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A Software Framework for Designing Material

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A SOFTWARE FRAMEWORK FOR DESIGNING MATERIALS

ECI Conference on Harnessing the Materials Genome

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& Granta Design Ltd

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Harnessing the Materials Genome

Aim of the MGI:

- Rapid development and insertion of new materials?

Essential components of the solution:

- Material structure and property prediction software
- Material design methodologies and tools

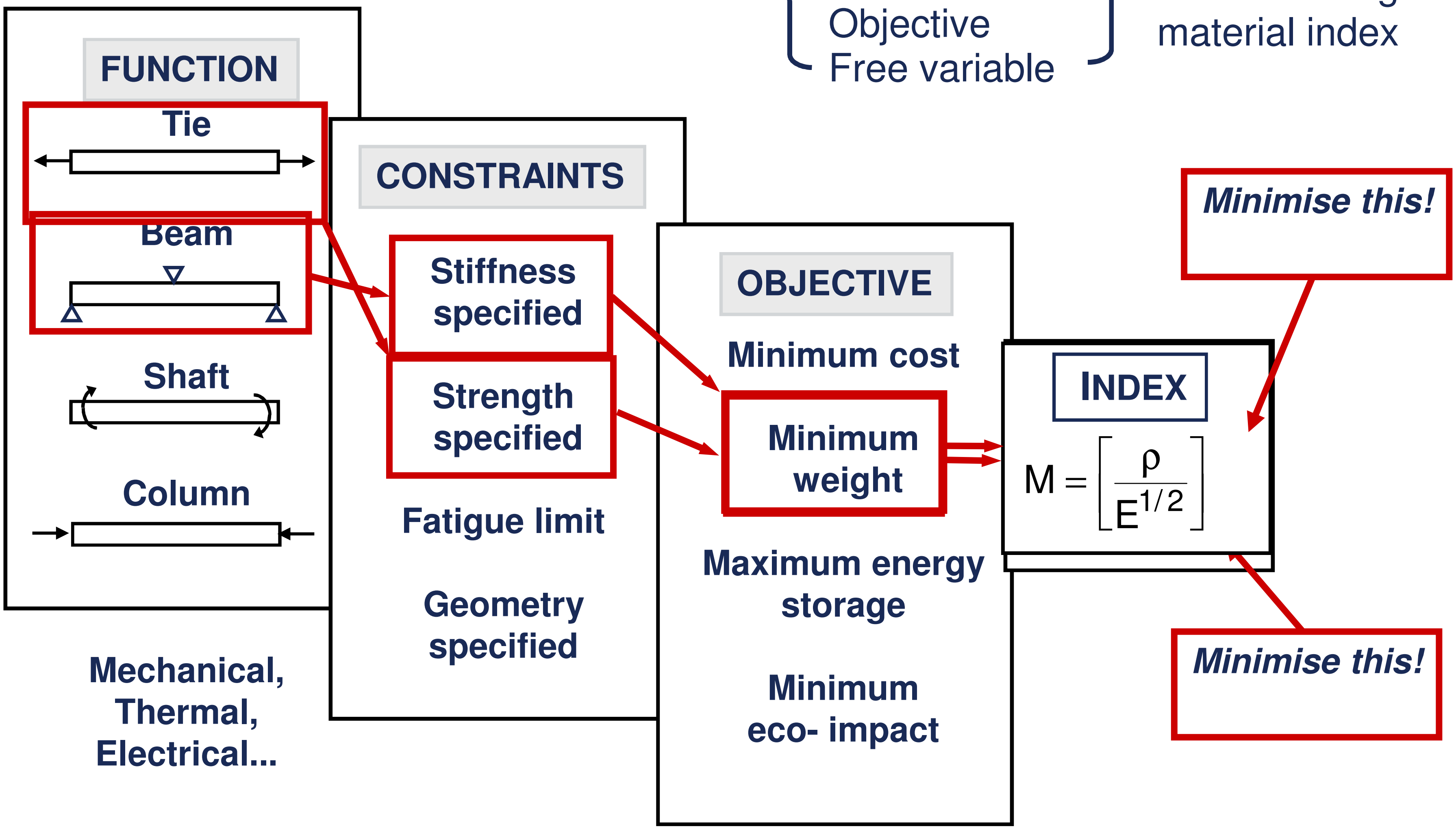
Analogy – Mechanical Product Development...

- Developed since 1960s, $20b per year industry
- Computer Aided Design (CAD):
  - Pro/Engineer (PTC); CATIA (Dassault); NX (Siemens); Inventor (Autodesk)...
- Product Lifecycle Management (PLM):
  - Windchill (PTC); ENOVIA (Dassault); Teamcenter (Siemens); PLM360 (Autodesk)...

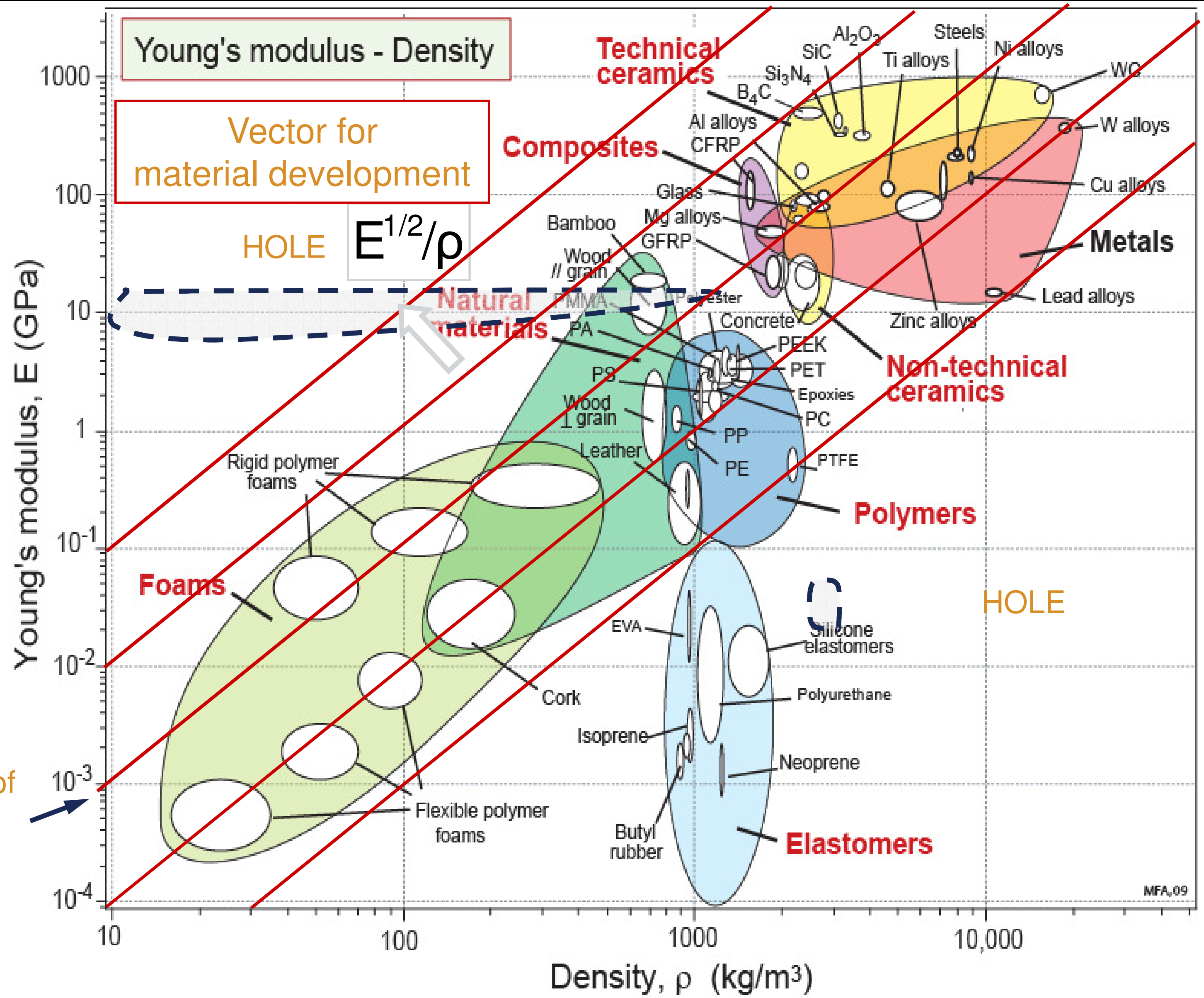
What are the equivalents of CAD and PLM for Materials Development?

Systematic Material Selection: 'Material indices'

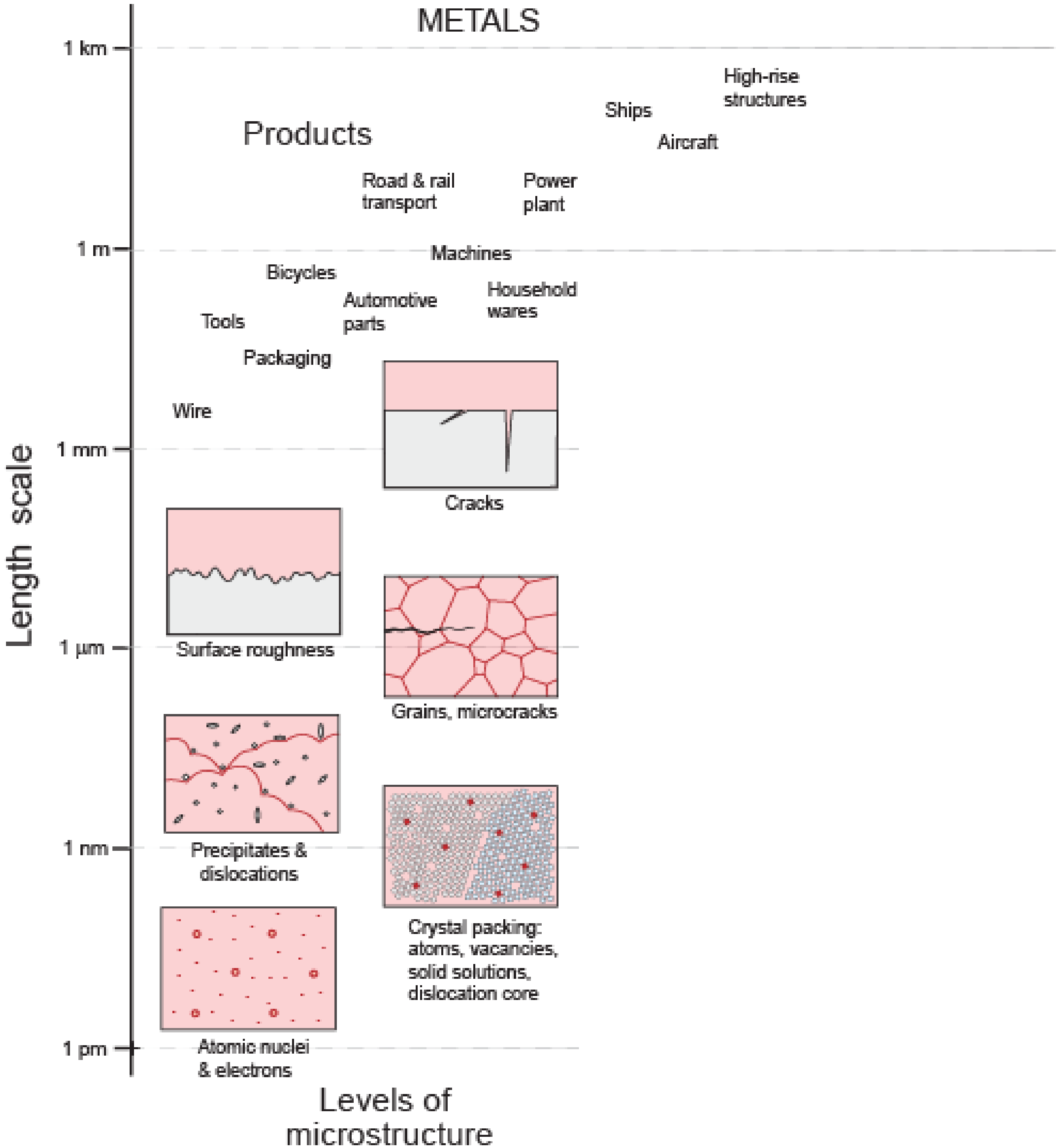
Each combination of { Function, Constraint, Objective, Free variable } has a characterising material index



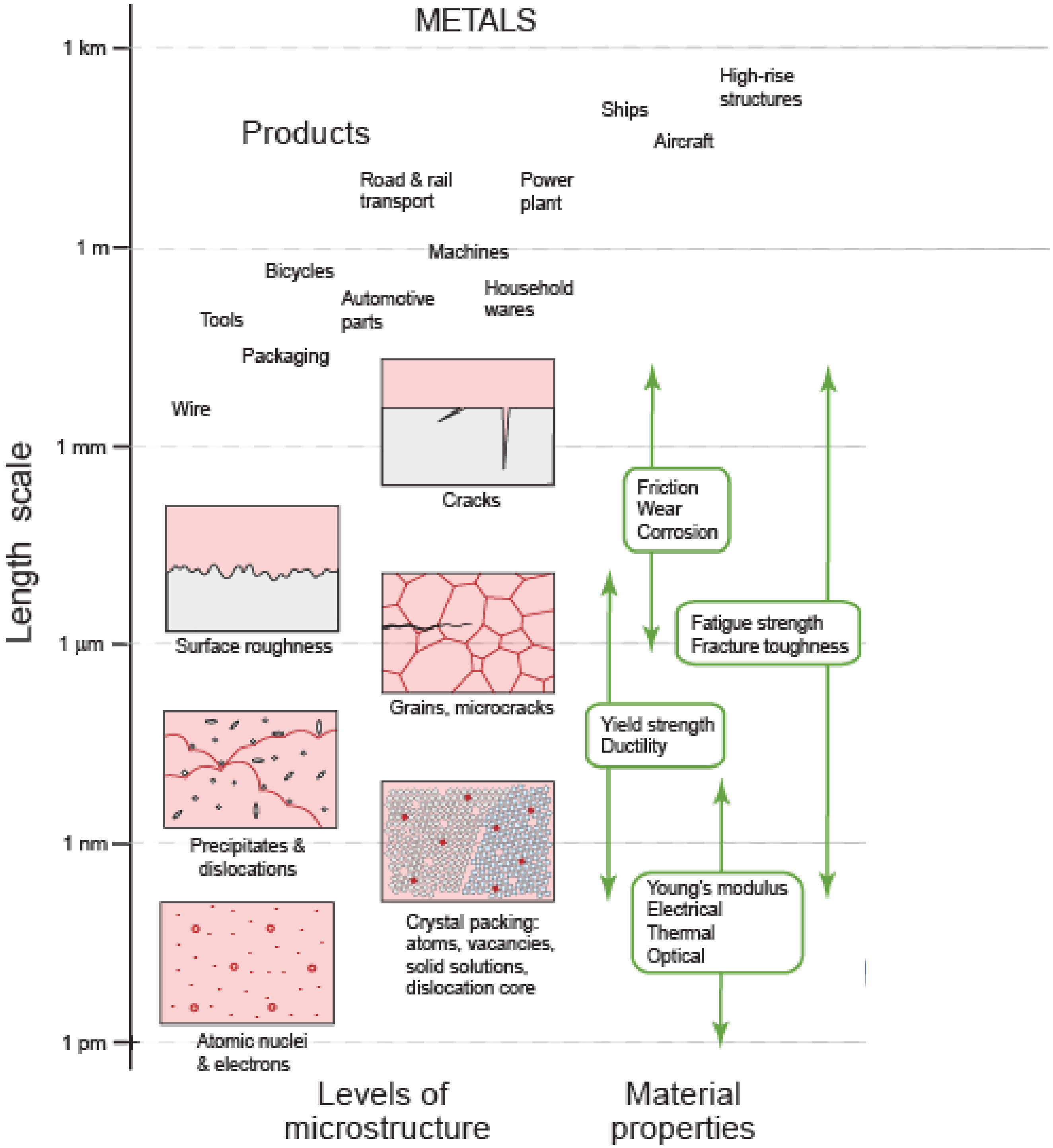
Modulus and Density



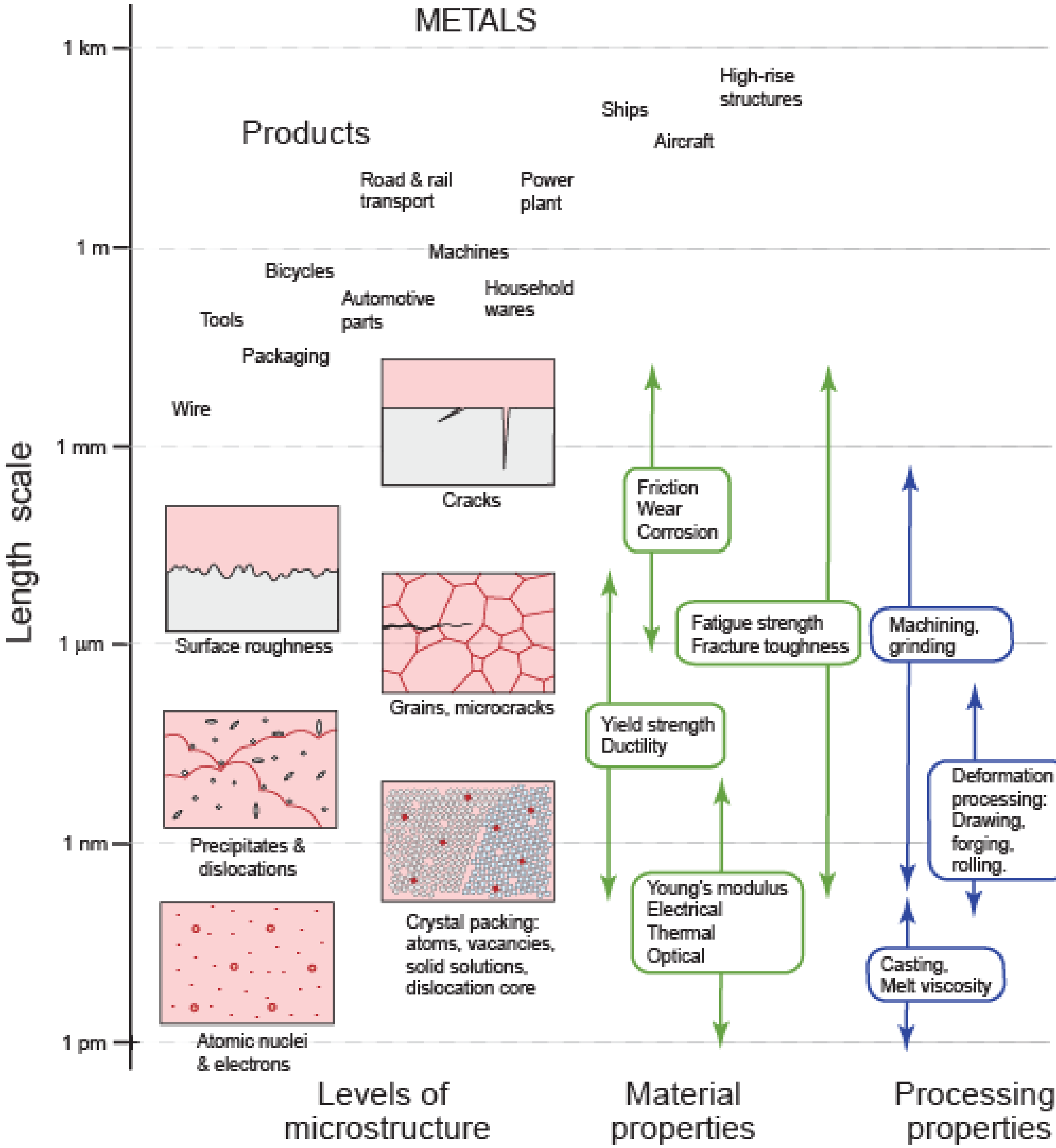
Contours of $E^{1/2}/\rho$



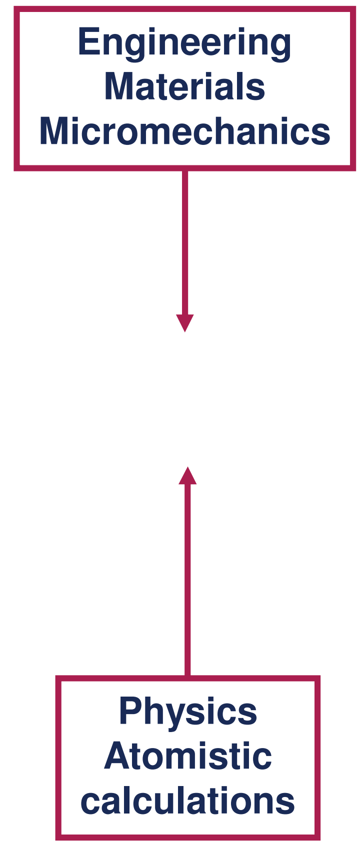
What Properties?



What Properties?

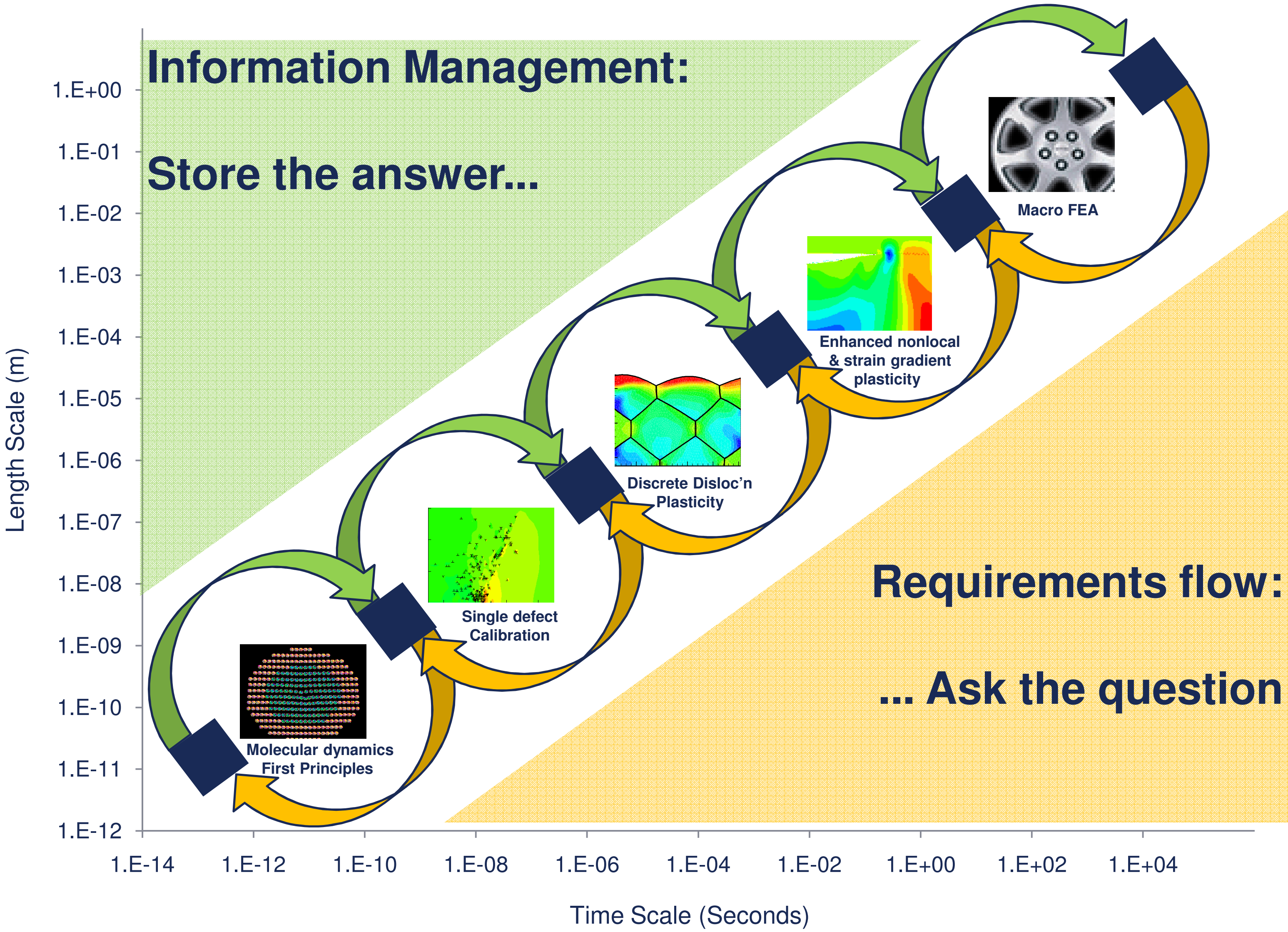


What Properties?

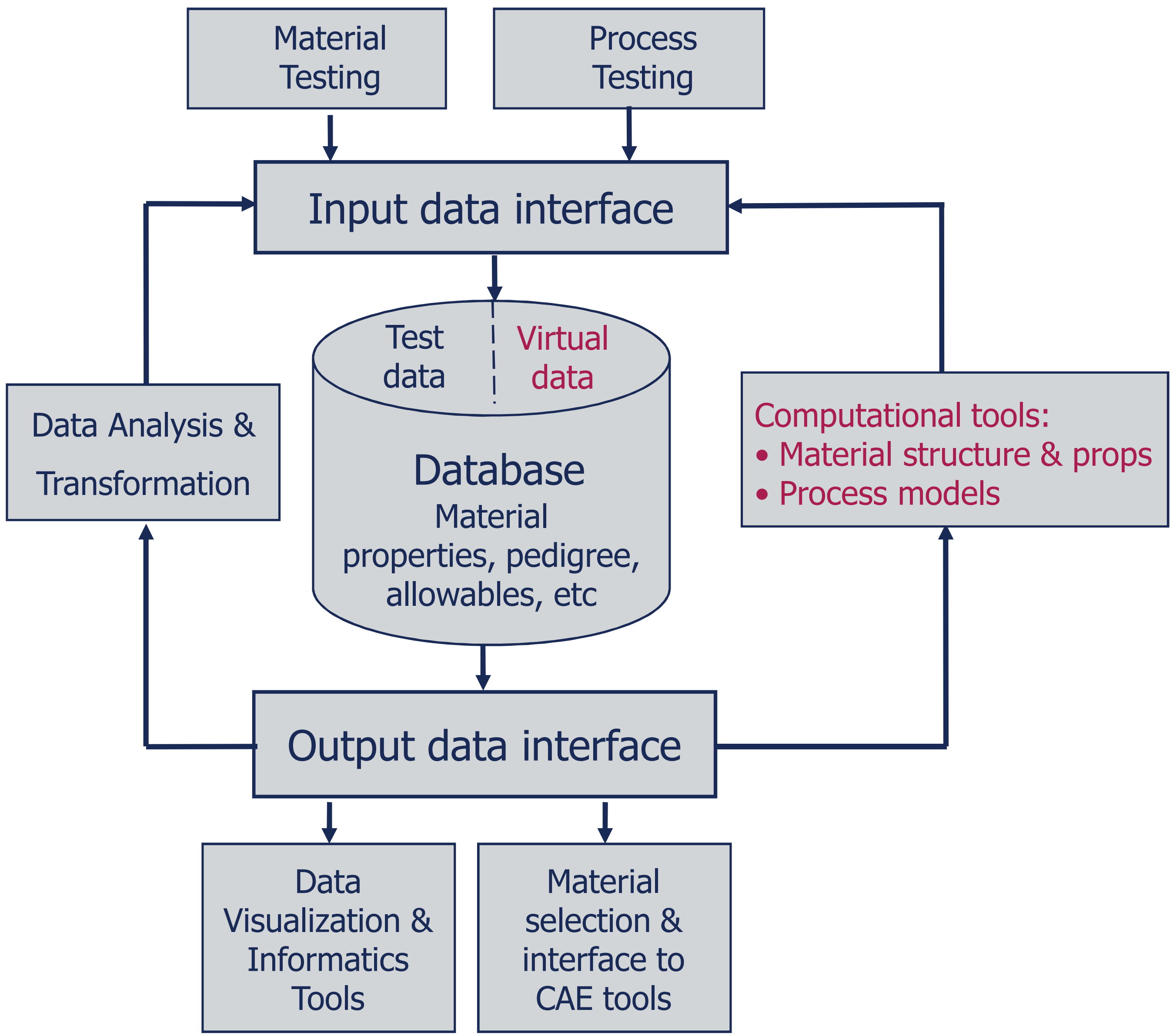


A Framework for Multiscale Modelling

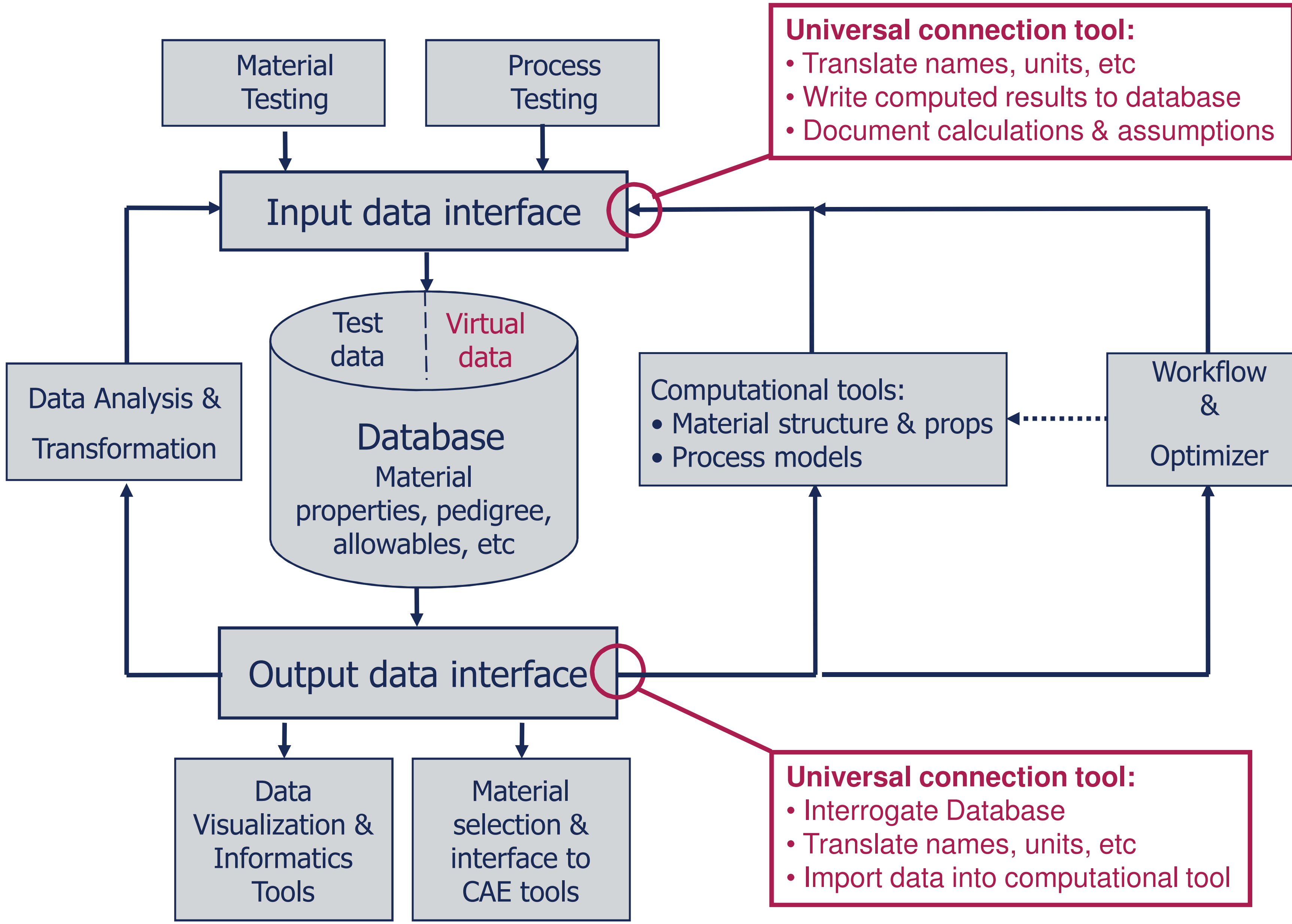
Multiscale Modelling



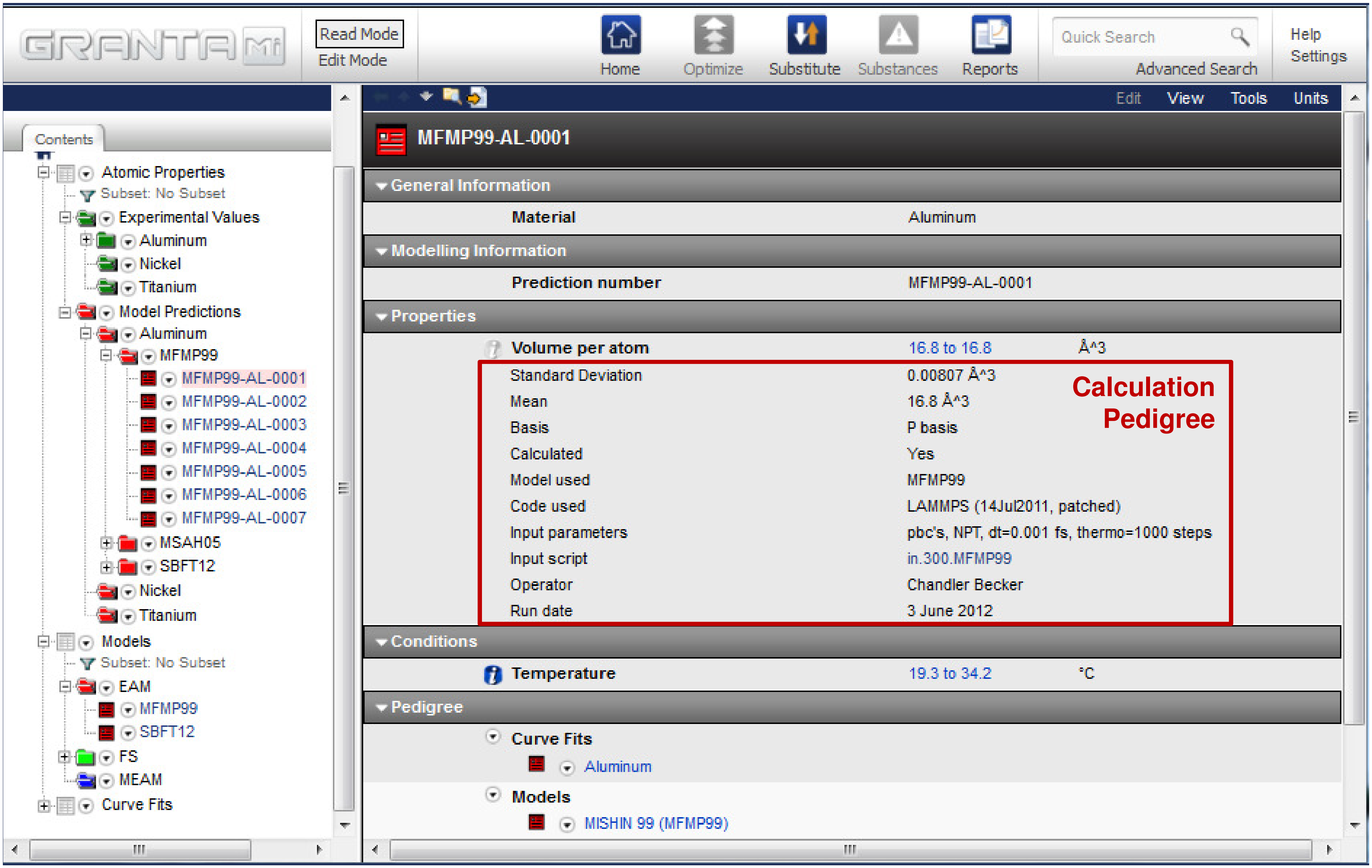
Proposed Architecture



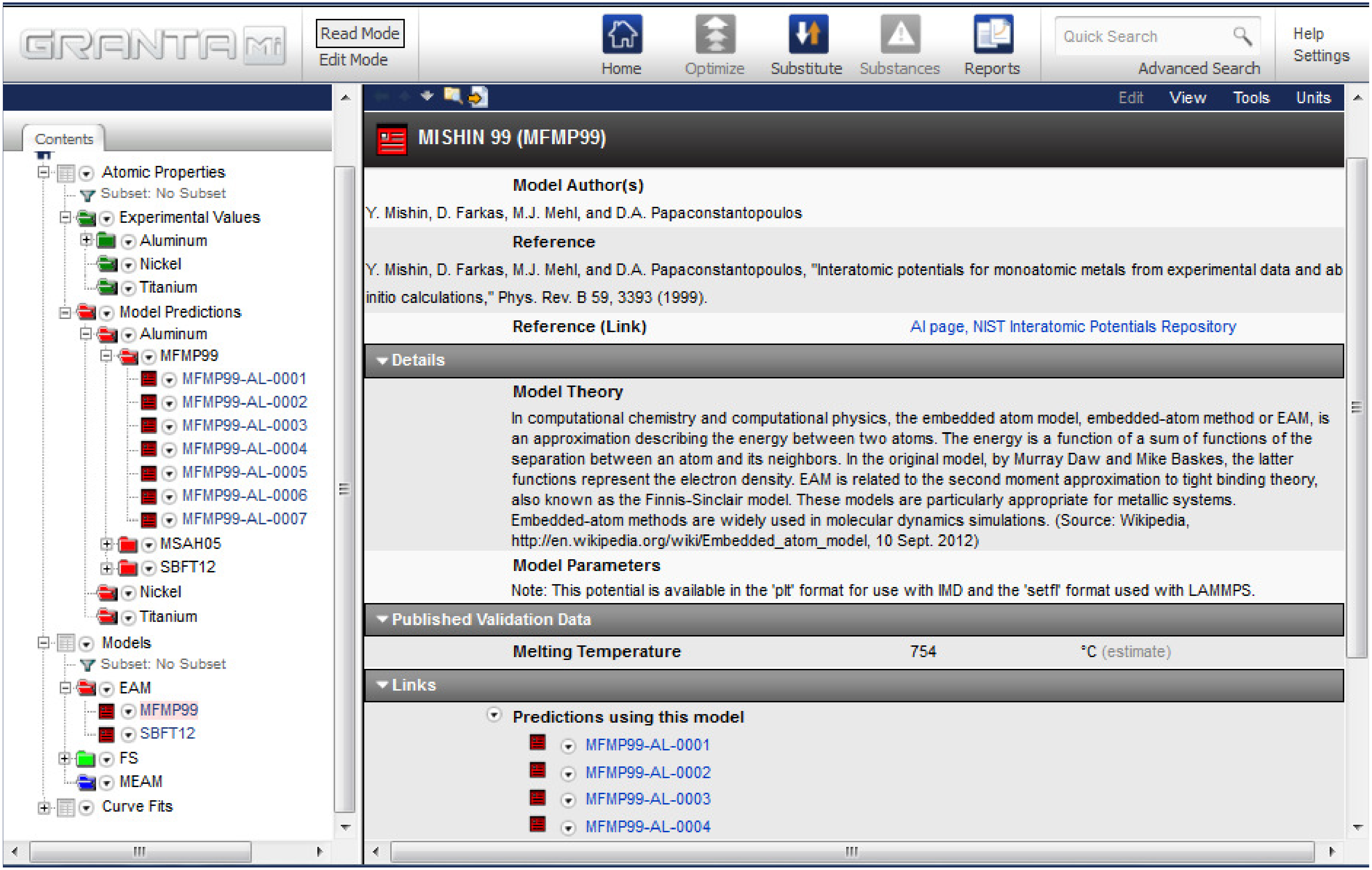
Proposed Architecture



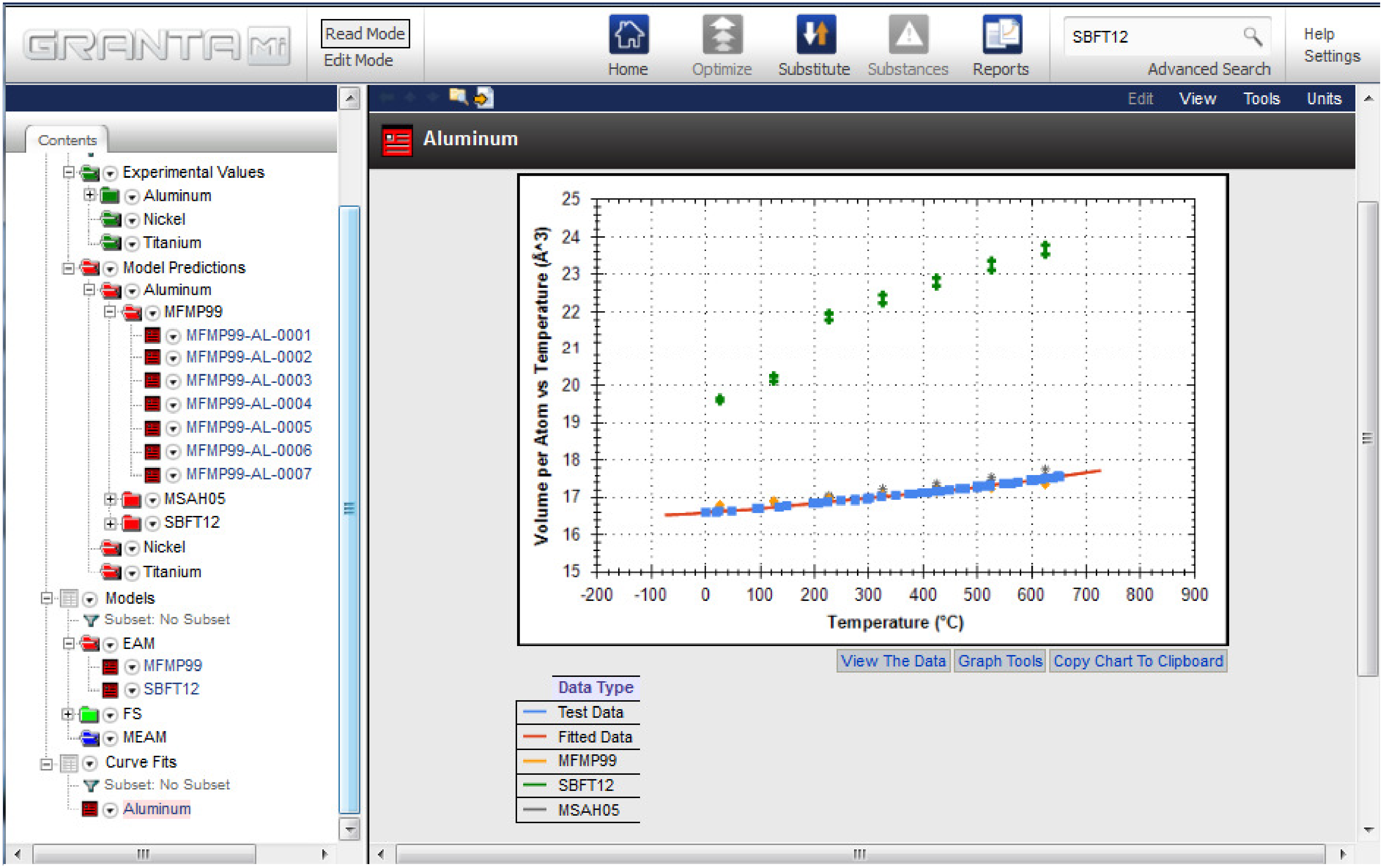
NIST Demo Atomistics Database Simulation Data



NIST Demo Atomistics Database
Model Description Record

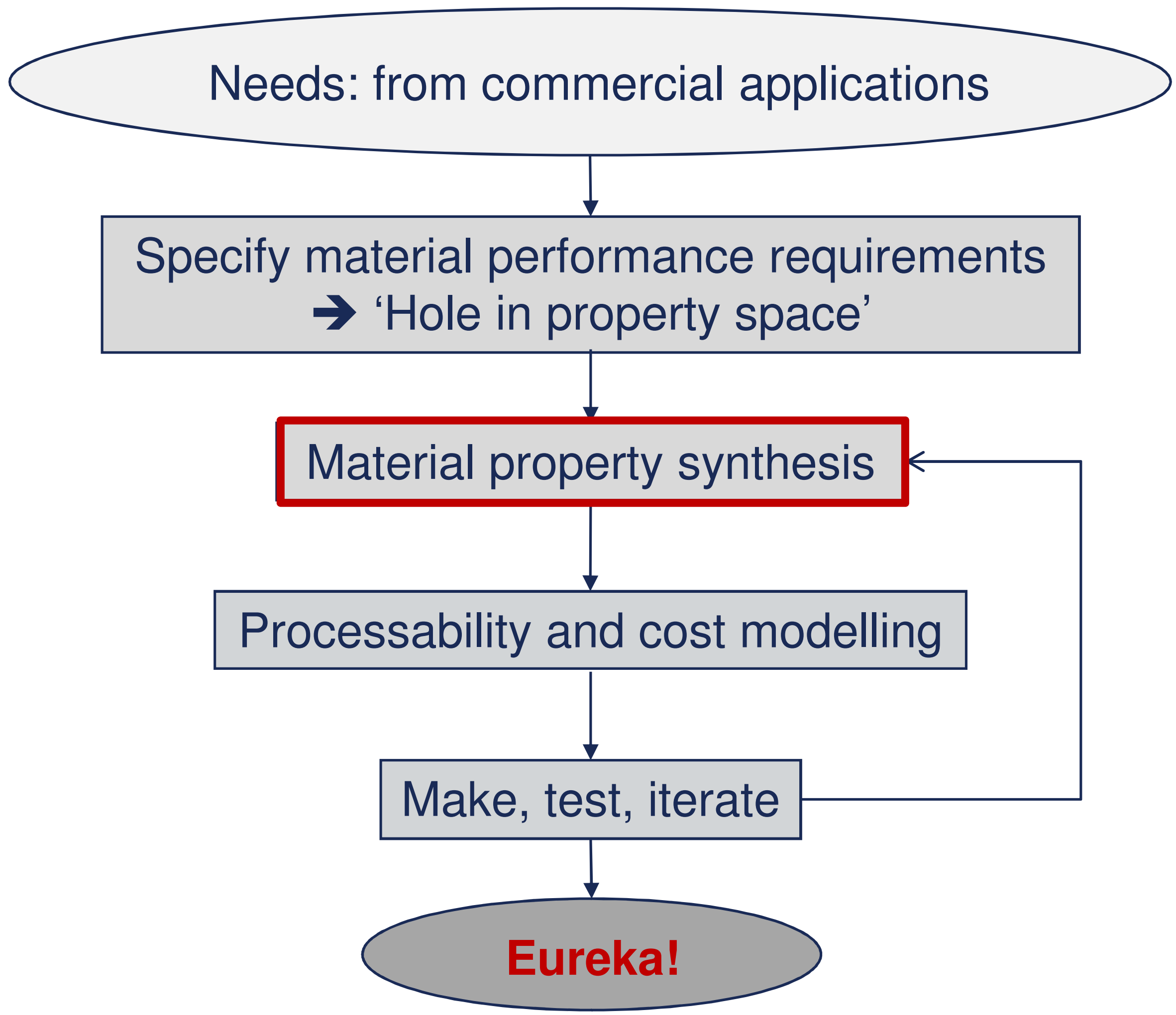


NIST Demo Atomistics Database
Validating models with experimental data



A Framework for Materials Design

Systematic Materials Design (CAD)



Research Framework: Material Property Synthesis

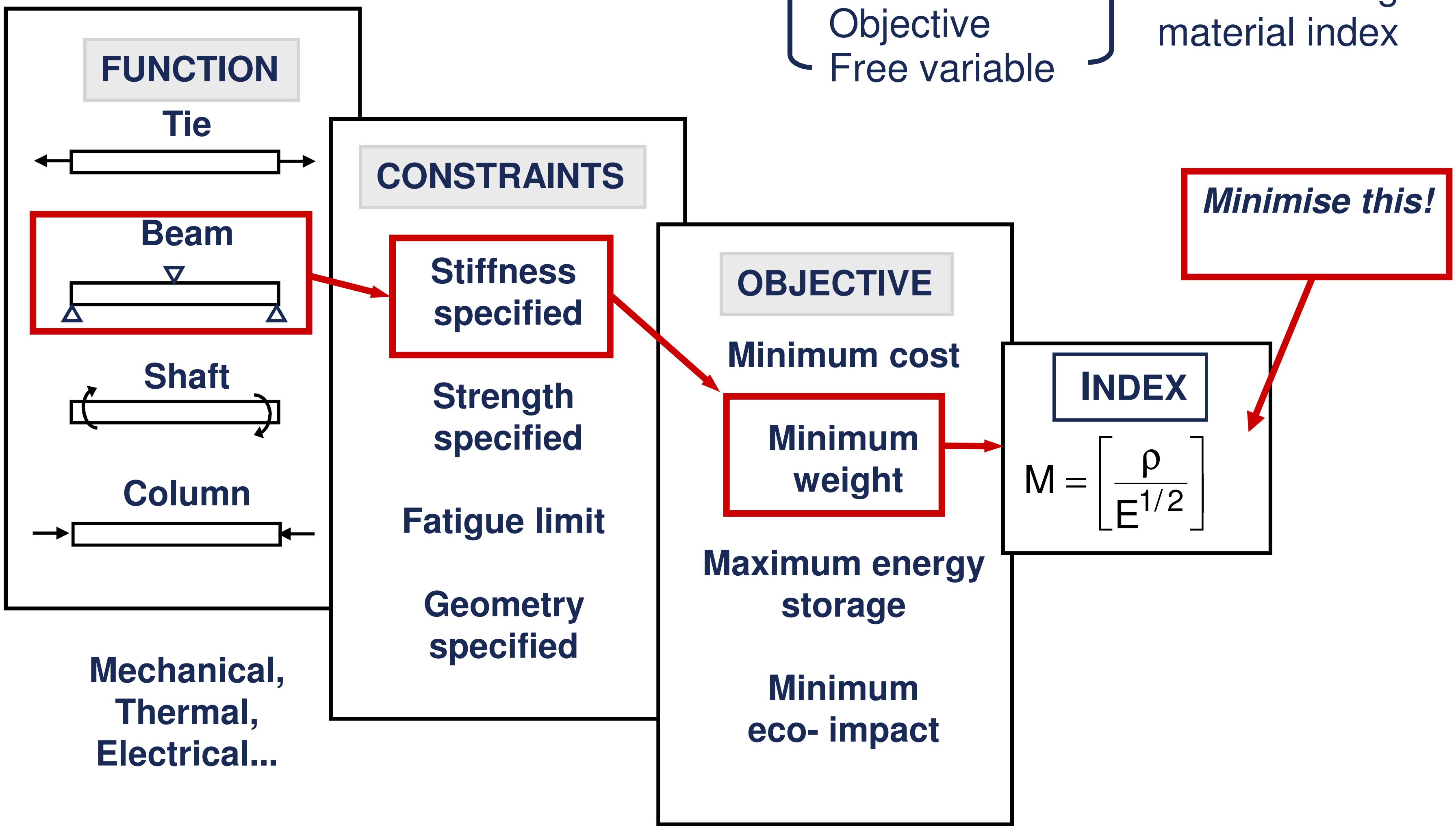
	Alloys	Polymers	Ceramics	Hybrids
1. Trajectory Guidance	Combination rules for alloy systems Select by Analogy 'Enlightened Empiricism' Neural Networks, etc			Material Property Charts & Indices
2. Compatibility	Atom size, solubility, structure, non-equilibrium systems, etc			'Manufactured' Compatibility
3. Microstructure Prediction	Thermodynamic models- eg CALPHAD method Meso phase models			Specified by designer
4. Property Prediction	Many modelling approaches at various length scales Quantum mechanics,dynamics Molecular mechanics and dynamics, Meso phase modelling			Micromechanical Models
5. Evaluation & Optimal Selection	Numerical and graphical methods			Graphical Optimization Methods

↑ **Case Study**

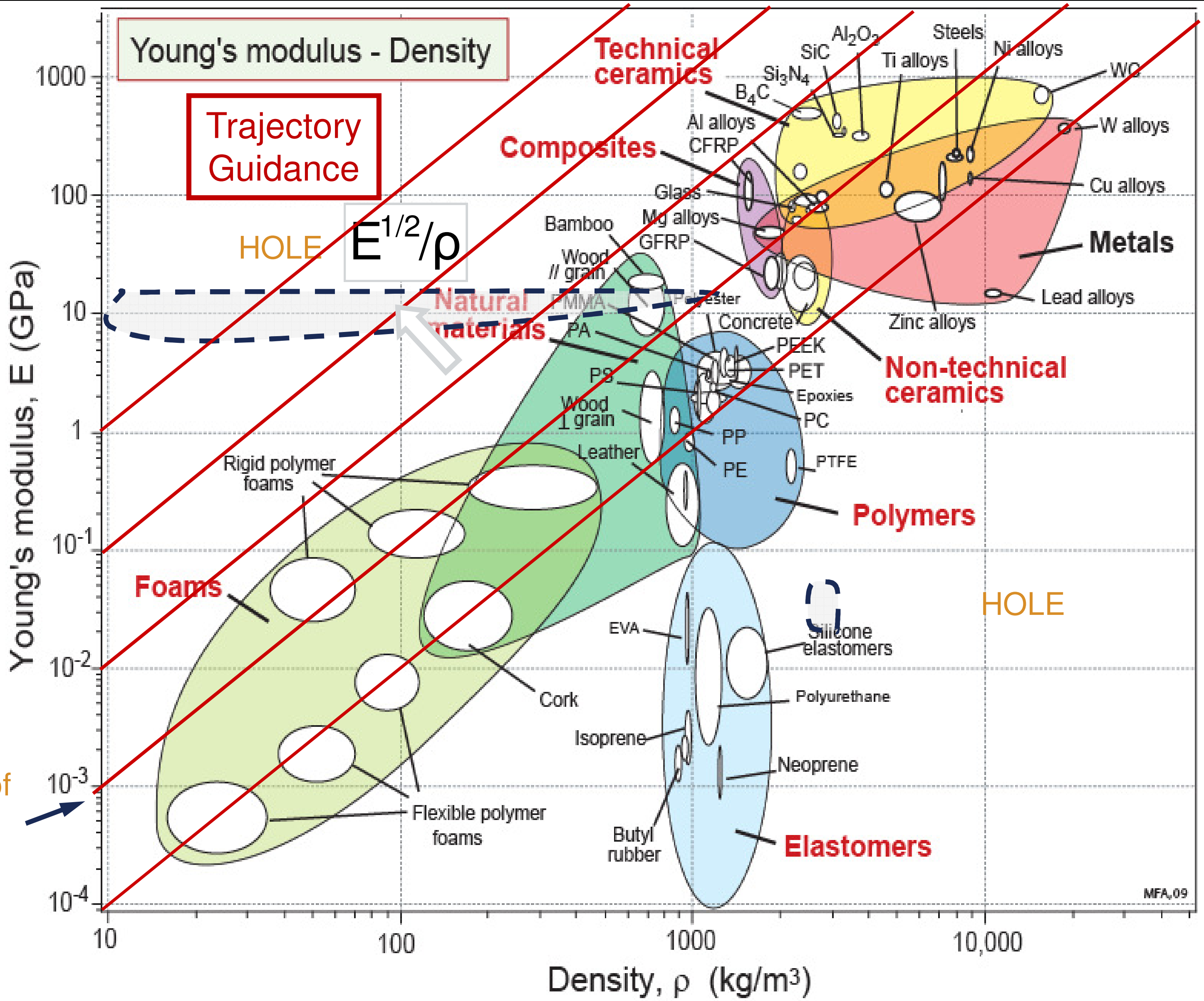
Case Study
Light, Stiff Panels: Hybrid Synthesis

Systematic Material Selection: 'Material indices'

Each combination of { Function, Constraint, Objective, Free variable } has a characterising material index



Modulus and Density



Contours of

$E^{1/2}/\rho$

Innovation through macrostructure

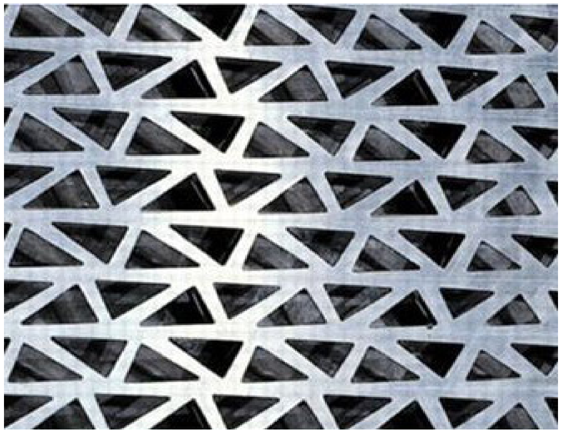
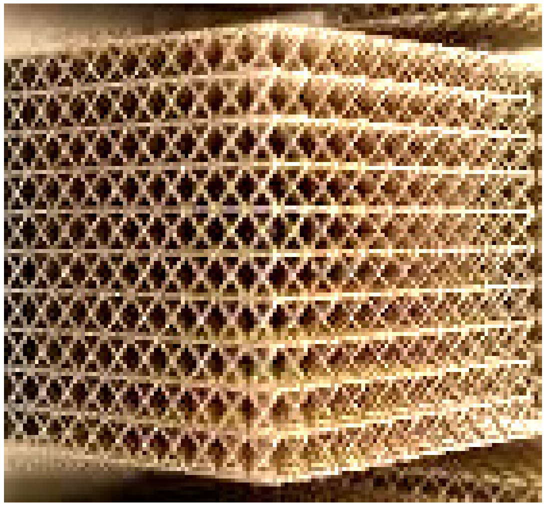
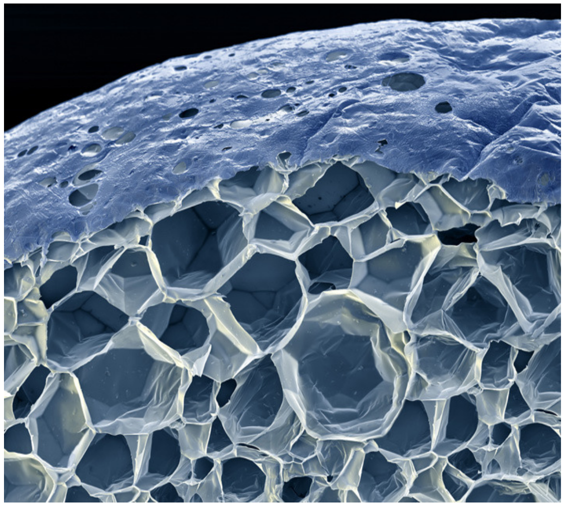
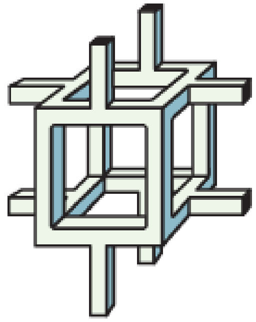

From “Manufacturing Material Effects”


Image courtesy Dr. Sacha Peters

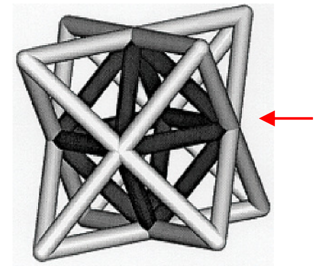

Courtesy University of Liverpool


BASF Neopor EPS foam

Configurations

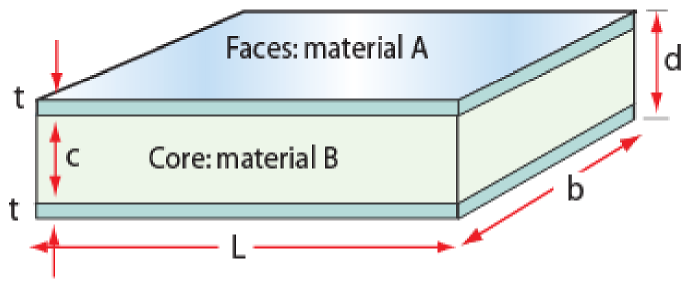


Foam cell



Triangulated cell faces

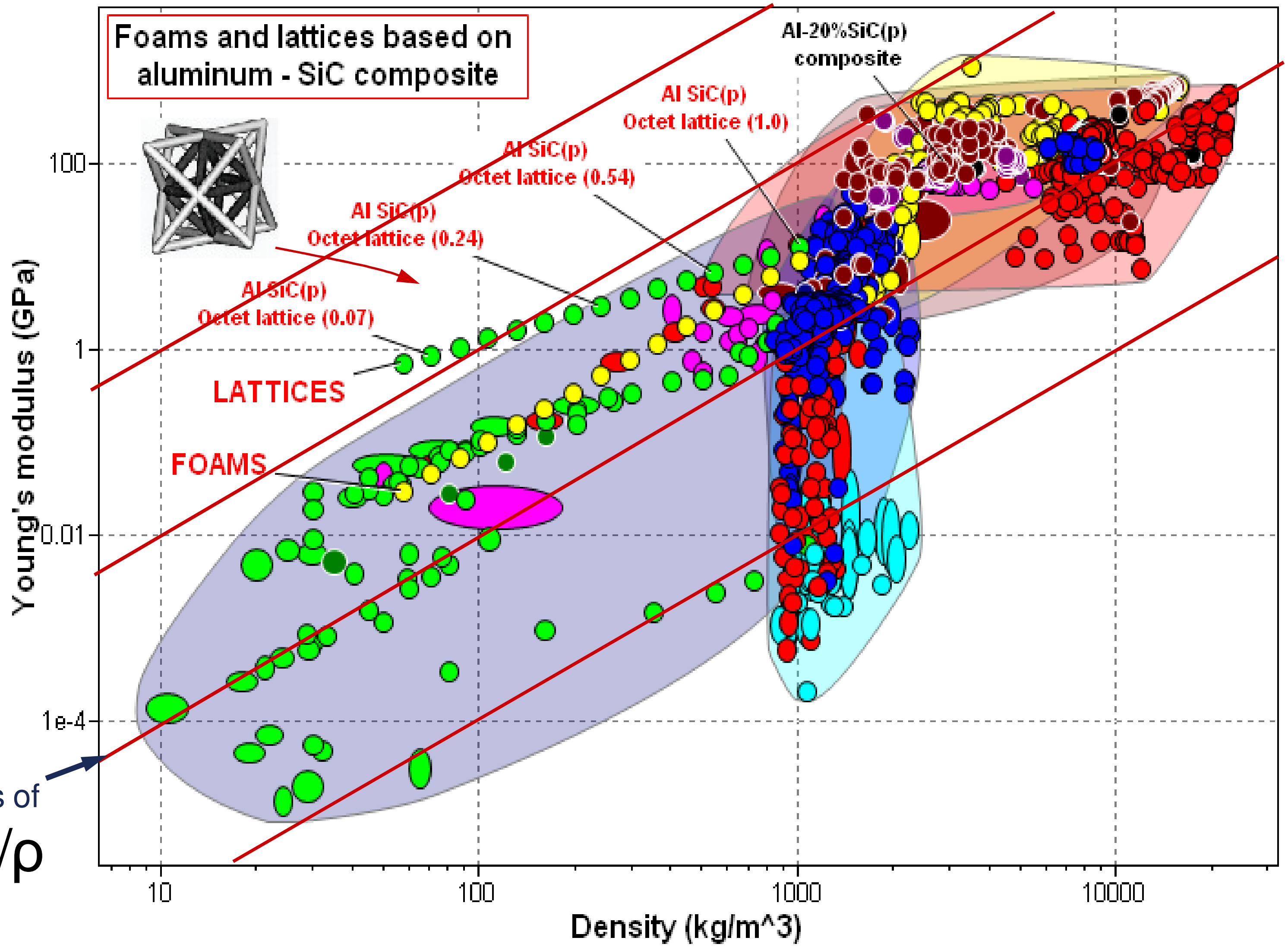
Lattice cell



Sandwich cell

Reliable models exist for their mechanical, thermal, electrical properties, acoustic properties

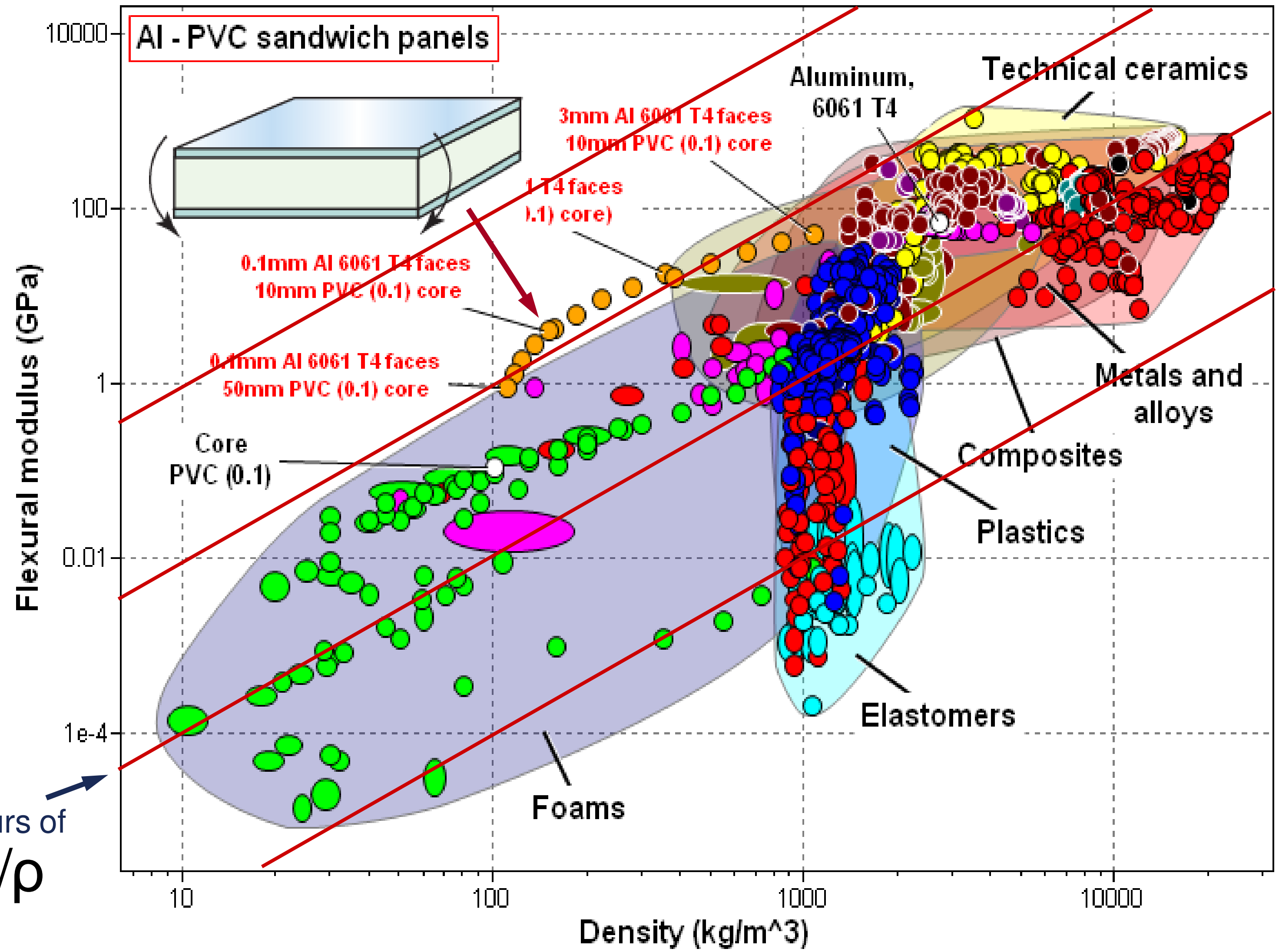
Expand material property space: Lattices



2800 materials

Contours of $E^{1/2}/\rho$

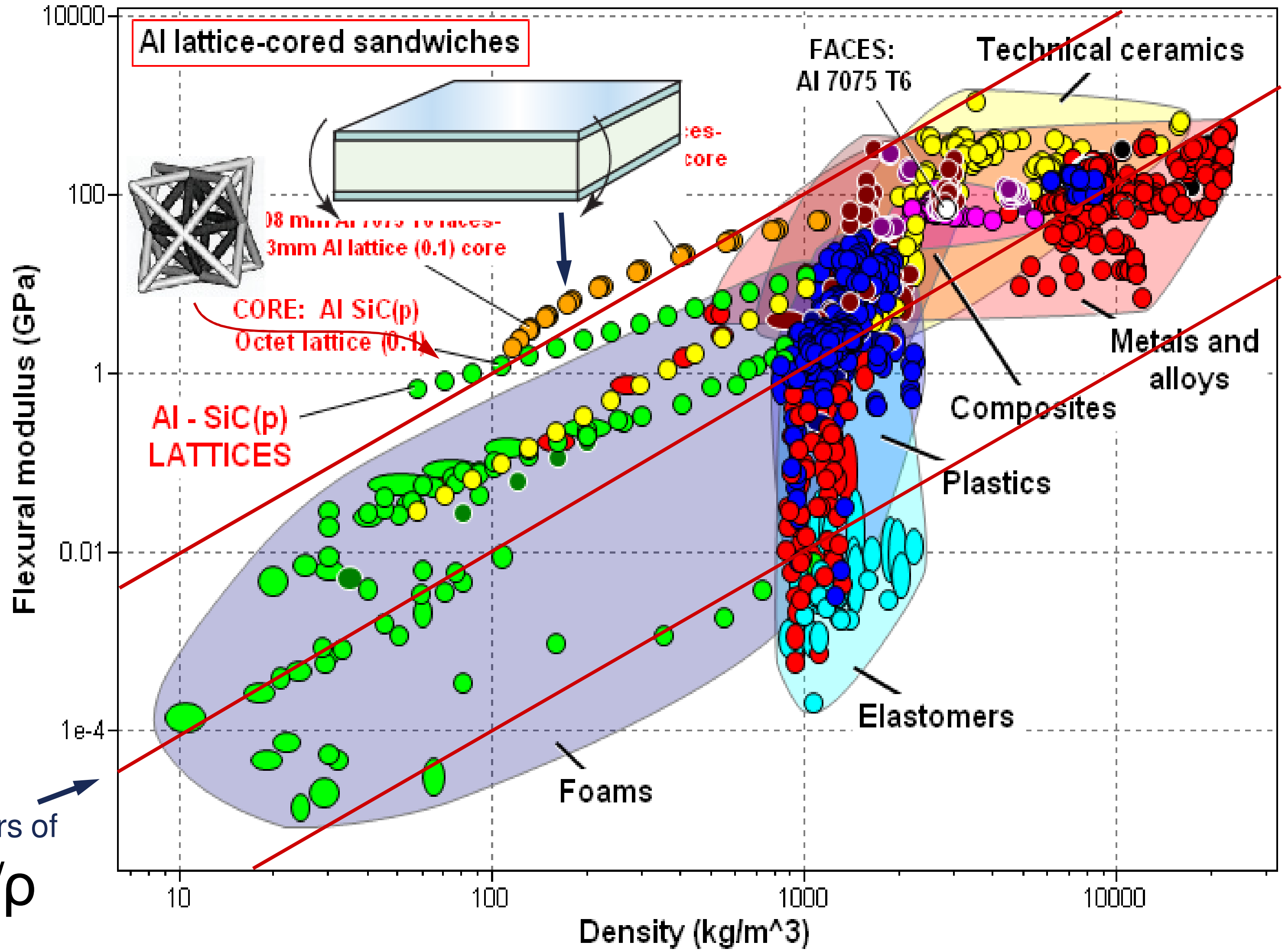
Expand material property space: Sandwiches



2800 materials

Contours of $E^{1/2}/\rho$

Expand material property space: Structures



2800 materials

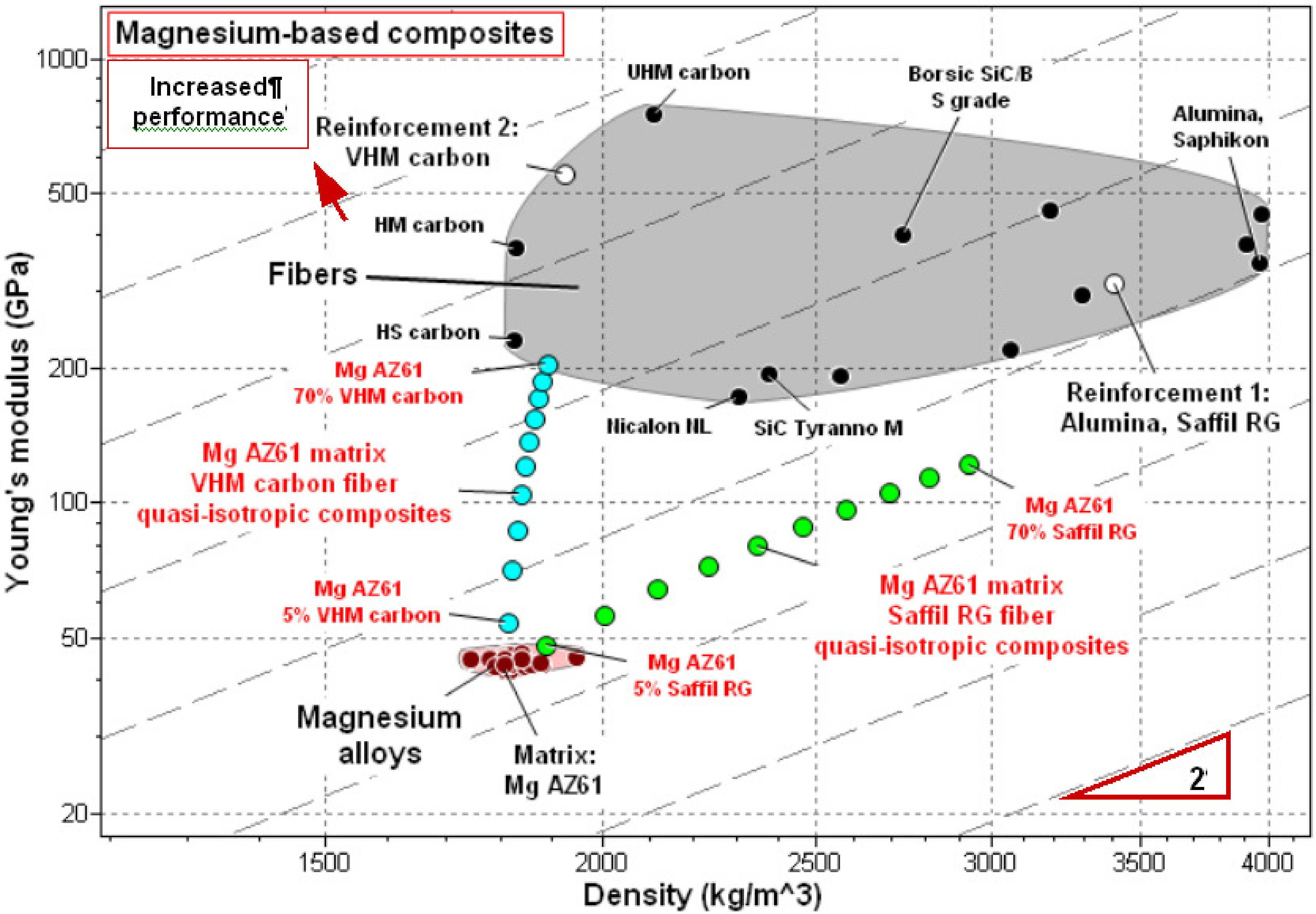
Contours of $E^{1/2}/\rho$

Conclusions

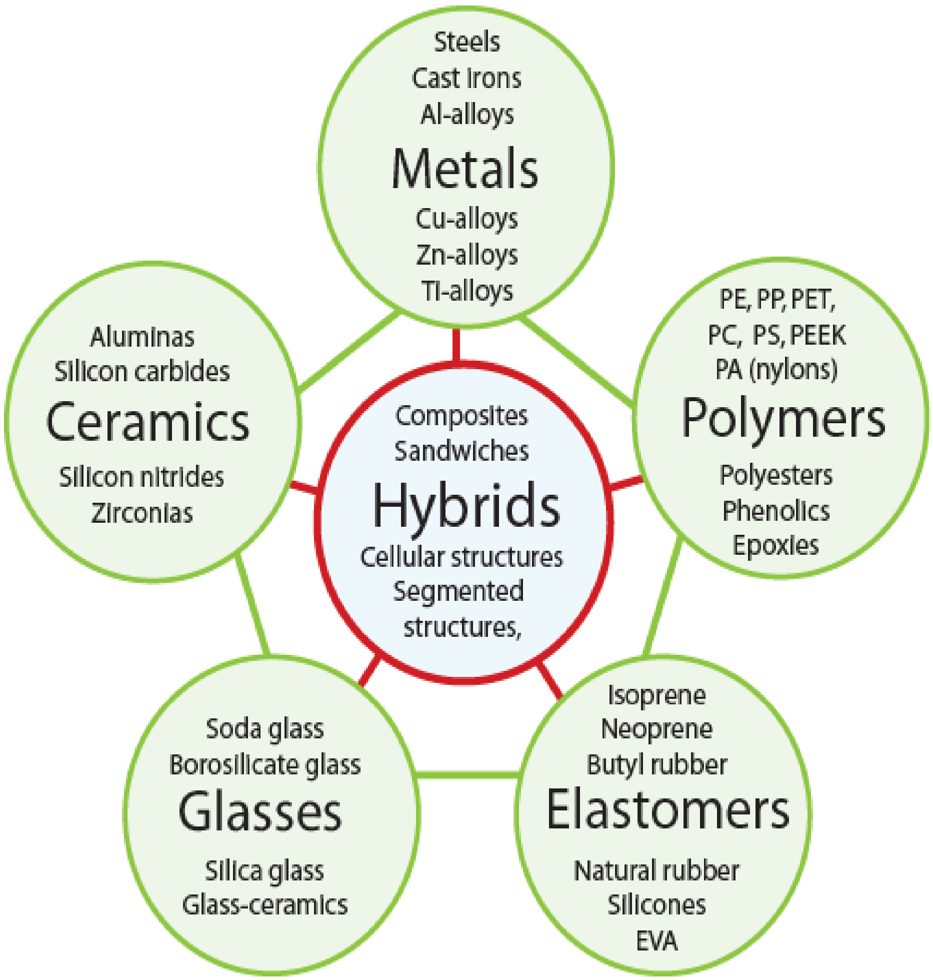
1. **Multiscale modelling:**
   - Is necessary to predict macro-scale properties
   - Is achievable in some areas, distant future in others
   - Co-managing simulation and test data is a good way forward
   - ➔ 'Materials Lifecycle Management' (MLM)
2. **Materials design:**
   - Individual software components exist, but not integrated
   - Proposed framework for 'Materials CAD': demonstrated for hybrid materials
3. **Research and Technology Development Needs:**
   - Development of a rich, open framework for integrating multiscale modelling tools and sharing of test data and virtual data
   - Data, interface and communications standards
   - Development of multiscale modelling 'recipes' for key material classes
   - Development materials design tools

➔ **A Grand Challenge…**

Example of hybrid synthesis



Hybrid materials



Design variables:

- Choice of materials
- Volume fractions
- Configuration
- Connectivity
- Scale

The hybrid synthesizer

- Explore configurations, with free material choice
- Explore structured-structures
- A shell: insert models for other configurations