Introduction to Data Workflows in ICMSE

May 12, 2015

Vasisht Venkatesh

David Furrer

2015 UCSB Workshop on Collection and Analysis of Big Data in 3D Materials Science

University of California – Santa Barbara
May 12th-14th 2015

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

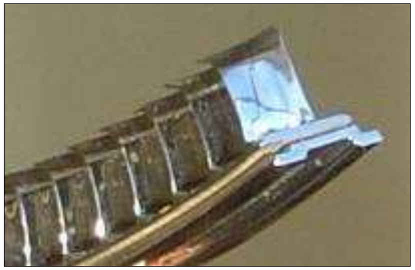
Freeform Fabrication of Parts

- Shorter Lead Times
- Eliminate Tooling

Alternatives to Castings

New Innovative Designs

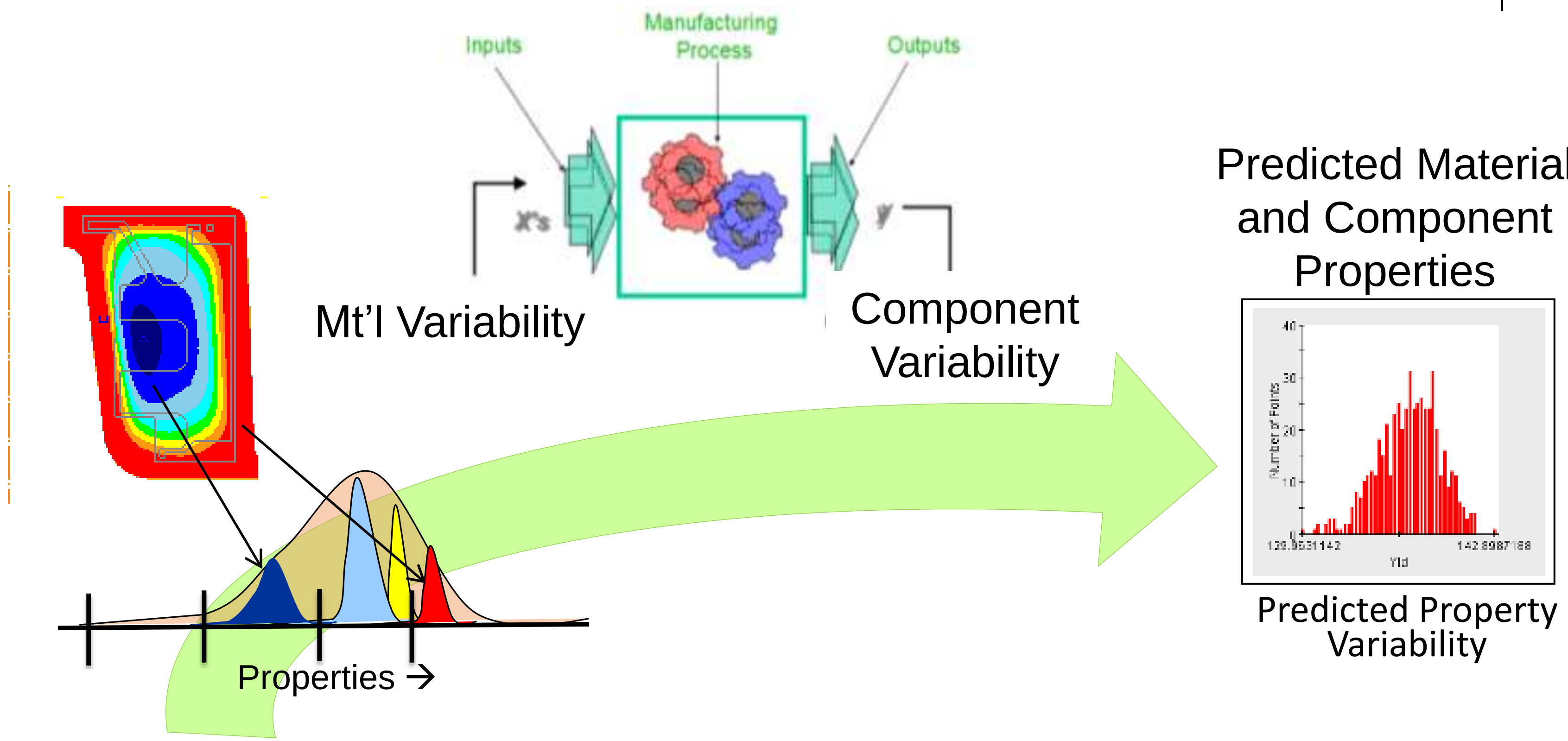
Powder Bed Technologies



Direct Metal Laser Sintering (DMLS)

Electron Beam Melting (EBM)

Predicting Material Capabilities

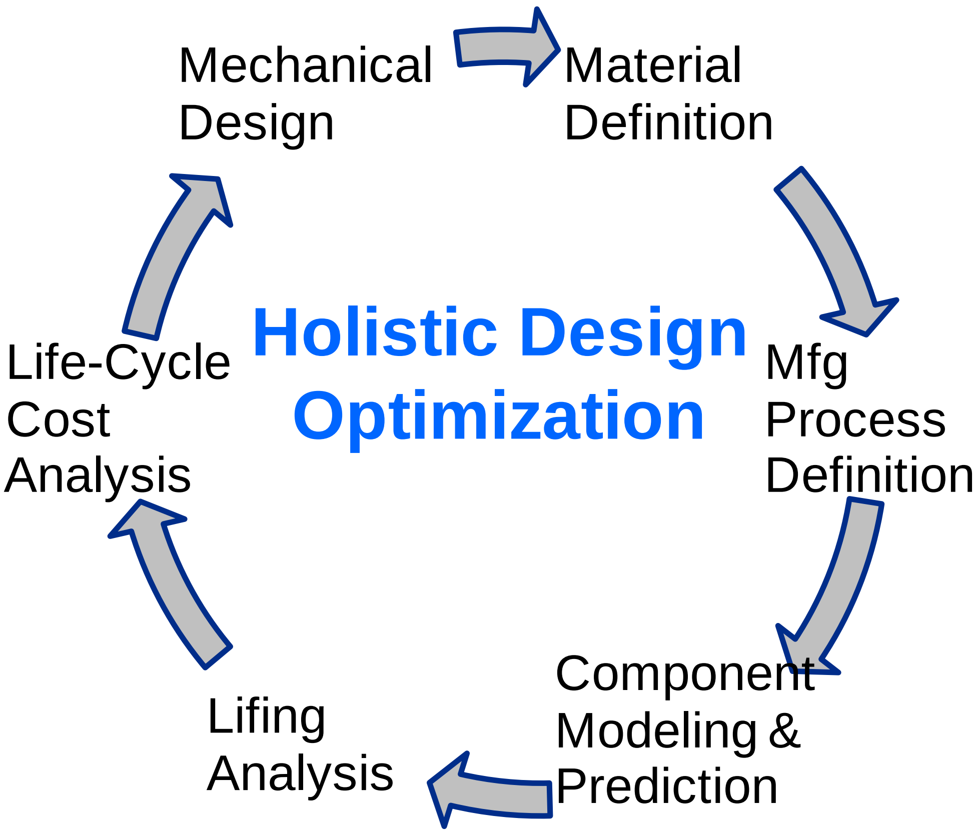


Measured Material Properties

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)

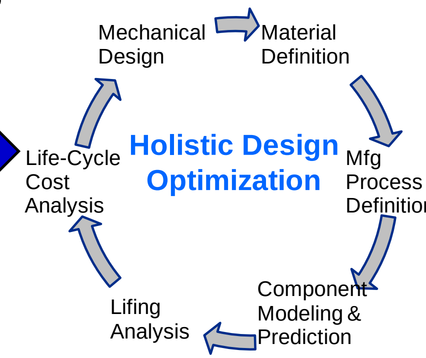
ICME Development Path

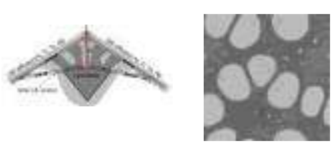
Capture benefits early and often

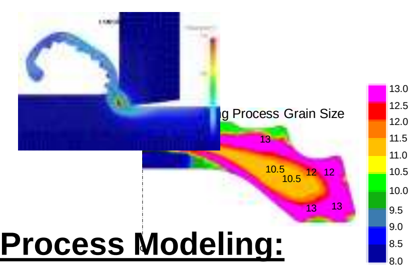
"Off-Ramps" for Developed Models with FIT-FOR-PURPOSE Capabilities

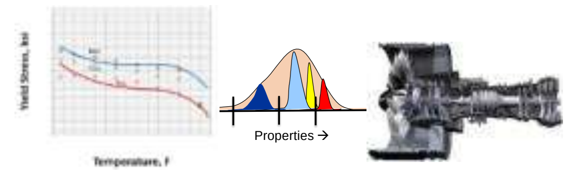
Model Development

Physic-based model application flow









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

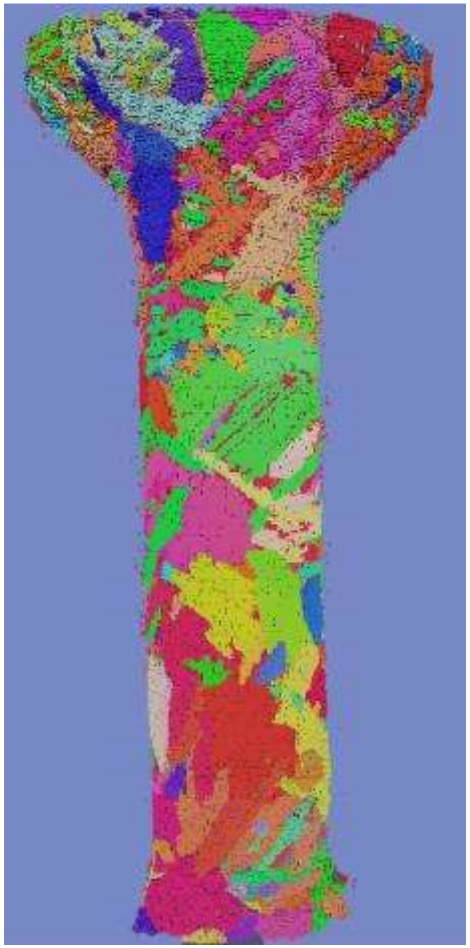
Mfg Process Modeling:
- Process Design / Optimization
- Design Rules and Tools

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

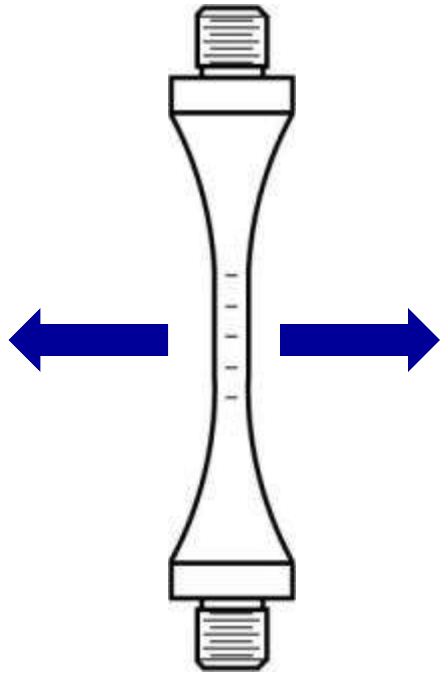
Interdisciplinary Applications

Local Applications → Global, "Holistic" Applications

Materials Data Perspectives



Materials Engineer



MIL-HBK-5H

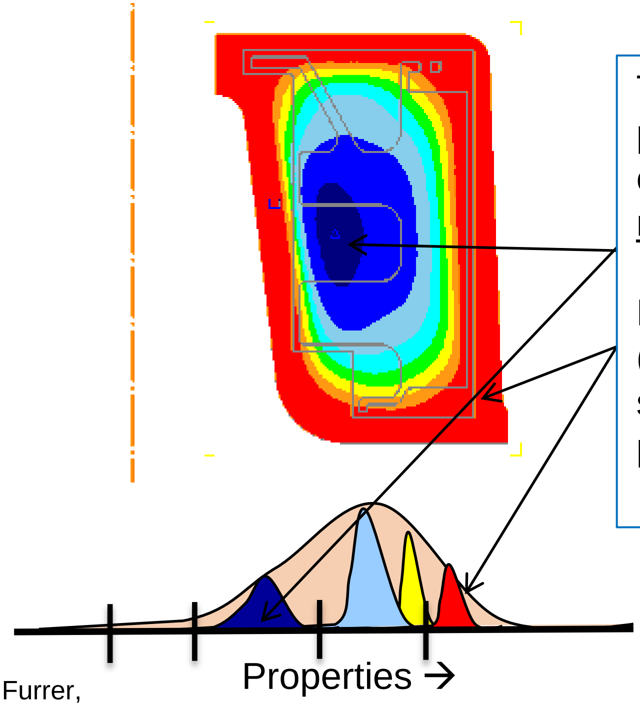
Table 5.4.1.0(b). Design Mechanical and Physical Properties of Ti-6Al-4V Sheet, Strip, and Plate

Specification	AMS 4911 and MIL-T-9046, Comp. AB-1					MIL-T-9046, Comp. AB-1			
Form	Sheet		Plate			Sheet, strip, and plate			
Condition	Annealed					Solution treated and aged			
Thickness, in.	≤ 0.1875		0.1875-2.000		2.001-4.000	≤ 0.1875	0.1875-0.750	0.751-1.000	1.001-2.000
Basis	A	B	A	B	S	S	S	S	S
Mechanical Properties:									
F_{tu}, ksi:									
L	134	139	130[a]	135	130	160	160	150	145
LT	134	139	130[a]	138	130	160	160	150	145
F_{ty}, ksi:									
L	126	131	120	125	120	145	145	140	135
LT	126	131	120[a]	131	120	145	145	140	135
F_{cy}, ksi:									
L	133	138	124	129	124	154	150	145	—
LT	135	141	130	142	130	162	—	—	—
F_{su}, ksi	87	90	79	84	79	100	93	87	—
F_{bru}, ksi:									
(e/D = 1.5)	213[b]	221[b]	206[b]	214[b]	206[b]	236	248	233	—
(e/D = 2.0)	272[b]	283[b]	260[b]	276[b]	260[b]	286	308	289	—
F_{bry}, ksi:									
(e/D = 1.5)	171[b]	178[b]	164[b]	179[b]	164[b]	210	210	203	—
(e/D = 2.0)	208[b]	217[b]	194[b]	212[b]	194[b]	232	243	235	—
e, percent (S-basis):									
L	8[c]	—	10	—	10	5[d]	8	6	6
LT	8[c]	—	10	—	10	5[d]	8	6	6
E, 10^3 ksi	16.0								
E_c, 10^3 ksi	16.4								
G, 10^3 ksi	6.2								
μ	0.31								
Physical Properties:									
ω, lb/in.^{3}	0.160								
C, K, and α	See Figure 4.5.1.0								

a The rounded T_{99} values are higher than specification values as follows: F_{tu}(L) = 131 ksi, F_{tu}(LT) = 132 ksi, and F_{ty}(LT) = 123 ksi.
b Bearing values are "dry pin" values per Section 1.4.7.1.
c 8%—0.025 to 0.062 in. and 10%—0.063 in. and above.
d 5%—0.050 in. and above; 4%—0.033 to 0.049 in. and 3%—0.032 in. and below.

Mechanical Engineer

Material Capabilities Definitions



True material capability and property distributions are controllable and reproducible; <u>not</u> "random variability".

Properties are a fn (chemistry, microstructure, stain, cooling rate, etc.); i.e. pedigree.

From D.Furrer, OPTIMoM Conf., 2010

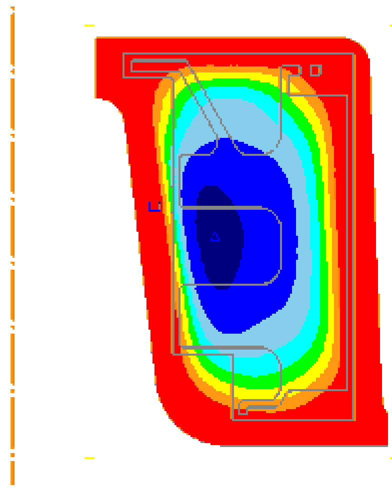
Materials properties are path dependent and are often "location-specific". Engineering specifications often treat entire material volume as single, homogeneous property capabilities.

Modeling and simulation can help enhance component property capability definitions

Efficient Testing and Qualification

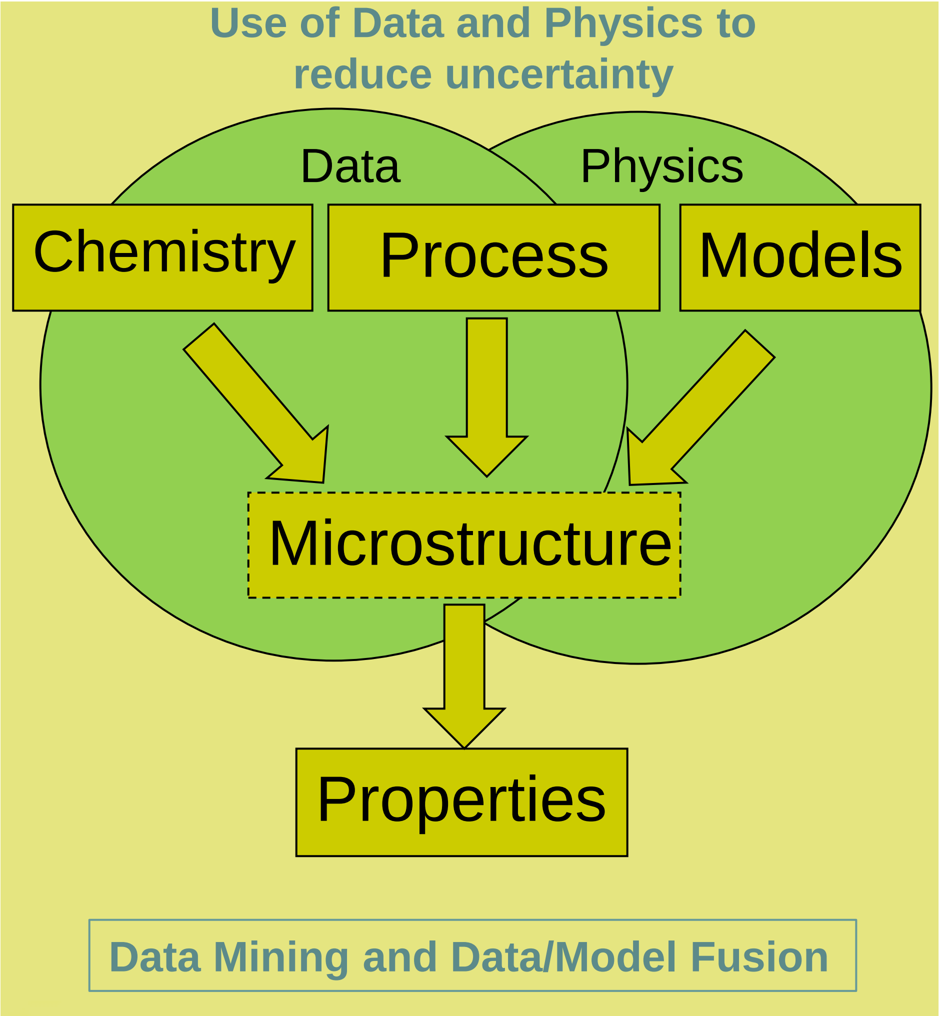
Production Testing

- 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



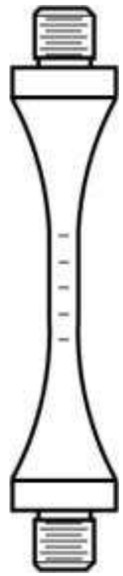
- Capture and Re-Use Materials Data and Meta-Data ("Digital Thread")
- Establish Enhanced Models to Support Future Materials Definitions and Design Functions
- Quantify Uncertainty of Models and Understanding to Minimize Future Testing

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

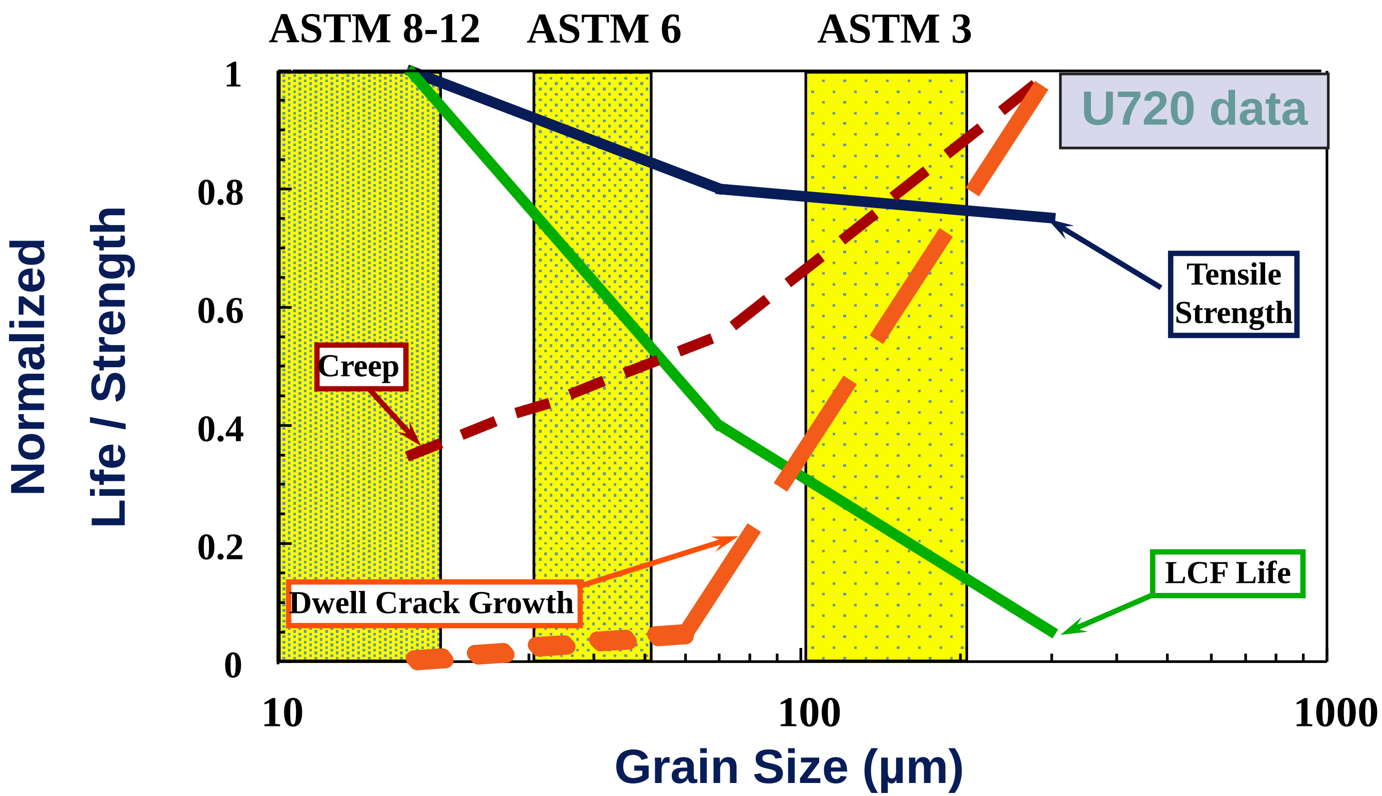
- Administrative Data
  - Charge Numbers
  - Purchase Order Approvers
  - Export requirements
  - Requestor
  - Test Engineer
  - Technical Contact
  - Program Description

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

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.)

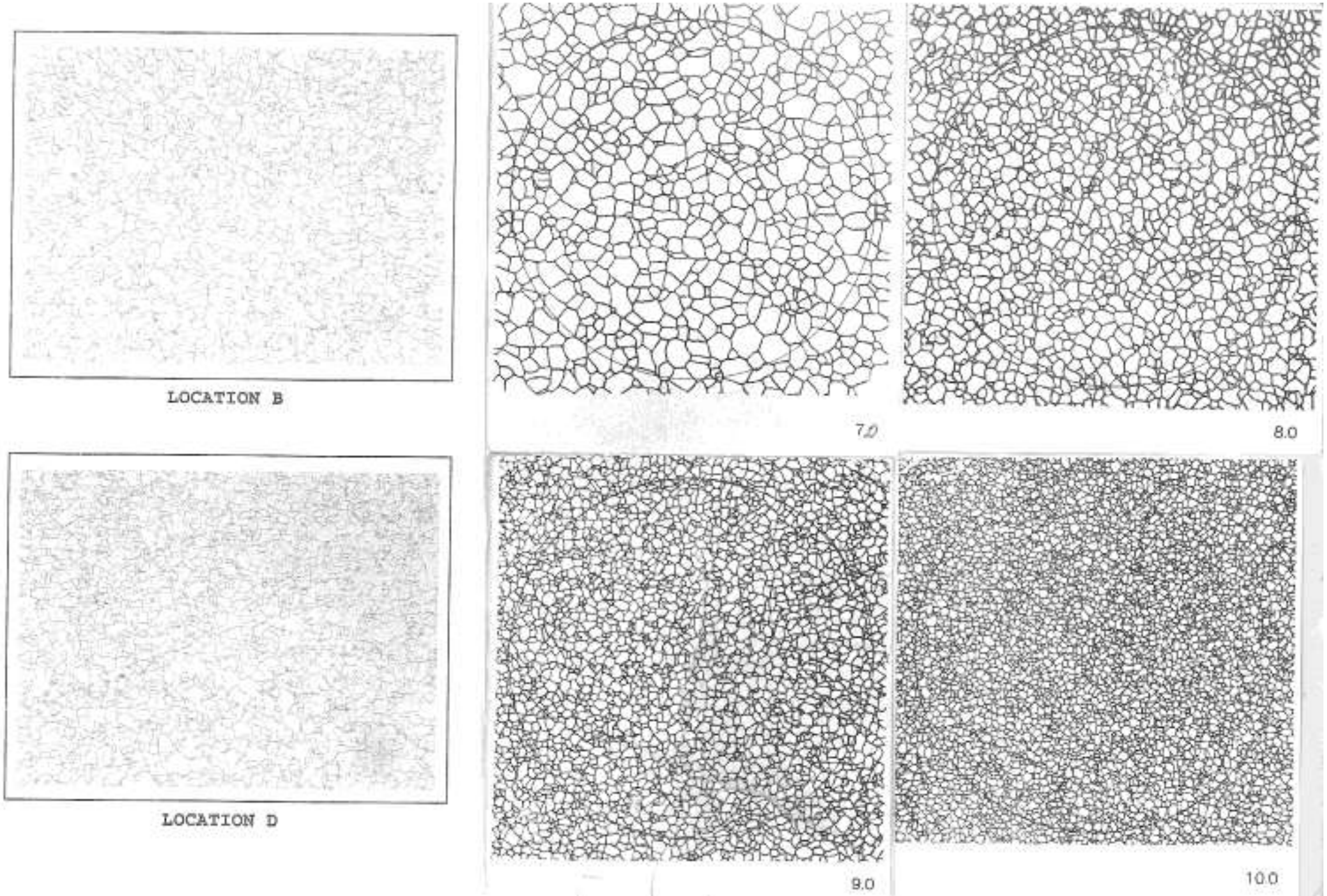
Grain Size Impacts are Powerful



Significant implications for processing choices

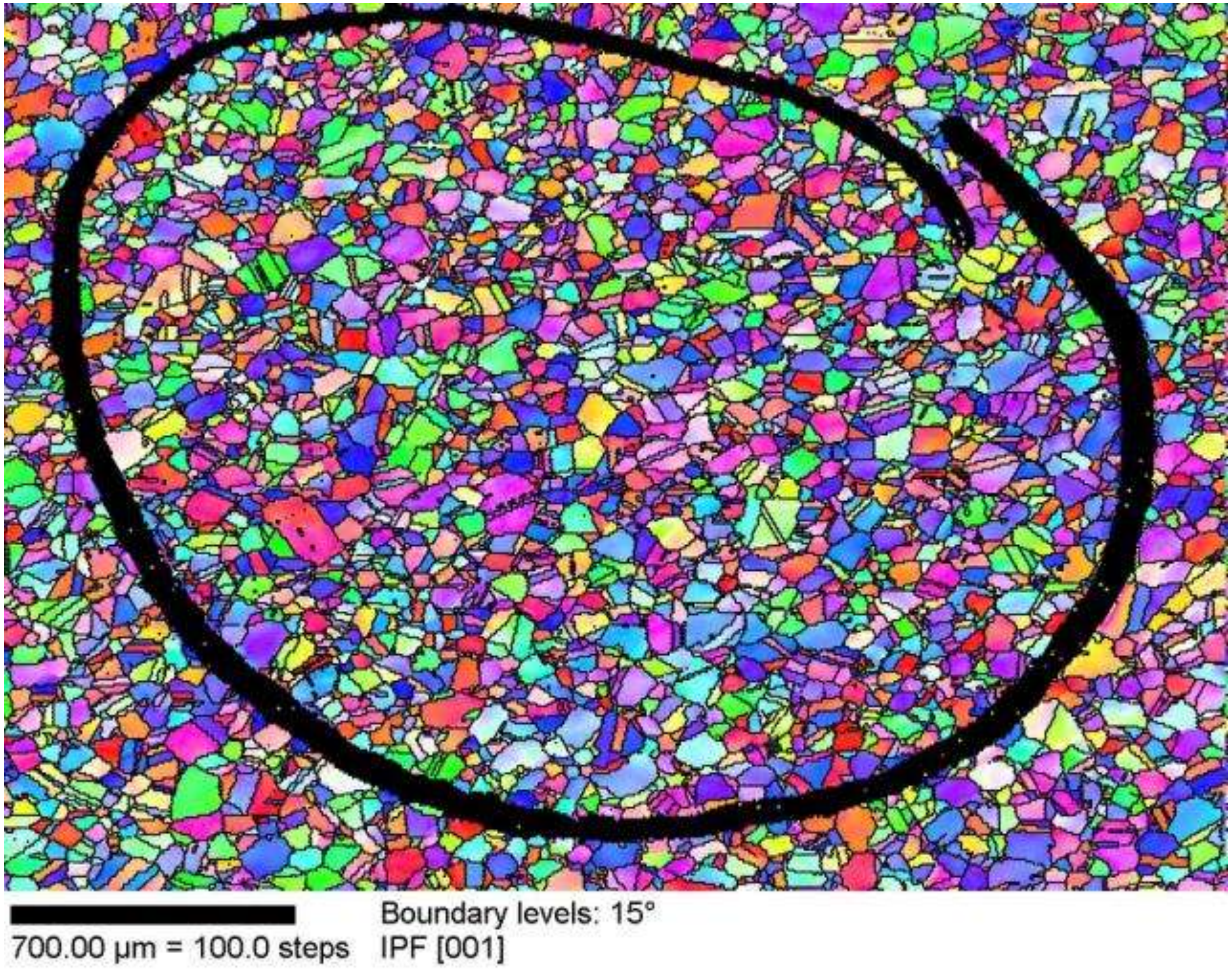
Source: J.Williams, OSU

ASTM E112 Grain Size By Comparison Method

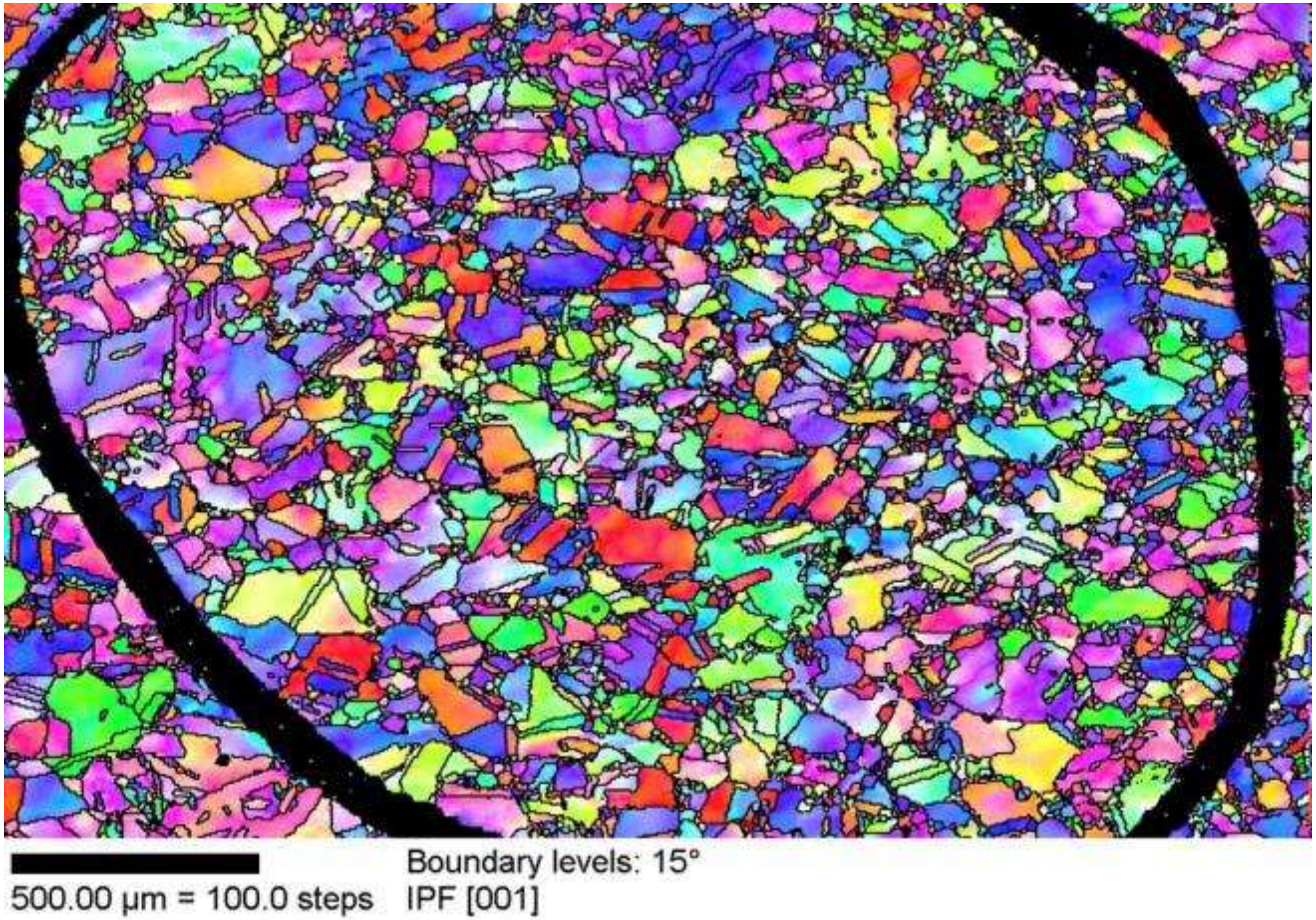


No Technical Data per the EAR or ITAR

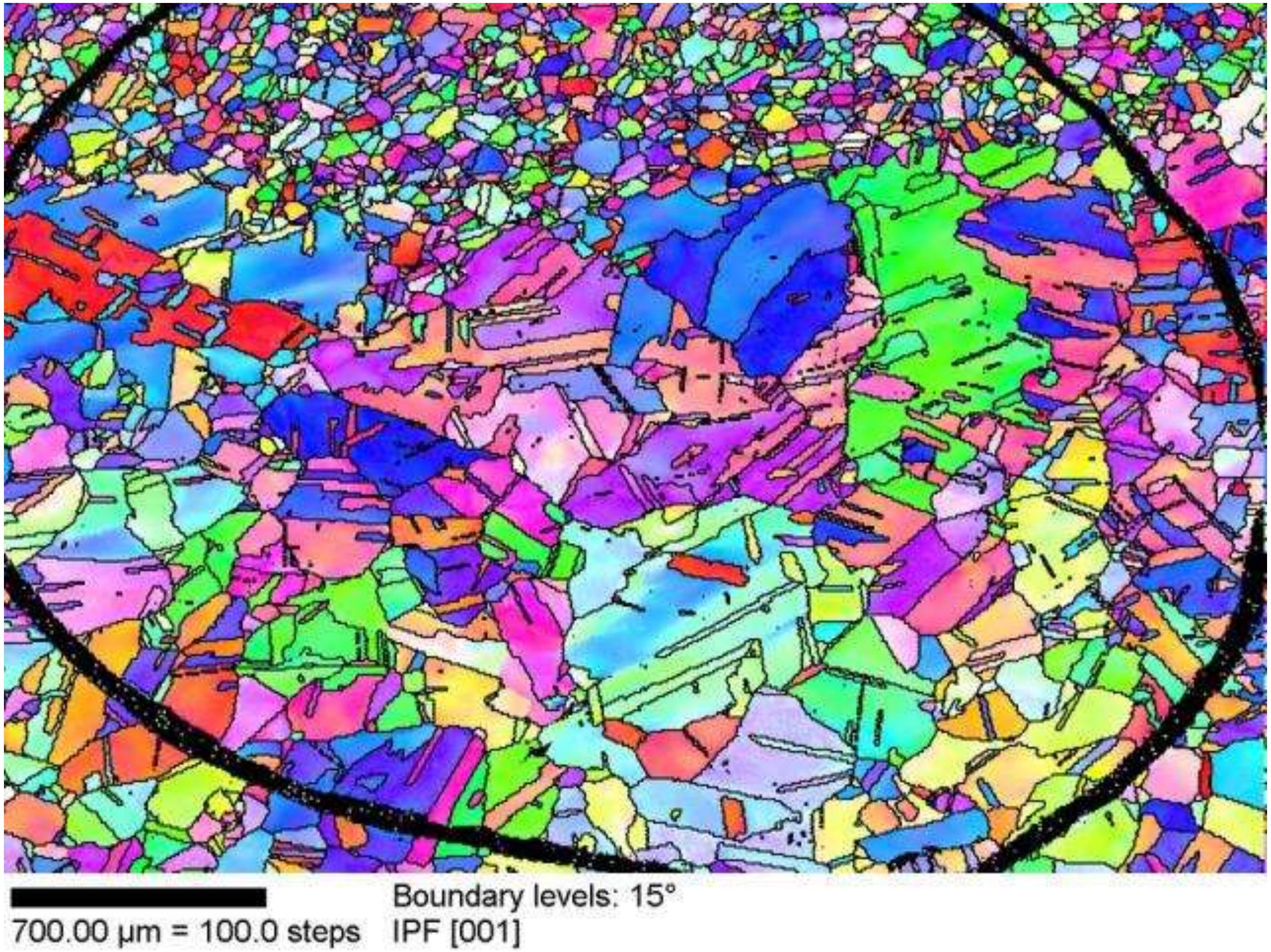
Grain Size Distribution in Waspaloy Material



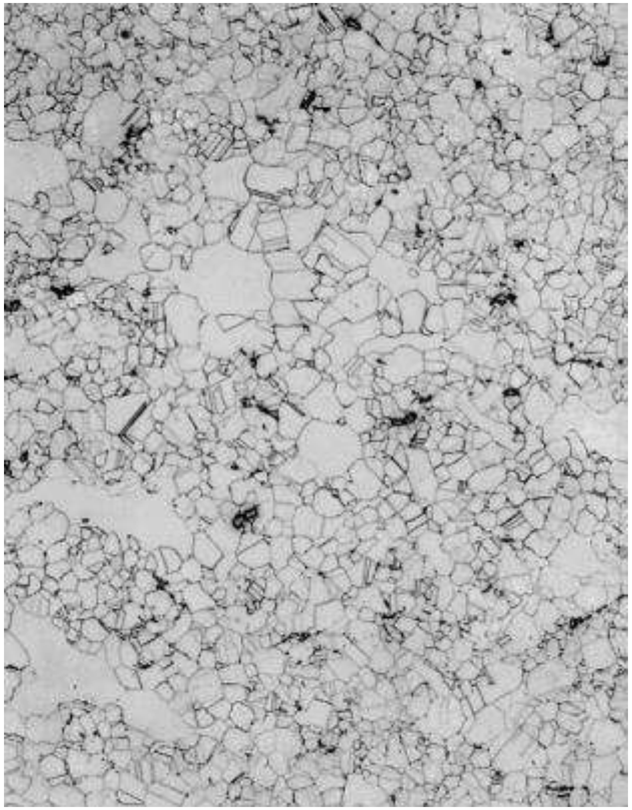
Necklaced Grain Structures in Waspaloy Material



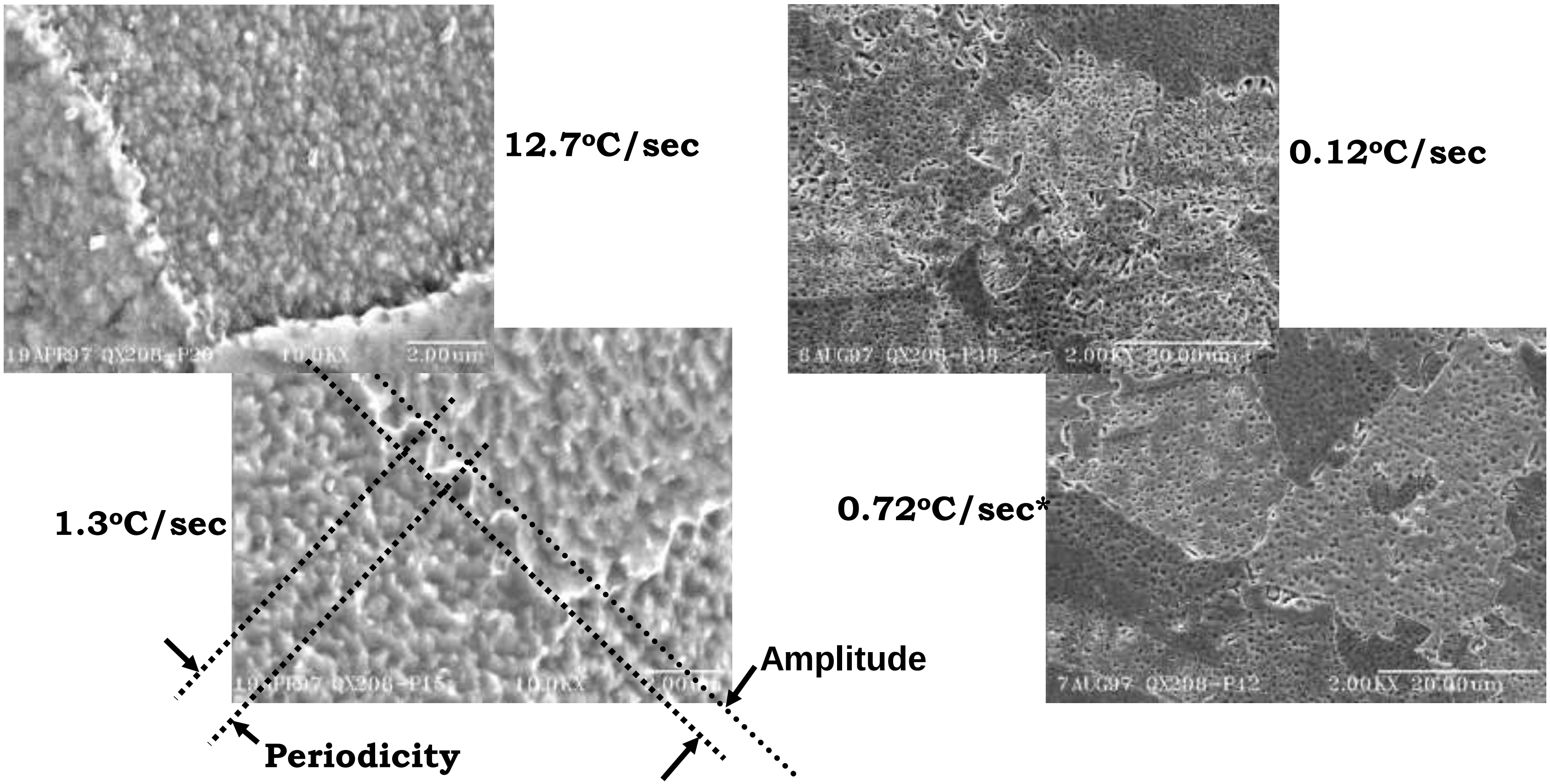
Non-Uniform Grain Size in Waspaloy Material



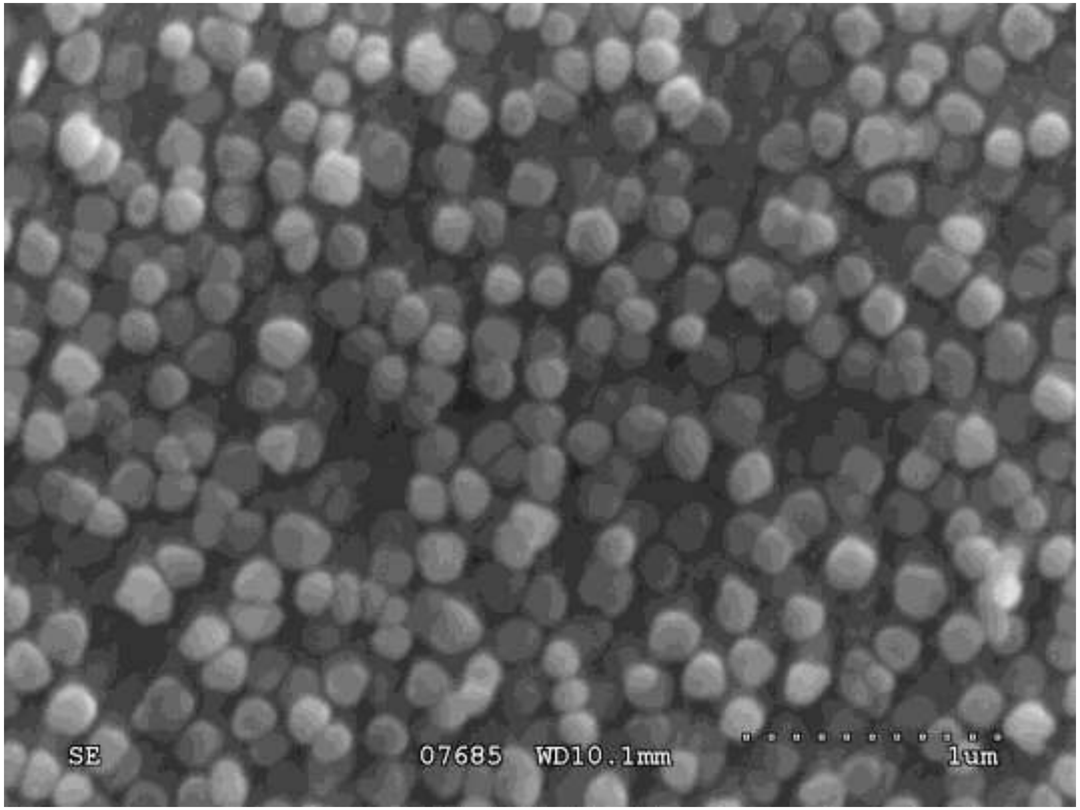
Optical and OIM Images of Partially Recrystallized Wapaloy



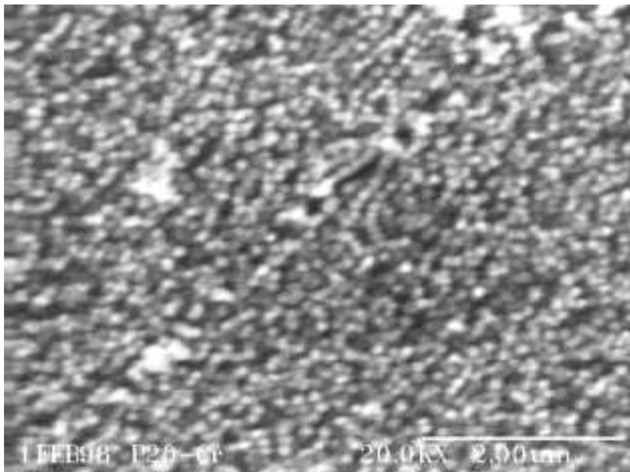
Grain Boundary Morphology in Superalloy U720



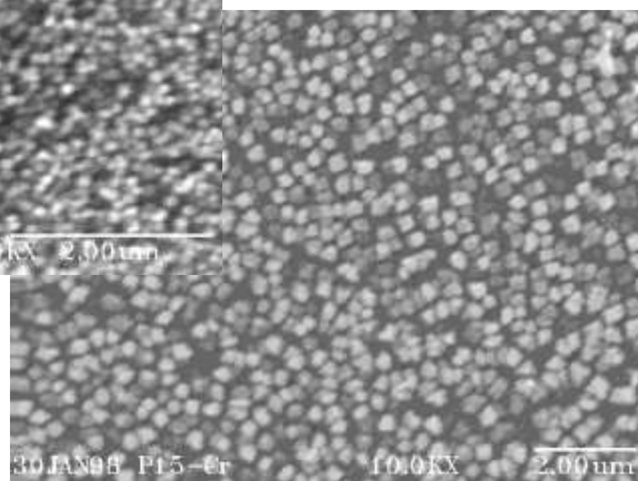
Gamma-Prime Size and Distribution in P/M Superalloy



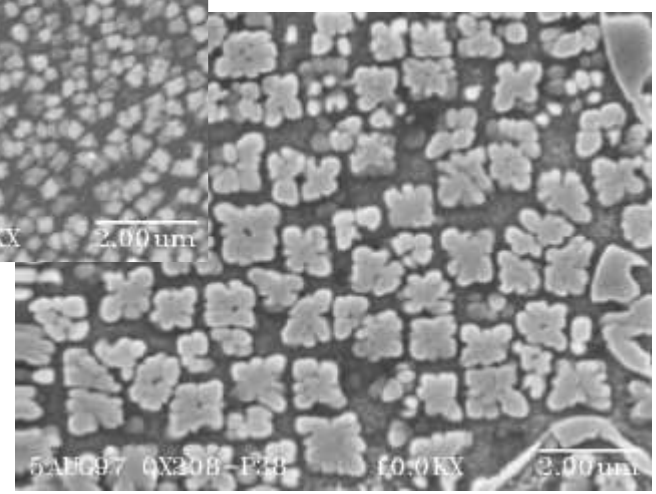
Gamma-Prime Precipitate Size as a Function of Cooling Rate



12.7°C/sec



1.3°C/sec



0.12°C/sec

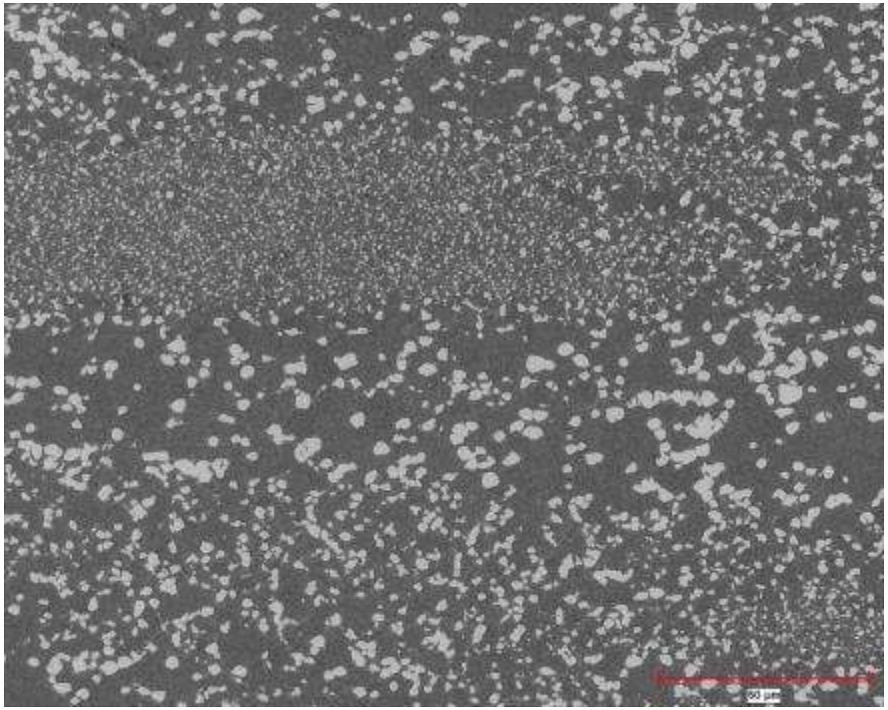
Gamma-Prime Morphology

Gamma-Prime Density

Gamma-Prime Size

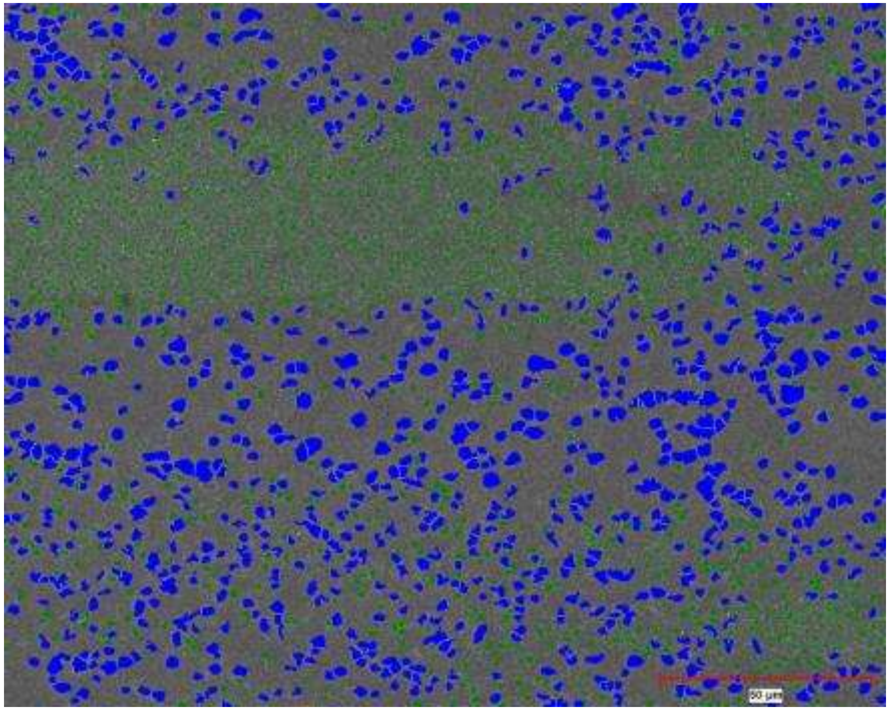
U720

Gamma-Prime Banding in Superalloy U720



Area Percent of Large Grains 12.7%

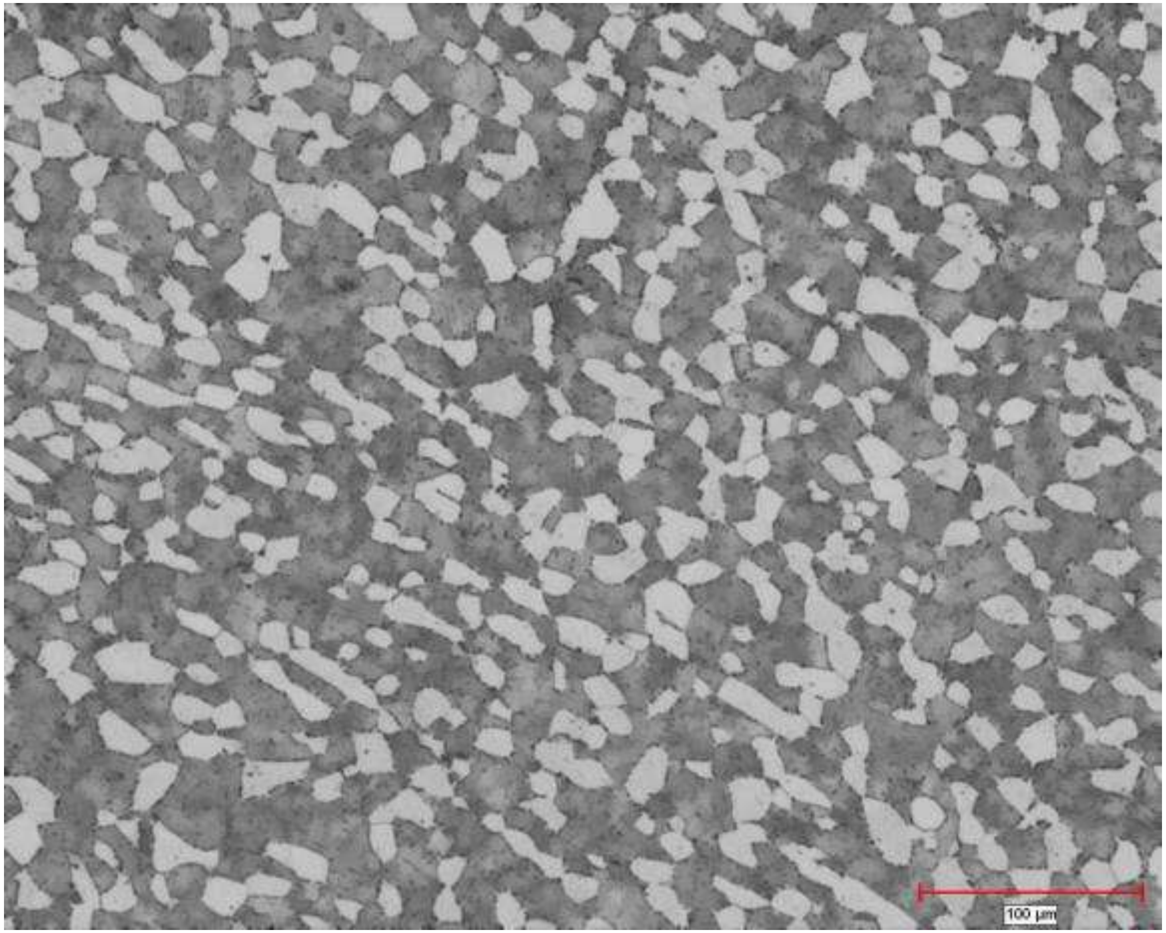
Area Percent of Small Grains 6.43



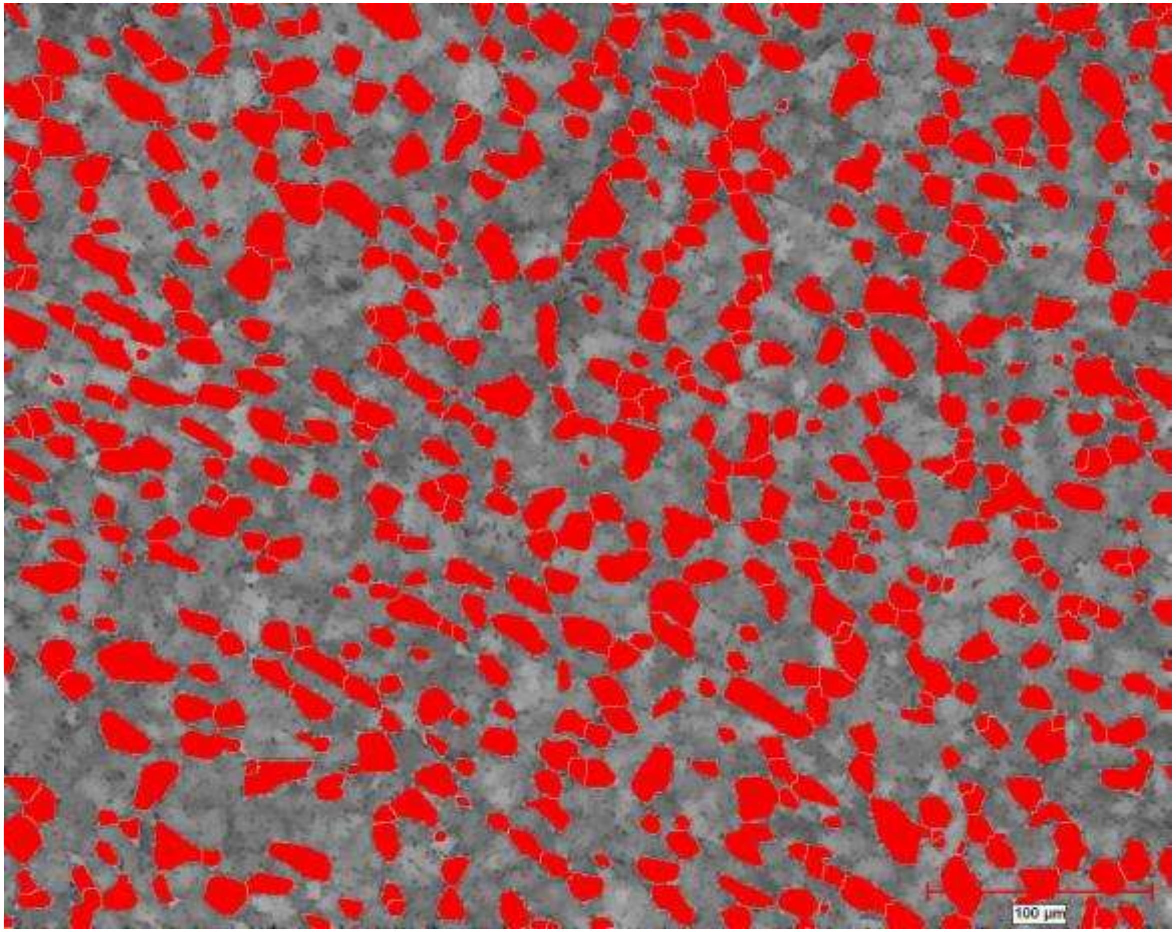
Average Size of Large Grains 5.25 um^2

Average Size of Small Grains 0.626 um^2

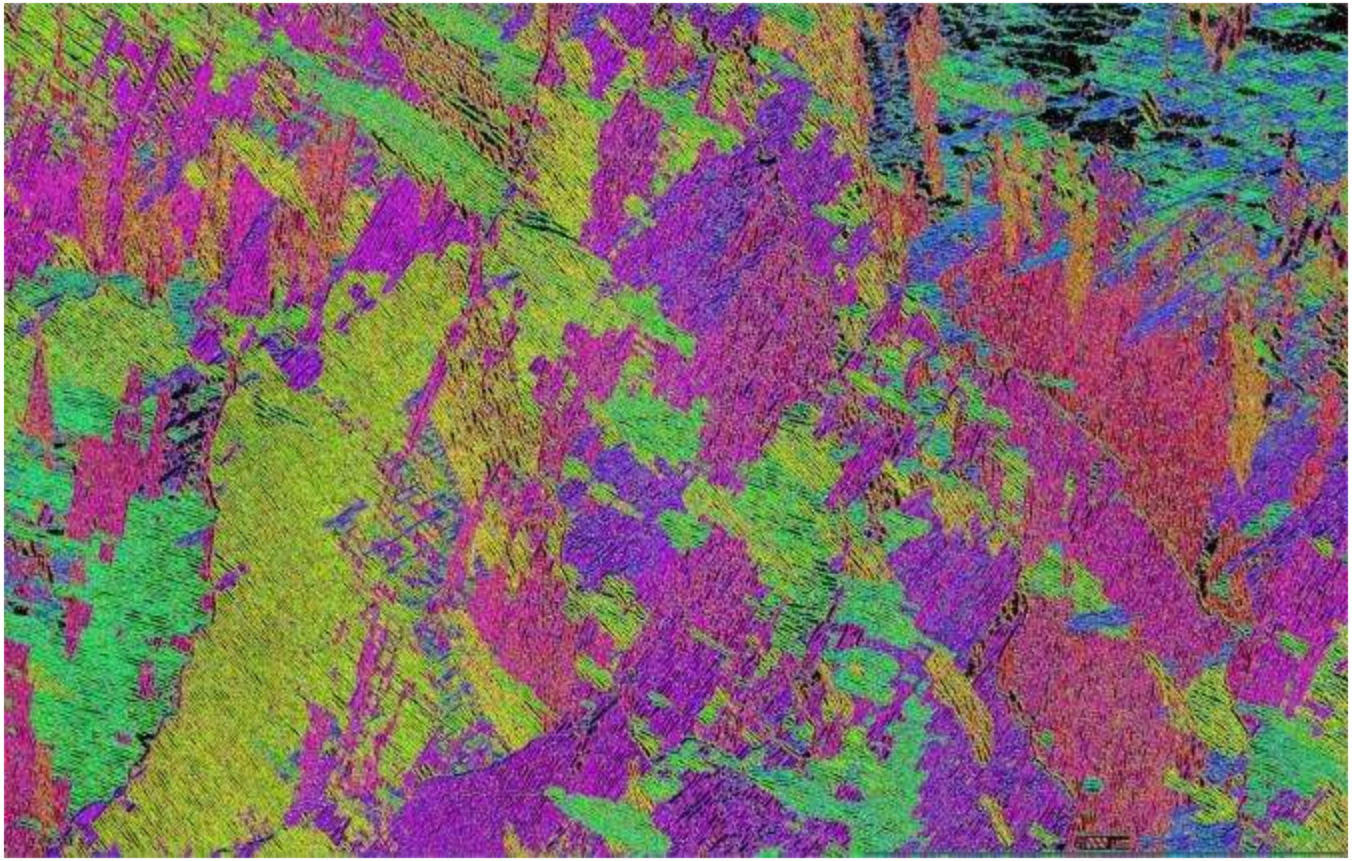
Primary Alpha Size and Volume Fraction in Titanium



Primary Alpha Size and Volume Fraction in Titanium

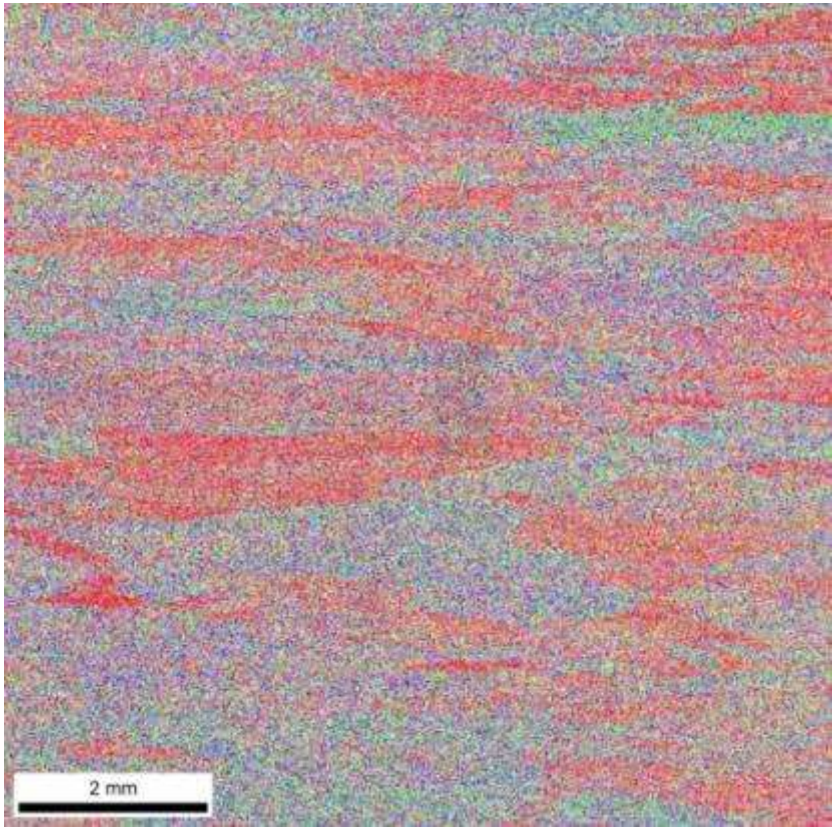


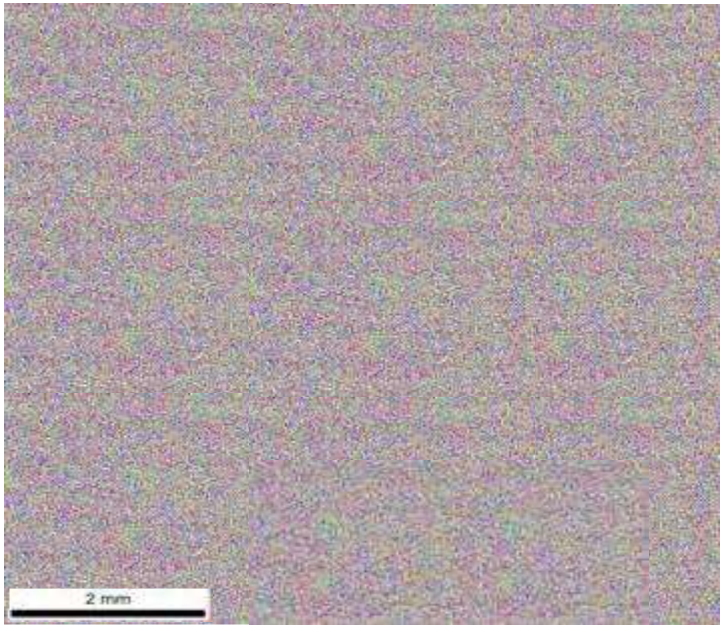
Optical Image Analysis of Ti Transformed Beta Structure



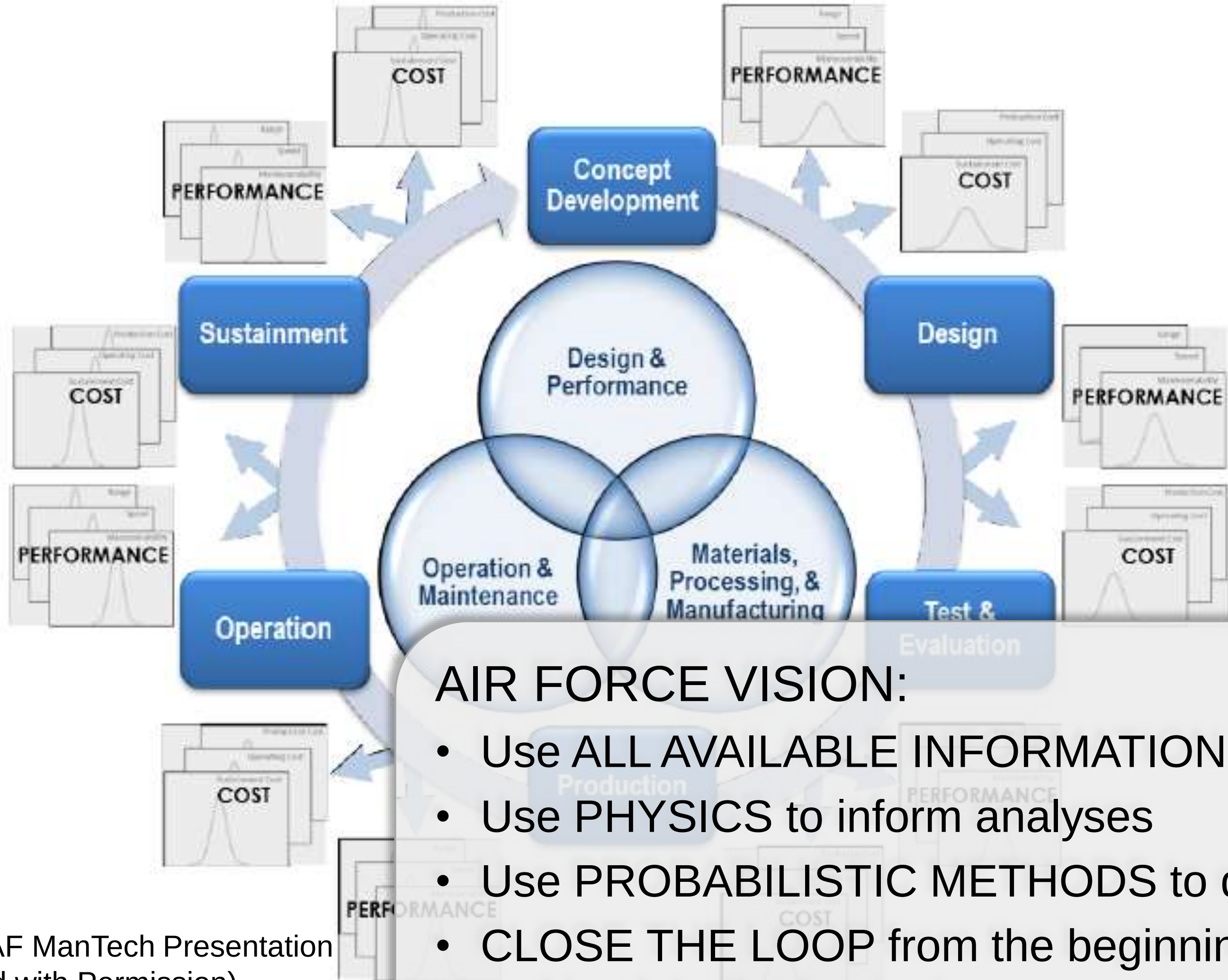
M. Dallair and D. Furrer, “Quantitative Metallography of Titanium Alloys”, Advanced Materials and Processes, December, 2004, pp. 25-28.

Micro-Texture in Titanium Alloys





Digital Thread - Air Force Vision

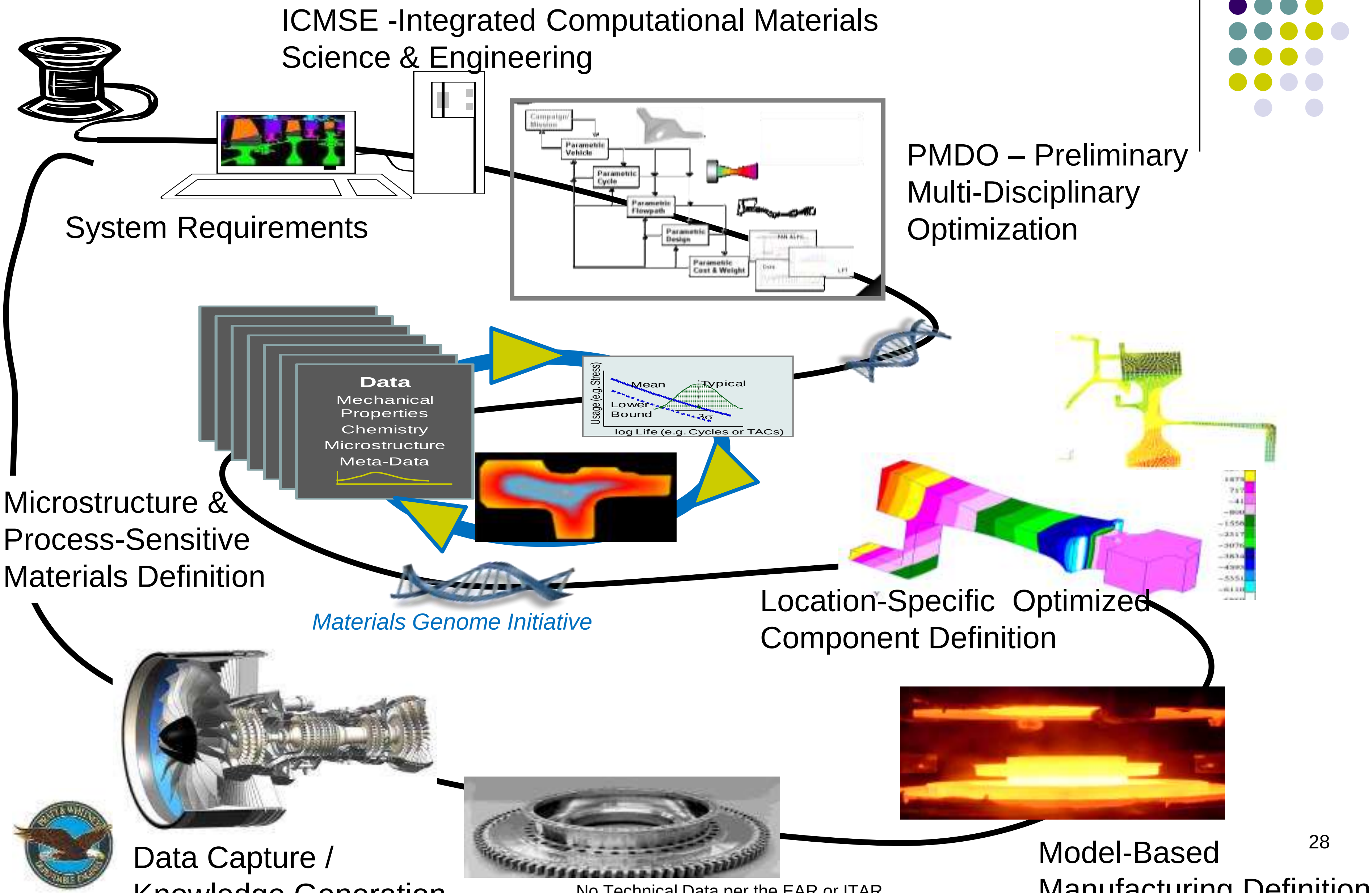


AIR FORCE VISION:

- 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)

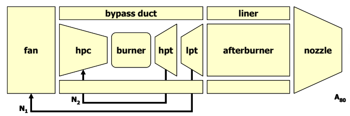
Turbine Disk Digital Thread



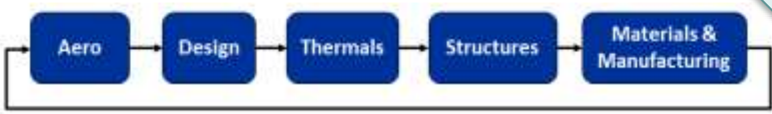
Digital Thread & Design for Variation Vision

Digital Thread Enables More Effective Decision Making Through DFV

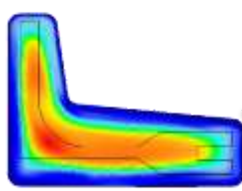
System Engineering Models



Multi-Disciplinary Automated Workflows



Materials and Manufacturing Process Modeling



Engineering System Design / Analysis

Reqts ↓ ↑ Capability

Engineering Component Design / Analysis

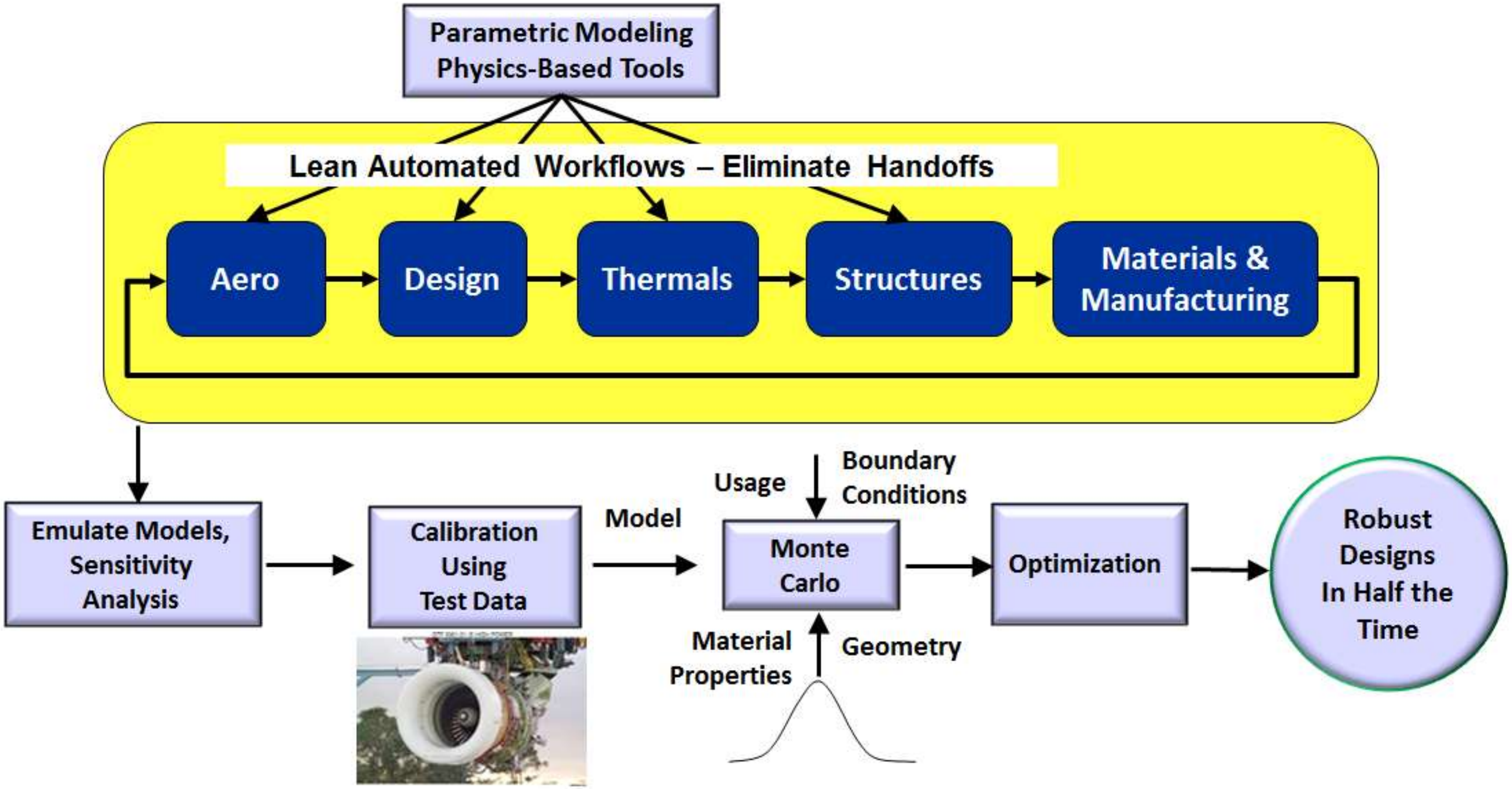
Reqts ↓ ↑ Capability

Manufacturing / Supply Chain

<u>Future State:</u>
Seamless Digital Thread Enables DFV

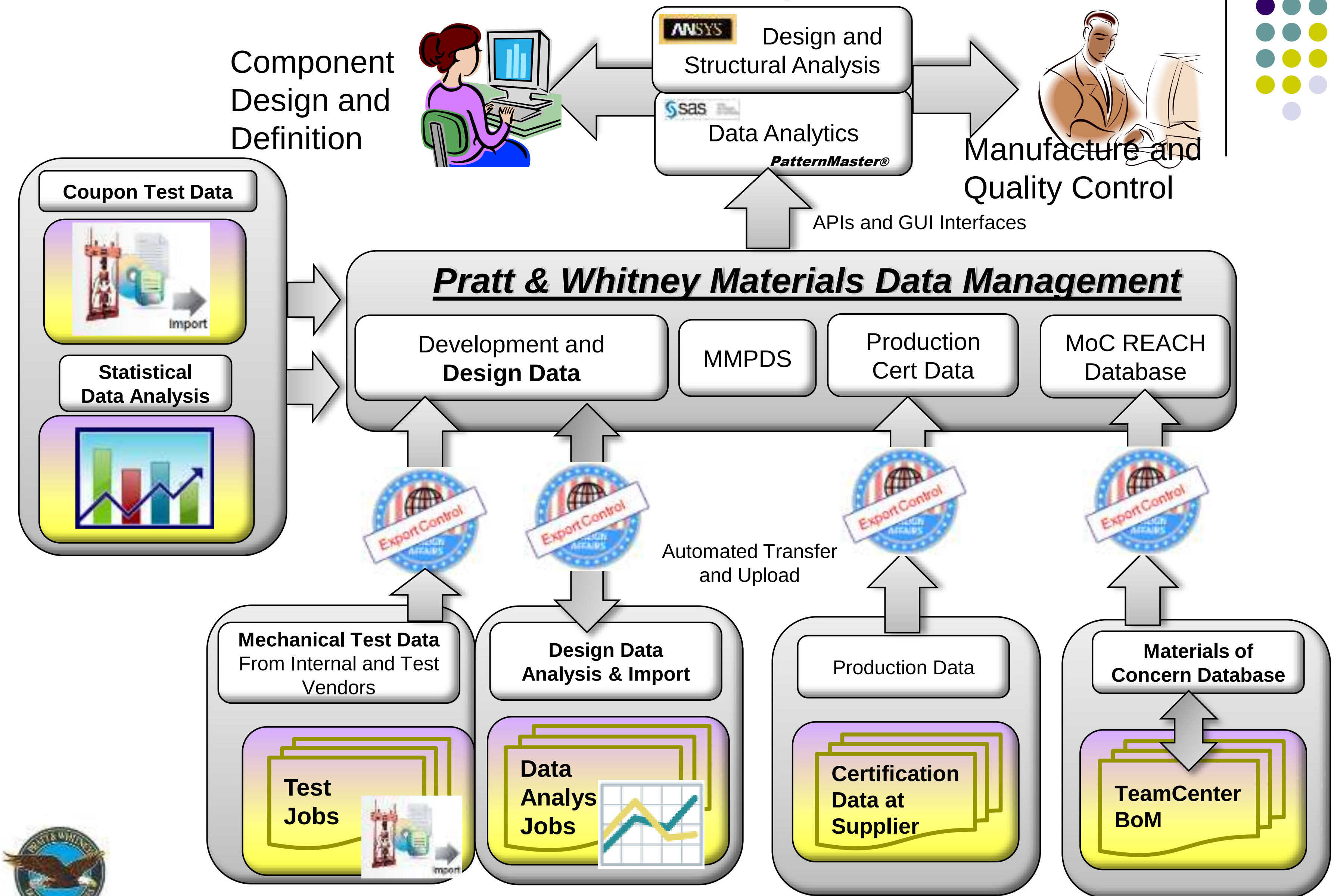
Goal is 50% reduction in development time with 90% elimination of quality non-conformance

Design for Variation



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

Materials Data Management



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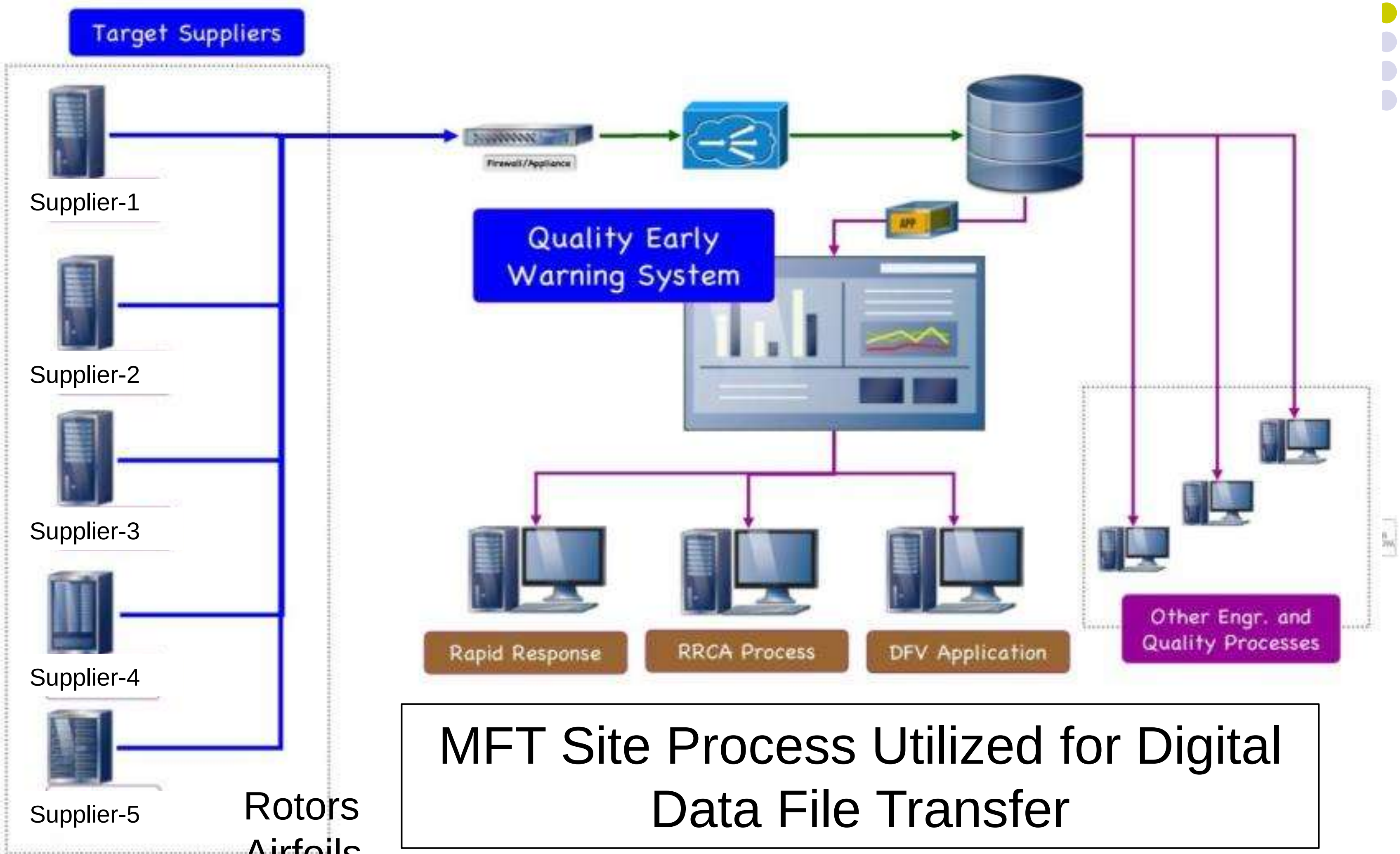
Materials Data Management



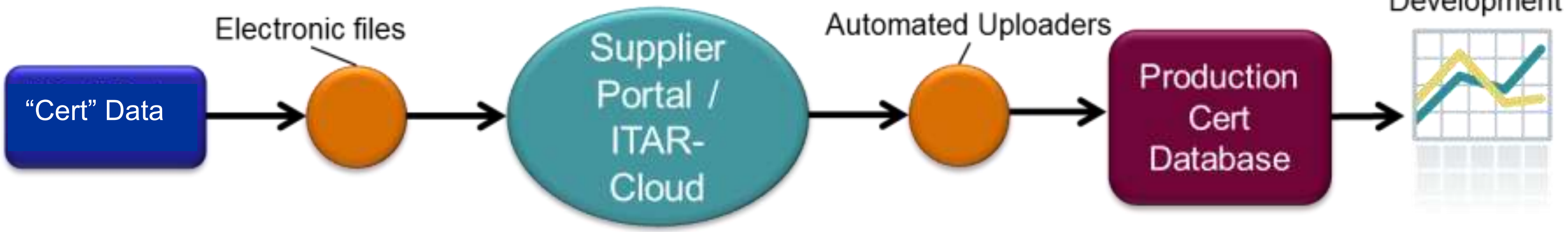
Rotors
Airfoils
Structural Castings

MFT Site Process Utilized for Digital Data File Transfer

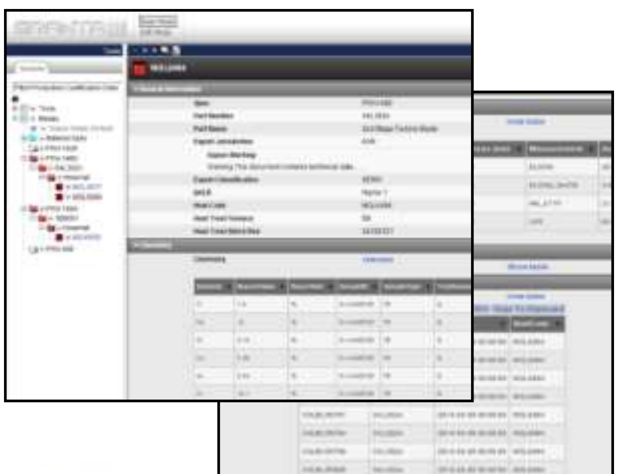
Materials Data Management Initiative

Data Captue Efforts showing Success

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



GRANTA-MI is Live



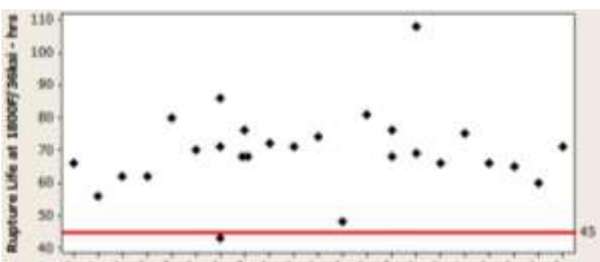
- Production Data Pilot Proving Digital Data Capture Is Possible
- Data has been Analyzed and Applied to Support and Establish Root Cause on Two Recent Materials QNs

Materials Data Management

Success from Data Analytics

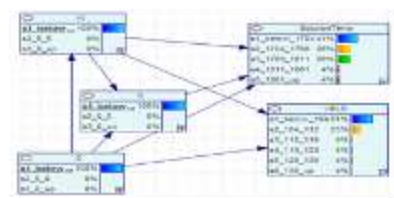
- Production data has been captured, analyzed, linked to models and applied to enhanced material definitions
  - Castings, Forgings
- Optimal chemistry range defined for several legacy alloys, which supports required manufacturing control

Production Data Capture



Quality Release Data

Data Analytics and Model Development

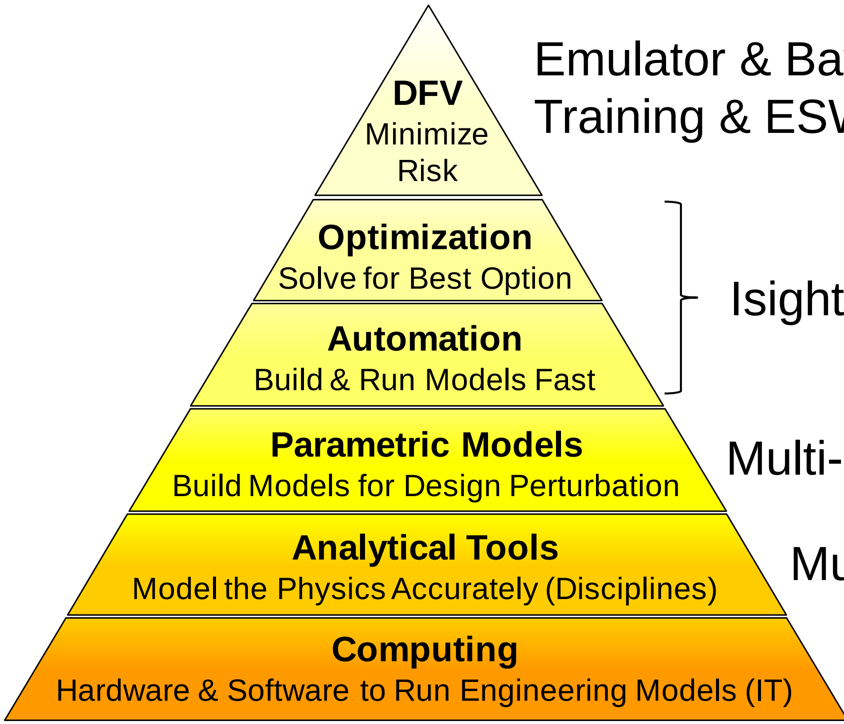


Enhanced Material Definition

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

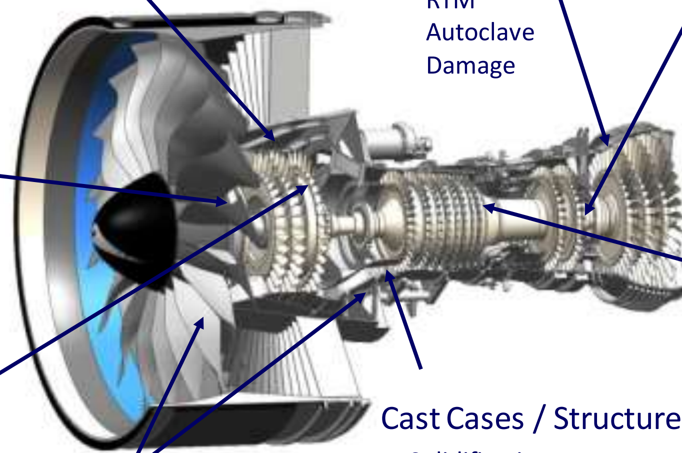
Internal Investment in Key Enablers Driving Broad Implementation of DFV

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

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