Computational Models in the Materials World
- We are nearly there....

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Pratt & Whitney

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AIAA Conference
April 10, 2013
Boston, Mass.
**Computational Models in the Materials World - We are nearly there...**

1. **REPORT DATE**
   10 APR 2013

2. **REPORT TYPE**

3. **DATES COVERED**
   00-00-2013 to 00-00-2013

4. **TITLE AND SUBTITLE**

5. **AUTHOR(S)**

6. **PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)**
   Pratt & Whitney, 400 Main Street, East Hartford, CT, 06118

7. **SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)**

8. **PERFORMING ORGANIZATION REPORT NUMBER**

9. **DISTRIBUTION/AVAILABILITY STATEMENT**
   Approved for public release; distribution unlimited

10. **ABSTRACT**

11. **SUBJECT TERMS**

12. **REPORT SECURITY CLASSIFICATION OF:**
    - Report: Unclassified
    - Abstract: Unclassified
    - This Page: Unclassified

13. **LIMITATION OF ABSTRACT**
    Same as Report (SAR)

14. **NUMBER OF PAGES**
    21

15. **RESPONSIBLE PERSON**
    - Report: Unclassified
    - Abstract: Unclassified
    - This Page: Unclassified
• Materials are critical for every engineered product
• Traditionally materials were developed by trial and error processes, separate from application requirements
• Materials are currently defined by static specifications based on empirical data
• Challenge and opportunity of Computational Materials Engineering is the linking of Materials, Manufacturing Processes and Component Designs
Evolution of System Efficiency

Thrust Specific Fuel Consumption (lb/hr/lb)

<table>
<thead>
<tr>
<th>Engine Type</th>
<th>Certification Date</th>
<th>BPR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Turbojet</td>
<td></td>
<td></td>
</tr>
<tr>
<td>707 (JT3C)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>B727 (JT8D)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Low Bypass Turbofan</td>
<td></td>
<td>1.1 to 1.8</td>
</tr>
<tr>
<td>747 (JT9D)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>767 PW4000 94&quot;</td>
<td></td>
<td></td>
</tr>
<tr>
<td>737</td>
<td></td>
<td></td>
</tr>
<tr>
<td>777 PW4000</td>
<td></td>
<td></td>
</tr>
<tr>
<td>High Bypass Turbofan</td>
<td></td>
<td>4.5 – 5.5</td>
</tr>
<tr>
<td>747 (JT9D)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>767 PW4000 94&quot;</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A320 (V2500)</td>
<td></td>
<td></td>
</tr>
<tr>
<td>A380</td>
<td></td>
<td>BPR &gt; 6</td>
</tr>
</tbody>
</table>

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Propulsion History

Propulsion Innovations Enabled by Materials and Processing Technology

J58 Powered SR-71
- DS blades, Cast & Wrought disks, 1st Gen Thermal Spray TBC coatings

JT9D powered Boeing 747
- 1st Gen SC blades, 1st Gen PM disk, 1st Gen EB-PVD TBC

F100 Powered F-15 / F-16
- 2nd Gen SC blades, Aluminide coatings, 2nd Gen PM/fracture tolerant disk

F119 Powered F-22
- LFW Ti IBR, Dual Property Ni Disk, TBC blades, Burn resistant Ti, CatArc Metallic Coatings

F135 Powered F-35
- Dual Property 3rd Gen PM disk, High modulus blade, 2nd Gen TBC coating

PW1133G Powered A320neo
- 4th Gen PM disk alloy, Hybrid metallic airfoils, 3rd Gen TBC

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Ni Superalloy Turbine Airfoils: Significant Advances in Alloys and Casting Processes

Alloy Temperature Capability (°F)

Base

Equiaxed

Columnar

Single Crystal


IN100 B1900 PWA 1422 MM247 PWA 1426 PWA 1480 PWA 1484 PWA 1487 PWA 1497

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Key Technology Advances for Turbine Airfoil Materials

ICME is another technology to “break the curve”

Turbine Temperature Increase

Time ➔

Base

Convective Cooling

Film Cooling

Thermal Barrier Coatings

Advanced Casting

Material Technology

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Mechanical Properties = fn (chemistry and microstructure)

Microstructure = fn (chemistry and processing)

Processing = fn (component geometry)

Materials, Manufacturing Methods and Component Design are Strongly Coupled

ICME - Integrated Computational Materials Engineering
What a Tensile Test Looks Like…

To a Materials Engineer

To a Mechanical Engineer

MIL-HBK-5H

Table 5.4.1.0(b). Design Mechanical and Physical Properties of Ti-6Al-4V Sheet, Strip, and Plate

<table>
<thead>
<tr>
<th>Specification</th>
<th>AMS 4011 and MIL-T-6046, Comp. AB-1</th>
<th>MIL-T-6046, Comp. AB-1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Form</td>
<td>Sheet</td>
<td>Plate</td>
</tr>
<tr>
<td>Condition</td>
<td>Annealed</td>
<td>Solution treated and aged</td>
</tr>
<tr>
<td>Thickness, in.</td>
<td>0.001-0.085</td>
<td>0.085-0.200</td>
</tr>
<tr>
<td>Basis</td>
<td>A</td>
<td>B</td>
</tr>
<tr>
<td>Mechanical Properties:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$F_{Y}^{	ext{min}}$</td>
<td>L</td>
<td>134</td>
</tr>
<tr>
<td>LT</td>
<td>134</td>
<td>139</td>
</tr>
<tr>
<td>$F_{Y}^{	ext{max}}$</td>
<td>L</td>
<td>126</td>
</tr>
<tr>
<td>LT</td>
<td>126</td>
<td>131</td>
</tr>
<tr>
<td>$F_{U}^{	ext{min}}$</td>
<td>L</td>
<td>133</td>
</tr>
<tr>
<td>LT</td>
<td>135</td>
<td>141</td>
</tr>
<tr>
<td>$F_{U}^{	ext{max}}$</td>
<td>L</td>
<td>87</td>
</tr>
<tr>
<td>LT</td>
<td>87</td>
<td>90</td>
</tr>
<tr>
<td>$F_{U}^{	ext{max}-	ext{bent}}$</td>
<td>(e/D = 1.0)</td>
<td>213</td>
</tr>
<tr>
<td>(e/D = 2.0)</td>
<td>272</td>
<td>283</td>
</tr>
<tr>
<td>$F_{U}^{	ext{max}-	ext{bent}}$</td>
<td>(e/D = 1.5)</td>
<td>171</td>
</tr>
<tr>
<td>(e/D = 2.0)</td>
<td>209</td>
<td>217</td>
</tr>
<tr>
<td>$e_{p}$, percent (9-basis):</td>
<td></td>
<td></td>
</tr>
<tr>
<td>L</td>
<td>8%</td>
<td>10</td>
</tr>
<tr>
<td>LT</td>
<td>8%</td>
<td>10</td>
</tr>
<tr>
<td>Physical Properties:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$E$, $10^5$ ksi</td>
<td>16.0</td>
<td></td>
</tr>
<tr>
<td>$E$, $10^6$ ksi</td>
<td>16.4</td>
<td></td>
</tr>
<tr>
<td>$G$, $10^6$ ksi</td>
<td>6.2</td>
<td></td>
</tr>
<tr>
<td>$n$</td>
<td>0.31</td>
<td></td>
</tr>
<tr>
<td>0.160</td>
<td></td>
<td></td>
</tr>
<tr>
<td>See Figure 4.5.1.0</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

a The rounded $F_{y}$ values are higher than specification values as follows: $F_{y}(L) = 131$ ksi, $F_{y}(LT) = 132$ ksi, and $F_{y}(LT) = 133$ ksi.

b Values are in psi.

c $a_{0}=0.025$ to 0.062 in., and 0.063 in. and above

d $a_{0}=-0.025$ to 0.062 in., and 0.063 in. and above

e $a_{0}=-0.003$ to 0.045 in., and 0.046 in. and above

No Technical Data per the EAR and ITAR

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True material capability and property distributions are controllable and reproducible; not “random variability”.

Properties are a function of chemistry, microstructure, stain, cooling rate, etc.; i.e. pedigree.

Materials properties are path dependent and are often “location-specific”. Engineering specifications often treat entire material volume as single, homogeneous property capabilities.

Modeling and simulation can help enhance component property capability definitions.
Traditional Materials Definitions

• Design Curves – Empirical; Data Driven
• Specifications
• Prints Notes
• Fixed Process Requirements

Requires Defining Material Equivalency and Methods to Differentiate Material of One Control Pedigree from Another
The Challenge: Need Models and Computational Infrastructure

Current materials definitions for design limit design flexibility and final component capabilities

There is a need for:

Model-Based Materials Definitions

Model-based material definitions enable location-specific prediction, analysis and optimization

Model-based materials definitions enable greater material, process and component definitions

Goal is prediction and control of capabilities
ICME Involved Linkage with Other Discipline Activities

Customer Requirements

Mechanical Design

Material Definition

Life-Cycle Cost Analysis

Holistic Design Optimization

Mfg Process Definition

Lifing Analysis

Component Modeling & Prediction

Product Definition

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No Technical Data per the EAR and ITAR
Goal is prediction and control of capabilities

Capture of developmental and production data to support model development

Properties → Traditional empirical property measurement and analysis migrating to materials models

Failure below control limit

Failure due to trending

Spec Min

UCL

LCL

Serial Number →

Predicted Material Properties

Predicted Material and Component Properties

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Material & Process Modeling Goals

• Develop Simulation Tools that Emulate Reality
• Develop Analytical Tools that Provide Insight in Material - Process - Property Relationships
• Implement Tools for Design and Manufacturing Benefits
  • Model-based Decisions
  • Tangible Improvements obtained based on Decisions

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Holistic Integration: Digital Thread

Example of Integrated Computational Materials & Mfg Engineering

PMDO – Preliminary Multi-Disciplinary Optimization

Location-Specific Optimized Component Definition

Data Capture / Knowledge Generation

Microstructure & Process-Sensitive Materials Definition

Materials Genome Initiative

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### Example of ICME Application

**Cost Benefit**

>50% Reduction in Design Cycle Time

**System Benefits**

- Feasibility of full design integration demonstrated
  - Over 600 design loop runs with coupled part geometry and material capability driving design evolution
  - Realistic case studies

<table>
<thead>
<tr>
<th>Case Study</th>
<th>Heat Treat</th>
<th>Forging</th>
<th>Part</th>
<th>Forge Wt</th>
<th>Part Wt</th>
<th>Burst Speed</th>
<th>Comments</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Constant</td>
<td>Variable</td>
<td>Variable</td>
<td>-18%</td>
<td>-15%</td>
<td>+6%</td>
<td>Current State of the Art</td>
</tr>
<tr>
<td>2</td>
<td>Variable</td>
<td>Variable</td>
<td>Constant</td>
<td>-11%</td>
<td>n/a</td>
<td>+12%</td>
<td>Final Part shape constrained</td>
</tr>
<tr>
<td>3</td>
<td>Variable</td>
<td>Variable</td>
<td>Variable</td>
<td>-21%</td>
<td>-19%</td>
<td>+19%</td>
<td>Full impact of tool</td>
</tr>
</tbody>
</table>

**Geared Turbofan Engine**

**Final disk shape before and after**

Variation in Weak Pairing Curve - Strong Pairing Curve Intersection by changing APB Energy and Volume Fraction Independently

\[
\sigma_c = f_1 \left[ (T_{\text{Hall}} + \sum \frac{d \gamma}{d C_i} \right] + f_2 \left( 0.43 \left( \frac{d C_i}{d C_{\text{average}}} \right) \right) + f_3 \left( 0.43 \left( \frac{d C_i}{d C_{\text{average}}} \right) \right) + f_4 \left( \frac{1}{2} \right) \left( \frac{d d C_i}{d C_{\text{average}}} \right)
\]

Yield of Primary \( \gamma \)

Shearing of Secondary \( \gamma \) (Pairs)

Shearing of Tertiary \( \gamma \) - Solid Solution Strengthening

Hall-Petch \( \gamma \) Phase

Hall-Petch Primary \( \gamma \)

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Integration of Computational Materials Science and Engineering is Complicated

- Materials
- Manufacturing
- Design
- Structures
- Quality
- Supply-Chain
Challenges to Effective ICME Deployment

• Accurate computational models
• Efficient simulation software tools
• Data and databases for model application
• Industry standard methods and protocols
• Computational methods for design linkages
• Well trained interdisciplinary workforce

Unique engineering skill sets are required to support each challenge
Computational Supply-Chain

A series of well-established, capable and viable organizations that provide necessary portions of the ICME Value Chain

- Fundamental Model Development
- Model Integration into Software Packages
- Maintenance of Software Tools
- Database Generation
- Application Engineering
- Customer Approval and Certification
- Education and Training
Conclusions

ICME: Potential for dramatic changes to development time, cost, and product capabilities.

Computational materials engineering enables virtual manufacture and component testing for optimization and risk mitigation.

Application of ICME has several challenges: trained practitioners; tools and methods; and computational infrastructure.
Any Questions?