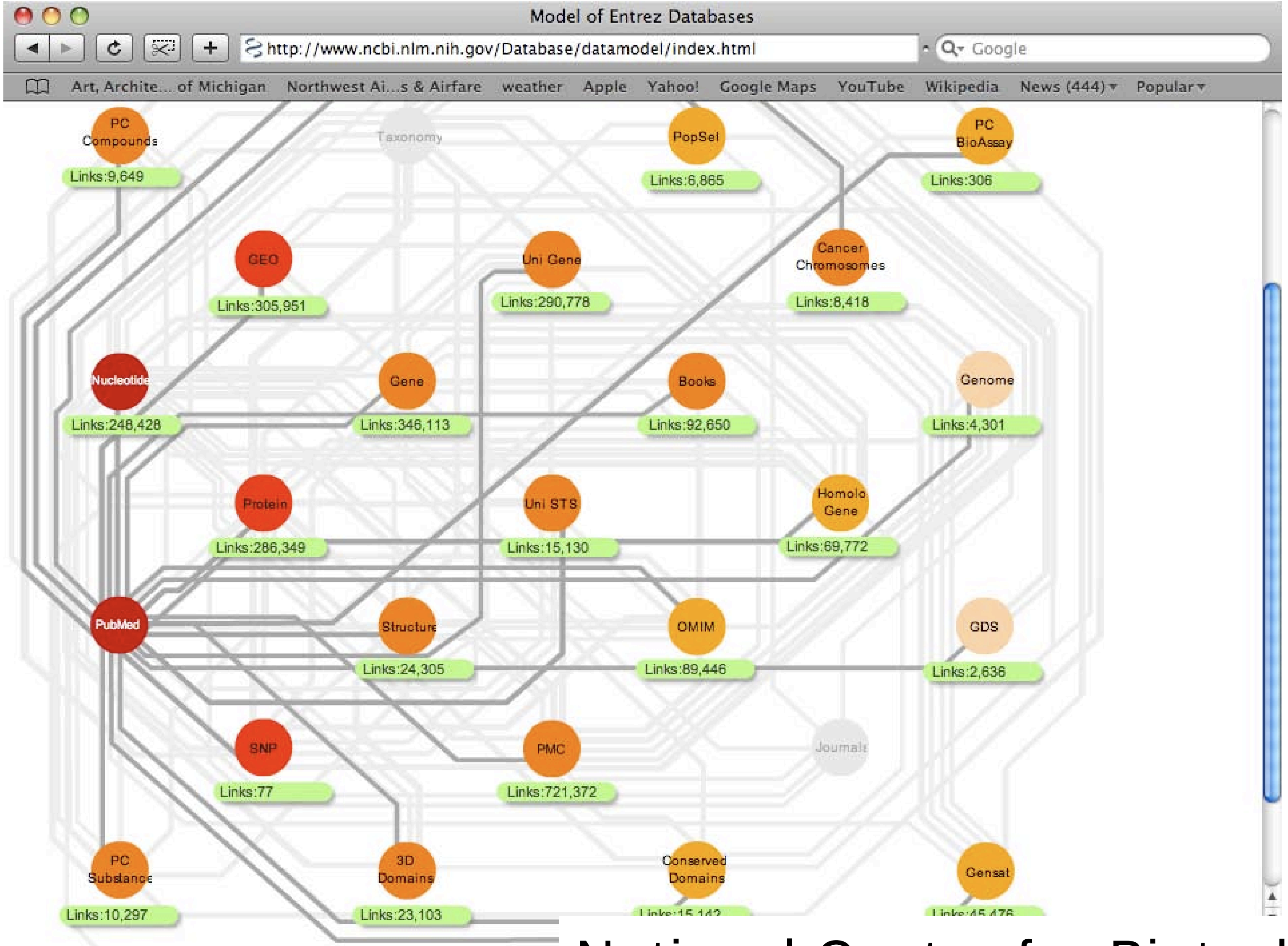
$10-40M per FEP (3-5 year funding)

Examples:

- 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

Lessons Learned from Other Fields

ICME Complexity and Magnitude Similar to Bioinformatics



Tools and linked databases to develop a better understanding of the molecular processes affecting health and disease

Curated Databases

NIH Requirement

National Center for Biotechnology Information (NCBI)

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)

The Vision

Within 10 – 20 year timeframe, **as a result of the coordination and targeted investment by stakeholders in the critical elements of ICME**:

- ICME will have reduced the materials development cycle from today's 10- to 20-year time frame to 2 or 3 years.
- ICME will have become established as a critical element in maintaining the competitiveness of the U.S. manufacturing base.
- ICME practitioners—a broad spectrum of scientists, engineers, and manufacturers—will have open access to a curated ICME cyberinfrastructure, including libraries of databases, tools, and models, thereby enabling the rapid design and optimization of new materials, manufacturing processes, and products.
- The materials scientist in academia performing traditional science-based inquiry will benefit from the assembled and networked data and tools. Discoveries will be easier.

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 (OSTP, DOD, DOE)
- Industrial interest
- Professional Society Interest: TMS, ASM, ASME, AIAA, AICHE?
- Academic Interest:
  - University Materials Council – Workshop on ICME & CMS
  - Three university ICME centers in the proposal stages (China, UK, US)

First World Congress on ICME

July 10-14, 2011 – Seven Springs, Pennsylvania

- **International Advisory Committee representing more than 15 countries**
- **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**

<u>Abstract Deadline: November 11</u>

Summary

- Integrated Computational Materials Engineering (ICME) offers a means to link:
  - ➢ Manufacturing, materials and design
  - ➢ Engineering and science
  - ➢ Information across disciplines
  - ➢ Theory, simulation and experiments
- Early case studies demonstrate a significant ROI for ICME
- To fully and efficiently realize the potential of ICME there is a need for a global infrastructure and coordinated efforts - a grand challenge!
- If successful, ICME will transform materials science and engineering and lead to increased competitiveness and national security