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An Information Architecture for ICME

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Granta Design

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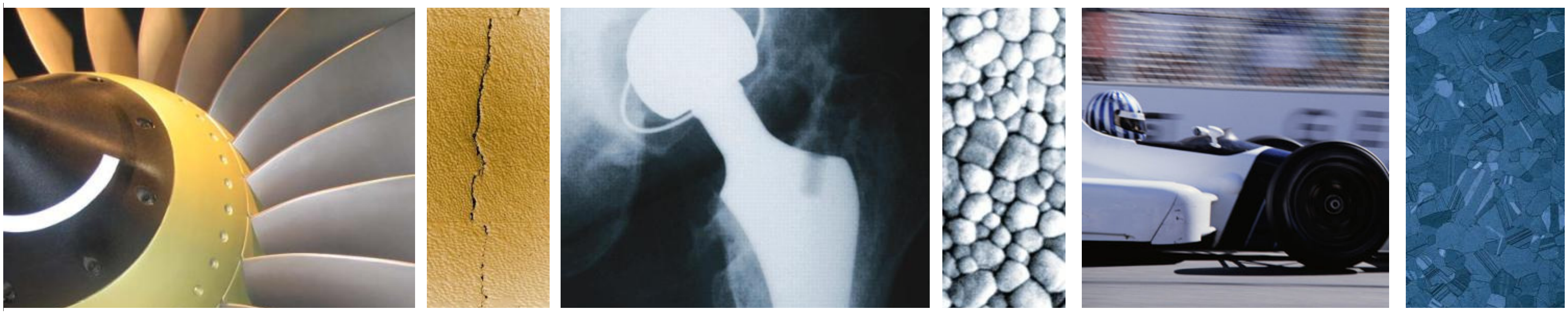

An information architecture for ICME

Will Marsden Ph.D

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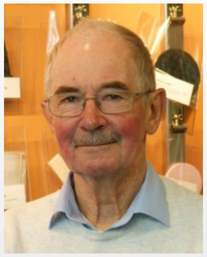

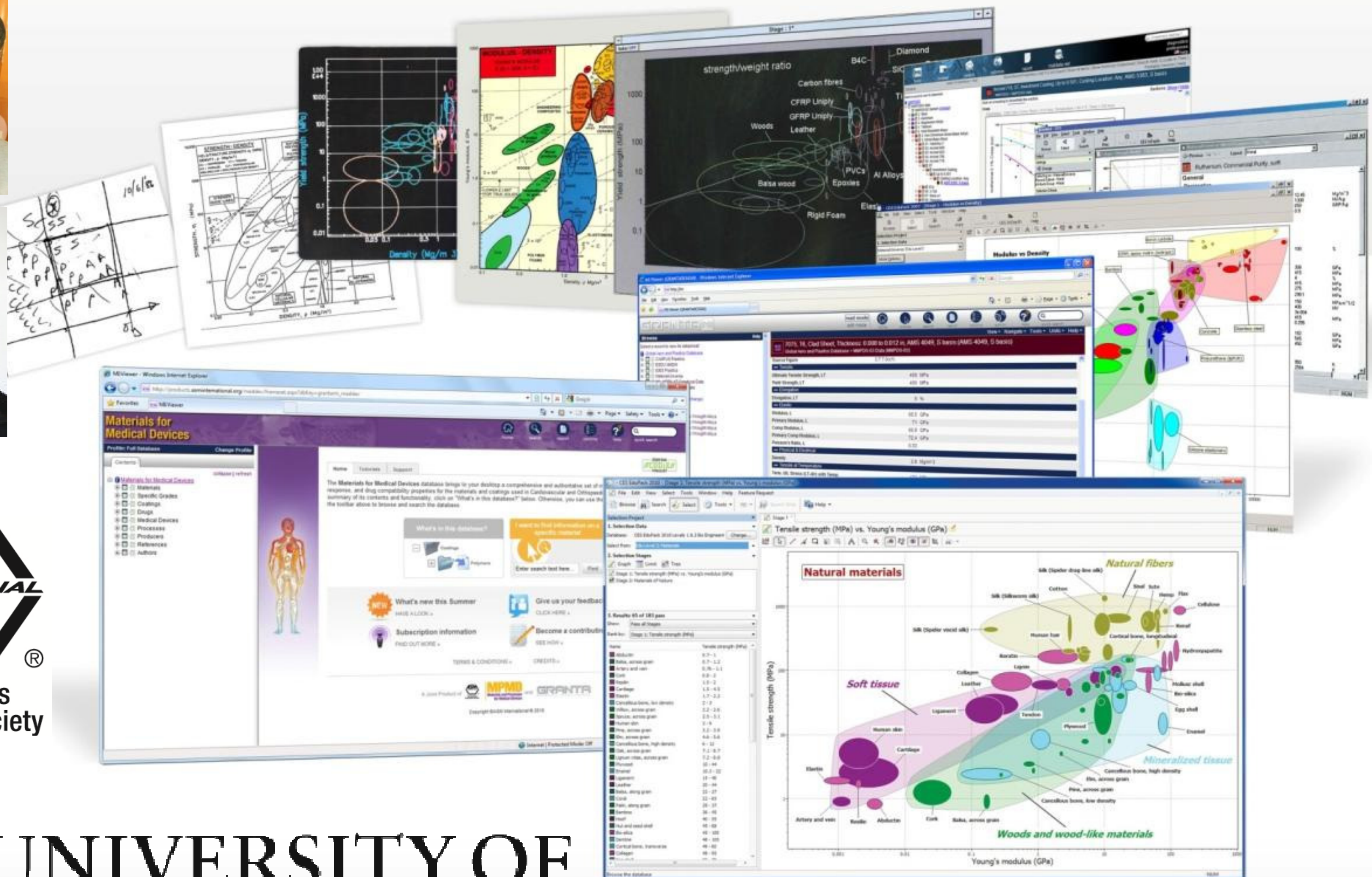

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The Materials Information Society

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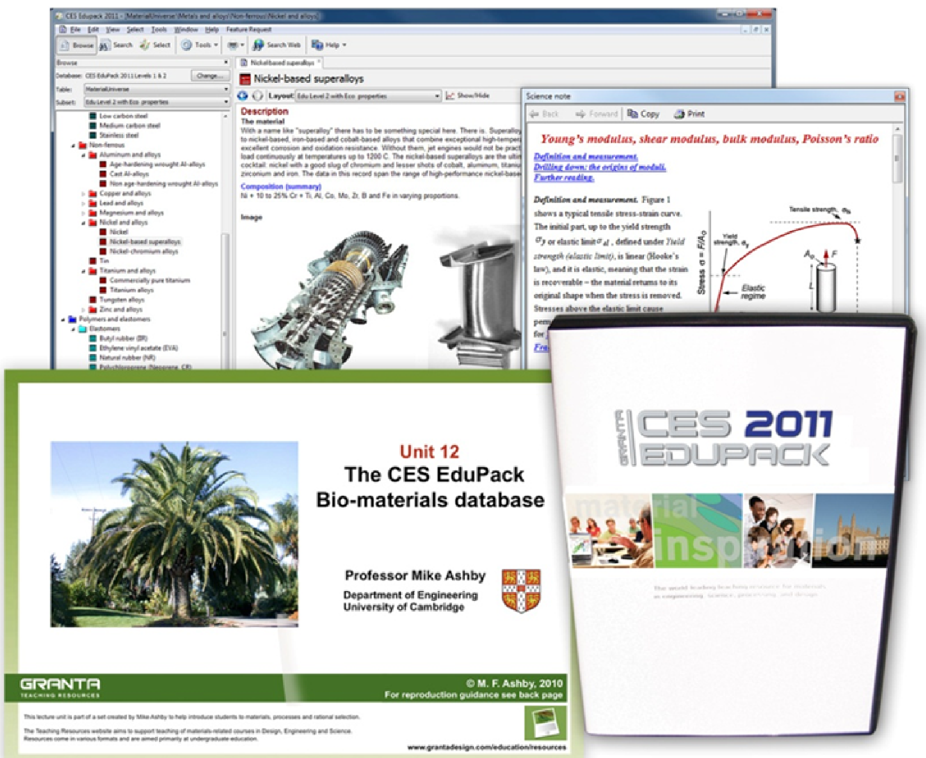
Granta for education

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



Materials Education Symposium, April 2011

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

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Granta for Industry

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- Automotive & transport
- Energy & nuclear
- Government & education
- High Technology
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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, …

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Some practical problems that we solve

Materials information management

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

Materials support for CAD, CAE…

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…

Materials decision support

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

Eco design & environmental regulations

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 CO_2 / energy, EoL…)

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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

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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

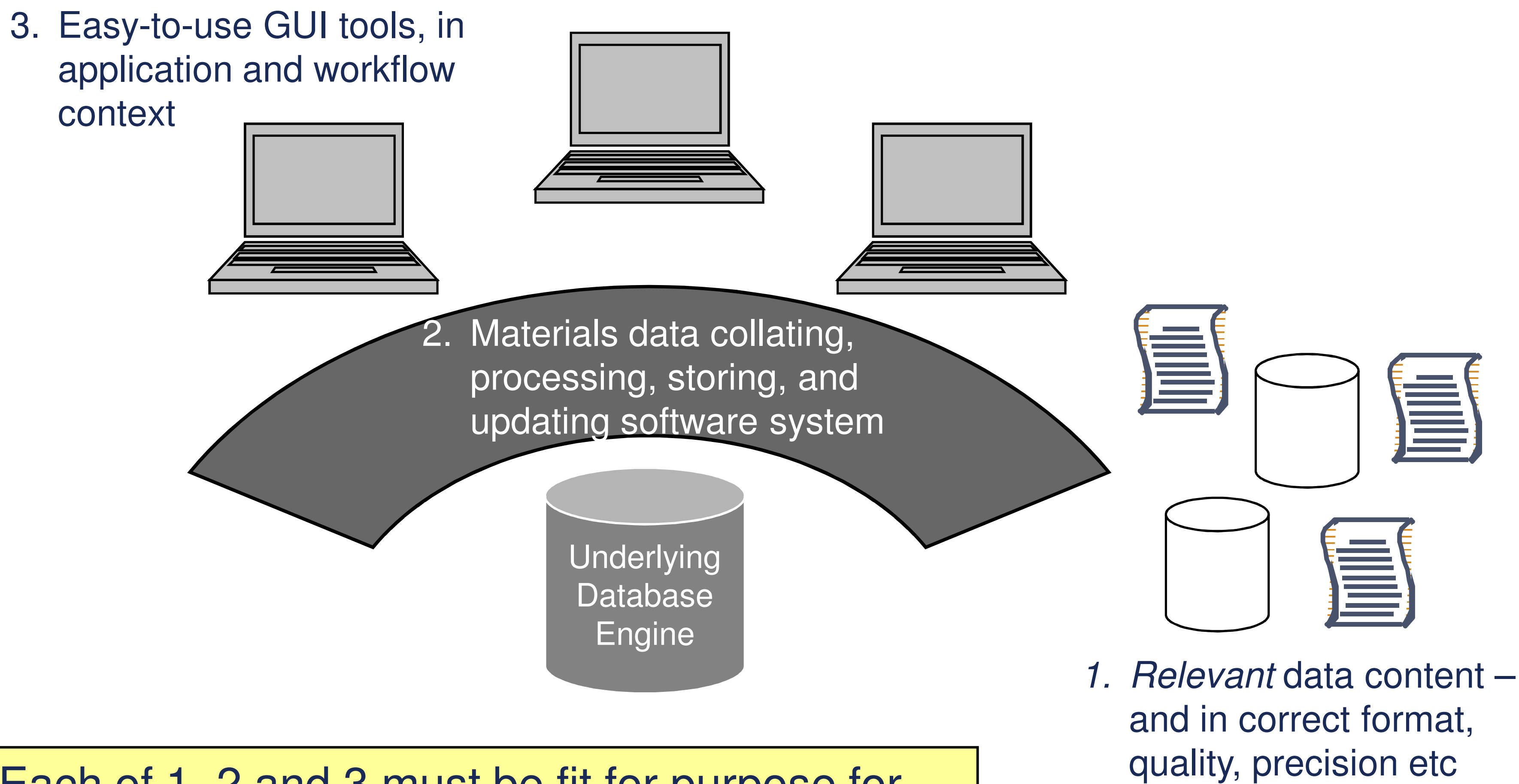
Medical devices

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

Materials suppliers

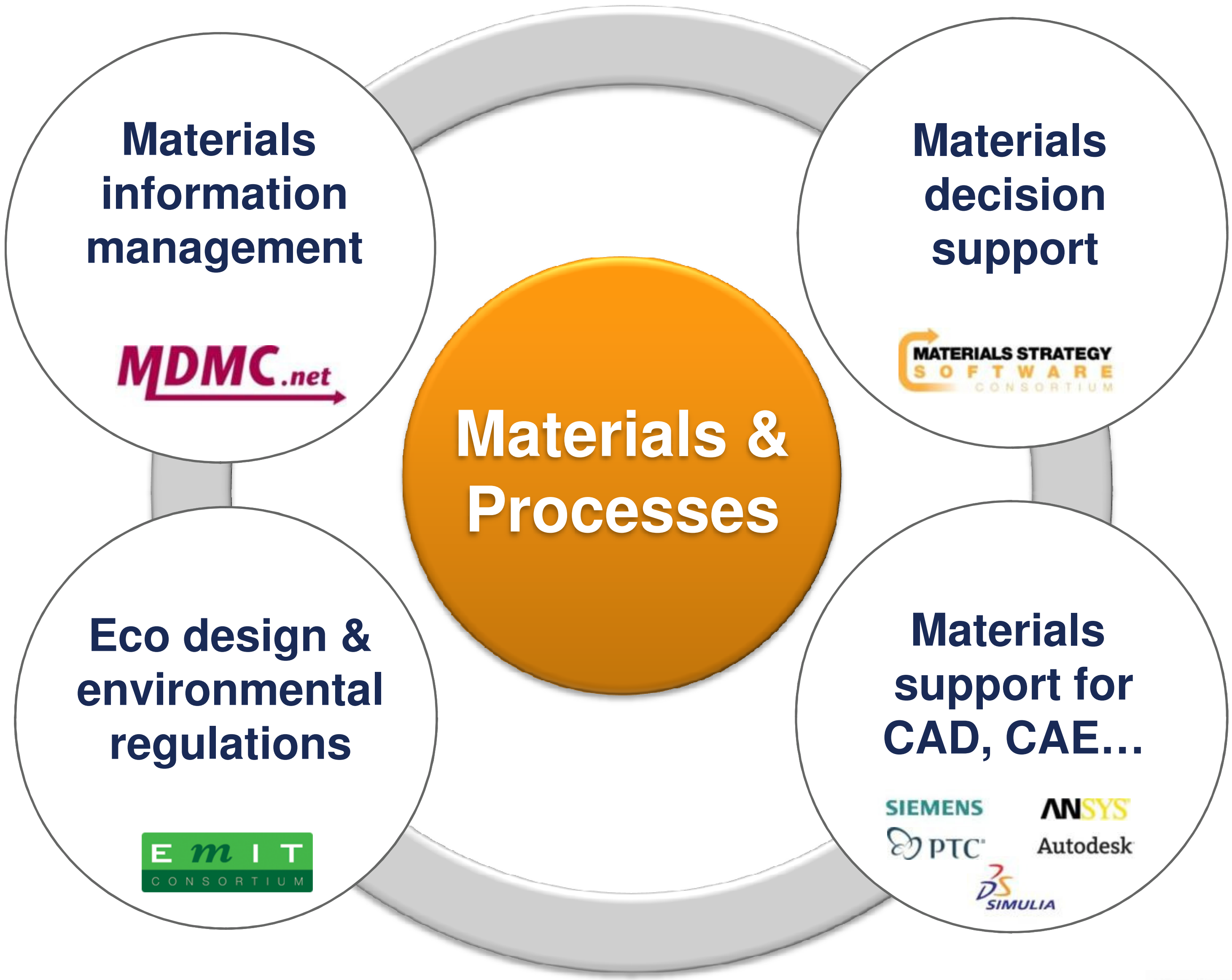
- Systematic method for identifying best applications for new materials

Materials information technology



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

Granta for industry



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Consortia

MDMC.net

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

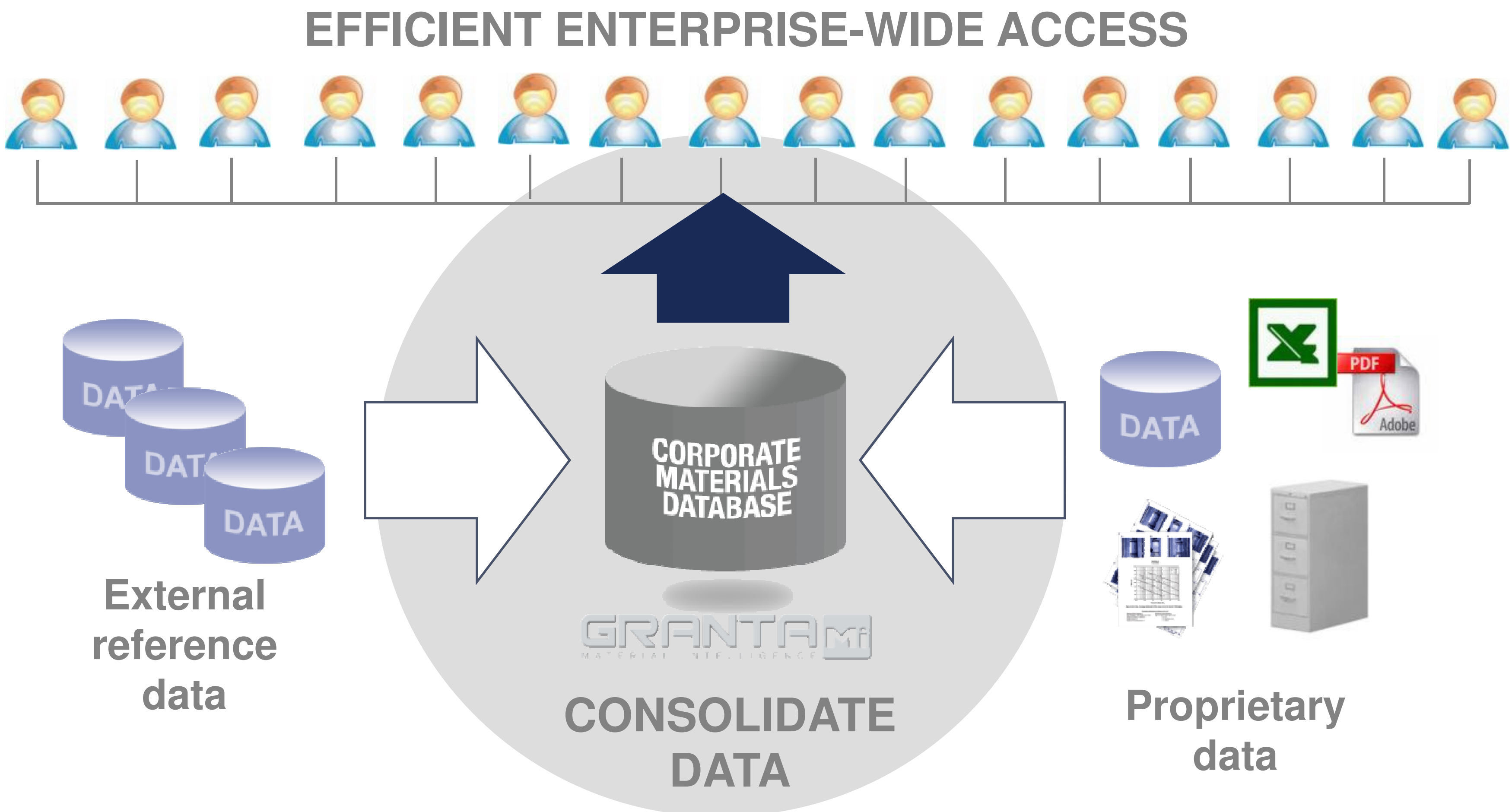
EMIT CONSORTIUM

Boeing
EADS Astrium Satellites
Emerson Electric
Eurocopter
Honeywell
Lockheed Martin
NASA
NPL
Rolls-Royce
Thales
US Army Res. Labs

MATERIALS STRATEGY SOFTWARE CONSORTIUM

Baker Hughes
DePuy
Emerson Electric
Ethicon Endosurgery
Moen Inc. (Fortune Brands)
NASA
Rhodia
Sulzer
TRW Automotive

Materials information management



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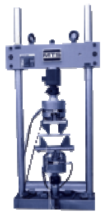
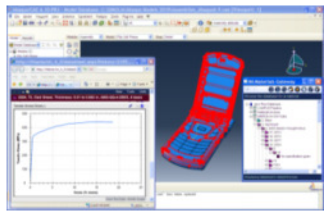
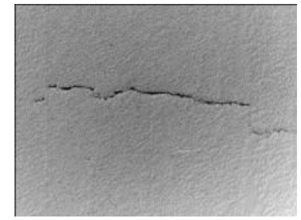
Examples of materials information







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

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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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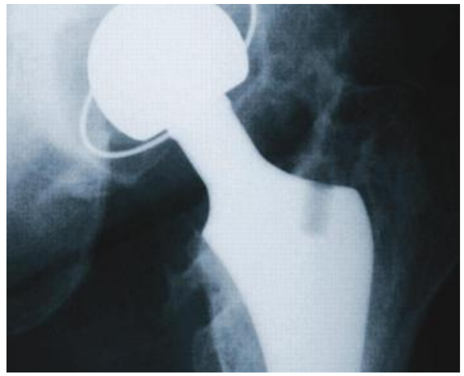
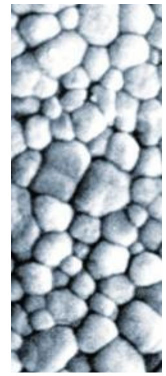



A composite example

MDMC Composites data schema

REPORTS
Full text original pdf files

COMPOSITE SYSTEM
General materials information - a record to matrix/reinforcement combo

MATERIAL PEDIGREE

Raw materials and process data
Constituent materials and process data
Intermediaries characterisation and process data
Laminate processing and lay-up data

Compiled reference data
Linked to Composite system and Test Results

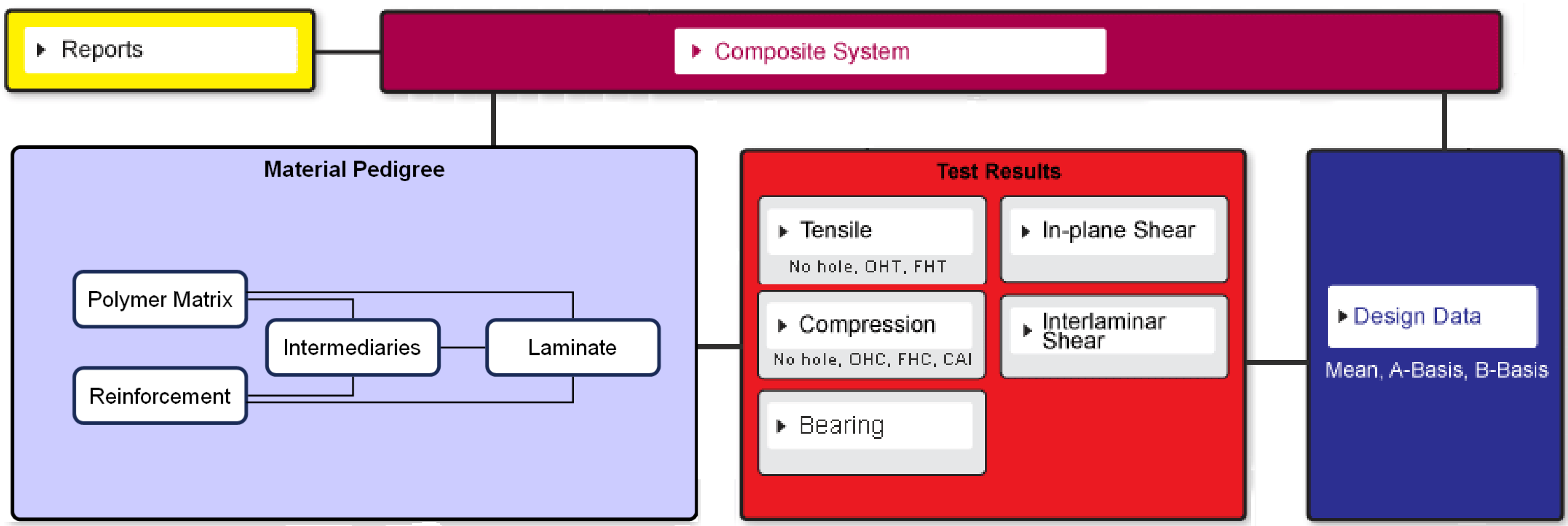
TEST RESULTS

Raw test data for each specimen
Can accommodate CAI and other 2-stage tests
Conditioning data stored with test data

DESIGN DATA

Statistically backed
A and B Basis
Linked to test and pedigree

Composite Data Flow



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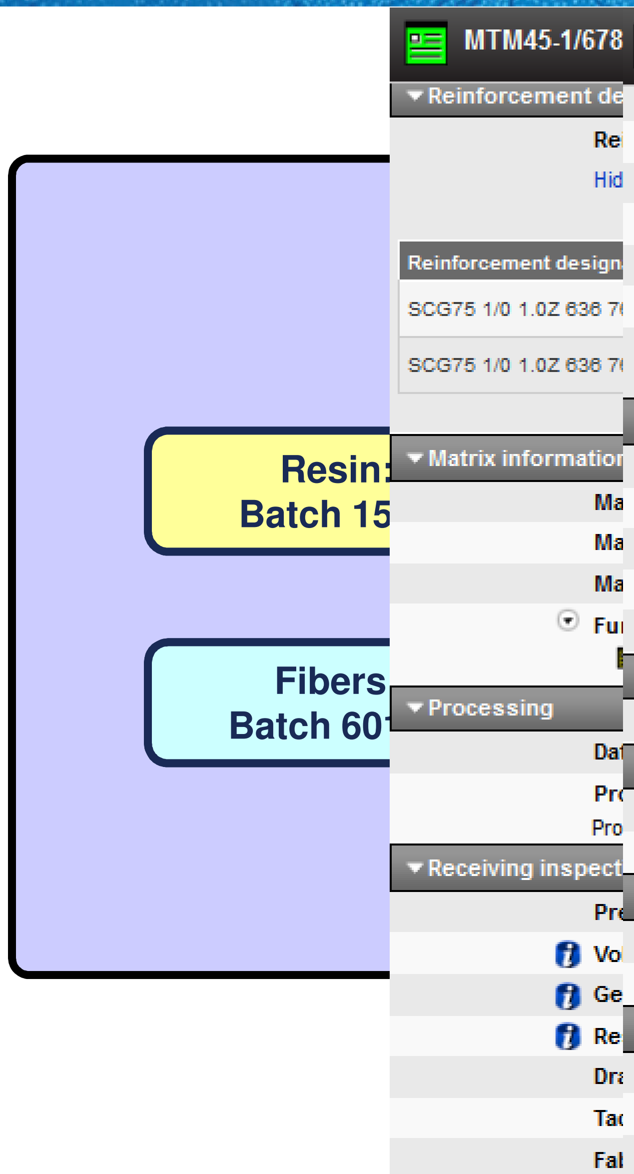
Traceability and processing history



MTM45-1/6781-35%RW, ACG, Panel: AITR1392-8HG-FHC1-D-MH1

Process	Prepreg lay-up	
Cure cycle		
Cure type	Oven	
Autoclave, oven, or press ID	Large Oven	
Initial applied vacuum	948	mb
Cure vacuum maintained throughout cure?	Yes	
Cure cycle phases Show table		
Post cure cycle phases Show table		
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

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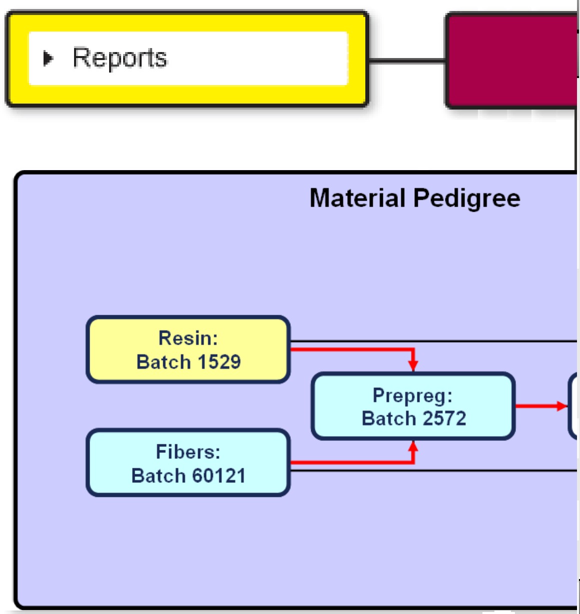
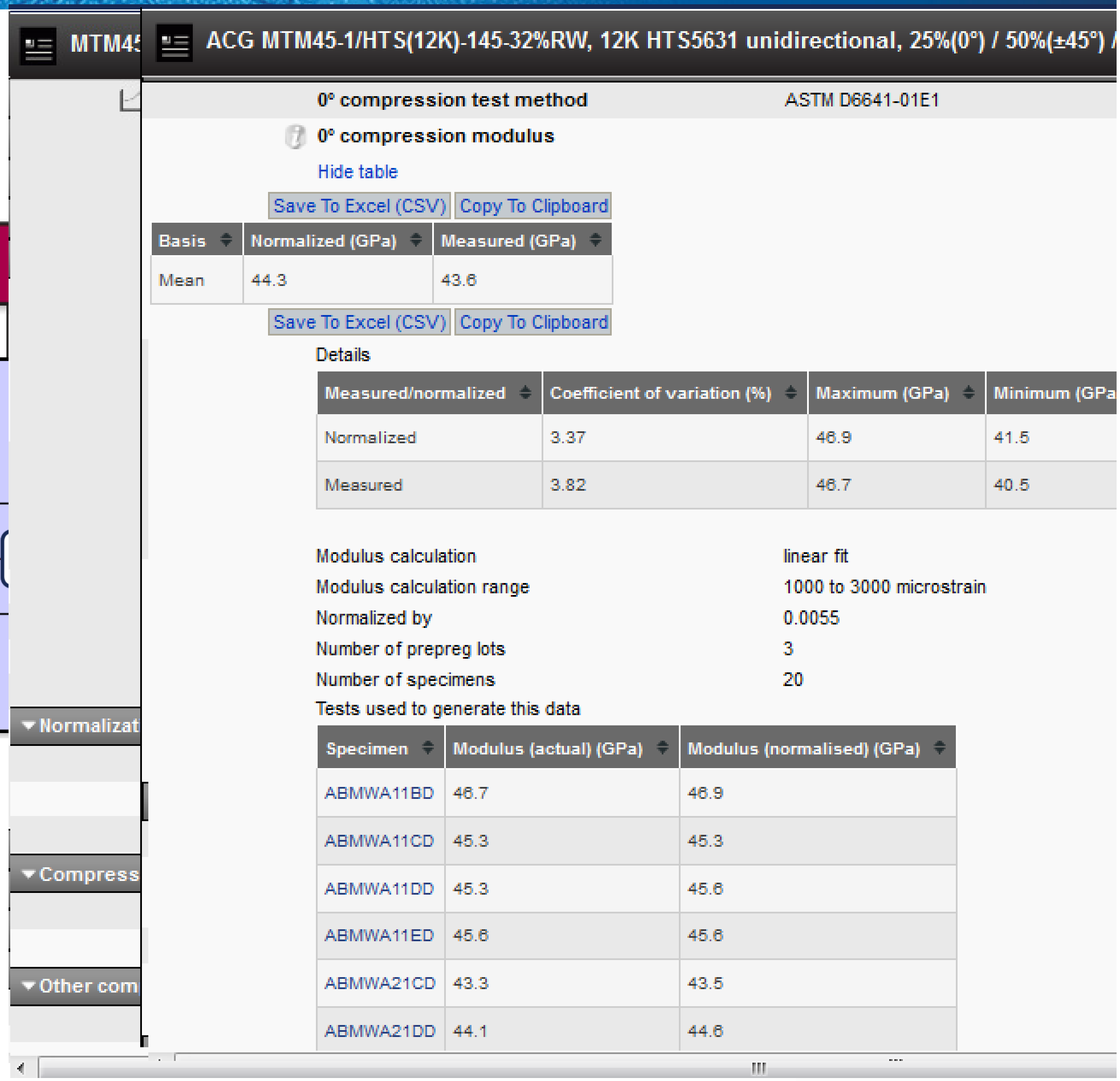
Test results and Design data





MTM45

Normalizat

Compress

Other com

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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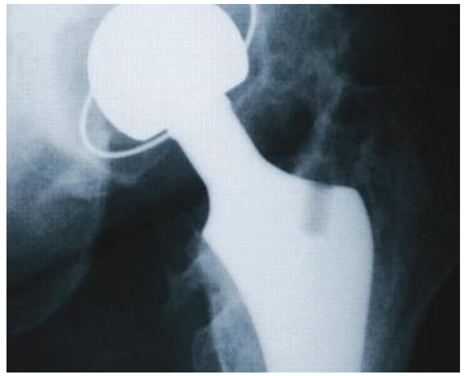
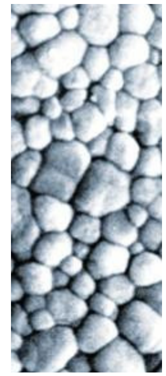

A metallic example

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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.

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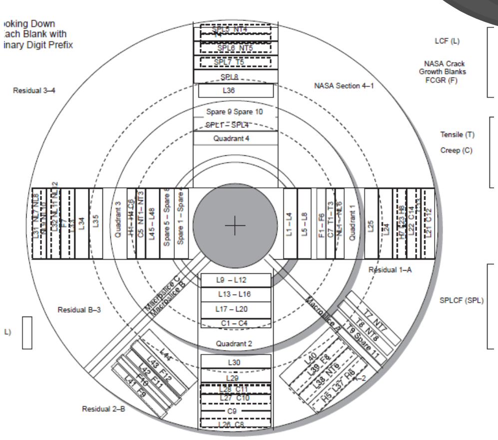
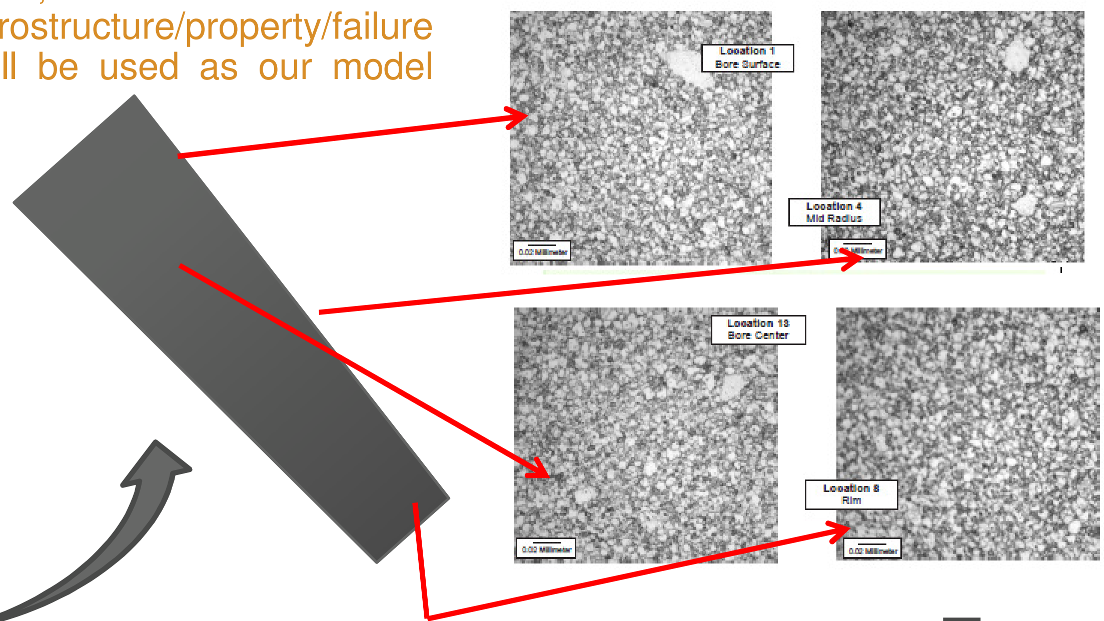
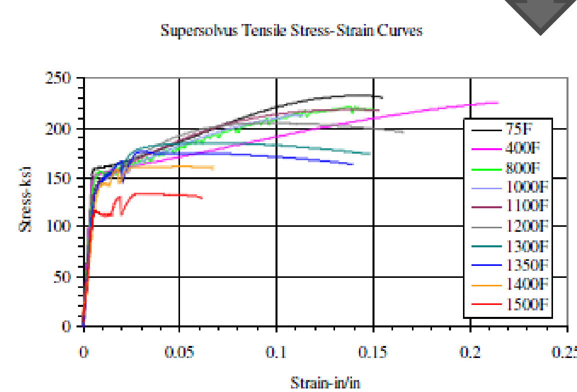




Pedigree of Location: Requires tracking of specimen location and microstructure

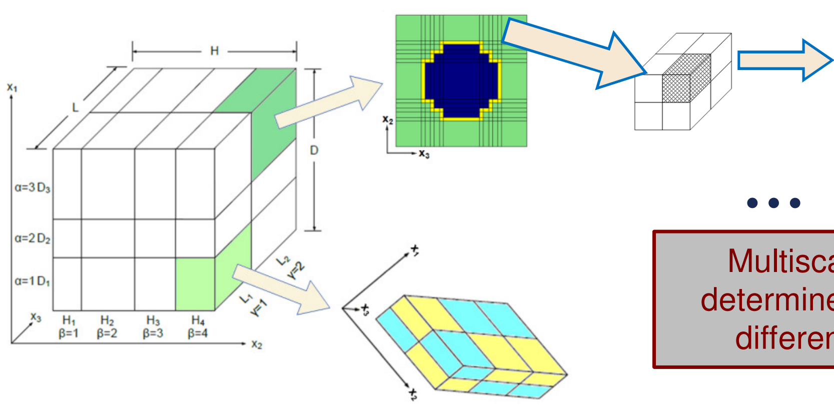


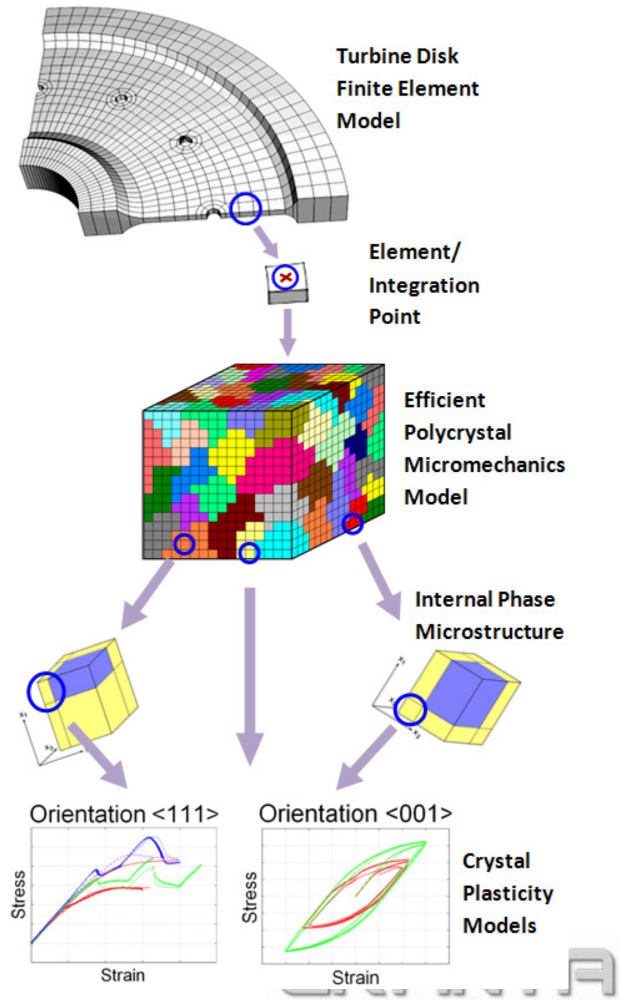
Efficient Multiscale Microstructural (EMMS) Modeling Tool

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

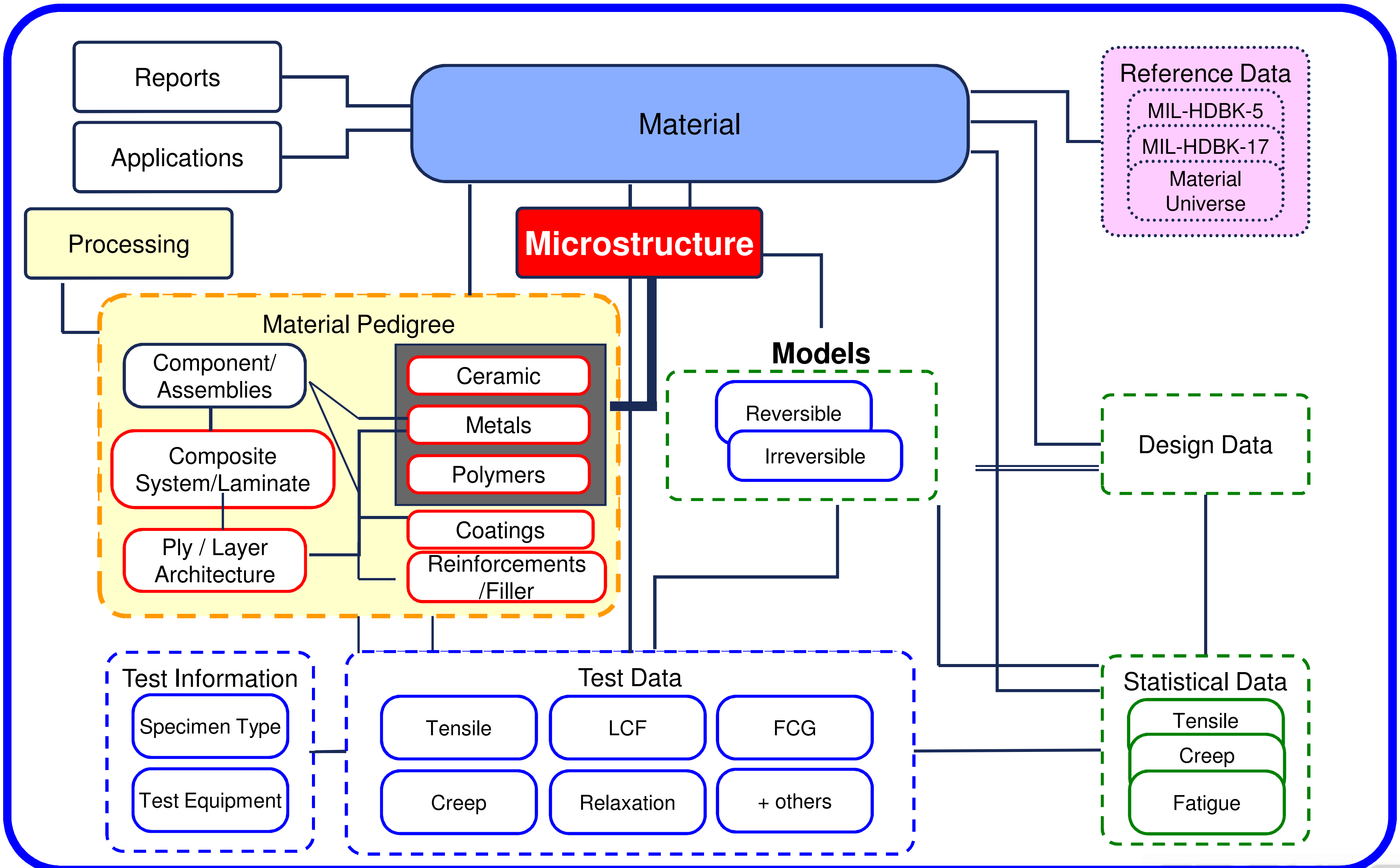




Multiscale analysis can determine local stresses at different length scales

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

MDMC Schema development



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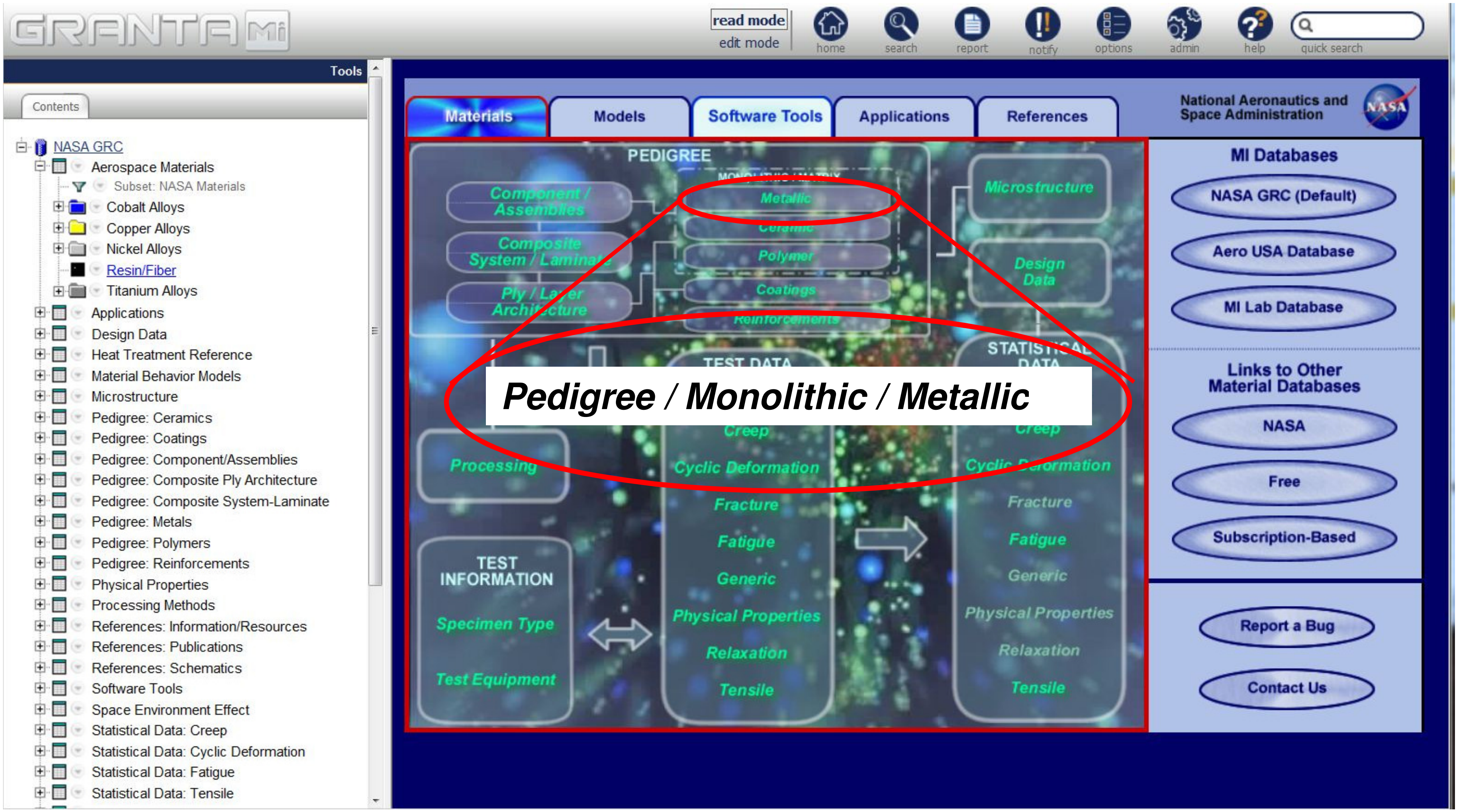
The NASA schema



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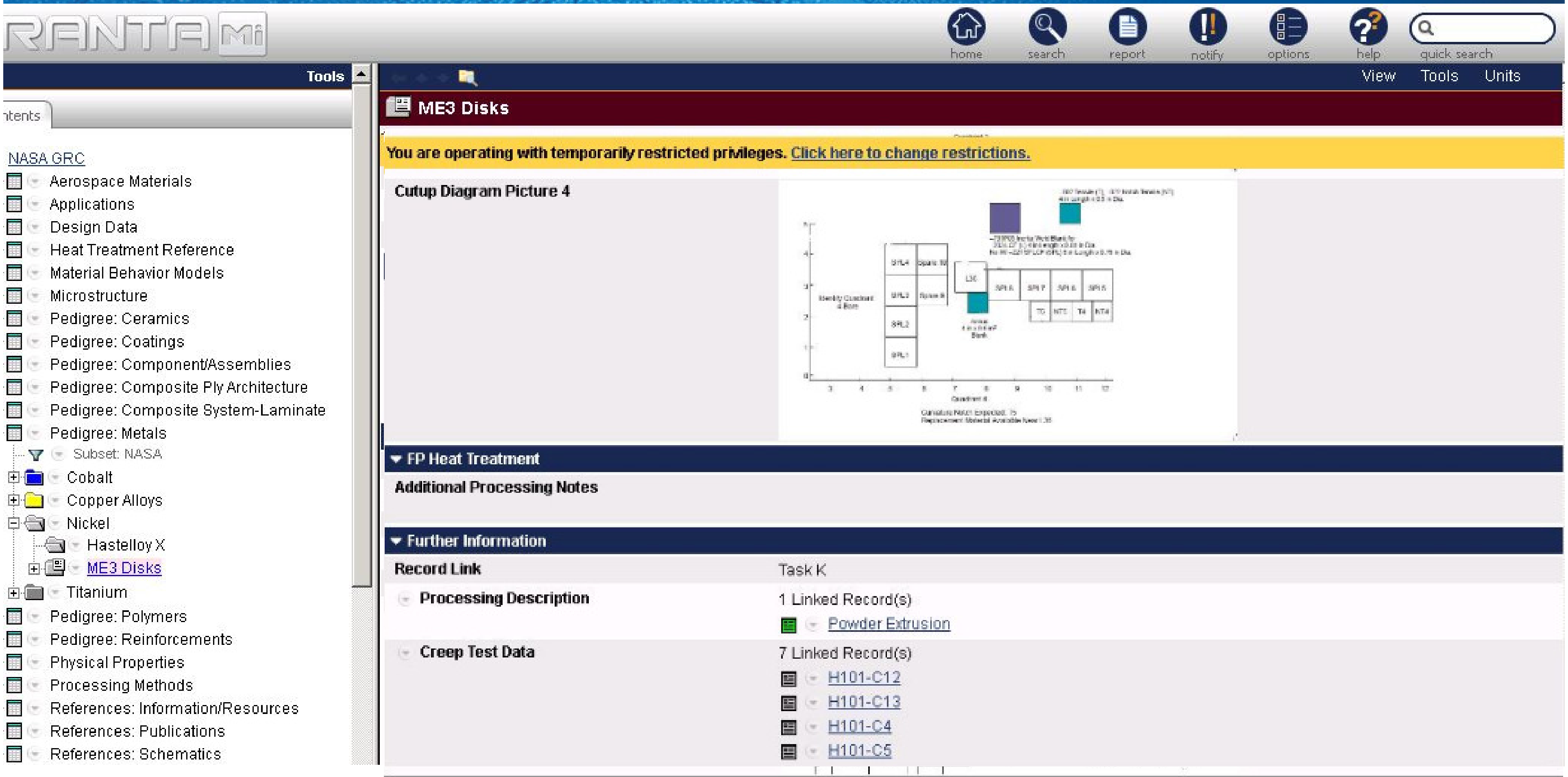
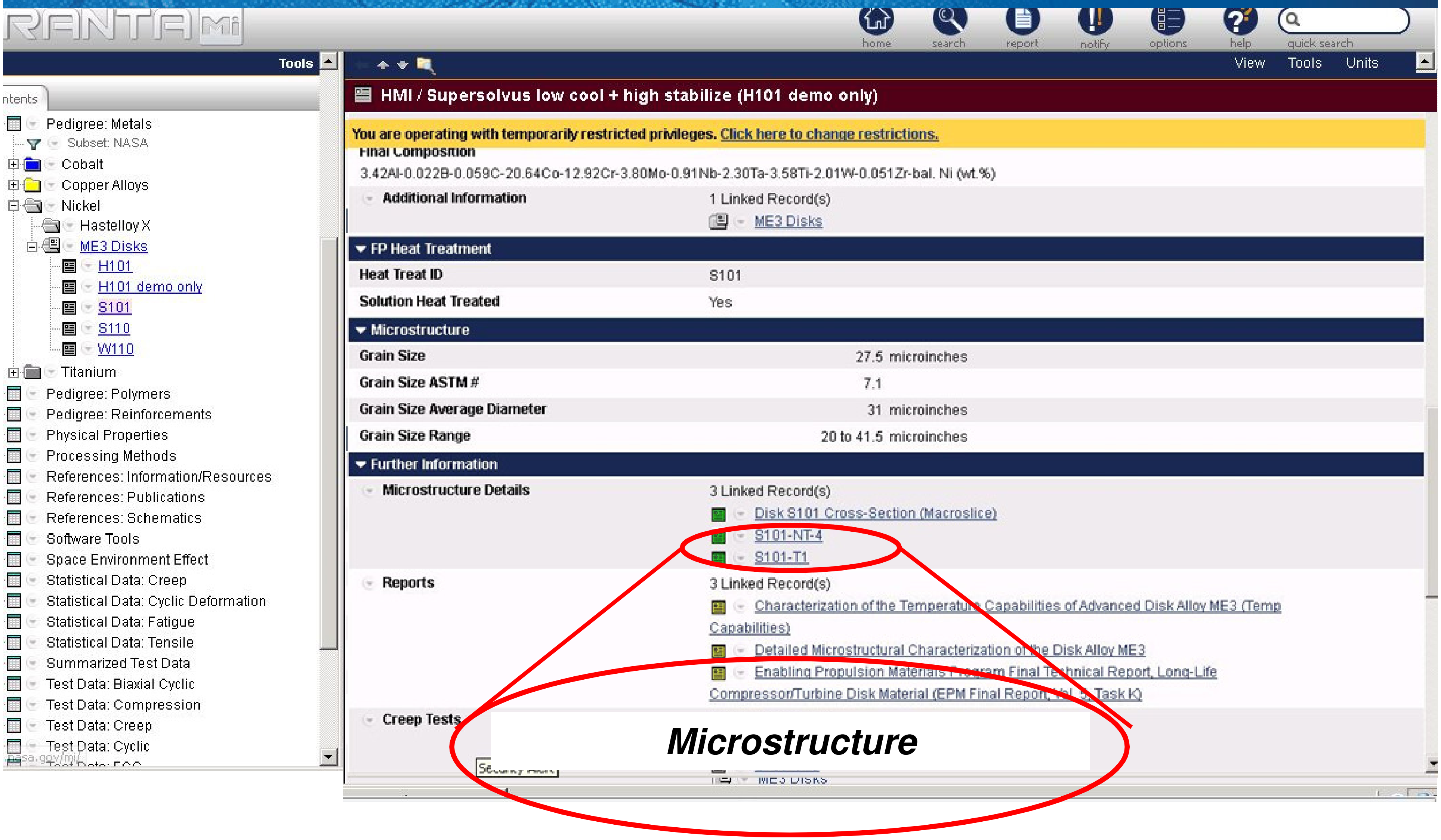
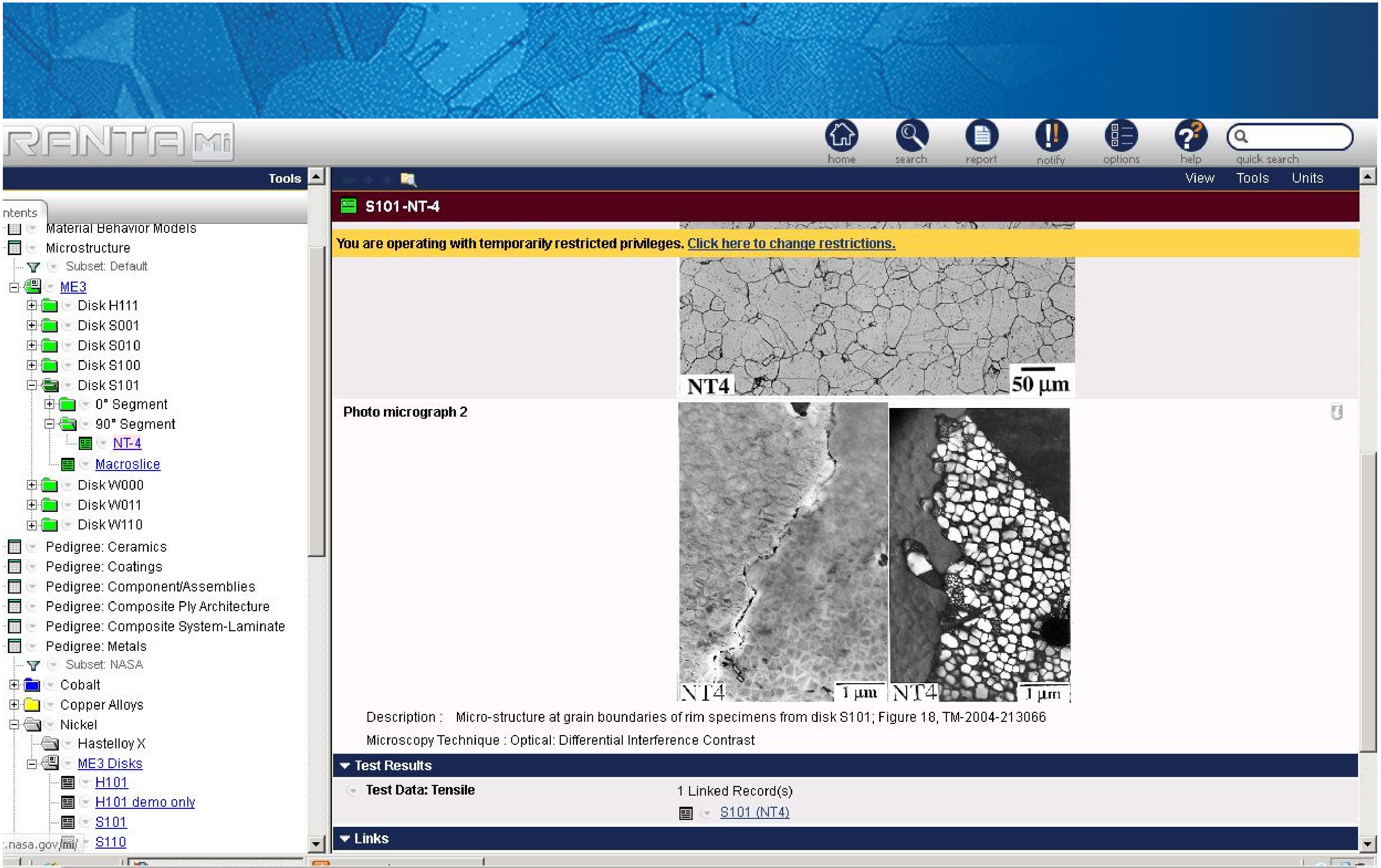
General disc info – cut-up diags etc



Processing data for specific discs




GRANTA Mi
home
search
report
notify
options
help
quick search
Tools
View
Tools
Units
ntents
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
.nasa.gov/mi/
S101-NT-4
You are operating with temporarily restricted privileges. Click here to change restrictions.
NT4
50 µm
Photo micrograph 2
NT4
1 µm
NT4
1 µm
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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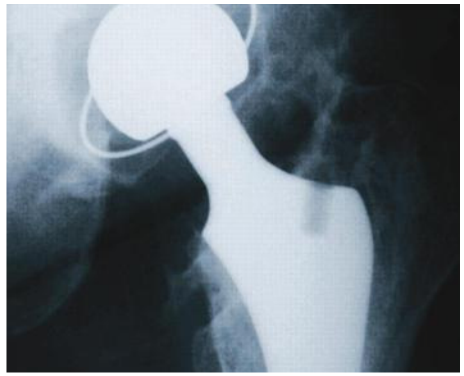
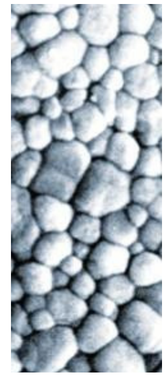
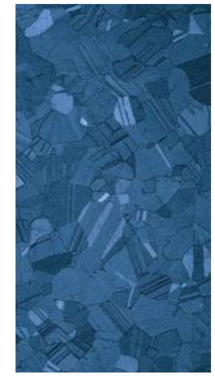
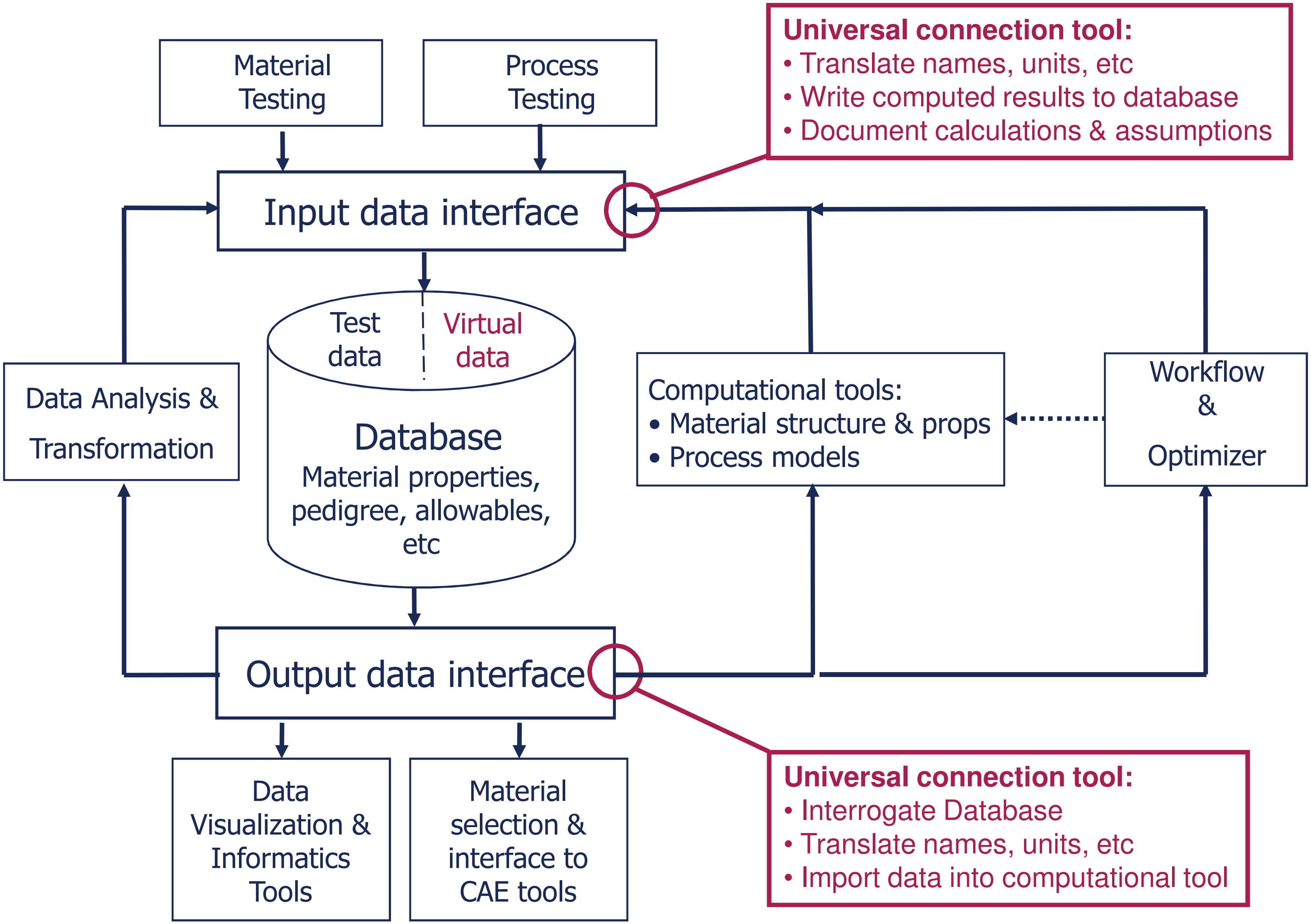



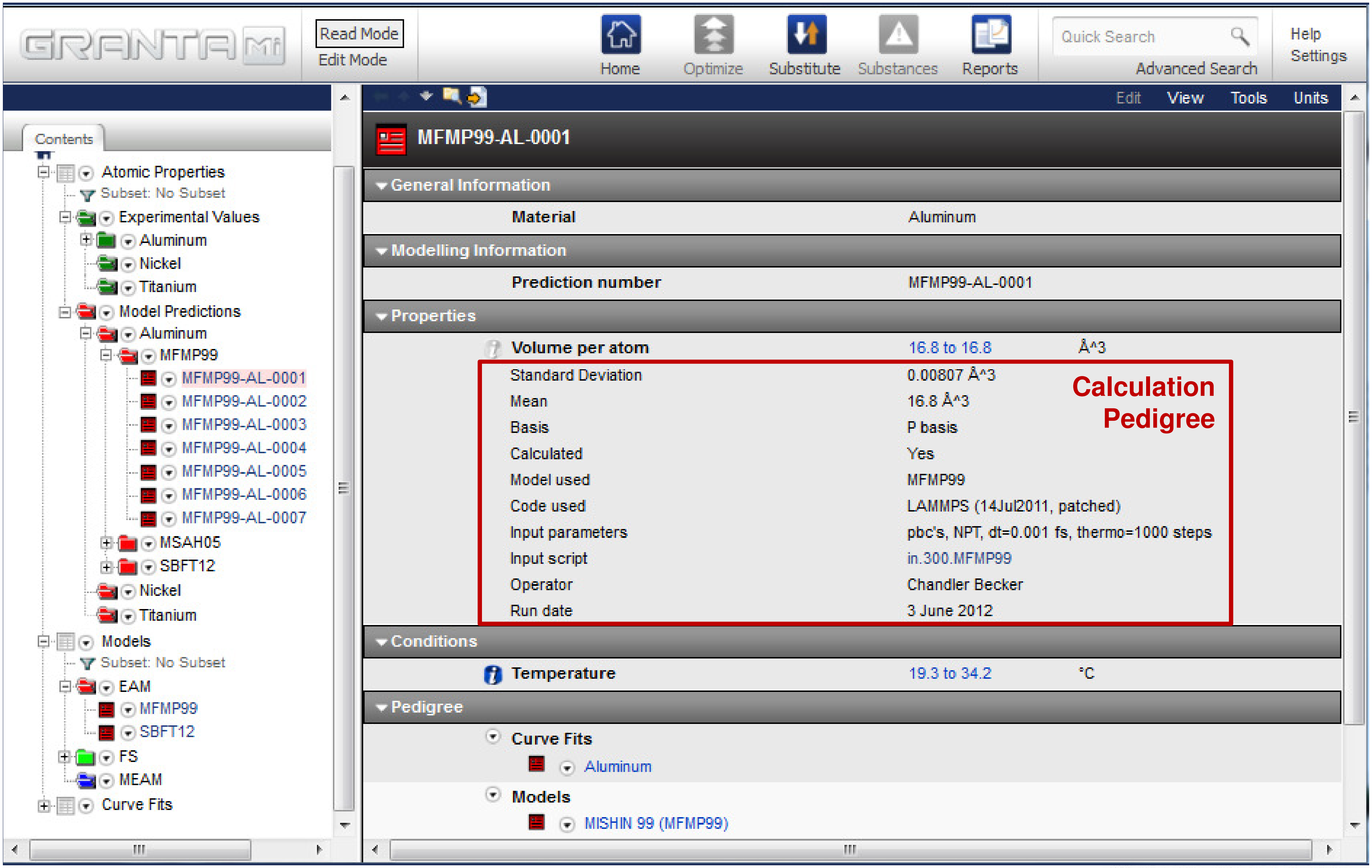


Where do the models come in??

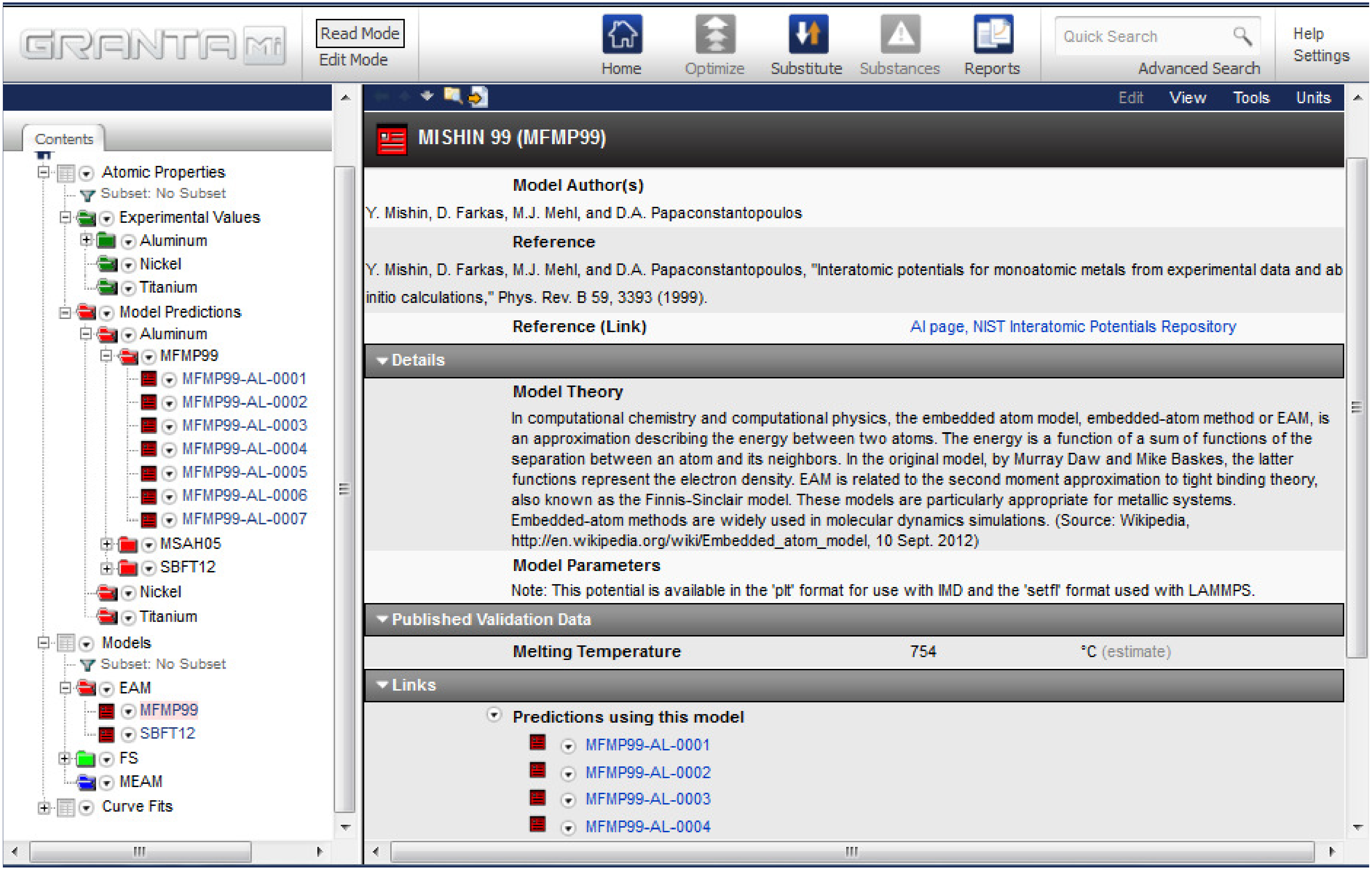
Proposed Architecture



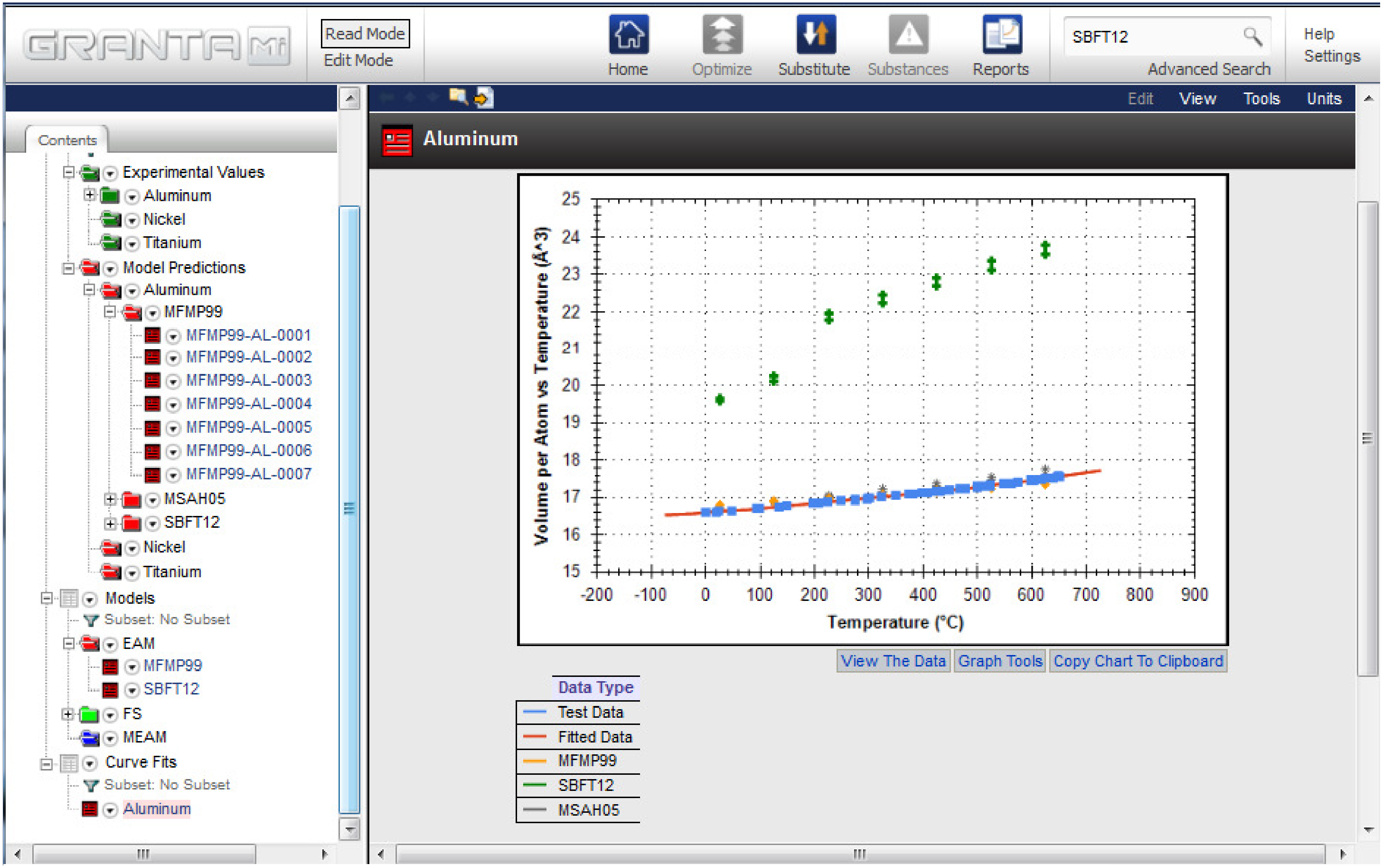
NIST Demo Atomistics Database
Simulation Data



NIST Demo Atomistics Database
Model Description Record



NIST Demo Atomistics Database
Validating models with experimental data



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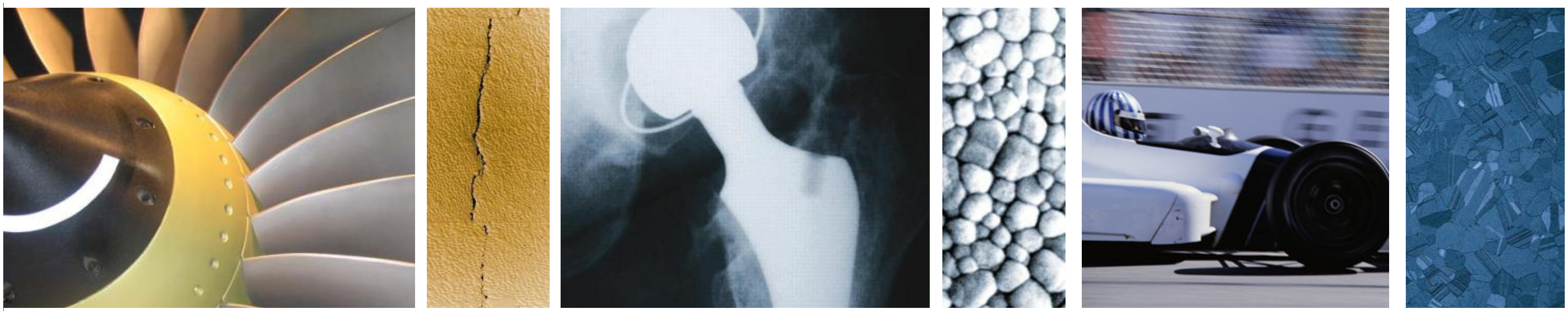

Where does MGI come into it?

Computational Materials Data Network

Three initiation projects

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

Computational Materials Data Network™

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

Computational Materials Data Network™

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

Computational Materials Data Network™

European Projects

Accelerated Metallurgy

- (i) new lightweight fuel-saving alloys (<4.5 g/cm3) for aerospace and automotive applications;
- (ii) new higher-temperature alloys (stable>1000 degC) for rockets, gas turbines, jet-engines, nuclear fusion;
- (iii) new high-Tc superconductor alloys (>30K) 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