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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

**David Cebon and Mike Ashby
University of Cambridge
& Granta Design Ltd**



- 1. Background**
- 2. A Framework for Multiscale Modeling**
- 3. A Framework for Materials Design**
- 4. Case Study – Hybrid Synthesis**
- 5. Conclusions**



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...

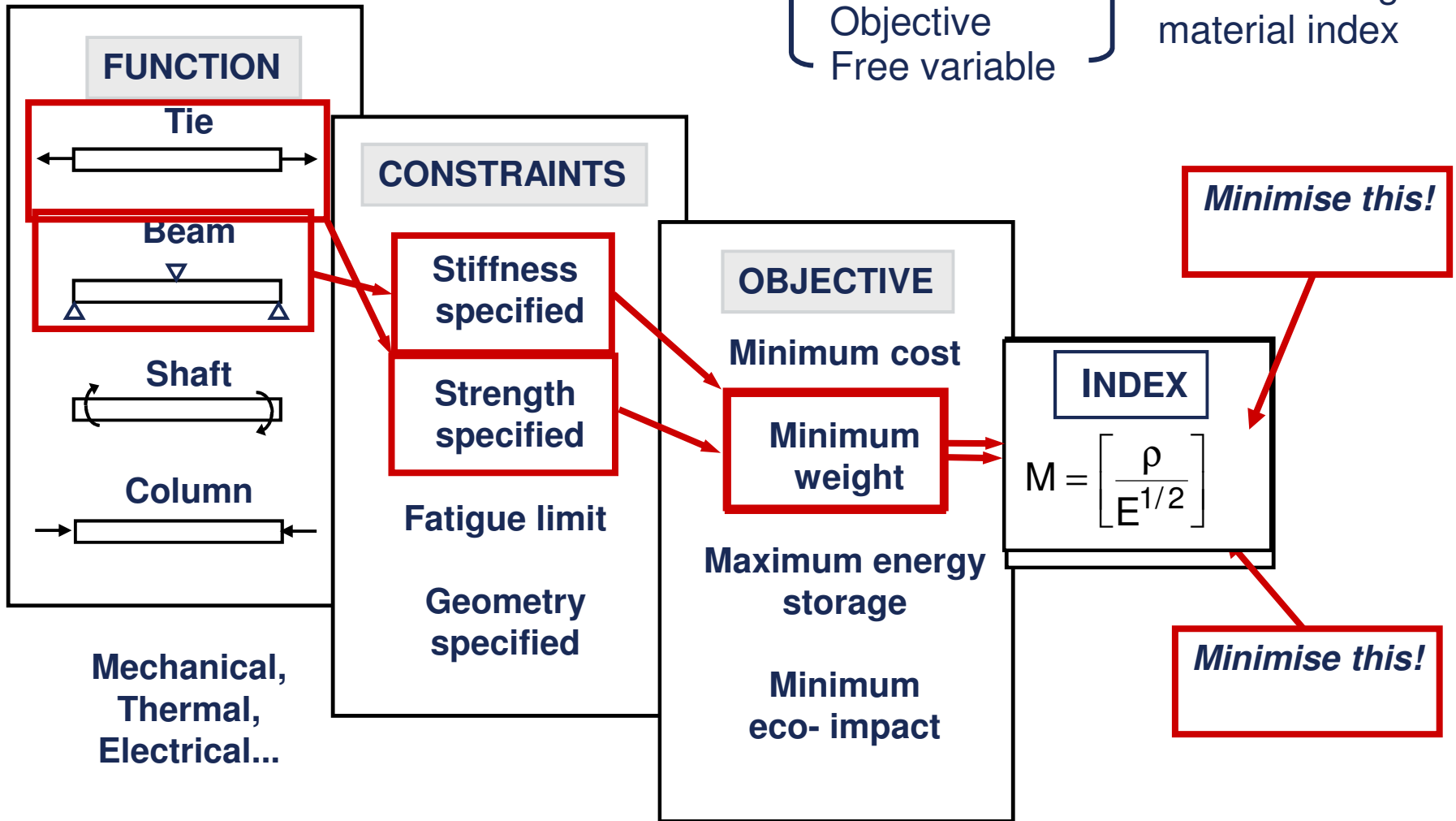
- **Developed since 1960s, \$20b per year industry**
- **Computer Aided Design (CAD):**
 - ▶ Pro/Engineer (PTC); CATIA (Dassault); NX (Siemens); Inventor (Autodesk)...
- **Product Lifecycle Management (PLM):**
 - ▶ Windchill (PTC); ENOVIA (Dassault); Teamcenter (Siemens); PLM360 (Autodesk)...

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

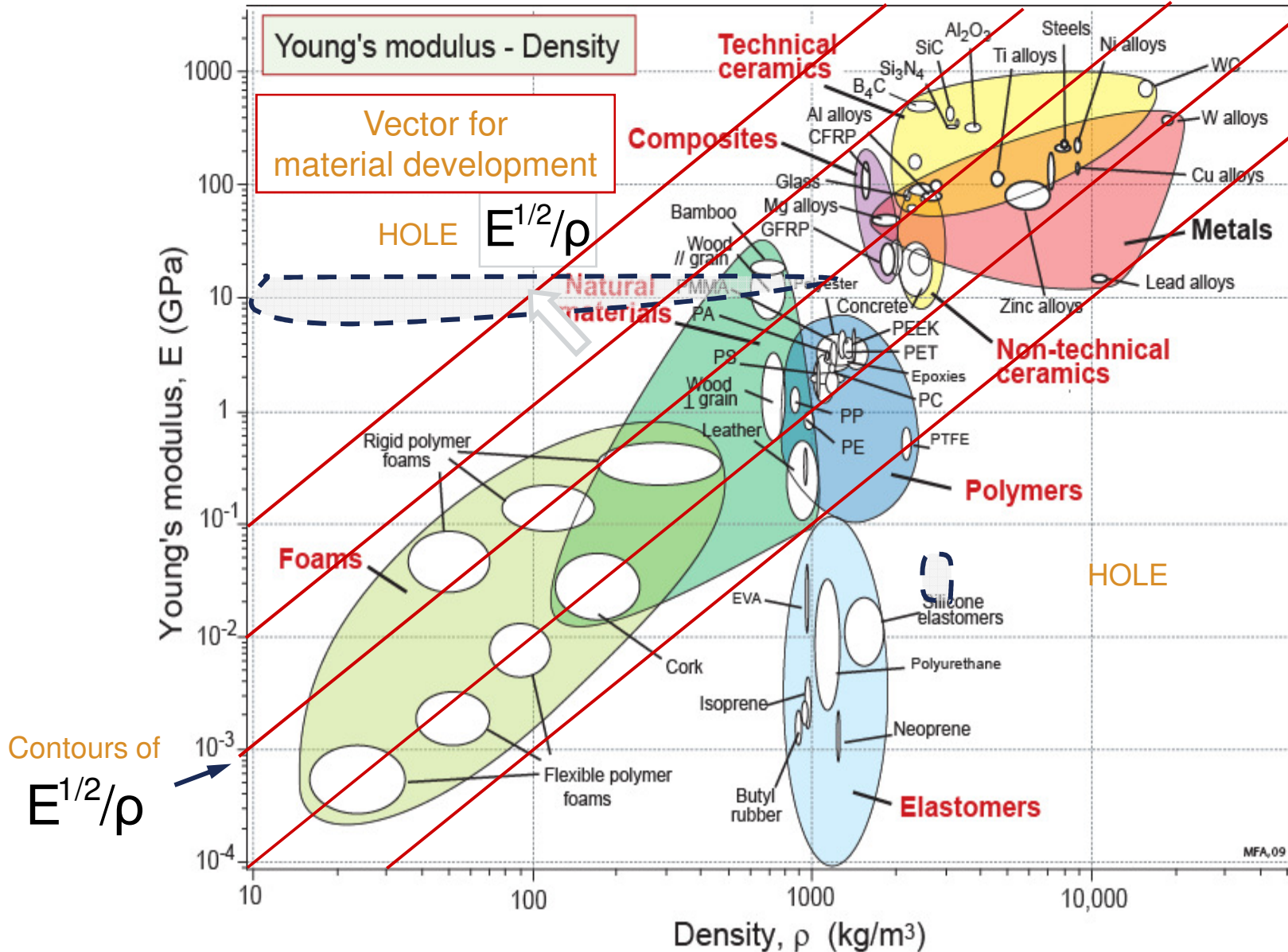
Systematic Material Selection: 'Material indices'

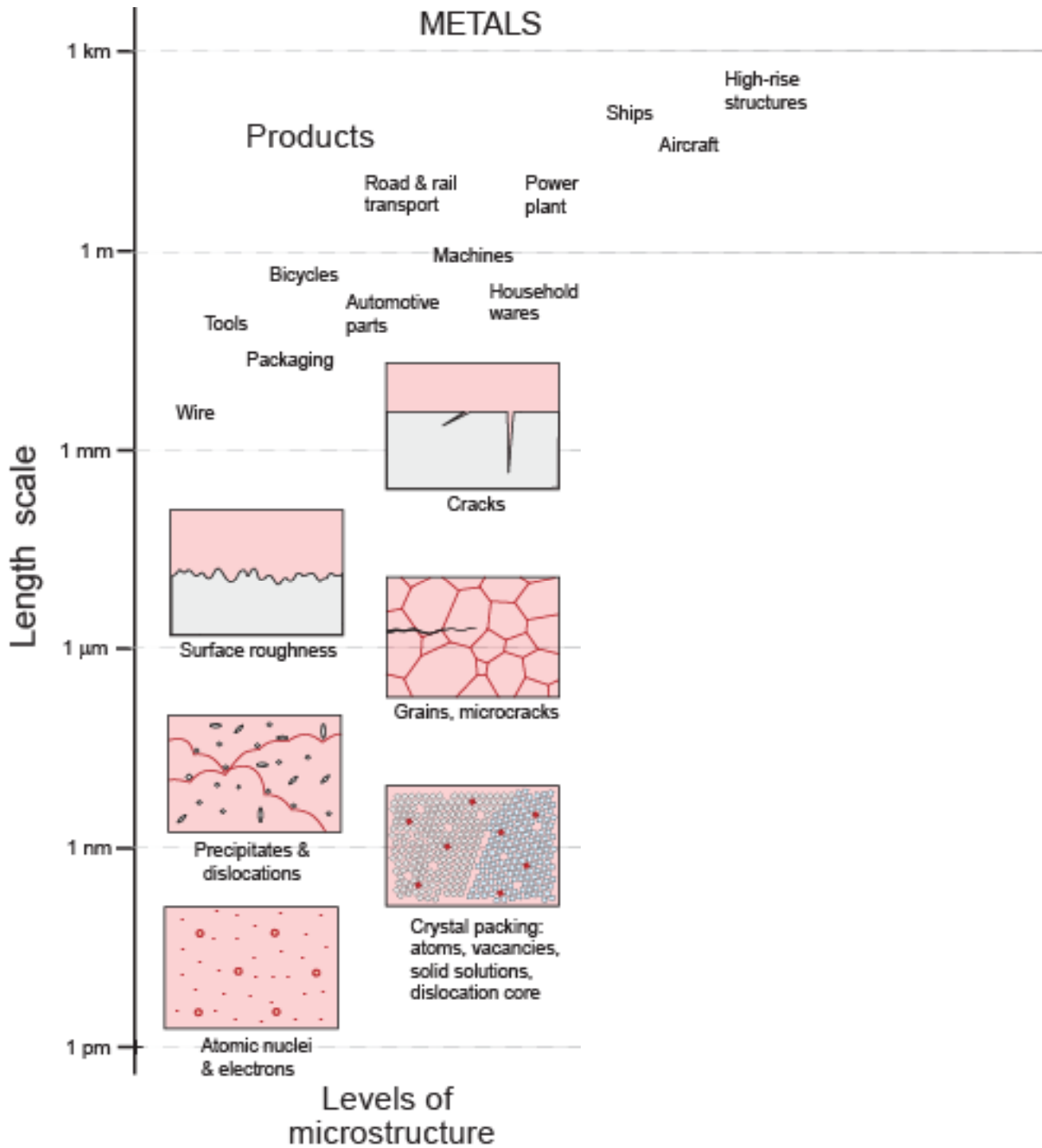


Each combination of $\left\{ \begin{array}{l} \text{Function} \\ \text{Constraint} \\ \text{Objective} \\ \text{Free variable} \end{array} \right\}$ has a characterising material index



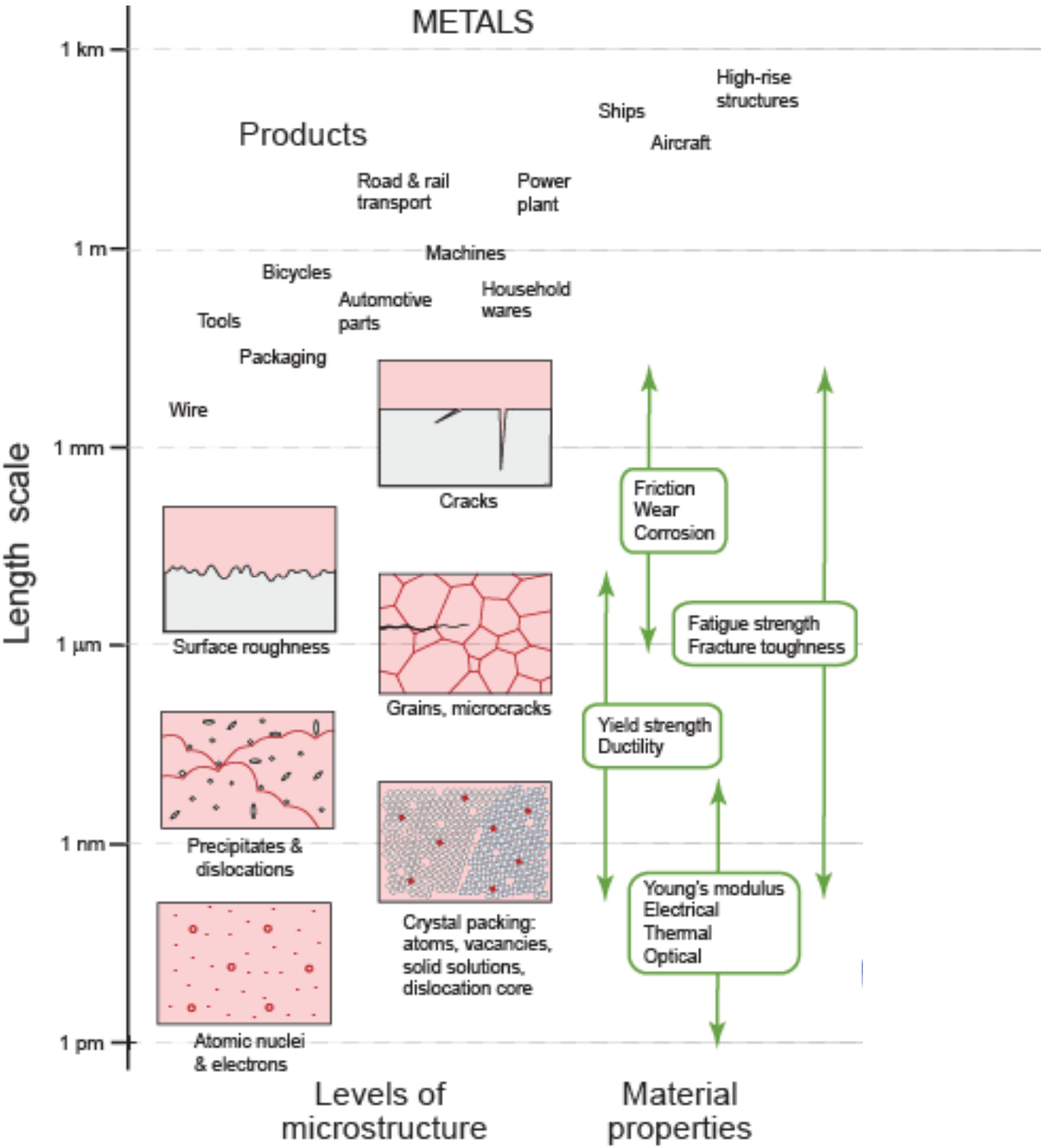
Modulus and Density

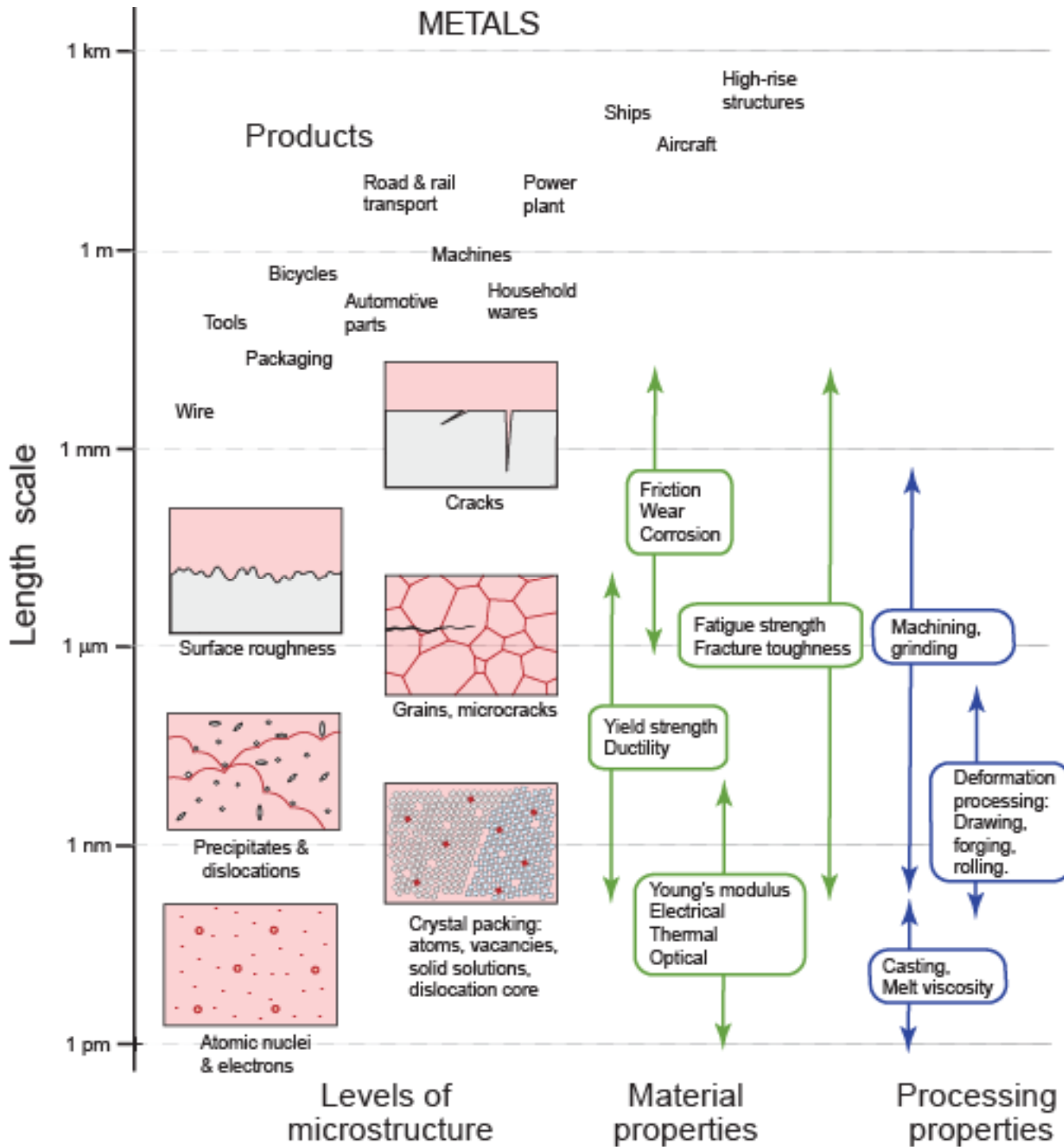




What Properties?

What Properties?





What Properties?

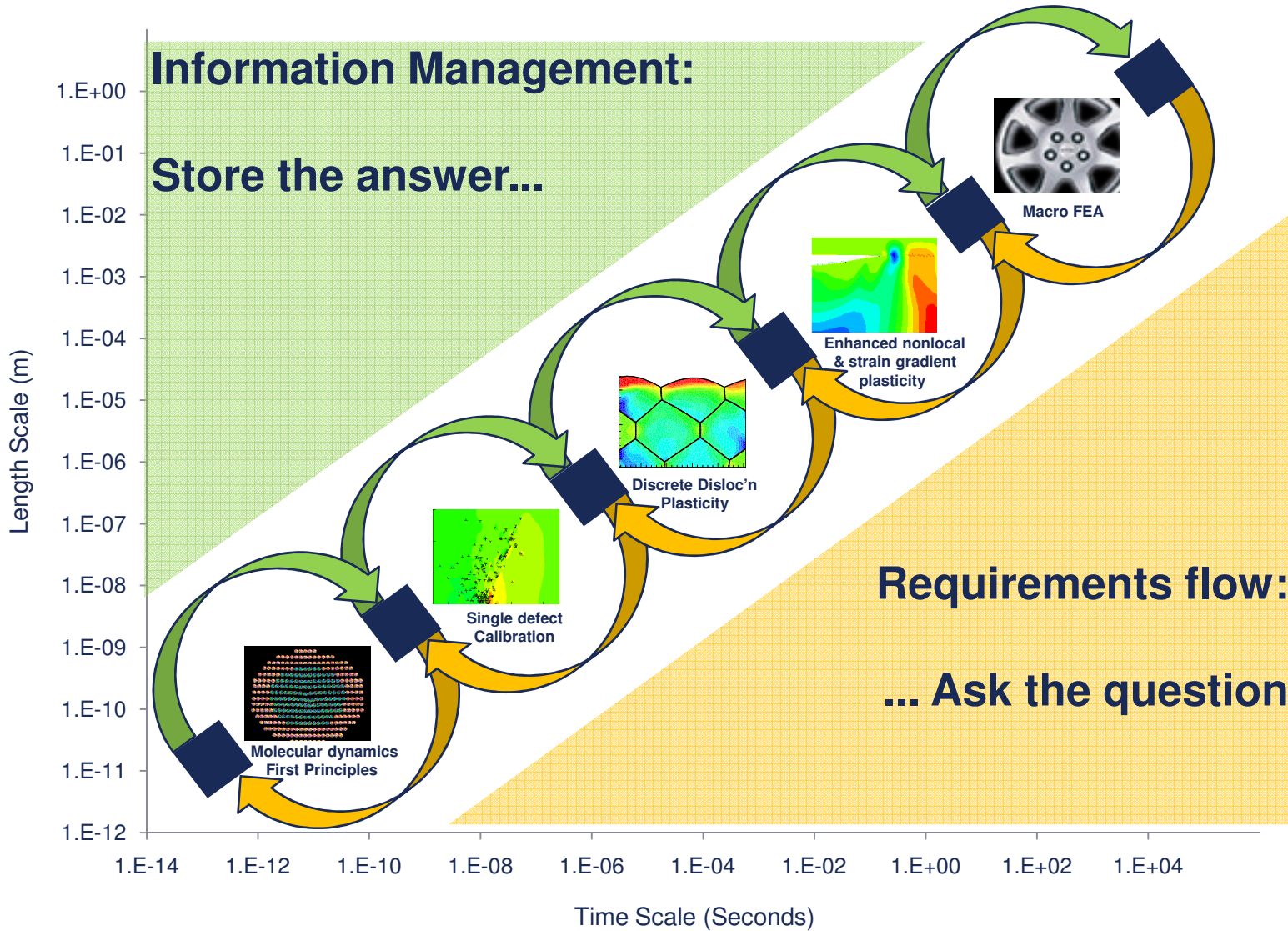
Engineering
Materials
Micromechanics

Physics
Atomistic
calculations

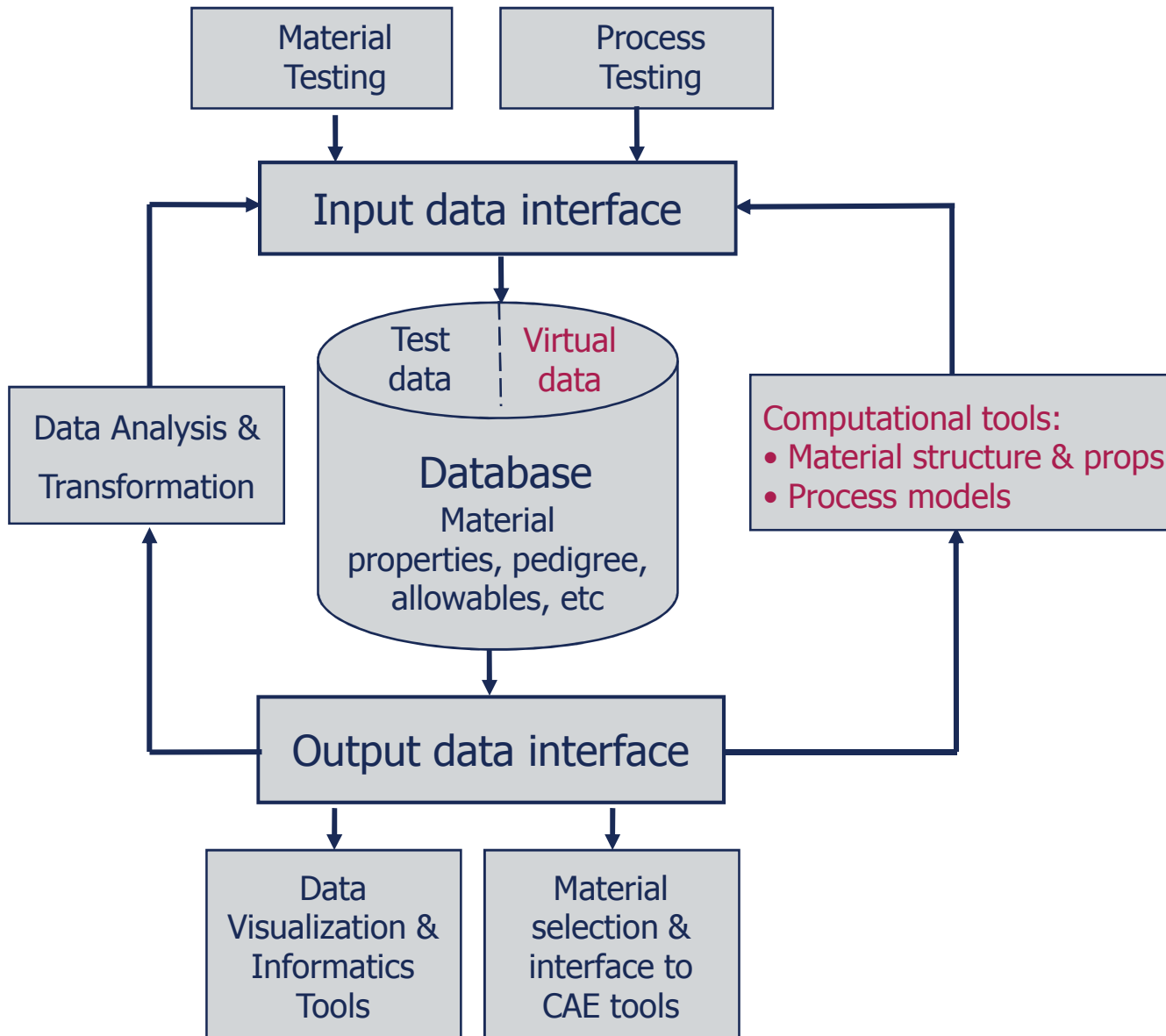


A Framework for Multiscale Modelling

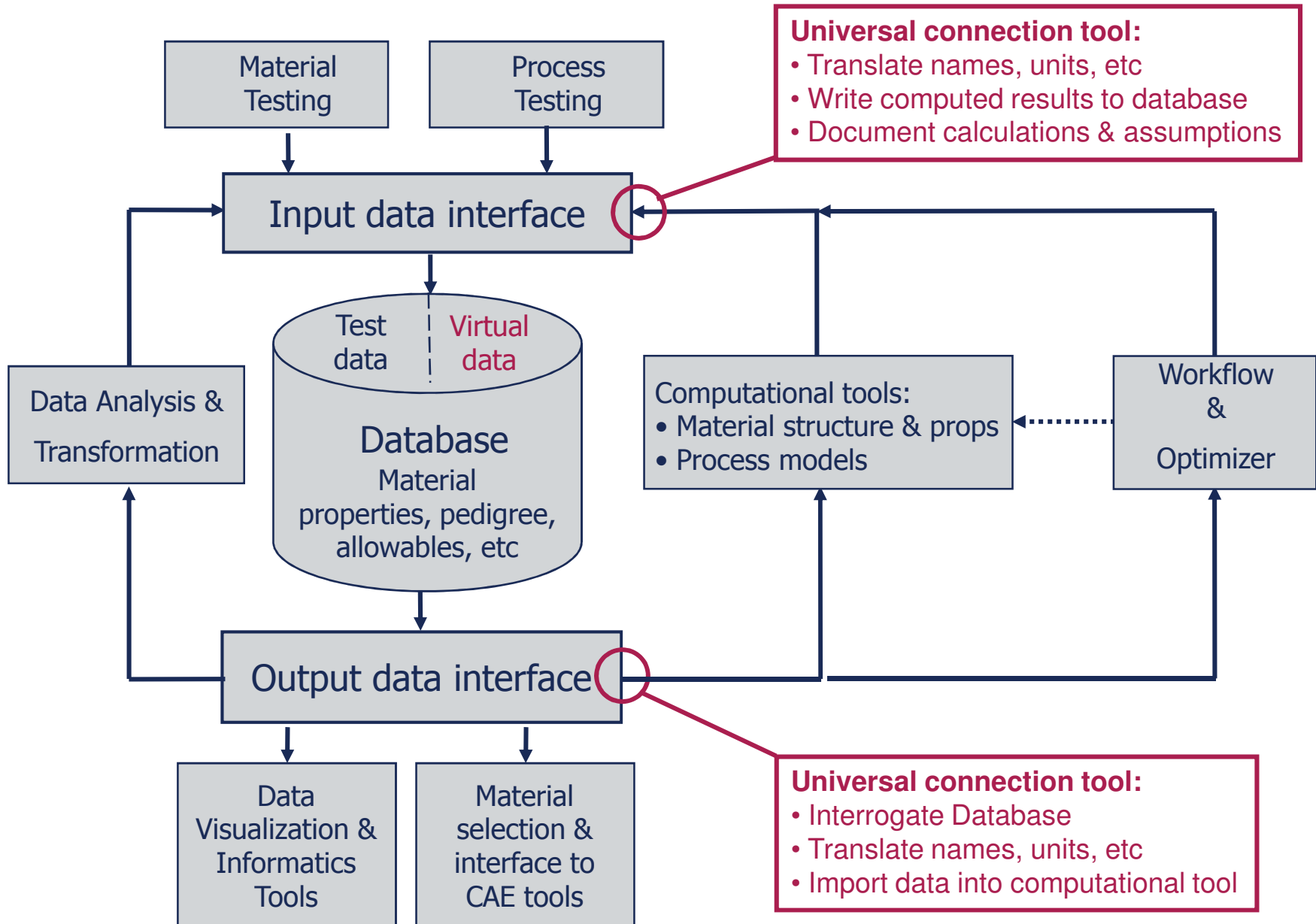
Multiscale Modelling



Proposed Architecture



Proposed Architecture



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	

Calculation Pedigree

Conditions

Temperature: 19.3 to 34.2 °C

Pedigree

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

NIST Demo Atomistics Database Model Description Record

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 - Curve Fits

MISHIN 99 (MFMP99)

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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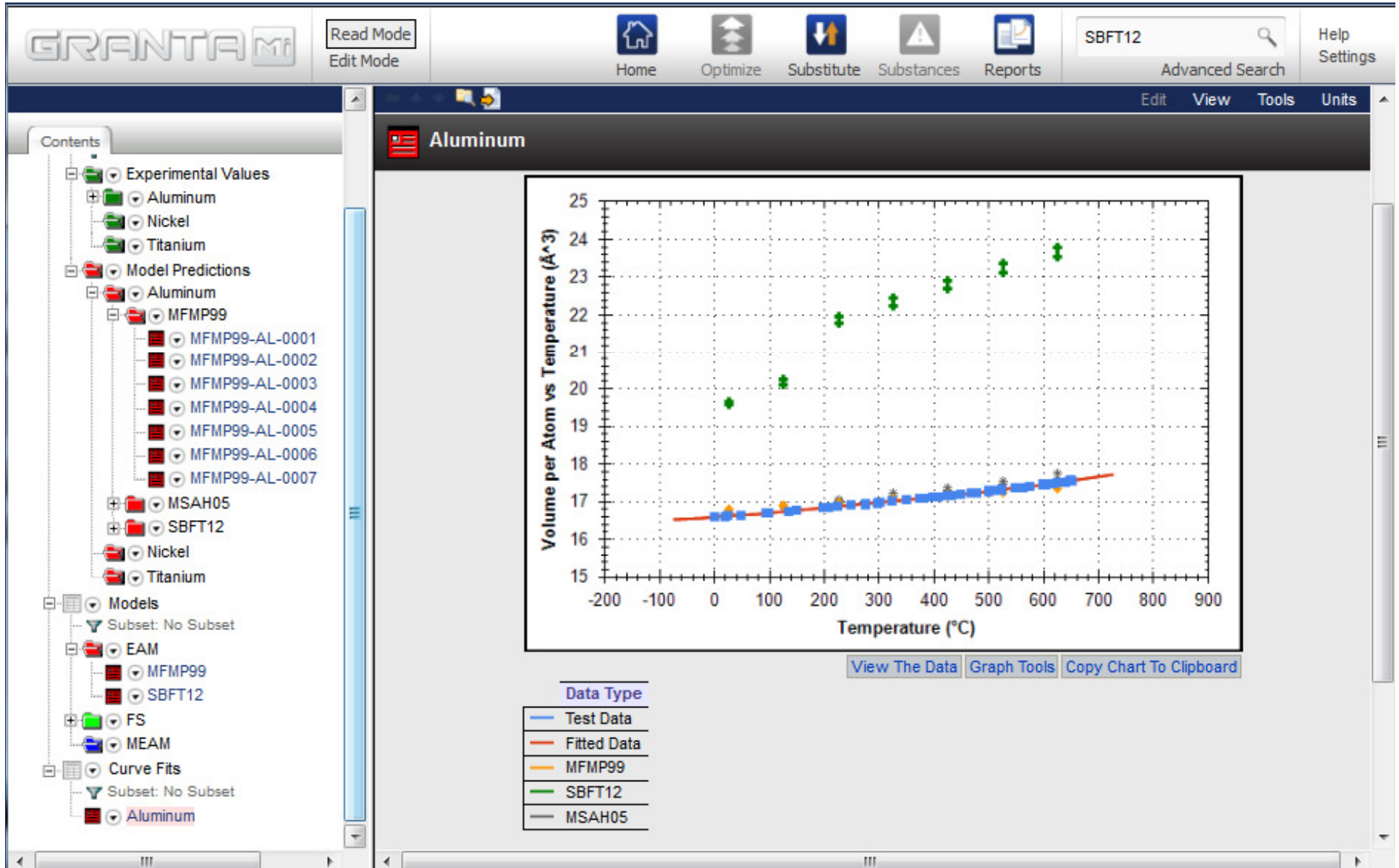
Links

Predictions using this model

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

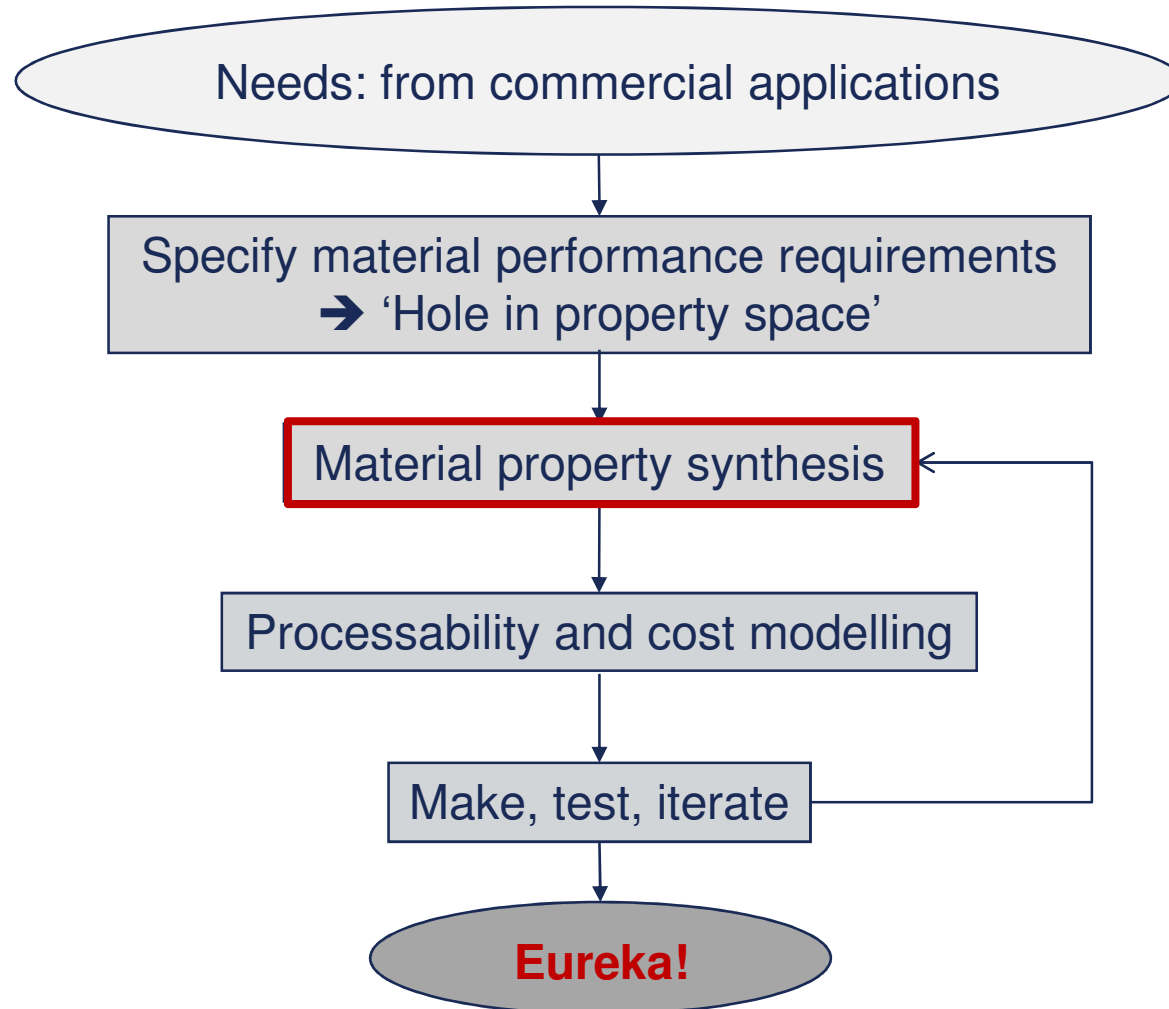
NIST Demo Atomistics Database

Validating models with experimental data





A Framework for Materials Design



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

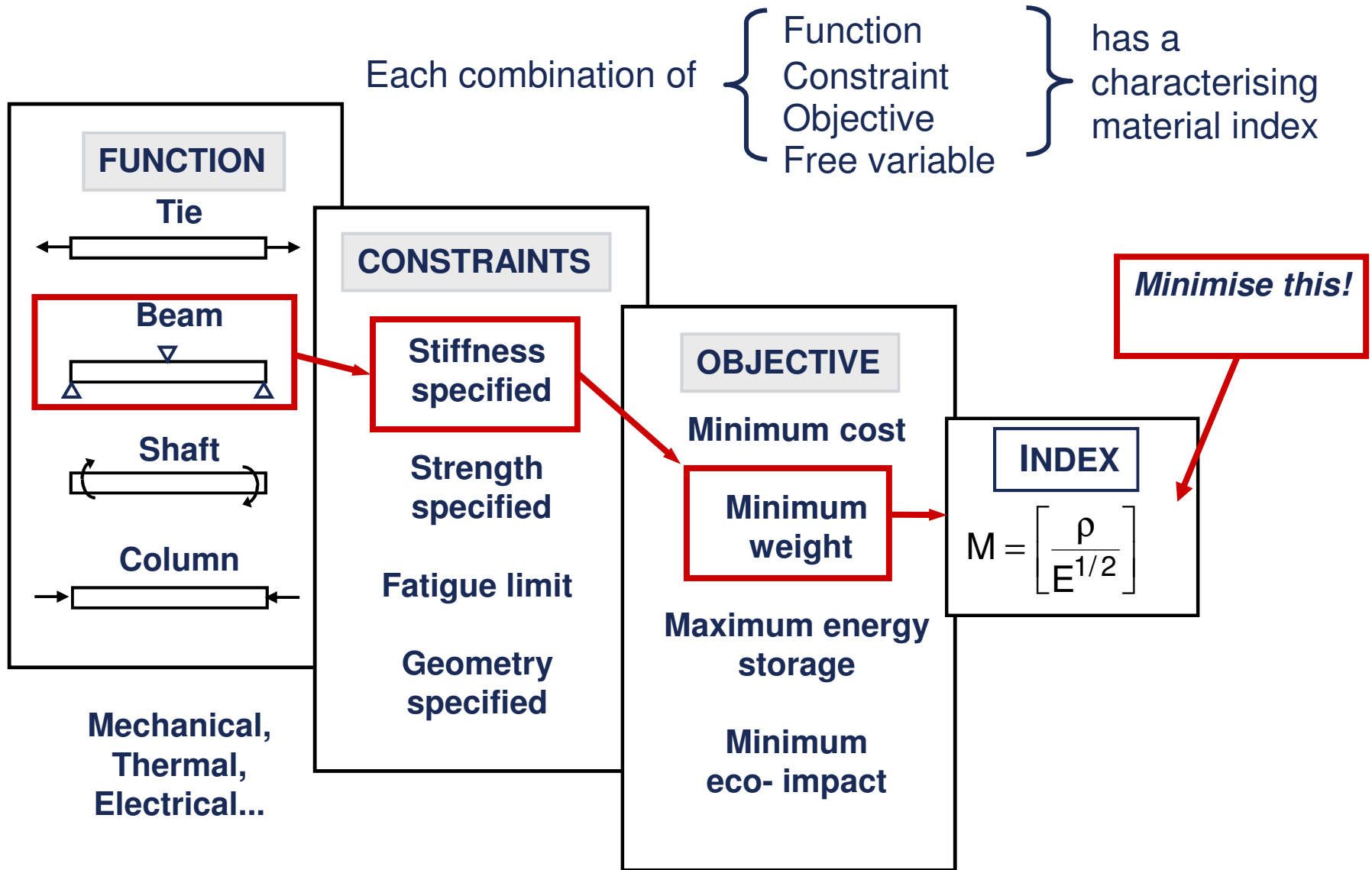
↑
Case Study



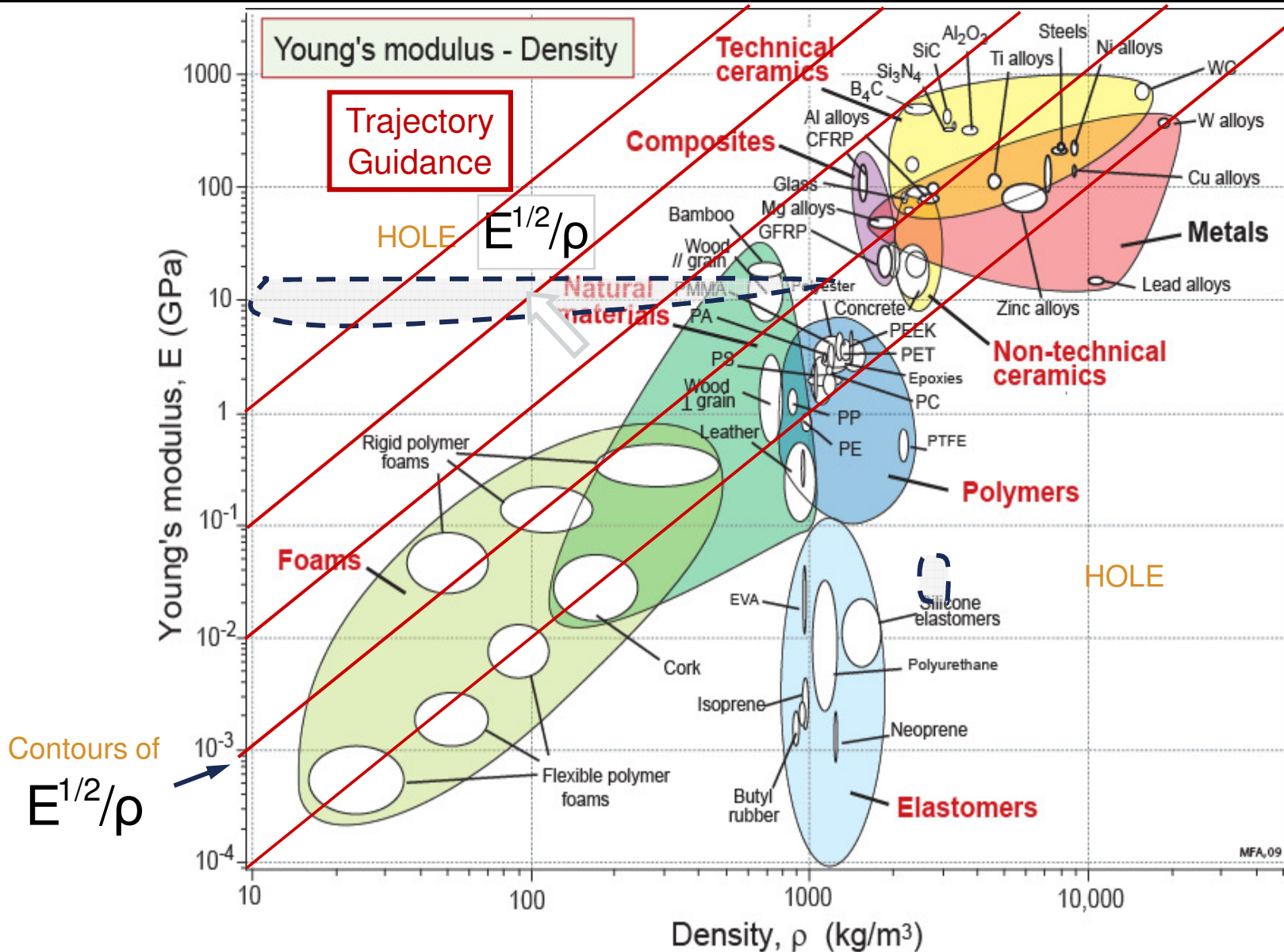
Case Study

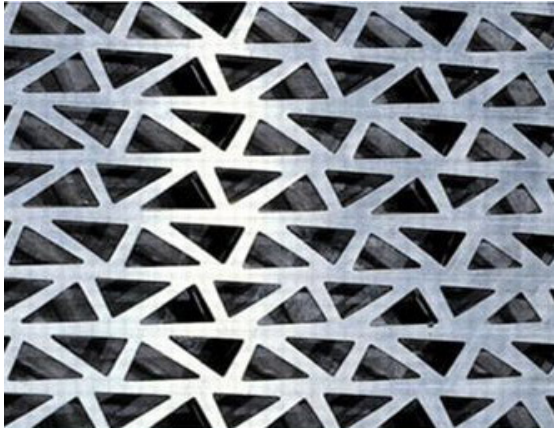
Light, Stiff Panels: Hybrid Synthesis

Systematic Material Selection: 'Material indices'



Modulus and Density

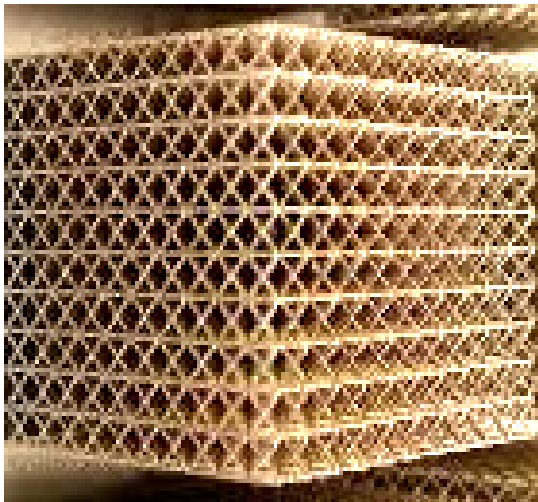




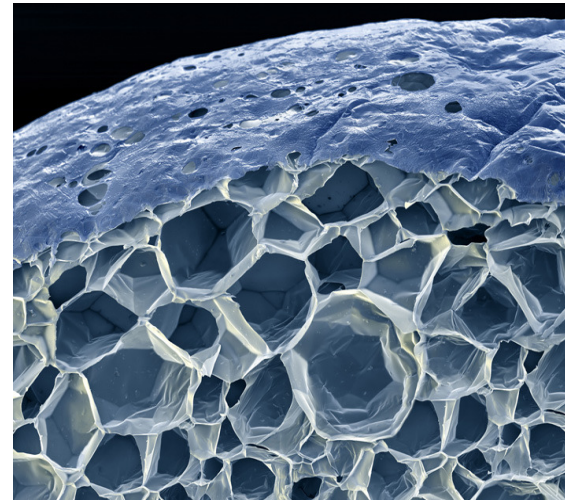
From "Manufacturing Material Effects"



Image courtesy Dr. Sacha Peters

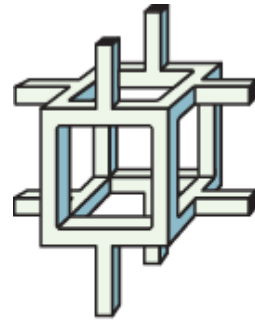


Courtesy University of Liverpool

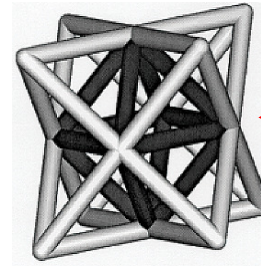


BASF Neopor EPS foam

Configurations

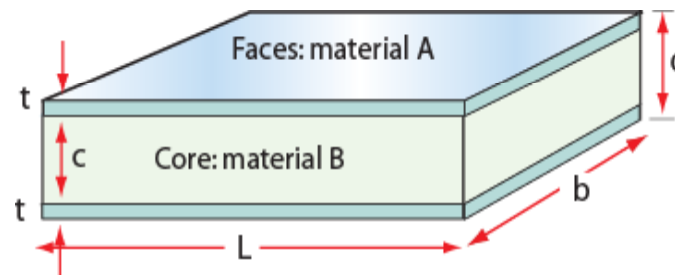


Foam cell



Lattice cell

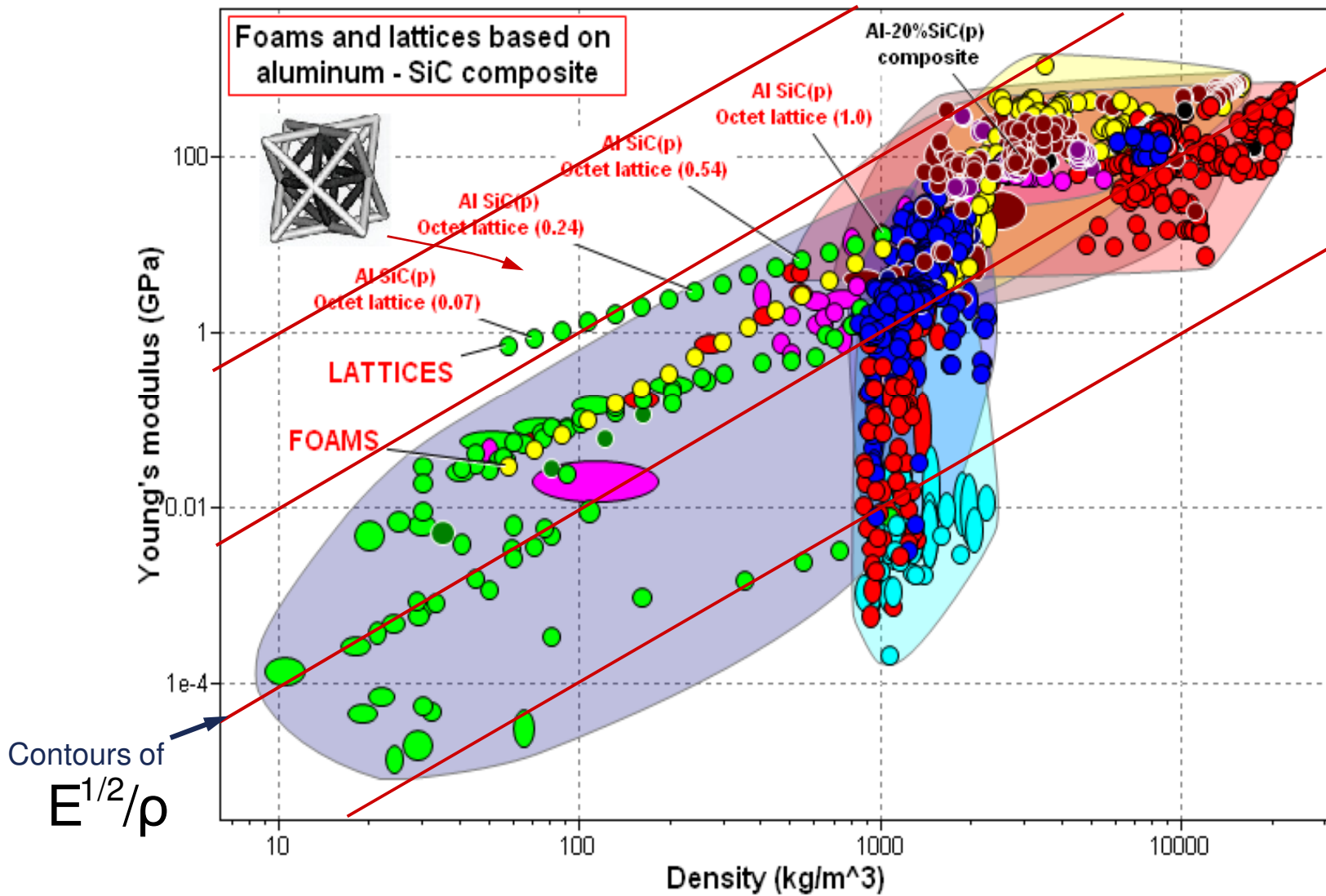
Triangulated
cell faces



Sandwich cell

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

Expand material property space: Lattices

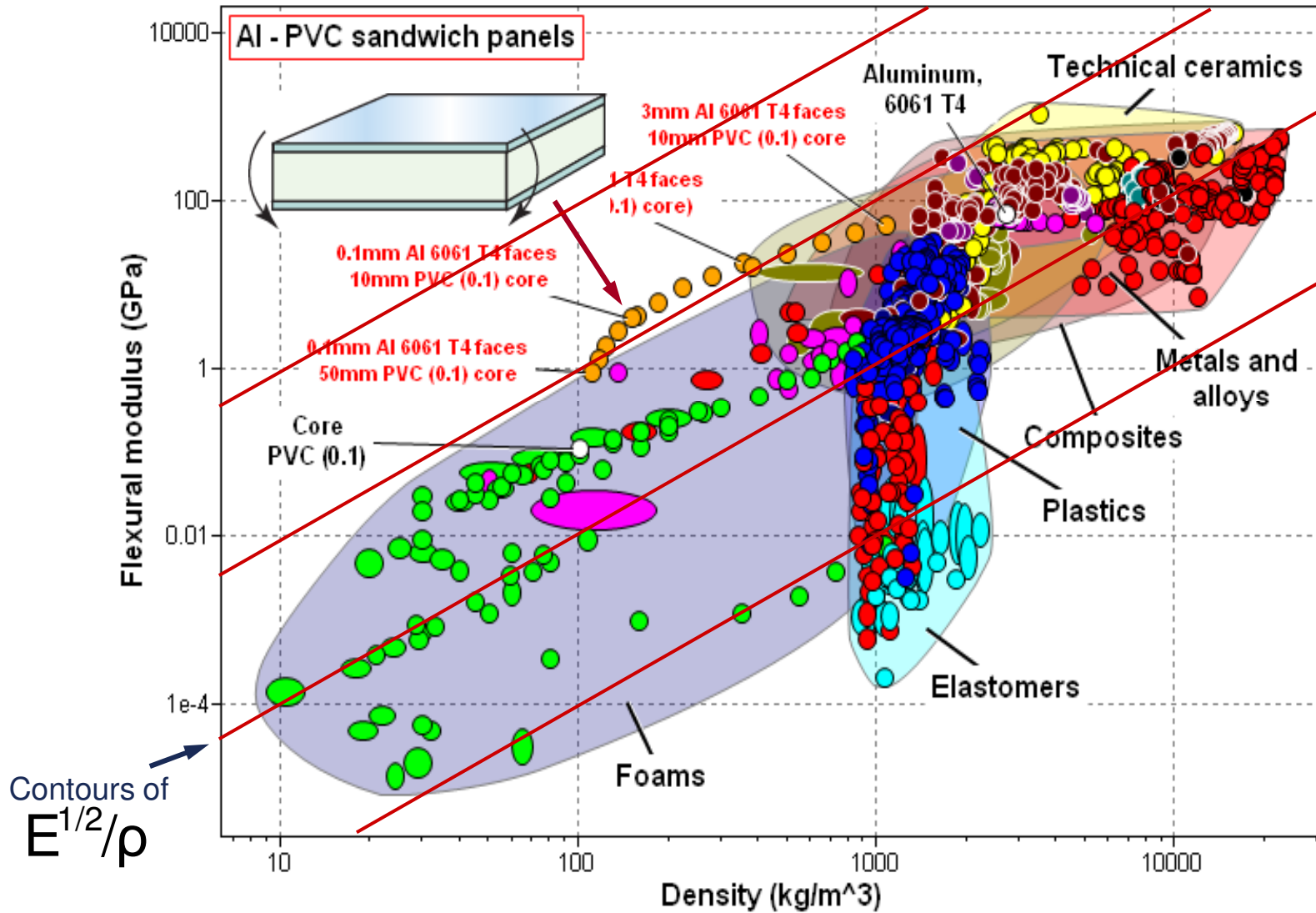


2800
materials

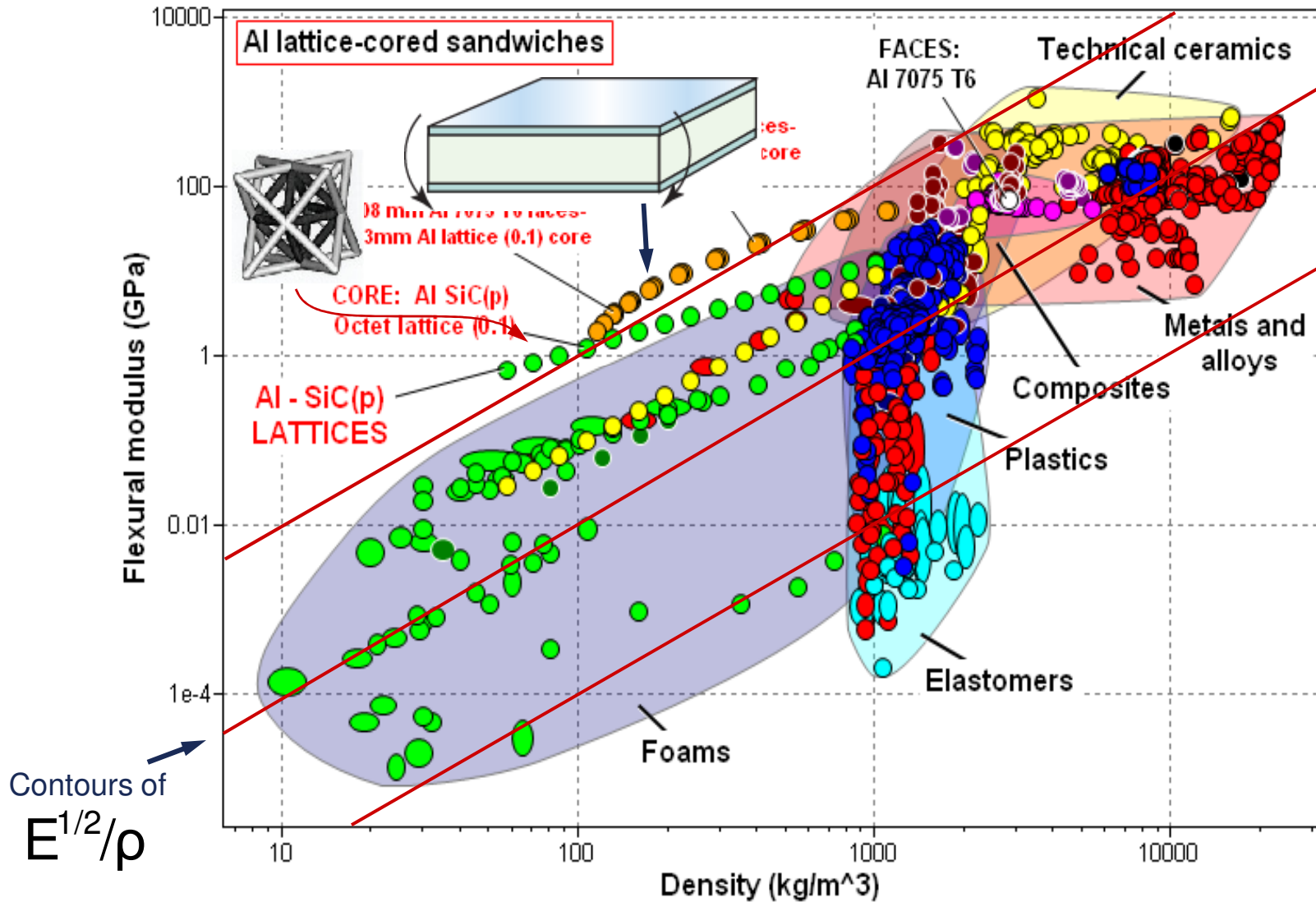
Expand material property space: Sandwiches



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materials



Expand material property space: Structures



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materials



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**

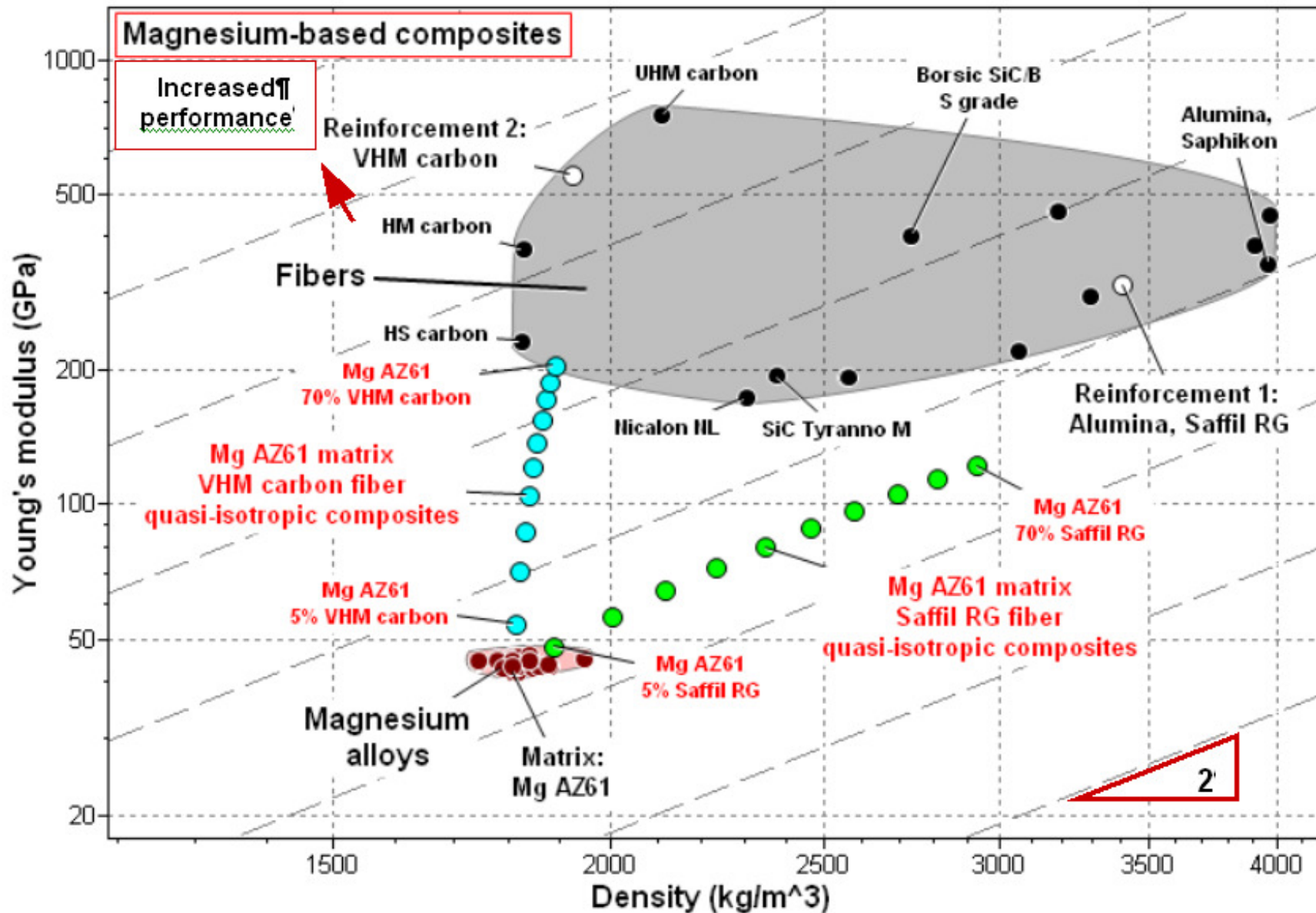
3. Research and Technology Development Needs:

- **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**

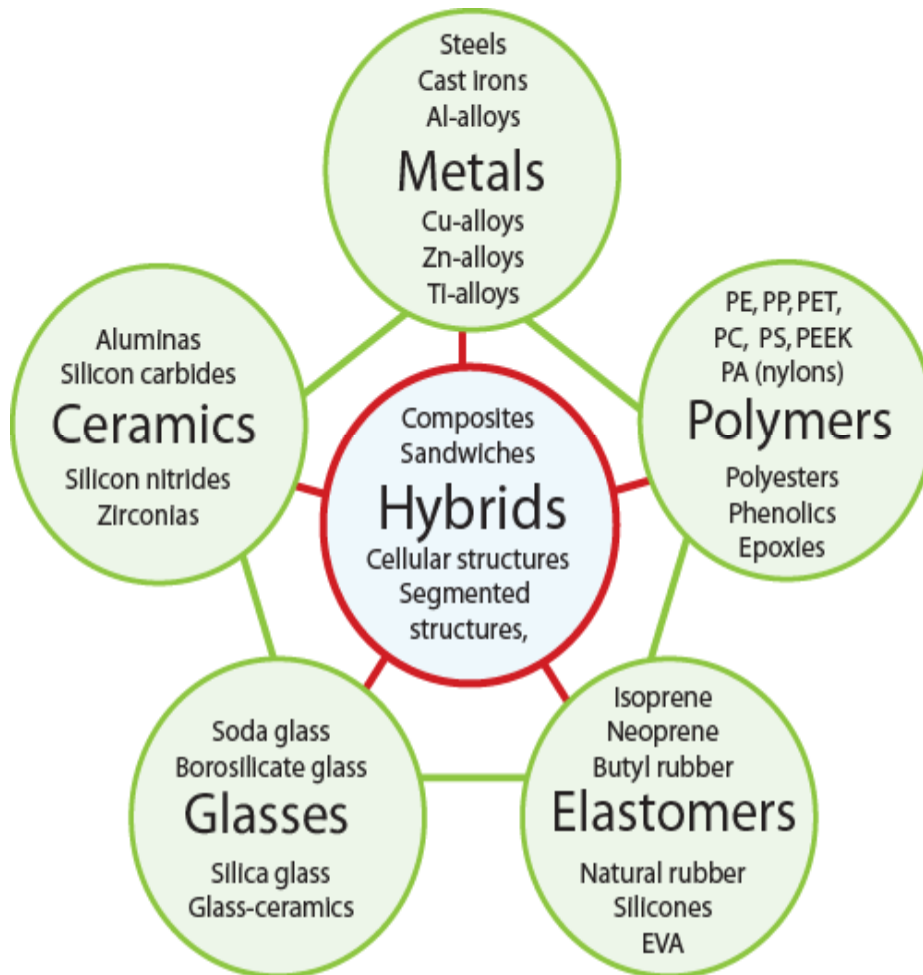
→ A Grand Challenge...



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