Introduction to Data Workflows in ICMSE

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No Technical Data per the EAR or ITAR
Data Workflows in ICMSE

- Materials and Process Development
- Material development
  - Data management plans
  - Characterizing controlling microstructural features
  - Data schema
- Model Development and Validation
  - Verification and Validation
  - Bayesian updating
- Production Data
  - Material and Model Monitoring
  - Model Enhancement
Additive Manufacturing: rapid, low cost, flexible

Freeform Fabrication of Parts
- Shorter Lead Times
- Eliminate Tooling

Alternatives to Castings

New Innovative Designs

Powder Bed Technologies
- Direct Metal Laser Sintering (DMLS)
- Electron Beam Melting (EBM)
Predicting Material Capabilities

Measured Material Properties → Predicted Property Variability

Mt’l Variability → Component Variability

Controlling Feature and Mechanism MUST be Understood
Computational Materials Modeling
Fit for purpose focus

Materials Modeling:
- Reduced cycle-time
- Capability optimization
- Enhanced material definition

Mfg Process Modeling:
- Reduced cycle-time
- Increased yield and product quality

Component Modeling:
- Location-specific optimization
- Optimize part weight/cost
- Maximized lifing capability

Integrated Computational Materials Engineering (ICME)
ICME Development Path
Capture benefits early and often

“Off-Ramps” for Developed Models with FIT-FOR-PURPOSE Capabilities

Physic-based model application flow

Materials Modeling:
- Material Design / Optimization
- Materials Definitions / Design Curves

Mfg Process Modeling:
- Process Design / Optimization
- Design Rules and Tools

Component Modeling:
- Component Design / Optimization
- System Design Optimization

Interdisciplinary Applications
Local Applications → Global, “Holistic” Applications

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Materials Data Perspectives

Table 5.4.1(b). Design Mechanical and Physical Properties of Ti-6Al-4V Sheet, Strip, and Plate

<table>
<thead>
<tr>
<th>Specification</th>
<th>AMS 4911 and MIL-T-9046, Comp. AB-1</th>
<th>MIL-T-9046, Comp. AB-1</th>
</tr>
</thead>
<tbody>
<tr>
<td>Form</td>
<td>Sheet, Plate</td>
<td>Sheet, strip, and plate</td>
</tr>
<tr>
<td>Condition</td>
<td>Annealed</td>
<td>Solution treated and aged</td>
</tr>
<tr>
<td>Thickness, in.</td>
<td>0.1250</td>
<td>0.0100 - 2.000</td>
</tr>
<tr>
<td>Basis</td>
<td>A, B, A, B</td>
<td>A, B, A, B</td>
</tr>
<tr>
<td>Mechanical Properties:</td>
<td></td>
<td></td>
</tr>
<tr>
<td>$F_y$, ksi</td>
<td>125</td>
<td>125</td>
</tr>
<tr>
<td>$F_u$, ksi</td>
<td>130</td>
<td>130</td>
</tr>
<tr>
<td>$F_m$, ksi</td>
<td>120</td>
<td>120</td>
</tr>
</tbody>
</table>

- $F_y$: Yield strength
- $F_u$: Ultimate tensile strength
- $F_m$: Maximum strength

MIL-HBK-5H

Materials Engineer

Mechanical Engineer

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Material Capabilities Definitions

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

Properties are a function (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.

From D. Furrer, OPTIMoM Conf., 2010
Efficient Testing and Qualification
Production Testing

- Model-Driven Test Plans
  - Evaluation of critical component locations/properties
  - Target sensitive locations that provide information about entire component
  - Reduced testing provides reduced costs and qualification cycle-time

Critical – All Data to be Captured and Integrated with Current Understanding
Materials Informatics

Use of Data and Physics to reduce uncertainty

- Capture and Re-Use Materials Data and Metadata ("Digital Thread")
- Establish Enhanced Models to Support Future Materials Definitions and Design Functions
- Quantify Uncertainty of Models and Understanding to Minimize Future Testing

Data Mining and Data/Model Fusion
Materials Data Management

**DEVELOPMENT DATA**

Specific data collected, stored & reported

- **Material Data**
  - Heat Code
  - Material Spec
  - Chemistry
  - Source
  - Part Number
  - Heat Treatment
  - Machining Source
  - Material Source
  - Expected Results

- **Test Data**
  - Test Conditions
    - Temp, Stress, Frequency, etc
  - Test Results
    - Life, Strength, Curves (da/dN vs dK, S-S, etc.)
  - Microstructure Results

- **Administrative Data**
  - Charge Numbers
  - Purchase Order Approvers
  - Export requirements
  - Requestor
  - Test Engineer
  - Technical Contact
  - Program Description

- **Tracking Data (barcode)**
  - Approvals & Time Stamp
  - Location & Time Stamp
  - Alerts to incoming work
  - Identify bottlenecks
  - Locate specimen
  - Job Status
  - Performance assessment

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Measurement of Microstructure

- Quantitative metallography is critical to enable understanding influence of limiting features
- Distribution of features and tails of distributions provide keys to material behavior
- Historical method to quantify microstructure are no longer acceptable; greater statistical treatment is needed (SVEs, etc.)
Grain Size Impacts are Powerful

Significant implications for processing choices

Source: J. Williams, OSU
ASTM E112 Grain Size By Comparison Method
Grain Size Distribution in Waspaloy Material
Necklaced Grain Structures in Waspaloy Material
Non-Uniform Grain Size in Waspaloy Material
Optical and OIM Images of Partially Recrystallized Wapaloy
Grain Boundary Morphology in Superalloy U720

12.7°C/sec

1.3°C/sec

0.72°C/sec

0.12°C/sec

Amplitude

Periodicity

19
Gamma-Prime Size and Distribution in P/M Superalloy
Gamma-Prime Precipitate Size as a Function of Cooling Rate

Gamma-Prime Morphology
Gamma-Prime Density
Gamma-Prime Size

U720

12.7°C/sec

1.3°C/sec

0.12°C/sec
Gamma-Prime Banding in Superalloy U720

Area Percent of Large Grains  12.7%
Area Percent of Small Grains  6.43

Average Size of Large Grains  5.25 um²
Average Size of Small Grains  0.626 um²
Primary Alpha Size and Volume Fraction in Titanium
Primary Alpha Size and Volume Fraction in Titanium
Optical Image Analysis of Ti Transformed Beta Structure

Micro-Texture in Titanium Alloys
Digital Thread - Air Force Vision

AIR FORCE VISION:
• Use ALL AVAILABLE INFORMATION in analyses
• Use PHYSICS to inform analyses
• Use PROBABILISTIC METHODS to quantify risks
• CLOSE THE LOOP from the beginning to the end and back to the beginning

Source: USAF ManTech Presentation (Used with Permission)
Turbine Disk Digital Thread

ICMSE - Integrated Computational Materials Science & Engineering

System Requirements

PMDO – Preliminary Multi-Disciplinary Optimization

Data
Mechanical Properties
Chemistry
Microstructure
Meta-Data

Microstructure & Process-Sensitive Materials Definition

Location-Specific Optimized Component Definition

Data Capture / Knowledge Generation

Materials Genome Initiative

Model-Based Manufacturing Definition

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Digital Thread & Design for Variation Vision

Digital Thread Enables More Effective Decision Making Through DFV

System Engineering Models

Multi-Disciplinary Automated Workflows

Materials and Manufacturing Process Modeling

Goal is 50% reduction in development time with 90% elimination of quality non-conformance

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Design for Variation

Parametric Modeling
Physics-Based Tools

Lean Automated Workflows – Eliminate Handoffs

Aero → Design → Thermals → Structures → Materials & Manufacturing

Emulate Models, Sensitivity Analysis → Calibration Using Test Data → Monte Carlo → Optimization

Usage → Boundary Conditions

Model → Material Properties → Geometry

DFV Enables Reduced Development & Part Costs by Aligning Models, Data, and Producibility

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Materials Data Management

Pratt & Whitney Materials Data Management

- Development and Design Data
- MMPDS
- Production Cert Data
- MoC REACH Database
- Automated Transfer and Upload
- Mechanical Test Data From Internal and Test Vendors
- Design Data Analysis & Import
- Production Data
- Materials of Concern Database

Component Design and Definition

- Coupon Test Data
- Statistical Data Analysis
- Test Jobs
- Data Analysis Jobs
- PatternMaster®

Design and Structural Analysis

Data Analytics

Manufacture and Quality Control APIs and GUI Interfaces

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Materials Data Management

MFT Site Process Utilized for Digital Data File Transfer

Supplier-1
Supplier-2
Supplier-3
Supplier-4
Supplier-5

Rotors
Airfoils
Structural Castings

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Materials Data Management Initiative

Data Capture Efforts showing Success

Data for over hundreds of thousands of serials captured to-date

GRANTA-MI is Live

- Production Data Pilot Proving Digital Data Capture Is Possible
- Data has been Analyzed and Applied to Support and Establish Root Cause on Two Recent Materials QNs

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Materials Data Management

Success from Data Analytics

- Production data has been captured, analyzed, linked to models and applied to enhanced material definitions
  - Castings, Forgings
- Optimal chemistry range defined for several legacy alloys, which supports required manufacturing control

Production Data Capture

Data Analytics and Model Development

Enhanced Material Definition

Quality Release Data

Improved Quality and Capabilities through Continuous Learning
Design for Variation

Enabling Multi-Fidelity and Multi-Disciplinary Uncertainty Quantification

Emulator & Bayesian updating software/technology, Training & ESW

Isight & CCE software, Training & ESW

Multi-User CAD, multi-fidelity geometry modeling

Multi-fidelity physics-based models

Investment in high speed computing

Internal Investment in Key Enablers Driving Broad Implementation of DFV
Computational Materials Modeling

Enhance specific materials capabilities

Design for cost and manufacture

Rapid, robust materials definitions

Many Applications for Materials and Process Modeling within Turbine Engines

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Conclusions

• Prediction of material and component properties is a major element of ICME

• Understanding of weakest microstructural links and associated mechanisms is required

• Traditional characterization methods not acceptable for understanding limiting features relative to statistics and tails of distributions

• Appropriate length scales of SVEs required based on feature and mechanism

• “Big Data” and data analytics are critical elements of ICME