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An Information Architecture for ICME

William Marsden
Granta Design

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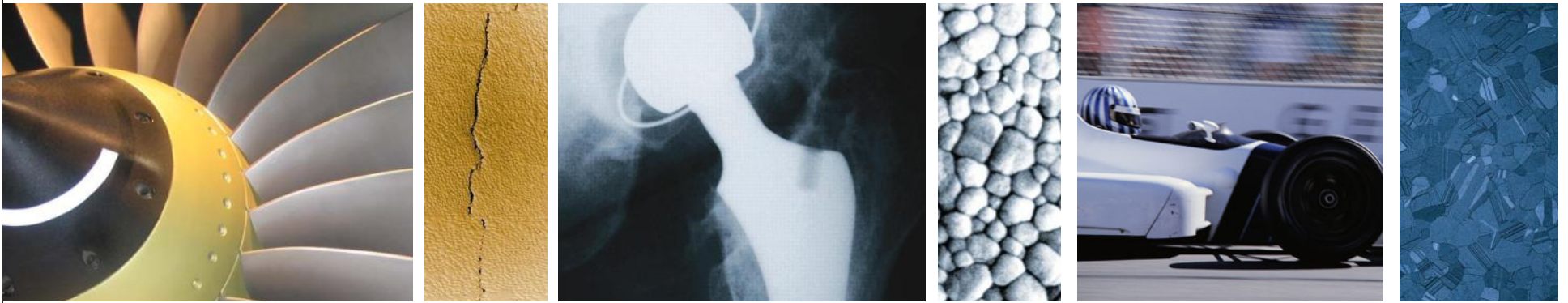
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MATERIAL INTELLIGENCE

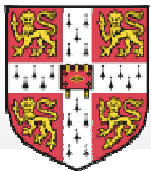
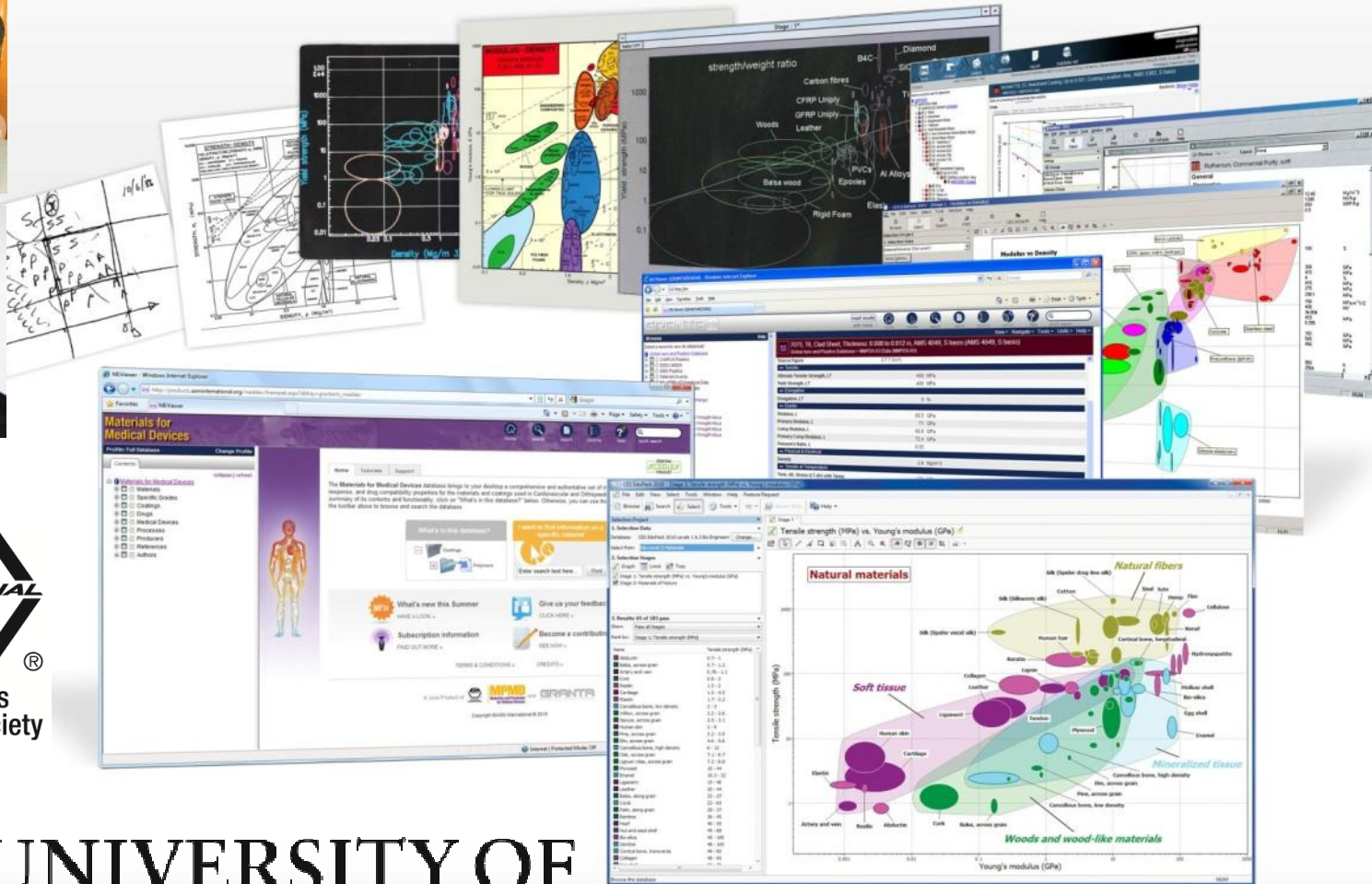
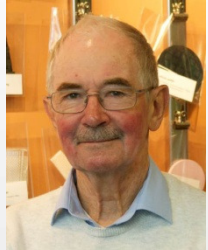


An information architecture for ICME

Will Marsden Ph.D

www.grantadesign.com

Granta Design—innovating since 1994



UNIVERSITY OF CAMBRIDGE



Granta for education

Granta's CES EduPack is used to support teaching of materials & processes at **800** universities and colleges worldwide



The screenshot shows the CES EduPack 2011 software interface. The left pane displays a hierarchical materials database with categories like 'Low carbon steel', 'Medium carbon steel', 'High carbon steel', 'Non-ferrous', 'Aluminum and alloys', 'Copper and alloys', 'Lead and alloys', 'Magnesium and alloys', 'Nickel', 'Nickel-based superalloys', 'Titanium and alloys', 'Commerciually pure titanium', 'Tungsten alloys', 'Zinc and alloys', 'Polymers and elastomers', and 'Composites'. The main window displays a 'Science note' for 'Nickel-based superalloys'. The note includes a description, composition summary, and a stress-strain curve. The curve shows a yield strength σ_y , an elastic limit σ_e , and a tensile strength σ_b . The text below the curve states: 'Figure 1 shows a typical tensile stress-strain curve. The solid part, up to the yield strength σ_y or elastic limit σ_e , defined under Yield strength (elastic limit), is linear (Hooke's law), and it is elastic, meaning that the strain is recoverable - the material returns to its original shape when the stress is removed. Stresses above the elastic limit cause permanent deformation.'



The presentation slide for Unit 12, 'The CES EduPack Bio-materials database', features a photograph of a palm tree. The slide includes the text: 'Unit 12 The CES EduPack Bio-materials database', 'Professor Mike Ashby Department of Engineering University of Cambridge', and the Granta logo. At the bottom, it states: '© M. F. Ashby, 2010 For reproduction guidance see back page' and 'www.grantadesign.com/educationresources'.



Materials Education Symposium, April 2011

The next generation of engineers is familiar with Granta and its technology

Granta for Industry



Aerospace & defense



Automotive & transport



Energy & nuclear



Government & education



High Technology



Industrial / consumer equipment



Materials producers



Medical devices



Motorsports



Online publishing

**Airbus, Aubert & Duval, Boeing, Dow Chemical, Emerson, EADS
Astrium, Ferrari, GE, Honeywell, IHI, Intel, J&J, Moen / Fortune Brands,
MTI, NASA, Renault F1, Rolls-Royce, Schlumberger, Timken, ...**

Some practical problems that we solve

Materials
information
management

Materials
support for
CAD, CAE...

Materials
decision
support

Eco design &
environmental
regulations

1. We lose materials property data or waste time finding it
2. I want to consolidate our materials (test) data in one place
3. We need to improve our monitoring of materials in production
4. We need to derive design data from large sets of material tests
5. I want to deploy corporate materials data to engineers
6. I need to get the correct data into my FEA, CAD, etc...
7. We'd like to publish materials information to our customers
8. I often need to find a cheaper material to do the same job
9. Our company wants to limit proliferation of material choices
10. We'd like to help designers make rational materials decisions
11. We need to position our materials against competition
12. We need environmental design (REACH, low CO₂ / energy, EoL...)

What is Materials Information Technology?

Materials Information Technology

- Everything that computers do in the collating, analysing, managing and deploying of materials information
- The “back office” of everything that happens to materials information, its derivation and use, to ensure that ultimately the optimum material is specified for every application
- The lifecycle management of every property of every material relevant to an organisation, including:
 - ▶ The tools required by the authors of that information, to help them capture it, collate it, analyse and process it, publish it and maintain it
 - ▶ The tools required by the users of that information, to help them apply it appropriately, including:
 - Making optimum decisions in materials selection and substitution, and
 - Using the correct information in design and simulation

Different applications have different needs

Aerospace

- Derivation of design allowables from test data, with full auditability

Automotive (components), and general manufacturing

- Cost avoidance by materials rationalization
- Explore trade-off between function, cost and environmental impact

Automotive (body)

- Provision of non-linear data for forming and crash CAE codes

Medical devices

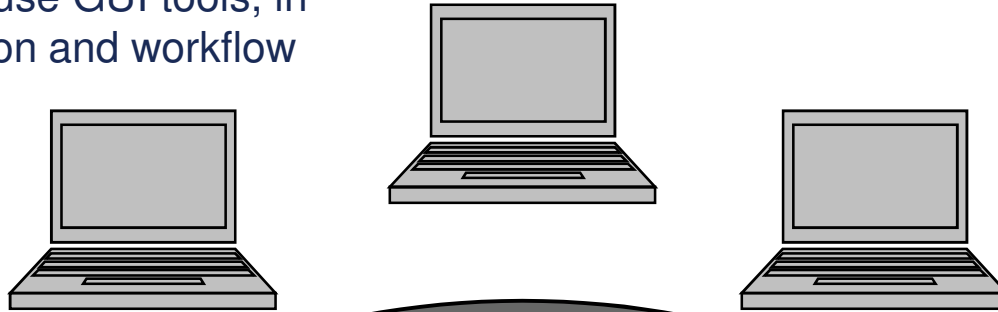
- Knowledge of materials usage in predicate (ie already-approved) devices
- Considering engineering properties alongside biological response

Materials suppliers

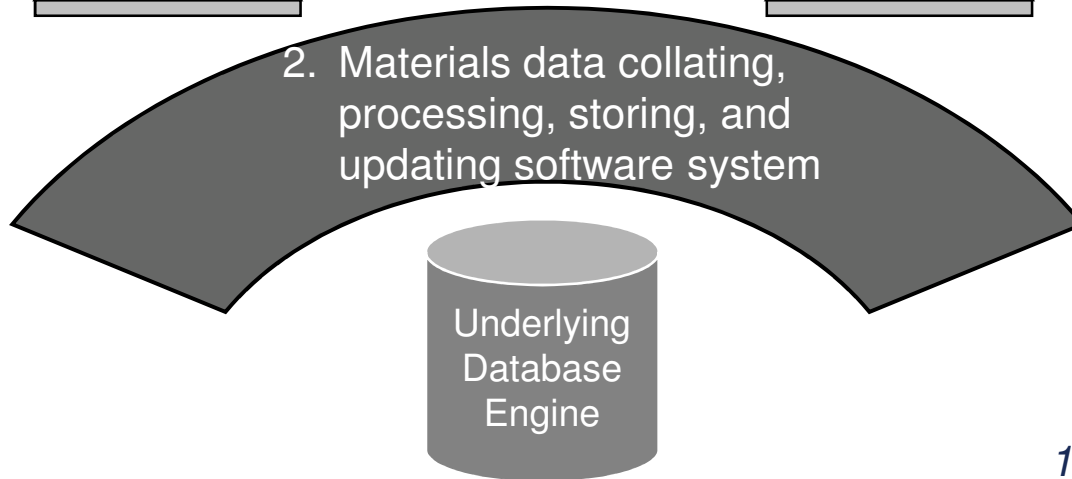
- Systematic method for identifying best applications for new materials

Materials information technology

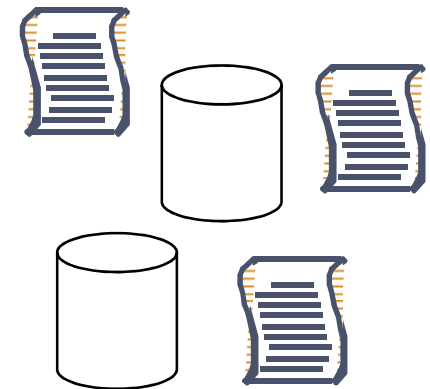
3. Easy-to-use GUI tools, in application and workflow context



2. Materials data collating, processing, storing, and updating software system



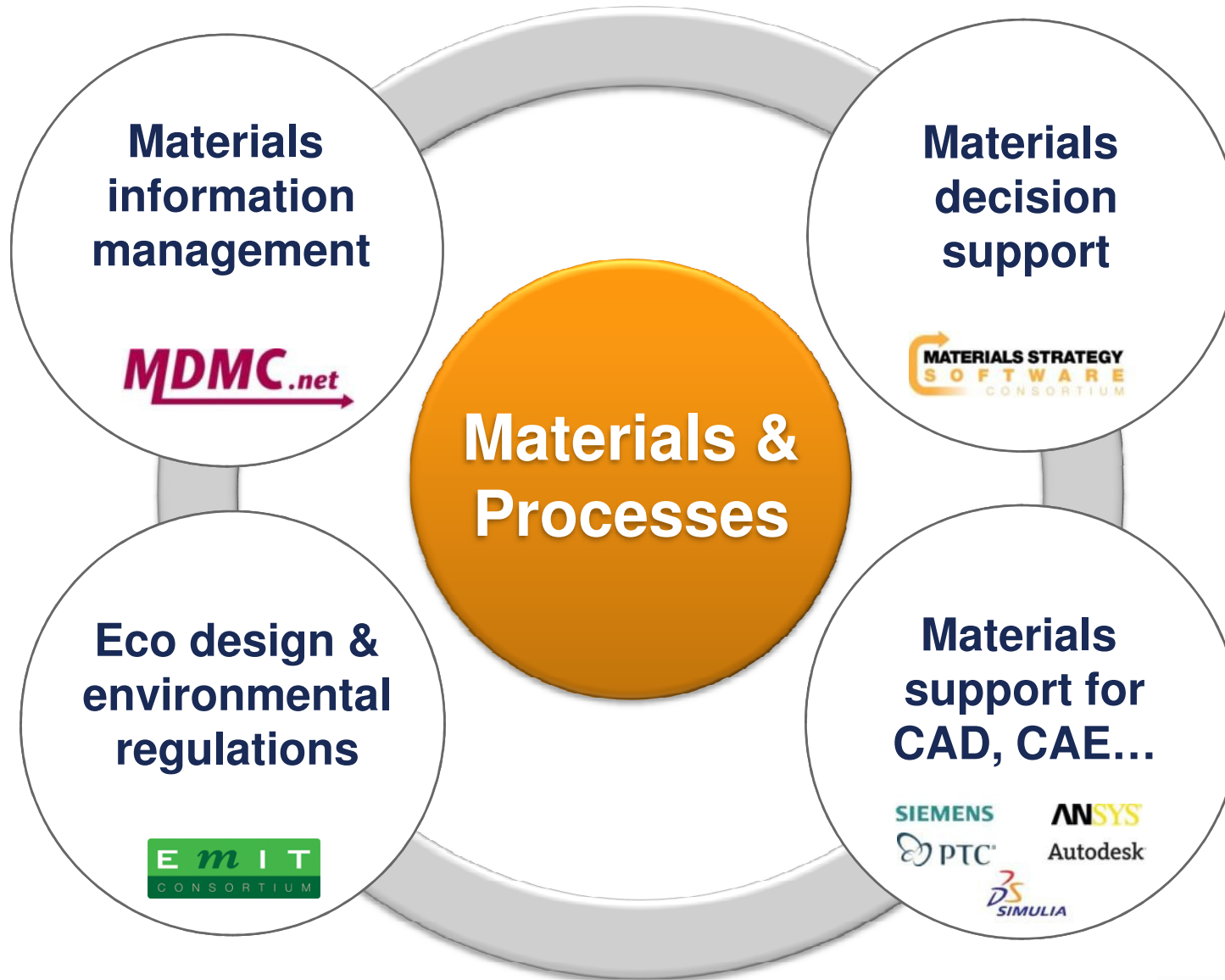
Underlying
Database
Engine



1. *Relevant* data content – and in correct format, quality, precision etc

- Each of 1, 2 and 3 must be fit for purpose for relevant stakeholder(s)
 - (Data producers *and* data users)

Granta for industry



Consortia



AWE
Boeing
Honeywell Aerospace
GE - Aviation
GE - Energy
Lockheed Martin
Los Alamos Nat Labs
NASA
Northrop Grumman
Oak Ridge Nat Labs
Raytheon
Rolls-Royce
Sandia Nat Labs
US Navy SWC
US Army Research Labs



Boeing
EADS Astrium Satellites
Emerson Electric
Eurocopter
Honeywell

Lockheed Martin
NASA
NPL
Rolls-Royce
Thales
US Army Res. Labs

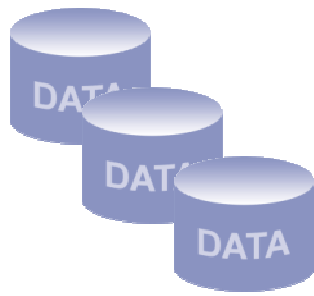
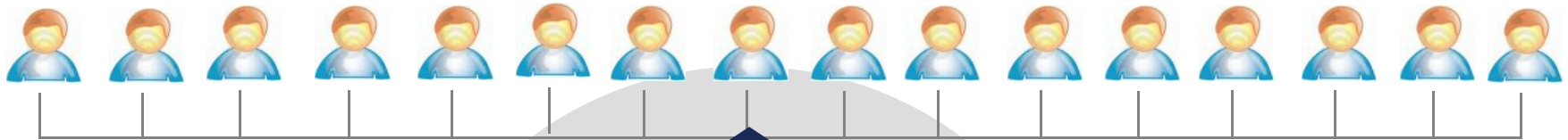


Baker Hughes
DePuy
Emerson Electric
Ethicon Endosurgery

Moen Inc. (Fortune Brands)
NASA
Rhodia
Sulzer
TRW Automotive

Materials information management

EFFICIENT ENTERPRISE-WIDE ACCESS

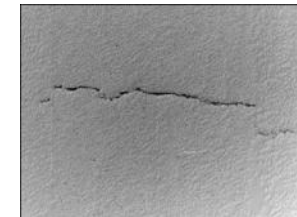
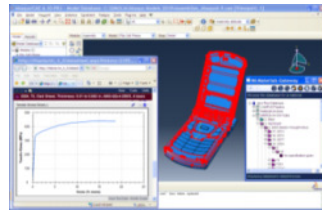


External
reference
data



Proprietary
data

Examples of materials information



Research

Materials R&D

- Testing
- Characterisation
- Statistical analysis
- Reports
- Certification
- Environmental impact
- Model Verification
- Model Validation

Design

Decision support data

- Certified design data
- Reference data
(Properties, cost, eco)
- Purchasing specs
- Preferred materials
- Restricted substances

Production

Materials QA

- Batch testing
- SPC data
- Comparison with specs
- Process improvement

In-service & End-of-life

Materials Performance

- Failure reports
- In-service testing
- Empirical knowledge
- Materials substitution
- Cost reduction
- Materials aging
- Recycling & disposal

Materials information technology differentiators

Not just materials assigned to products – but rather *all* materials relevant to an organization

Not just half a dozen engineering properties – but rather *all* attributes (could be 100's per material)

Lifecycle management on many of these individual properties – a level of granularity and focus not appropriate for a product-oriented system

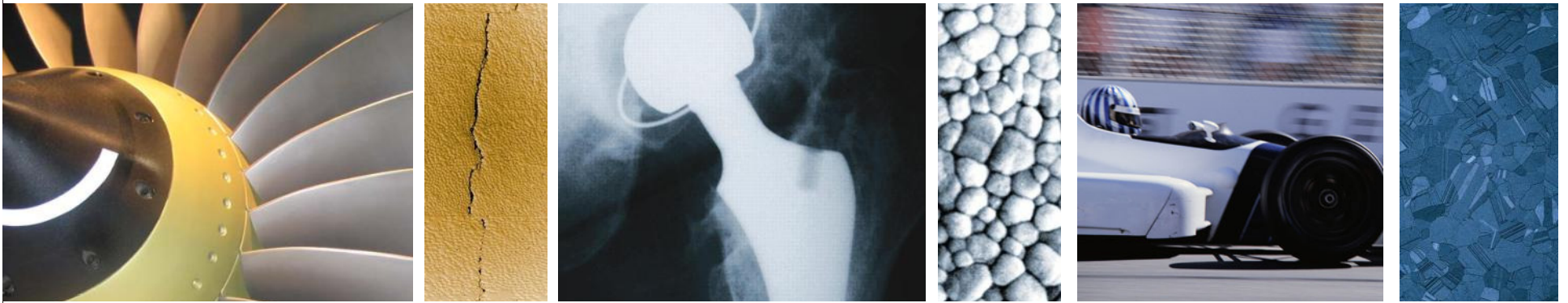
Living data – materials information is NOT a static catalog or library

Property authoring as well as data management – engineering software functionality specified by the MDMC

Incorporates expert guidance tools for data users – reports/dashboards, and selection and substitution

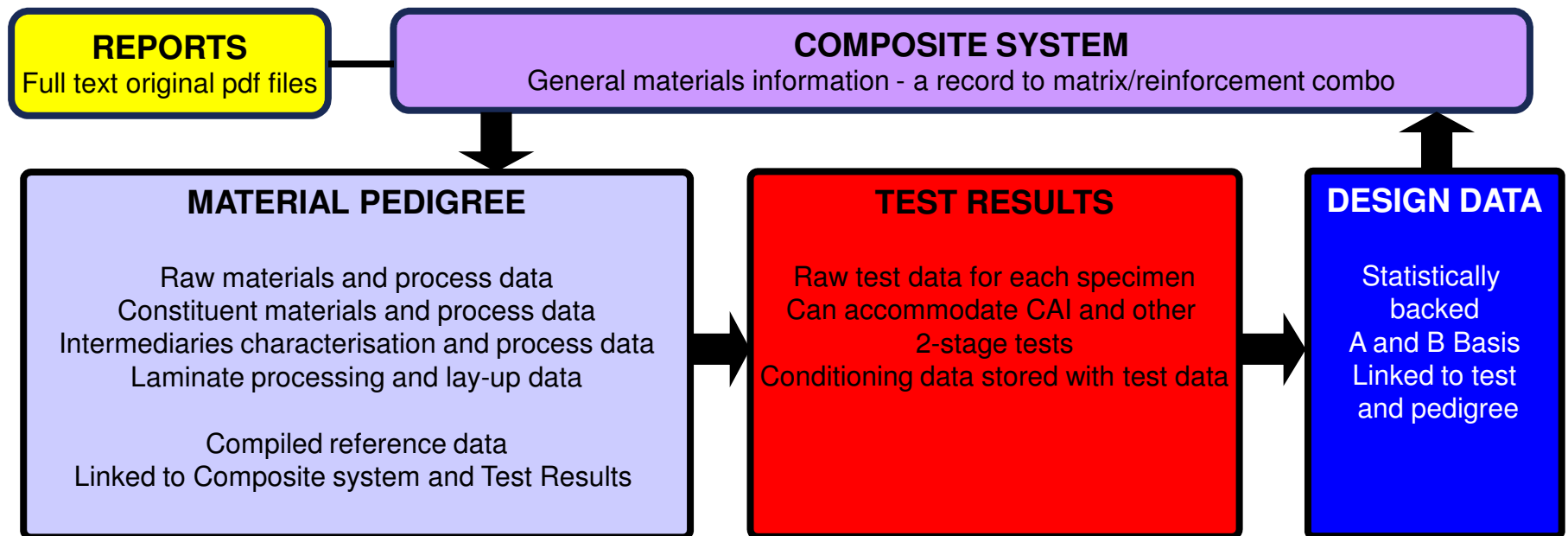
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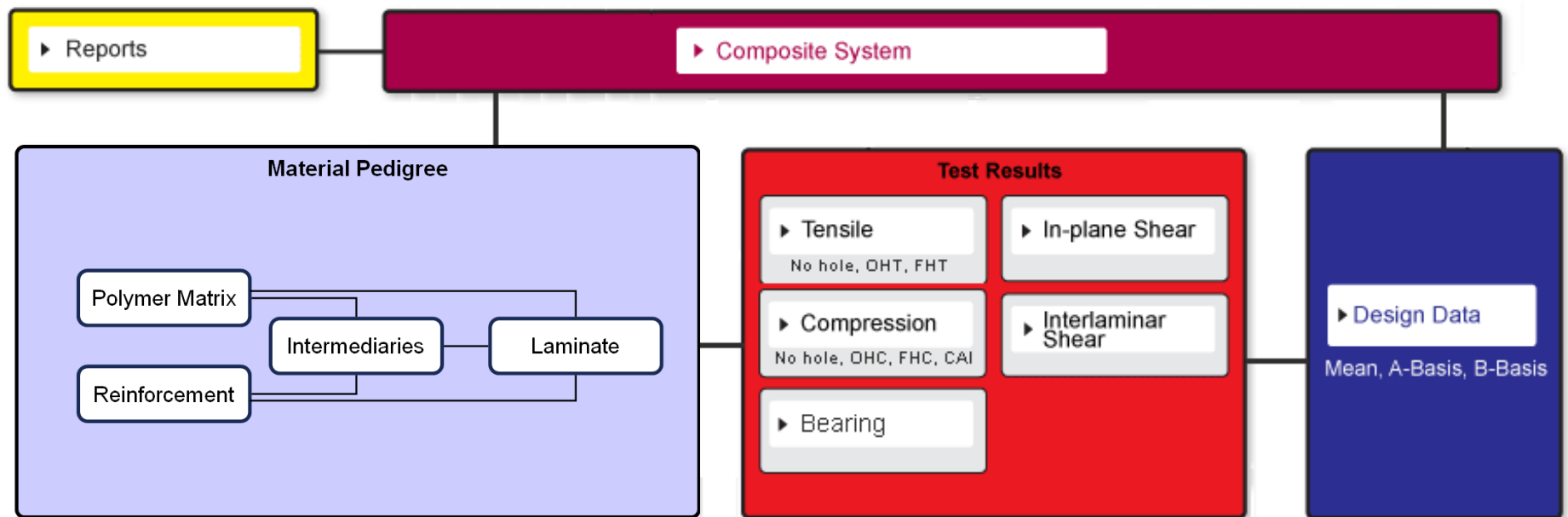


A composite example

MDMC Composites data schema



Composite Data Flow



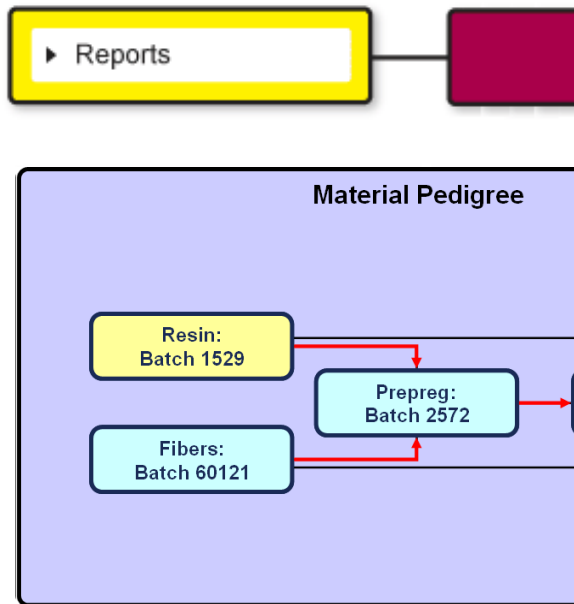
Traceability and processing history

Resin
Batch 15

Fibers
Batch 60

MTM45-1/678		MTM45-1/6781-35%RW, ACG, Panel: AITR1392-8HG-FHC1-D-MH1	
Reinforcement design	Process	Prepreg lay-up	
SCG75 1/0 1.0Z 638 71	Cure cycle		
SCG75 1/0 1.0Z 638 71	Cure type	Oven	
	Autoclave, oven, or press ID	Large Oven	
	Initial applied vacuum	948	mb
	Cure vacuum maintained throughout cure?	Yes	
	Cure cycle phases		
	Post cure cycle phases		
	Receiving inspection		
	Panel thickness, average (measured)	3.17	mm
	Laminate density (measured)	1.79	g/cm ³
	Total reinforcement volume fraction (measured)	46.1	%
	Total matrix weight fraction, %wt (measured)	35.3 to 36.2	%
	Volatile content (measured)	0.22	%
	Ply thickness, average (measured)	0.263	mm
	Cured ply thickness (measured)	0.262	mm
	Traceability		
	Document reference	CAM-RP-2009-001 Rev. A	
	Original report	Qualification Material Property Data Report, CAM-RP-2009-001 Rev. A	
	Tests performed on this panel		
	Density (measured)	2.46	g/cm ³
	Linear density (measured)	0.0000669	kg/m
	Tensile strength (measured)	1890	MPa

Test results and Design data



MTM45 ACG MTM45-1/HTS(12K)-145-32%RW, 12K HTS5631 unidirectional, 25%(0°) / 50%(±45°)

0° compression test method ASTM D6641-01E1

0° compression modulus

[Hide table](#)

[Save To Excel \(CSV\)](#) [Copy To Clipboard](#)

Basis	Normalized (GPa)	Measured (GPa)
Mean	44.3	43.6

[Save To Excel \(CSV\)](#) [Copy To Clipboard](#)

Details

Measured/normalized	Coefficient of variation (%)	Maximum (GPa)	Minimum (GPa)
Normalized	3.37	46.9	41.5
Measured	3.82	46.7	40.5

Modulus calculation linear fit

Modulus calculation range 1000 to 3000 microstrain

Normalized by 0.0055

Number of prepreg lots 3

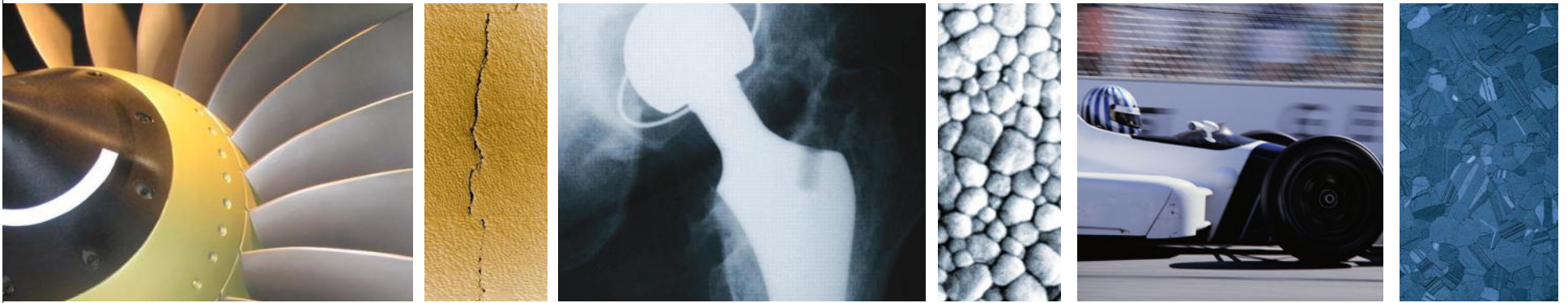
Number of specimens 20

Tests used to generate this data

Specimen	Modulus (actual) (GPa)	Modulus (normalised) (GPa)
ABMWA11BD	46.7	46.9
ABMWA11CD	45.3	45.3
ABMWA11DD	45.3	45.6
ABMWA11ED	45.6	45.6
ABMWA21CD	43.3	43.5
ABMWA21DD	44.1	44.6

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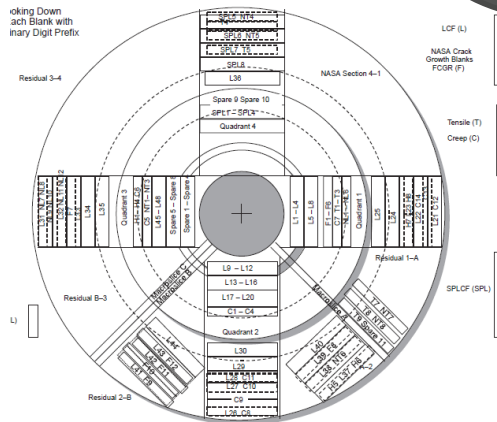
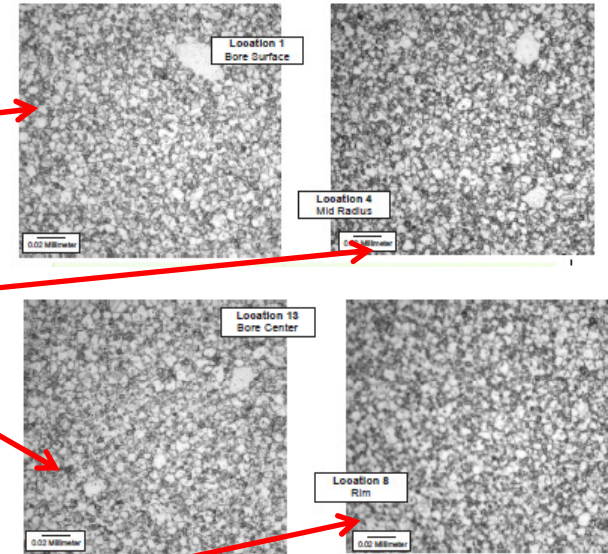
MATERIAL INTELLIGENCE



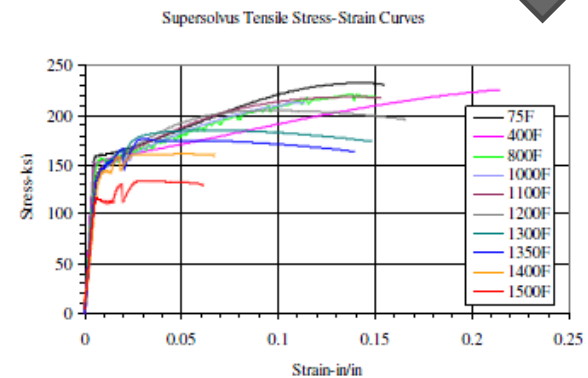
A metallic example

Identified Data Schema to Enable Data mining of Microstructure / Property/ Performance Relationships (ICME: Create a Data Tsunami)

Accomplishment: Established data scheme for capturing and analyzing Nickel based superalloy, e.g. Me3, turbine disk material information necessary to enable microstructure/property/failure relationships. Me3 and LSHR materials will be used as our model systems to verify the robustness of approach.



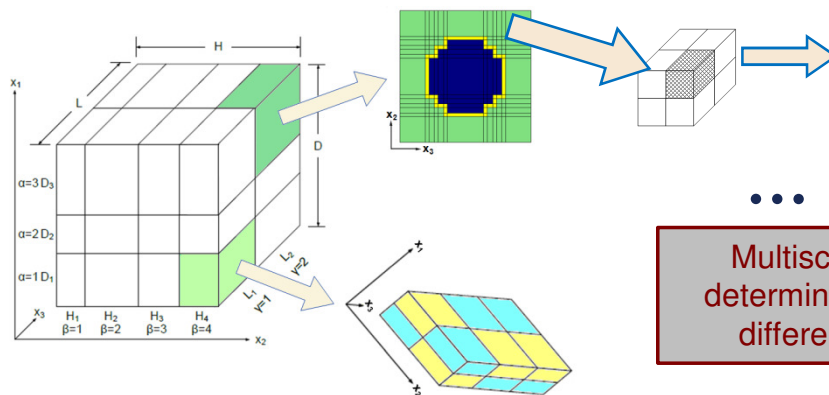
**Pedigree of Location:
Requires tracking of
specimen location and
microstructure**



Efficient Multiscale Microstructural (EMMS) Modeling Tool

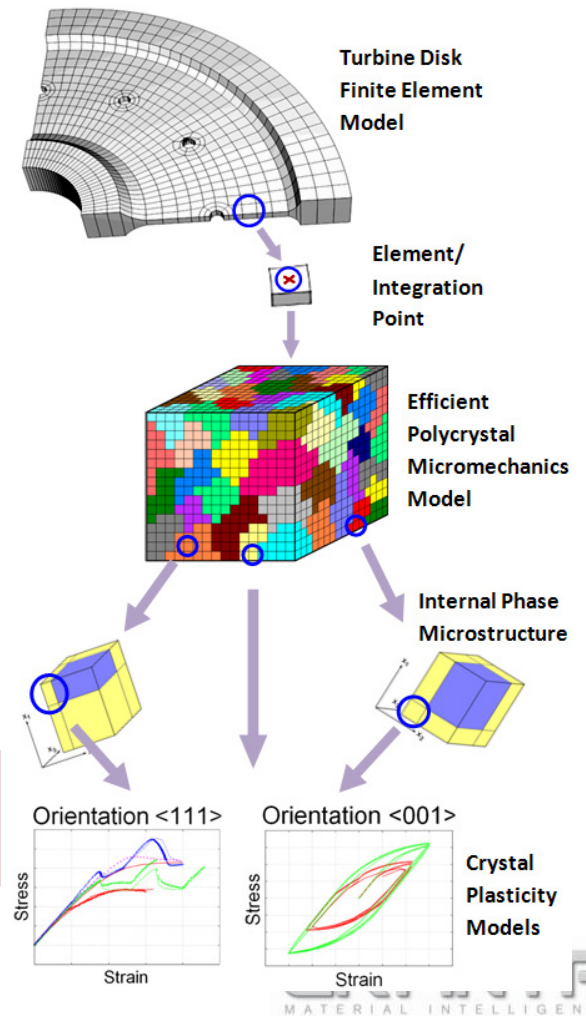
Utilizes NASA's ultra-efficient micromechanics methods to link grain and sub-grain behavior to the performance of the structure

- 100x100x100 RUC; EMMS (33 secs), FEA (hrs)
- EMMS 2-3 orders of magnitude faster
- Works for any arbitrary multiphase material
 - Elastic / Inelastic / Damage

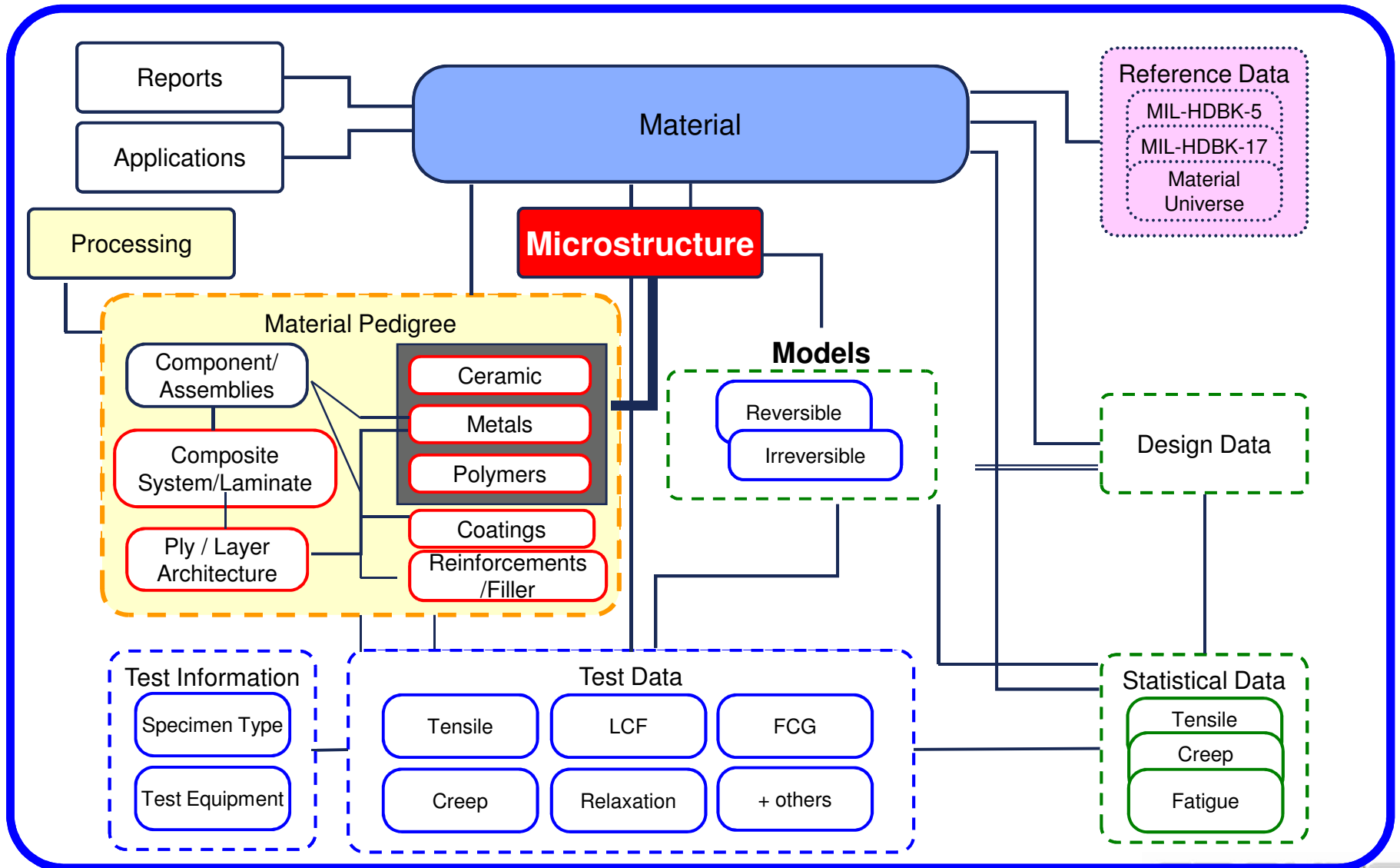


Multiscale analysis can determine local stresses at different length scales

$$\sigma^{\{\alpha\beta\gamma\}\{\beta g\}} = C^{\{\alpha\beta\gamma\}\{\beta g\}} A^{\{\alpha\beta\gamma\}\{\beta g\}} A_{tt}^{\{\alpha\beta\gamma\}} A_{ip}^{\{\beta\gamma\}} \Delta \epsilon$$



MDMC Schema development



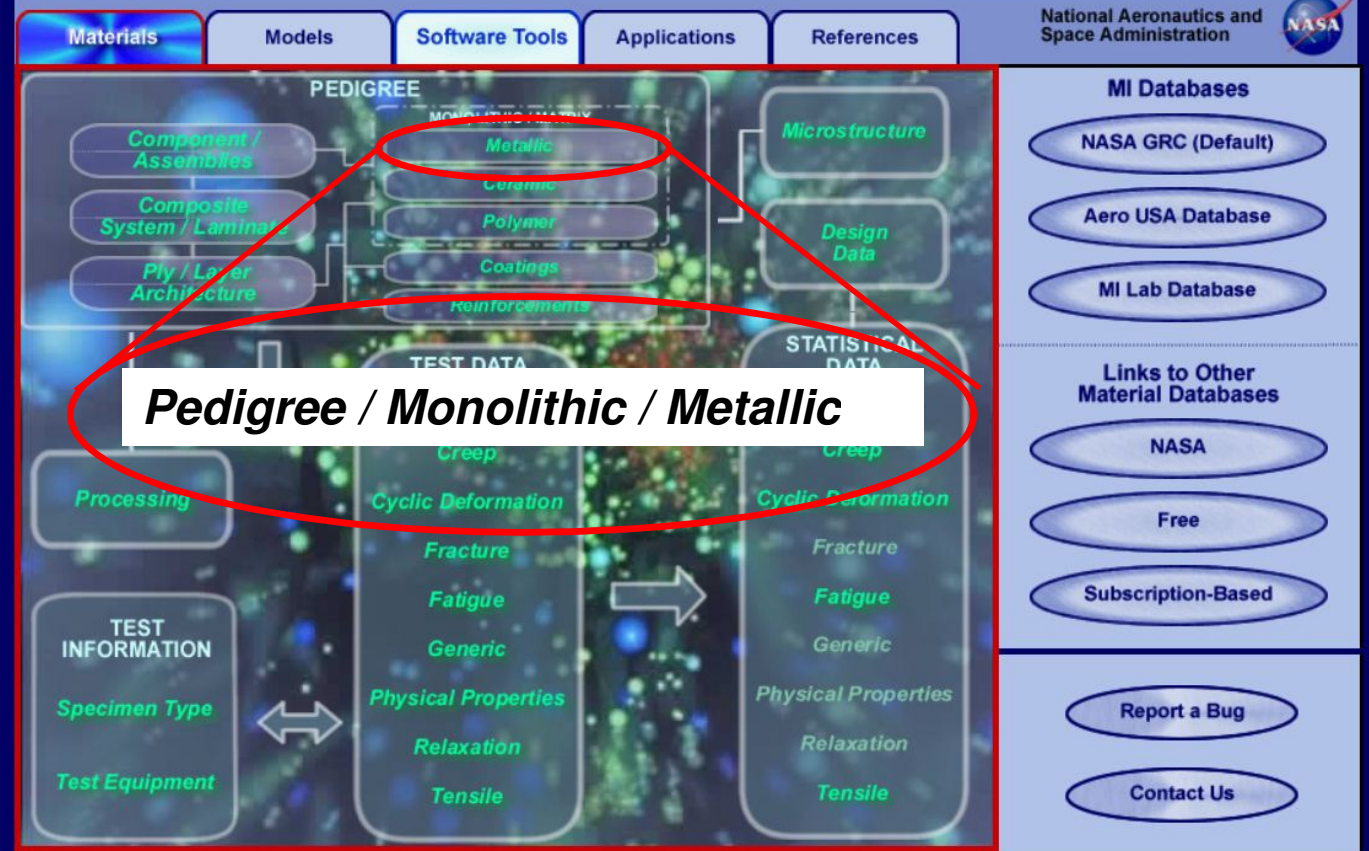
The NASA schema

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read mode
edit mode



- Tools
- Contents
- NASA GRC
 - Aerospace Materials
 - Subset: NASA Materials
 - Cobalt Alloys
 - Copper Alloys
 - Nickel Alloys
 - Resin/Fiber
 - Titanium Alloys
 - Applications
 - Design Data
 - Heat Treatment Reference
 - Material Behavior Models
 - Microstructure
 - Pedigree: Ceramics
 - Pedigree: Coatings
 - Pedigree: Component/Assemblies
 - Pedigree: Composite Ply Architecture
 - Pedigree: Composite System-Laminate
 - Pedigree: Metals
 - Pedigree: Polymers
 - Pedigree: Reinforcements
 - Physical Properties
 - Processing Methods
 - References: Information/Resources
 - References: Publications
 - References: Schematics
 - Software Tools
 - Space Environment Effect
 - Statistical Data: Creep
 - Statistical Data: Cyclic Deformation
 - Statistical Data: Fatigue
 - Statistical Data: Tensile



General disc info – cut-up diags etc

RANTAmi



View Tools Units

Tools

Contents

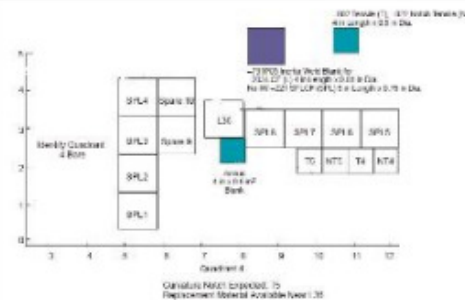
NASA.GRC

- [-] Aerospace Materials
- [-] Applications
- [-] Design Data
- [-] Heat Treatment Reference
- [-] Material Behavior Models
- [-] Microstructure
- [-] Pedigree: Ceramics
- [-] Pedigree: Coatings
- [-] Pedigree: Component/Assemblies
- [-] Pedigree: Composite Ply Architecture
- [-] Pedigree: Composite System-Laminate
- [-] Pedigree: Metals
 - [-] Subset: NASA
 - [-] Cobalt
 - [-] Copper Alloys
 - [-] Nickel
 - [-] Hastelloy X
 - [-] ME3 Disks
 - [-] Titanium
 - [-] Pedigree: Polymers
 - [-] Pedigree: Reinforcements
 - [-] Physical Properties
 - [-] Processing Methods
 - [-] References: Information/Resources
 - [-] References: Publications
 - [-] References: Schematics

ME3 Disks

You are operating with temporarily restricted privileges. [Click here to change restrictions.](#)

Cutup Diagram Picture 4



FP Heat Treatment

Additional Processing Notes

Further Information

Record Link	Task K
Processing Description	1 Linked Record(s)
	Powder Extrusion
Creep Test Data	7 Linked Record(s)
	H101-C12
	H101-C13
	H101-C4
	H101-C5

Processing data for specific discs

The screenshot displays the GRANTA Mi software interface. On the left is a navigation tree with categories like 'Pedigree: Metals', 'Titanium', and 'Processing Methods'. The main window shows the material 'HMI / Supersolvus low cool + high stabilize (H101 demo only)'. A yellow warning banner at the top states: 'You are operating with temporarily restricted privileges. Click here to change restrictions.' Below this, the 'Final Composition' is listed as 3.42Al-0.0222B-0.059C-20.64Co-12.92Cr-3.80Mo-0.91Nb-2.30Ta-3.58Ti-2.01W-0.051Zr-bal. Ni (wt.%). The 'Additional Information' section shows '1 Linked Record(s)' for 'ME3 Disks'. The 'FP Heat Treatment' section includes 'Heat Treat ID: S101' and 'Solution Heat Treated: Yes'. The 'Microstructure' section lists 'Grain Size: 27.5 microinches', 'Grain Size ASTM #: 7.1', 'Grain Size Average Diameter: 31 microinches', and 'Grain Size Range: 20 to 41.5 microinches'. The 'Further Information' section contains three linked records under 'Microstructure Details': 'Disk S101 Cross-Section (Macroslice)', 'S101-NT-4', and 'S101-T1'. The 'Reports' section lists three linked records: 'Characterization of the Temperature Capabilities of Advanced Disk Alloy ME3 (Temp Capabilities)', 'Detailed Microstructural Characterization of the Disk Alloy ME3', and 'Enabling Propulsion Materials Program Final Technical Report, Long-Life Compressor/Turbine Disk Material (EPM Final Report, Vol. 1, Task I)'. A red circle highlights the 'Microstructure' section and its records. The word 'Microstructure' is written in large black text at the bottom of the red circle.

Microstructure

- Contents
 - Material Behavior Models
 - Microstructure
 - Subset: Default
 - ME3
 - Disk H111
 - Disk S001
 - Disk S010
 - Disk S100
 - Disk S101
 - 0° Segment
 - 90° Segment
 - NT-4
 - Macroslice
 - Disk W000
 - Disk W011
 - Disk W110
 - Pedigree: Ceramics
 - Pedigree: Coatings
 - Pedigree: Component/Assemblies
 - Pedigree: Composite Ply Architecture
 - Pedigree: Composite System-Laminate
 - Pedigree: Metals
 - Subset: NASA
 - Cobalt
 - Copper Alloys
 - Nickel
 - Hastelloy X
 - ME3_Disks
 - H101
 - H101_demo_only
 - S101
 - S110

S101-NT-4

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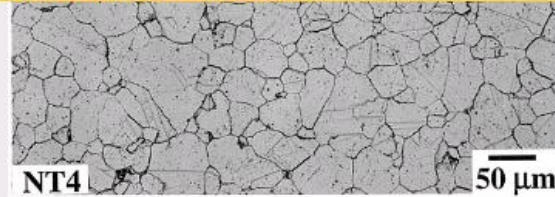
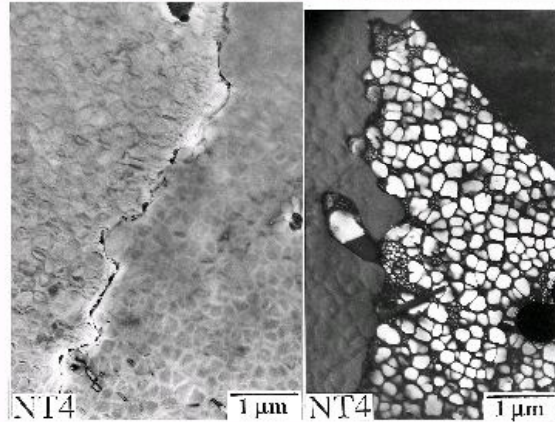


Photo micrograph 2



Description : Micro-structure at grain boundaries of rim specimens from disk S101; Figure 18, TM-2004-213066

Microscopy Technique : Optical: Differential Interference Contrast

Test Results

Test Data: Tensile

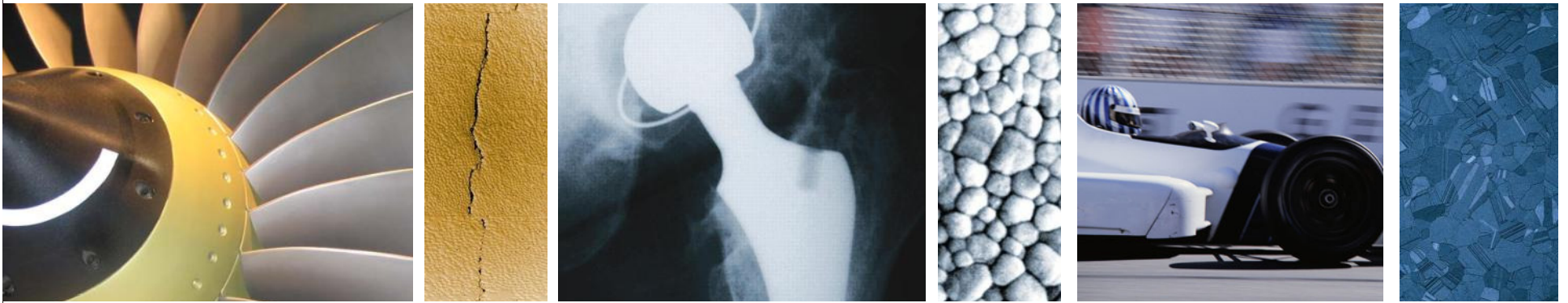
1 Linked Record(s)

S101 (NT4)

Links

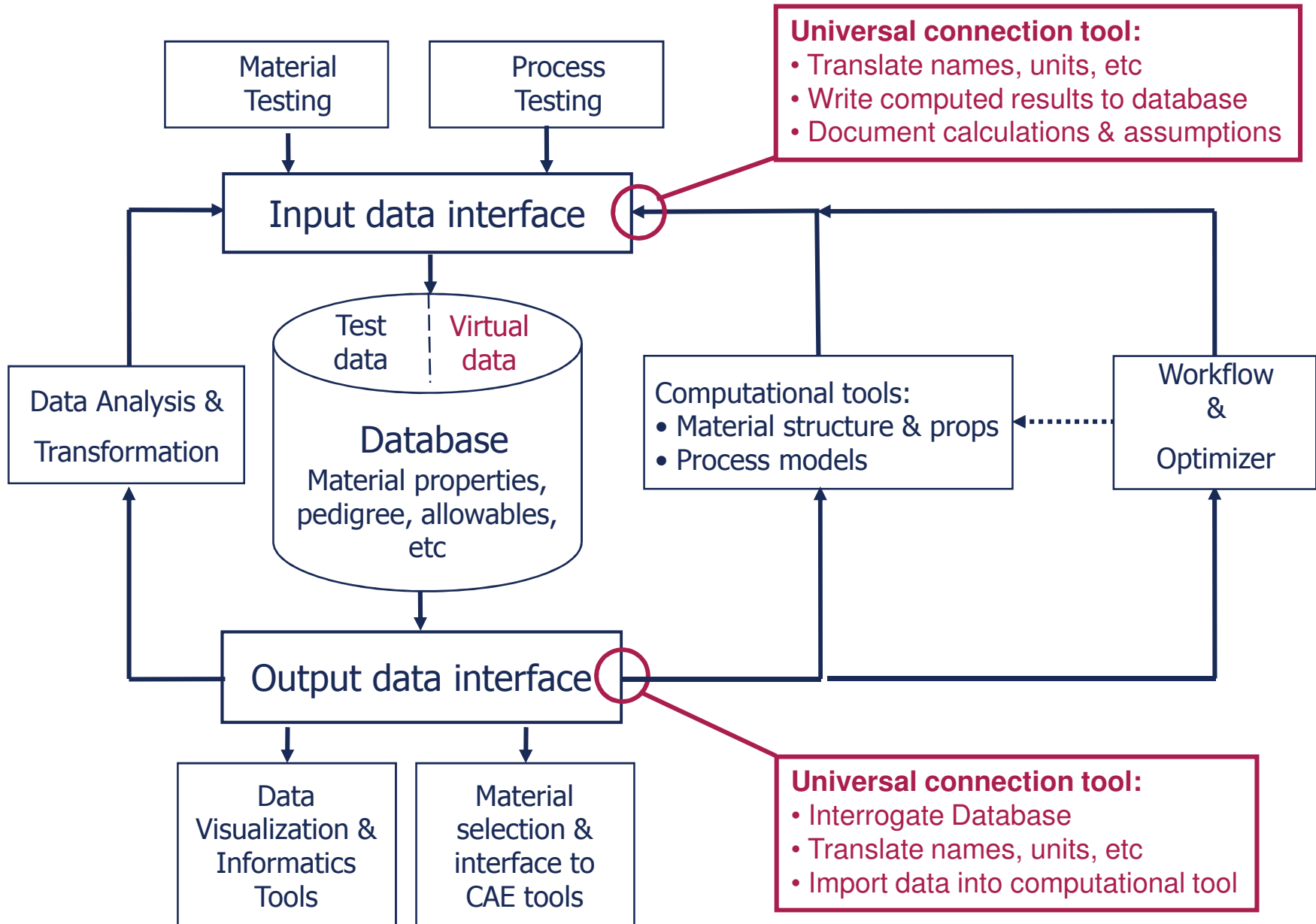
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Where do the models come in??

Proposed Architecture



NIST Demo Atomistics Database Simulation Data



GRANTA mi

Read Mode
Edit Mode

Home Optimize Substitute Substances Reports

Quick Search
Advanced Search

Help
Settings

Contents

- Atomic Properties
 - Subset: No Subset
- Experimental Values
 - Aluminum
 - Nickel
 - Titanium
- Model Predictions
 - Aluminum
 - MFMP99
 - MFMP99-AL-0001**
 - MFMP99-AL-0002
 - MFMP99-AL-0003
 - MFMP99-AL-0004
 - MFMP99-AL-0005
 - MFMP99-AL-0006
 - MFMP99-AL-0007
 - MSAH05
 - SBFT12
 - Nickel
 - Titanium
- Models
 - Subset: No Subset
 - EAM
 - MFMP99
 - SBFT12
 - FS
 - MEAM
 - Curve Fits

MFMP99-AL-0001

General Information

Material	Aluminum
----------	----------

Modelling Information

Prediction number	MFMP99-AL-0001
-------------------	----------------

Properties

Volume per atom	16.8 to 16.8	Å ³
Standard Deviation	0.00807 Å ³	
Mean	16.8 Å ³	
Basis	P basis	
Calculated	Yes	
Model used	MFMP99	
Code used	LAMMPS (14Jul2011, patched)	
Input parameters	pbs's, NPT, dt=0.001 fs, thermo=1000 steps	
Input script	in.300.MFMP99	
Operator	Chandler Becker	
Run date	3 June 2012	

Conditions

Temperature	19.3 to 34.2	°C
--------------------	--------------	----

Pedigree

- Curve Fits
 - Aluminum
- Models
 - MISHIN 99 (MFMP99)

Calculation Pedigree

NIST Demo Atomistics Database Model Description Record

NIST

GRANTA MI Read Mode Edit Mode Home Optimize Substitute Substances Reports Quick Search Advanced Search Help Settings

Contents

- Atomic Properties
 - Subset: No Subset
- Experimental Values
 - Aluminum
 - Nickel
 - Titanium
- Model Predictions
 - Aluminum
 - MFMP99
 - MFMP99-AL-0001
 - MFMP99-AL-0002
 - MFMP99-AL-0003
 - MFMP99-AL-0004
 - MFMP99-AL-0005
 - MFMP99-AL-0006
 - MFMP99-AL-0007
 - MSAH05
 - SBFT12
 - Nickel
 - Titanium
- Models
 - Subset: No Subset
 - EAM
 - MFMP99
 - SBFT12
 - FS
 - MEAM
 - Curve Fits

MISHIN 99 (MFMP99) Edit View Tools Units

Model Author(s)
Y. Mishin, D. Farkas, M.J. Mehl, and D.A. Papaconstantopoulos

Reference
Y. Mishin, D. Farkas, M.J. Mehl, and D.A. Papaconstantopoulos, "Interatomic potentials for monoatomic metals from experimental data and ab initio calculations," Phys. Rev. B 59, 3393 (1999).

Reference (Link) [AI page, NIST Interatomic Potentials Repository](#)

Details

Model Theory
In computational chemistry and computational physics, the embedded atom model, embedded-atom method or EAM, is an approximation describing the energy between two atoms. The energy is a function of a sum of functions of the separation between an atom and its neighbors. In the original model, by Murray Daw and Mike Baskes, the latter functions represent the electron density. EAM is related to the second moment approximation to tight binding theory, also known as the Finnis-Sinclair model. These models are particularly appropriate for metallic systems. Embedded-atom methods are widely used in molecular dynamics simulations. (Source: Wikipedia, http://en.wikipedia.org/wiki/Embedded_atom_model, 10 Sept. 2012)

Model Parameters
Note: This potential is available in the 'plt' format for use with IMD and the 'setfl' format used with LAMMPS.

Published Validation Data

Melting Temperature	754	°C (estimate)
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Links

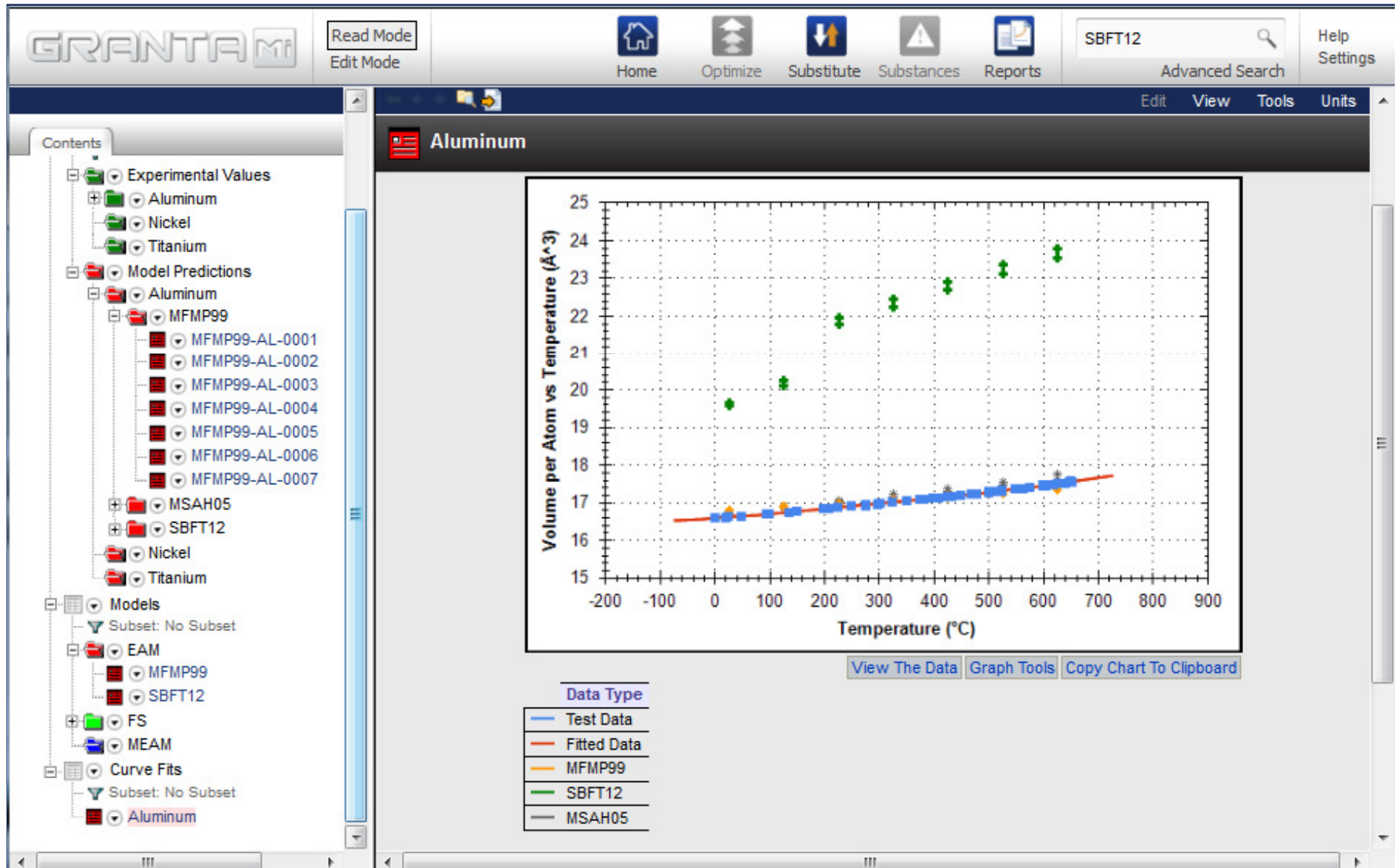
Predictions using this model

- MFMP99-AL-0001
- MFMP99-AL-0002
- MFMP99-AL-0003
- MFMP99-AL-0004

NIST Demo Atomistics Database

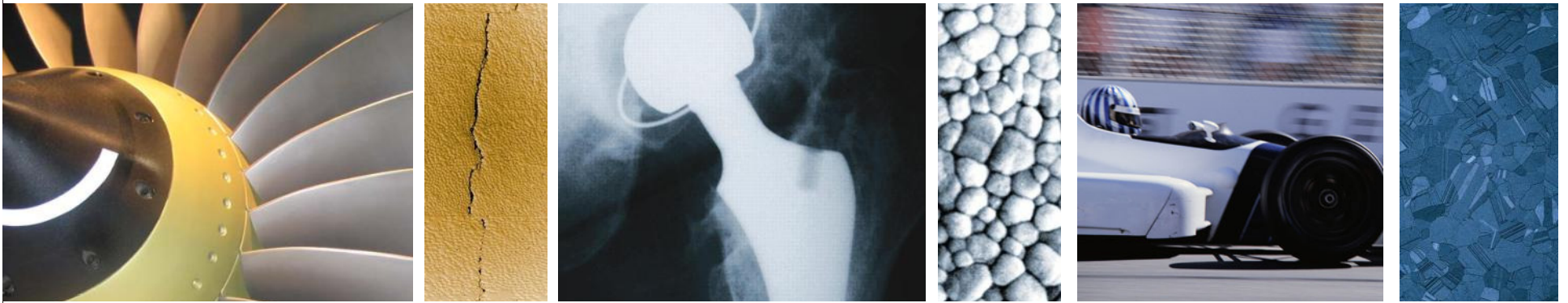
Validating models with experimental data

NIST



GRANTA

MATERIAL INTELLIGENCE



Where does MGI come into it?

Computational Materials Data Network

Three initiation projects

- Manufacturing in-process materials data
- Aerospace structural materials data
- National Materials Research Database



Manufacturing in-process materials data project

Focus on capturing and storing fully traceable in-process, high-temperature data

- such as yield stress and flow stress

Develop methodologies for providing this data for through process modeling

Understand how this can support supply chain data transfer

Aerospace structural materials data project

Based on the Materials Data Management Consortium (MDMC),

Propagate the ideas shown in the sample database for alloy ME3, a nickel-base superalloy,

Demonstrating data sharing across organizations.



National Materials Research Database

Recent trends indicate need to manage information in academic grants

- NSF
- EPSRC (UK)

Explore online data capture and dissemination of research generated at leading academic and government institutions

European Projects

Accelerated Metallurgy

- (i) new lightweight fuel-saving alloys ($<4.5 \text{ g/cm}^3$) for aerospace and automotive applications;
- (ii) new higher-temperature alloys (stable $>1000 \text{ degC}$) for rockets, gas turbines, jet-engines, nuclear fusion;
- (iii) new high- T_c superconductor alloys ($>30\text{K}$) that can be wire-drawn for electrical applications;
- (iv) new high-ZT thermoelectric alloys for converting waste heat directly into electricity;
- (v) new magnetic and magnetocaloric alloys for motors and refrigeration; and
- (vi) new phase-change alloys for high-density memory storage.

European Projects

Accelerated Metallurgy

- Automated, direct laser deposition (DLD) robotic alloy synthesis of specified previously unexplored alloy families
- combinatorial synthesis and testing of many thousands of unexplored alloy formulations
- 1000 times faster than conventional manual methods
- discrete mm-sized samples are submitted to a range of automated, standardised tests that will measure chemical, physical and mechanical properties
- All meta data and data will be stored in a Virtual Alloy Library
- The Virtual Alloy Library will be coupled with computer codes (eg neural network models) in order to extract and map out the key trends linking **process, composition, structure and properties**.

Conclusions

Materials information management is a mature technology utilised in multiple sectors across the globe

Granta and our systems support many projects in the MGI arena

ASM is actively supporting 3 MGI projects

- Manufacturing in-process materials data
- Aerospace structural materials data
- National Materials Research Database