

Progettazione di Materiali e Processi

Università degli Studi di Trieste
Facoltà di Ingegneria

Corso di Laurea in Ingegneria Chimica e dei Materiali
A.A. 2021-22

PRODUCT (MATERIALS) AND PROCESS DESIGN

Intro

- Design, Product, Process
- Product Design; Process Design; Product and Process Design
- Material, process, shape, properties, function

Design process

- Example
- Fundamentals
- Identification of needs (market; coevolution; true need)
- Types of design
- **Design tools**
 - **Databases**
 - **Analytical tools**
 - Simulation tools

- **Selection and design of materials and processes**
 - **Tools for optimal systematic selection**
 - Design of materials: case studies (nano, meso, microstructures; hybrid materials; composites)
- **Design and optimization of chemical processes**
- **Advanced tools and methods** (ad-hoc lectures and seminars: FEM, product/process economics, Life Cycle Assessment, ...)
- **Special topic seminars** (Intellectual Property, product evaluation, materials in industrial design, theory of scenarios, rapid plant assessment, material selection in engines, design for recycle, refurbish, reuse)

Progettazione di Materiali e Processi

Modulo 1

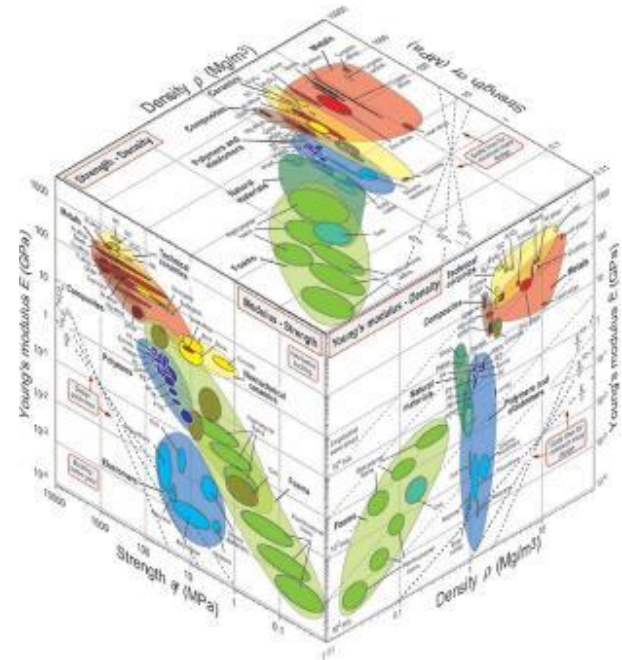
Selezione sistematica di materiali e processi

Lezione 1

- Strategia di selezione
- Database di materiali e processi

In this lecture...

- Selection strategy
- Review of important material properties
- Types of materials data
- Organizing a materials database
- Example of materials data table
- Representing materials properties (tables; 1D, 2D, 3D graphs)
- Selection tools:
 - Table comparison
 - Screening: 1D, 2D, multi-D (limit tool); simple property, multiproperty
 - Objective-driven: material index (examples)



The selection strategy

Selection (and design) of materials

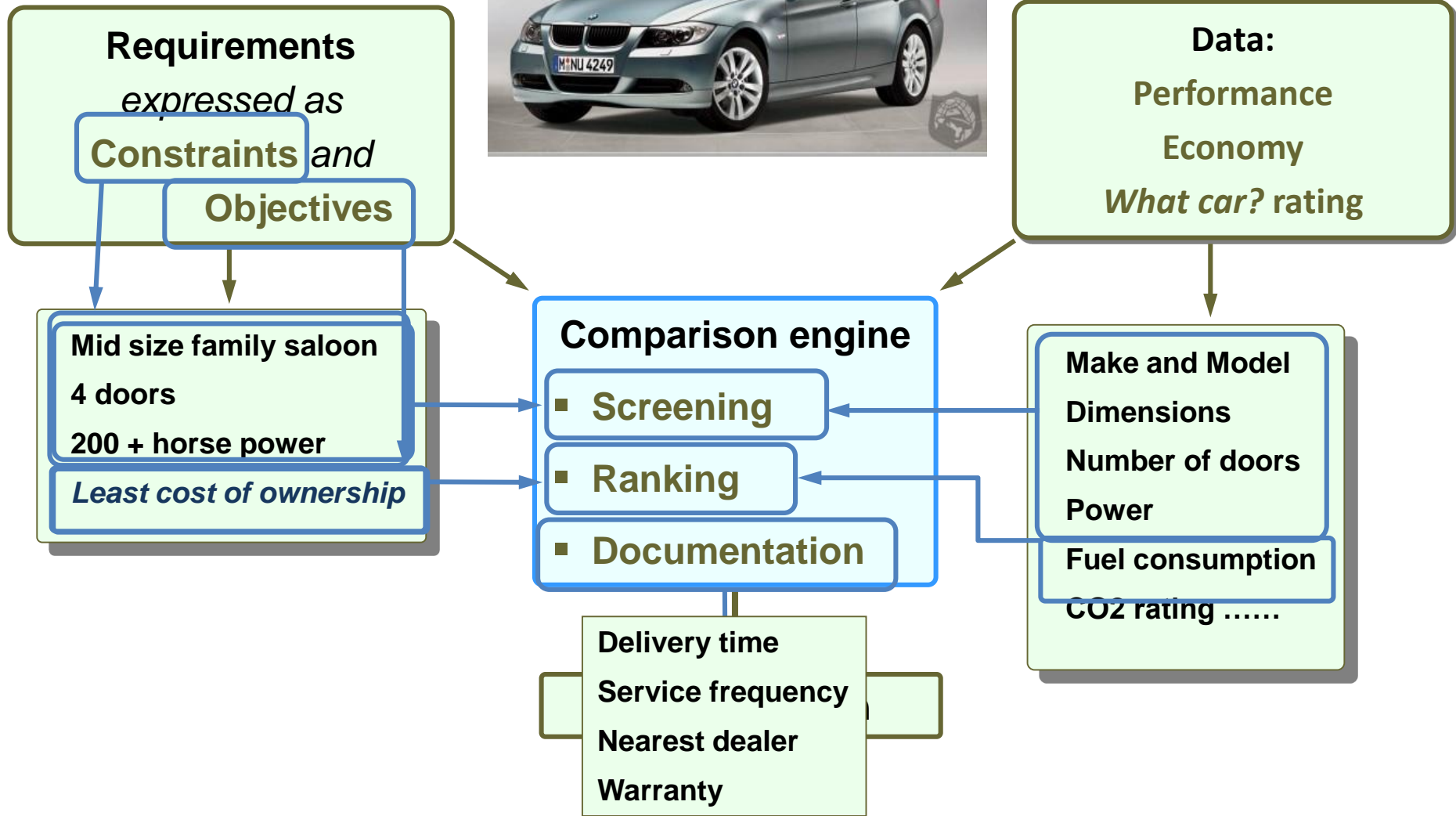
Selection and Design of materials and processes:

- Dynamic
- An opportunity
- From heuristic to systematic
- Interconnection with [shape, function, properties](#)

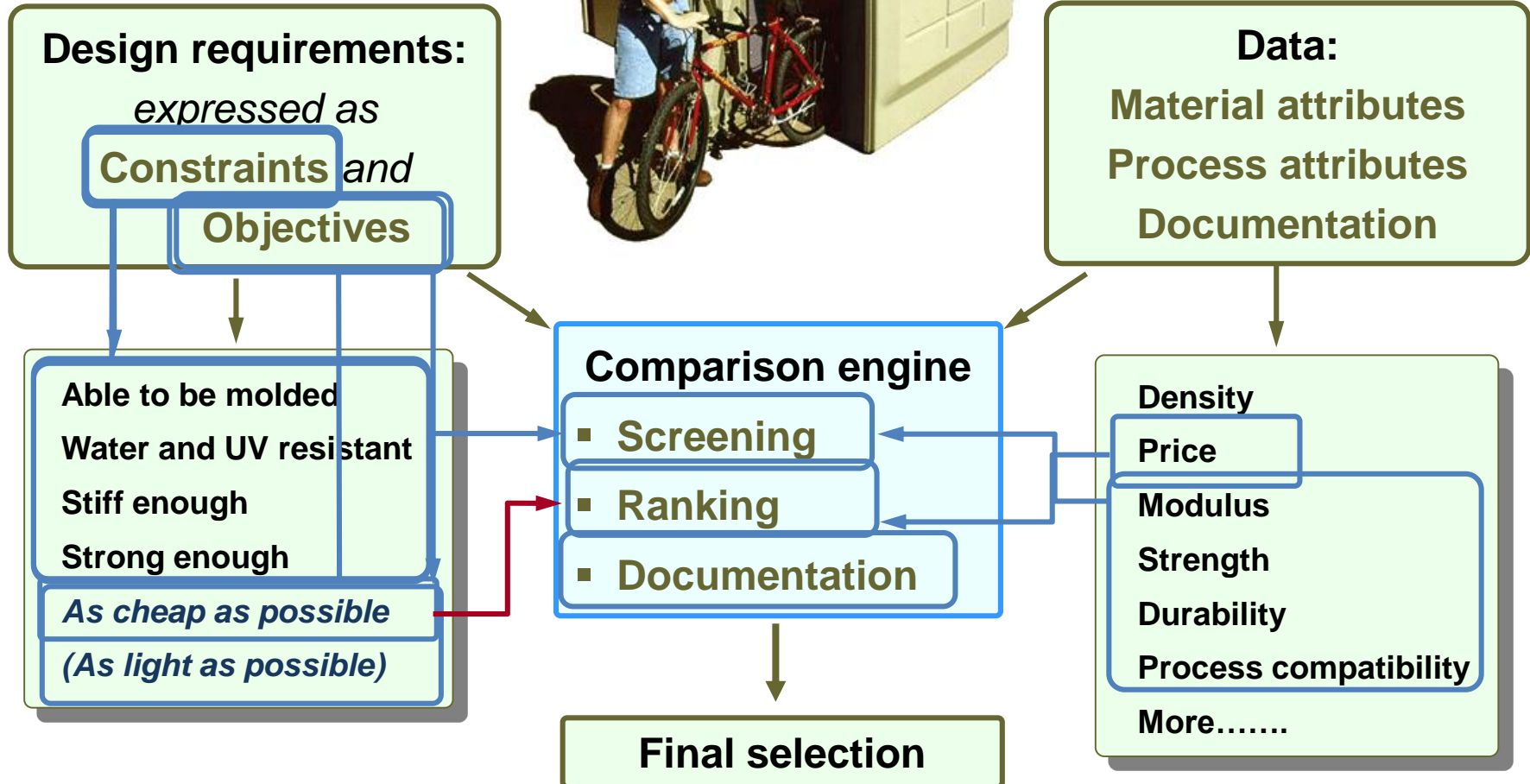
OUR GOAL: Design-led materials selection

The selection strategy: cars (function: ...?)

What do I want from a car?



The selection strategy: materials



Translation

Translation: “express design requirements as constraints and objectives”

Design requirements

Constraints

What essential conditions must it meet ?

- ***Be strong enough***
- ***Conduct electricity***
- ***Tolerate 250 C***
- ***Be able to be cast***

Objectives

What measure of performance is to be maximized or minimized ?

- ***Mass***
- ***Volume***
- ***Eco-impact***
- ***Cost***

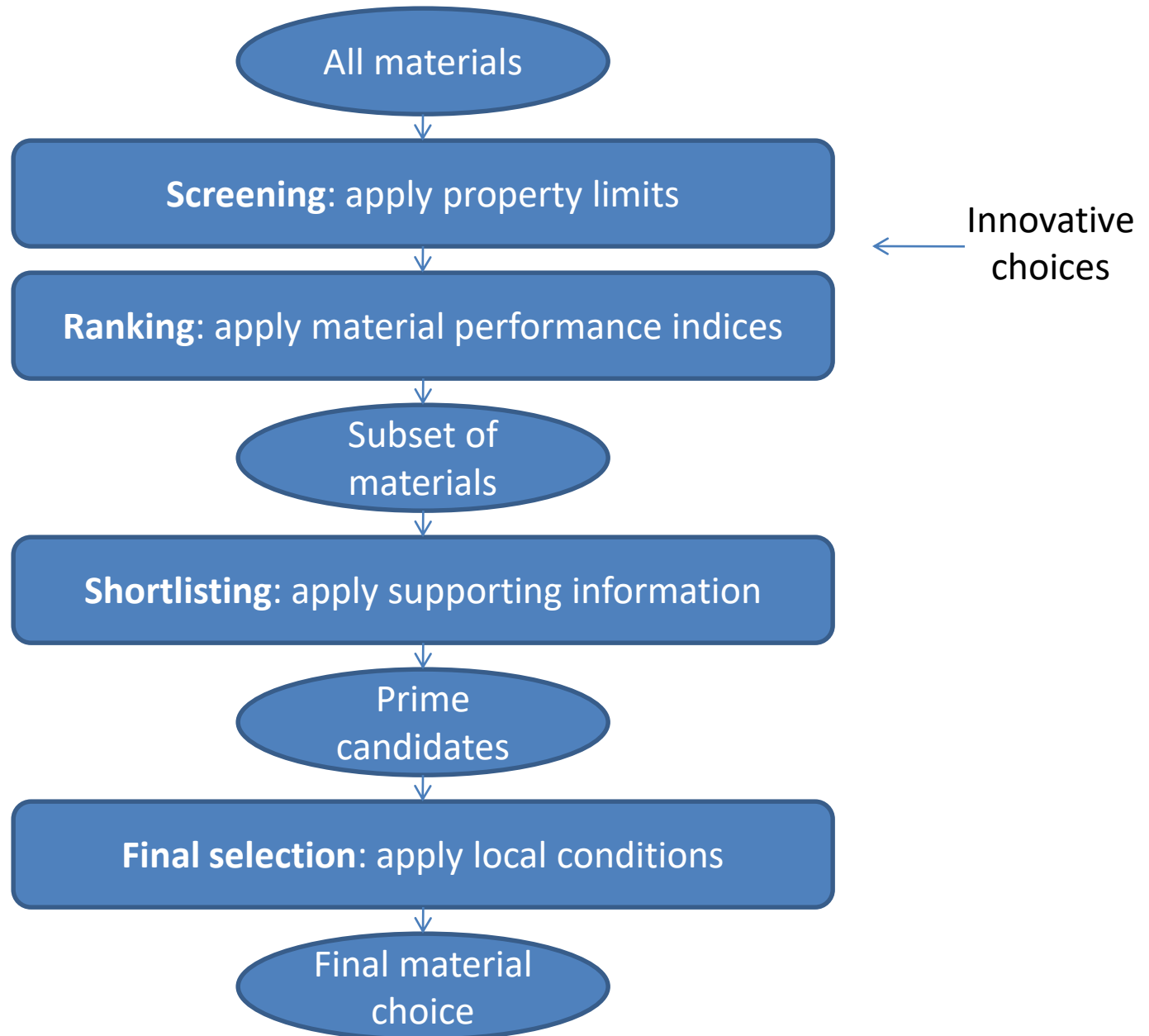
Screening: “use constraints to eliminate materials that can’t do the job”

Function – Objectives - Constraints

Function	What does the component do? e.g.: support load, seal, transmit heat, bicycle fork, etc.
Objective	What do we want to maximize (minimize)? e.g.: minimize cost, maximize energy storage, minimize weight, etc.
Constraints	What conditions must be met? (non-negotiable or negotiable) e.g. geometry, resist a certain load, resist a certain environment, etc.

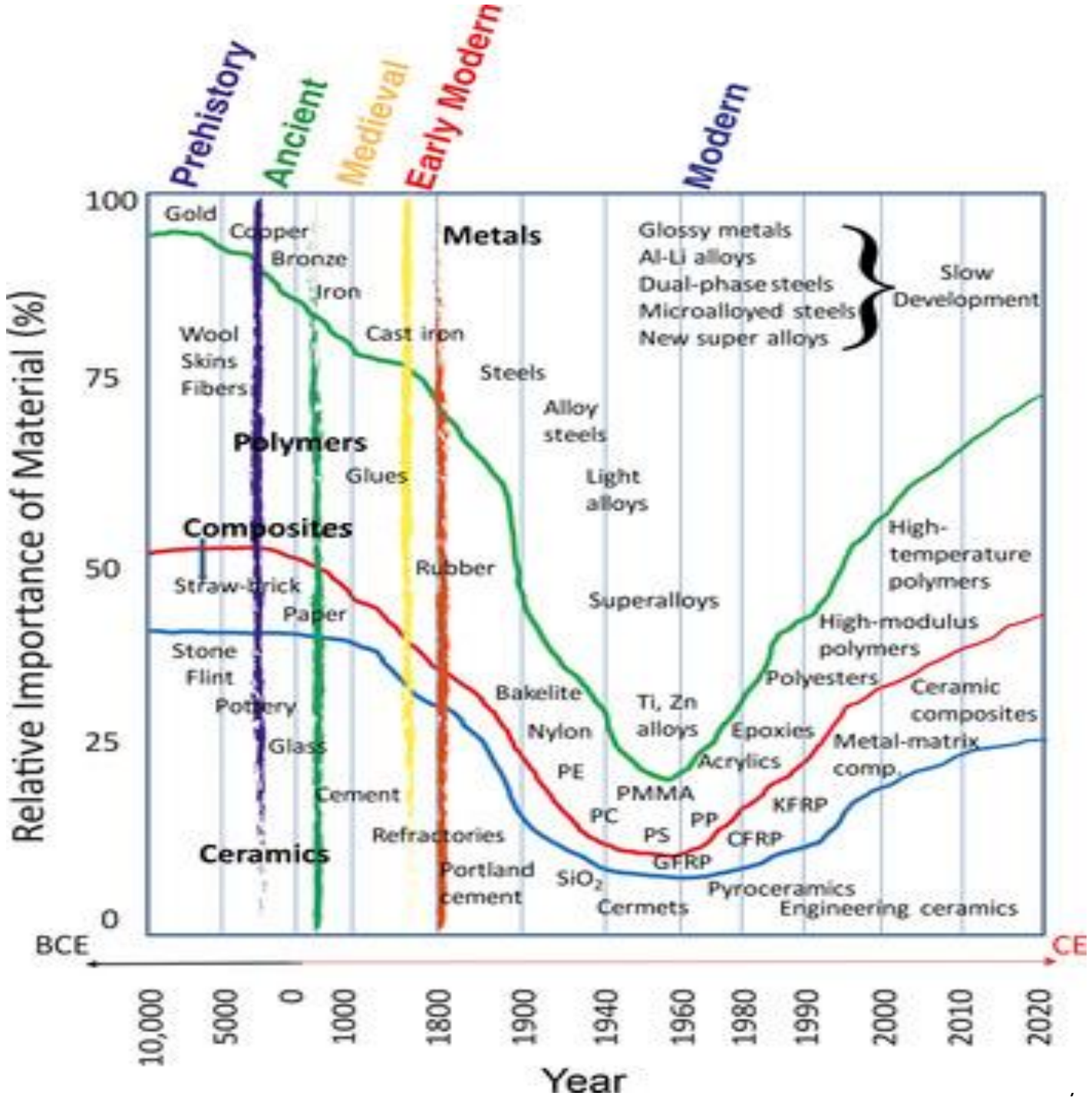
- Some functions are implicitly understood (e.g. tie, beam, shaft, column)
- Constraints often translate to property limits (temperature, conductivity, cost, ...)
- Some constraints are more complex (e.g. stiffness, strength, etc.) as they are coupled with geometry -> need of a specific objective
- **Material indices** help unravel such complexity

The selection process

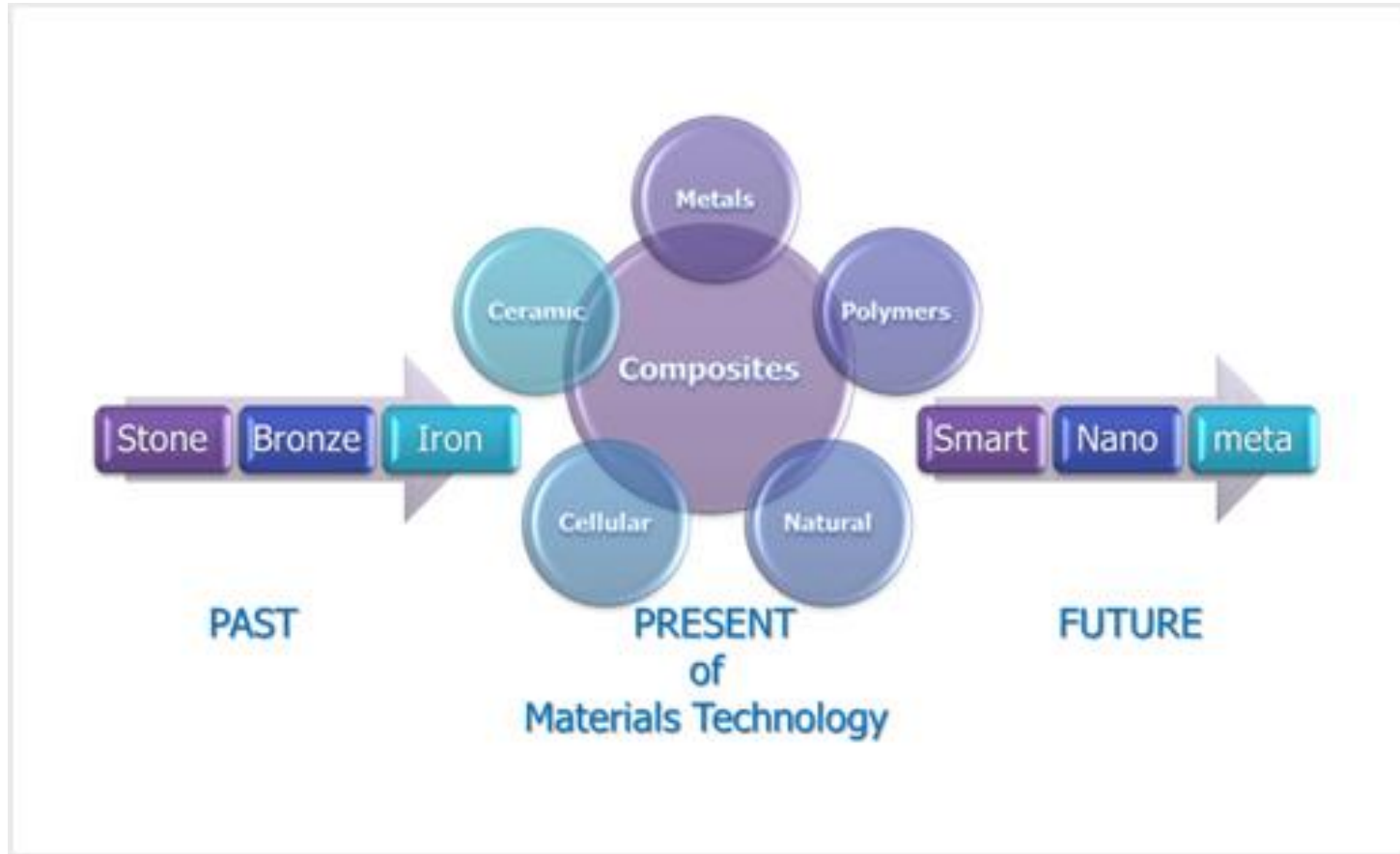


Databases for materials and processes

Evolution of Materials



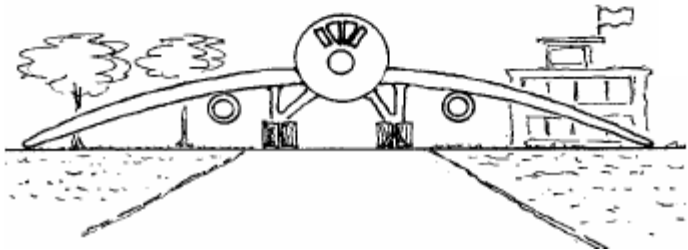
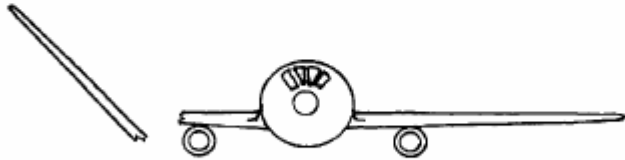
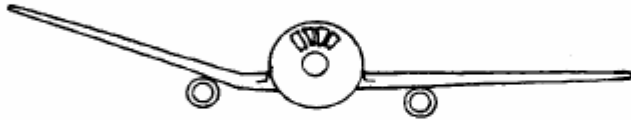
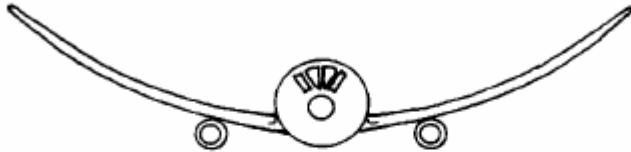
Evolution of Materials



Material properties

Class	Property	Order of magnitude
General	Cost	€/kg, €/m ³
	Density	
Mechanical	Elastic moduli (Young, Shear, Bulk)	
	Strength (yield, ultimate, fracture, MOR)	
	Resilience	
	Hardness	
	Fracture Toughness	
	Damping (Loss coefficient)	
	Fatigue limit	
Thermal	Thermal conductivity	
	Thermal diffusivity	
	Specific heat	
	Melting point	
	Glass temperature	
	Thermal expansion coefficient	
	Creep resistance	
Wear	Wear constant	
Corrosion	Corrosion rate	
Oxidation	Parabolic rate constant	

Mechanical Properties



Material Properties

Class	Property	Order of magnitude
General	Cost	€/kg, €/m ³
	Density	0.1 – 20 10 ³ kg/m ³
Mechanical	Elastic moduli (Young, Shear, Bulk)	0.01 – 1000 GPa
	Strength (yield, ultimate, fracture, MOR)	up to 2000 MPa
	Resilience	up to MPa
	Hardness	H (MPa) ~ 3σ _f Hv (kg mm ⁻²) = H/10
	Fracture Toughness	0.1 – 300 MPa m ^{0.5}
	Damping (Loss coefficient)	10 ⁻⁶ - 10
	Fatigue limit	up to 600 MPa
Thermal	Thermal conductivity	0.02 – 1000 W/m K
	Thermal diffusivity	5 10 ⁻⁸ – 5 10 ⁻³ m ² /s
	Specific heat	10 ³ J/kg K
	Melting point	20 – 4300 °C
	Glass temperature	-70 – 220 °C (polymers); 150 – 1200 °C (glasses)
	Thermal expansion coefficient	1 - 500 μm/m K
	Creep resistance	
Wear	Wear constant	
Corrosion	Corrosion rate	
Oxidation	Parabolic rate constant	

Materials Data

- **Numeric:**

properties measured by numbers:
density, modulus, cost
...other properties

Can extrude?

Good or bad
in sea water?

Design
guide
lines

Case
studies

Failure
analyses

Established
applications

Supplier
information

FE modules

Standards
and codes
(ISO 14000)

Sector-specific
approval
(FDA, MilSpec)

- **Non-numeric:** properties measured by
yes - no (Boolean) or
poor-average-good type (Rankings)

- **Supporting information,
specific:** what is the experience with the
material?

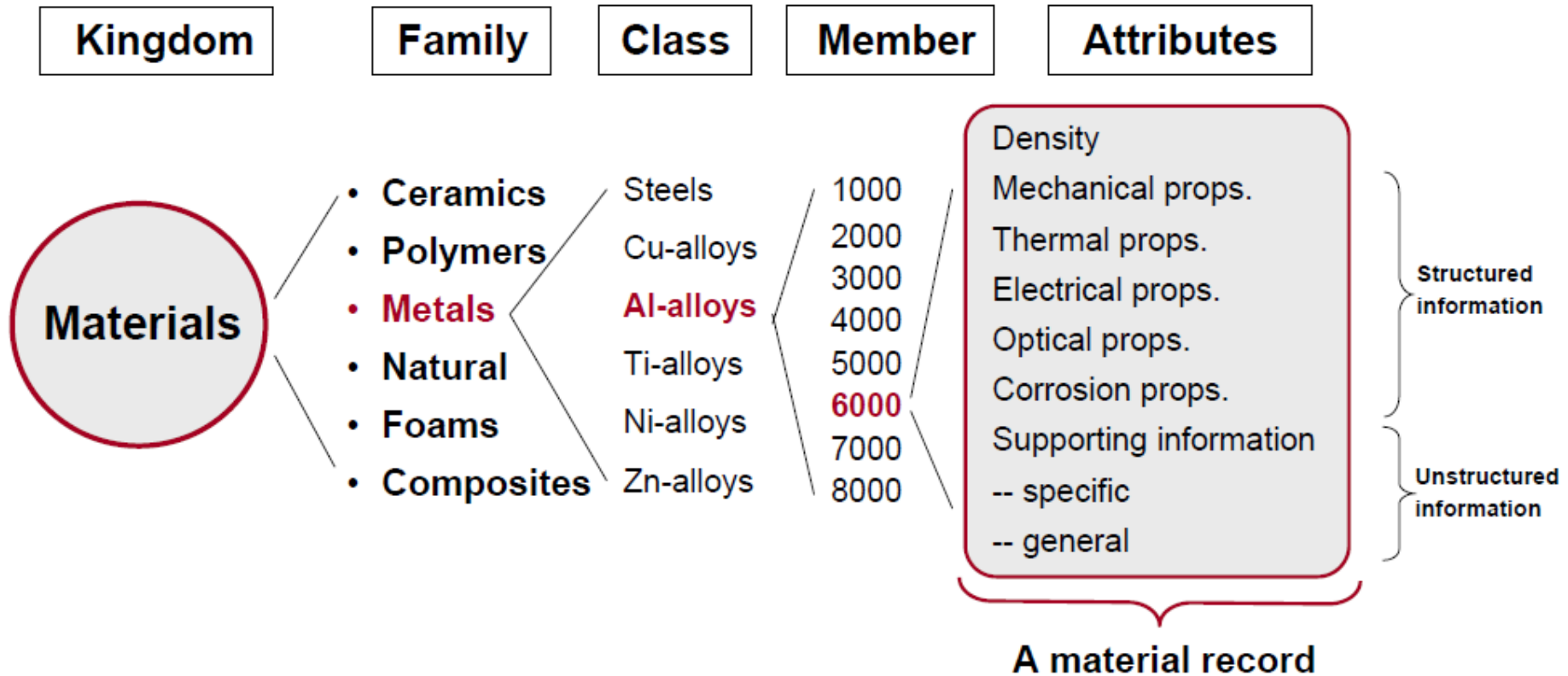
- **Supporting information,
general:** what else do you need to know?

“Structured” and “Unstructured” data

Handbooks,
data sheets

Reports, papers,
the Web

Materials Data



Some Material Databases

- Maptis
 - **NIST**
 - **CES**
 - Matweb
 - **Matbase**
 - Matnavi (NIMS)
 - Some more, application specific
-
- Datasheet

Materials Data

Example of material property table

CES Selector 2012 - [MaterialUniverse:\Ceramics and glasses\Non-technical ceramics\Cement and concrete\Concrete]

File Edit View Select Tools Window Help Feature Request

Browse Search Select Tools Eco Audit Synthesizer Search Web Help

Database: Basic Edition Change...
Table: MaterialUniverse
Subset: All materials

High density concrete

High density concrete

Layout: All attributes Show/Hide

MaterialUniverse

- Ceramics and glasses
 - Glasses
 - Non-technical ceramics
 - Cement and concrete
 - Cement
 - Concrete
 - Aerated concrete
 - Asphalt concrete
 - High density concrete
 - High volume fly ash concrete
 - Lightweight (0.9-1.4)
 - Normal density (2.2-2.6)
 - Reactive powder concrete
 - Plaster of paris
 - Fired clays
 - Minerals and stone
 - Technical ceramics
 - Fibers and particulates
 - Hybrids: composites, foams, honeycombs, natural materials
 - Metals and alloys
 - Polymers: plastics, elastomers

General properties

Designation
High Density Concrete

Density	4.9e3	-	5.5e3	kg/m ³
Porosity (closed)	0			%
Porosity (open)	0.1	-	0.15	%
Price	* 0.182	-	0.225	EUR/kg

Composition overview
Composition (summary)
.58:1.4.6:6.4 Water:OPC:Fine:Coarse (Aggregate=Baryte or Steel Shot)

Base	Other
------	-------

Composition detail (metals, ceramics and glasses)

Al ₂ O ₃ (alumina)	0.36	%
C (carbon)	0.15	%
CaO (calcia)	5.17	%
Fe (iron)	50.3	%
Fe ₂ O ₃ (ferric oxide)	0.26	%
H ₂ O (water)	4.61	%
MgO (magnesia)	0.2	%
Mn (manganese)	0.38	%
P (phosphorus)	0.01	%
S (sulfur)	0.01	%
SiO ₂ (silica)	38.2	%
Other oxide	0.29	%

Bio-data

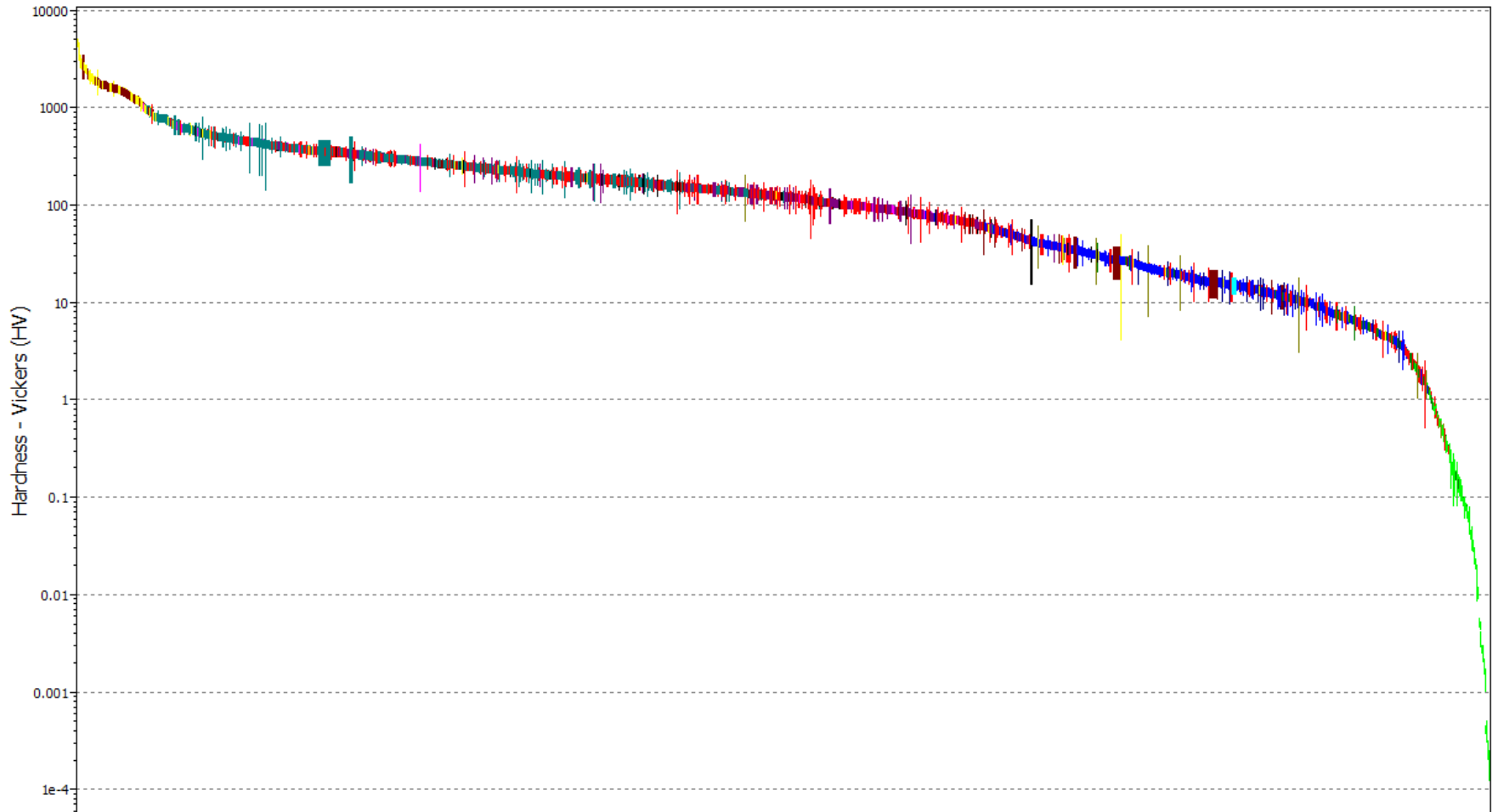
RoHS (EU) compliant grades?	✓
Toxicity rating	Non-toxic

Mechanical properties

Young's modulus	* 40.2	-	41.6	GPa
Flexural modulus	* 40.2	-	41.6	GPa
Shear modulus	* 16.5	-	17	GPa
Bulk modulus	* 23.9	-	24.8	GPa
Poisson's ratio	0.2	-	0.24	
Shape factor	3			

Materials Data

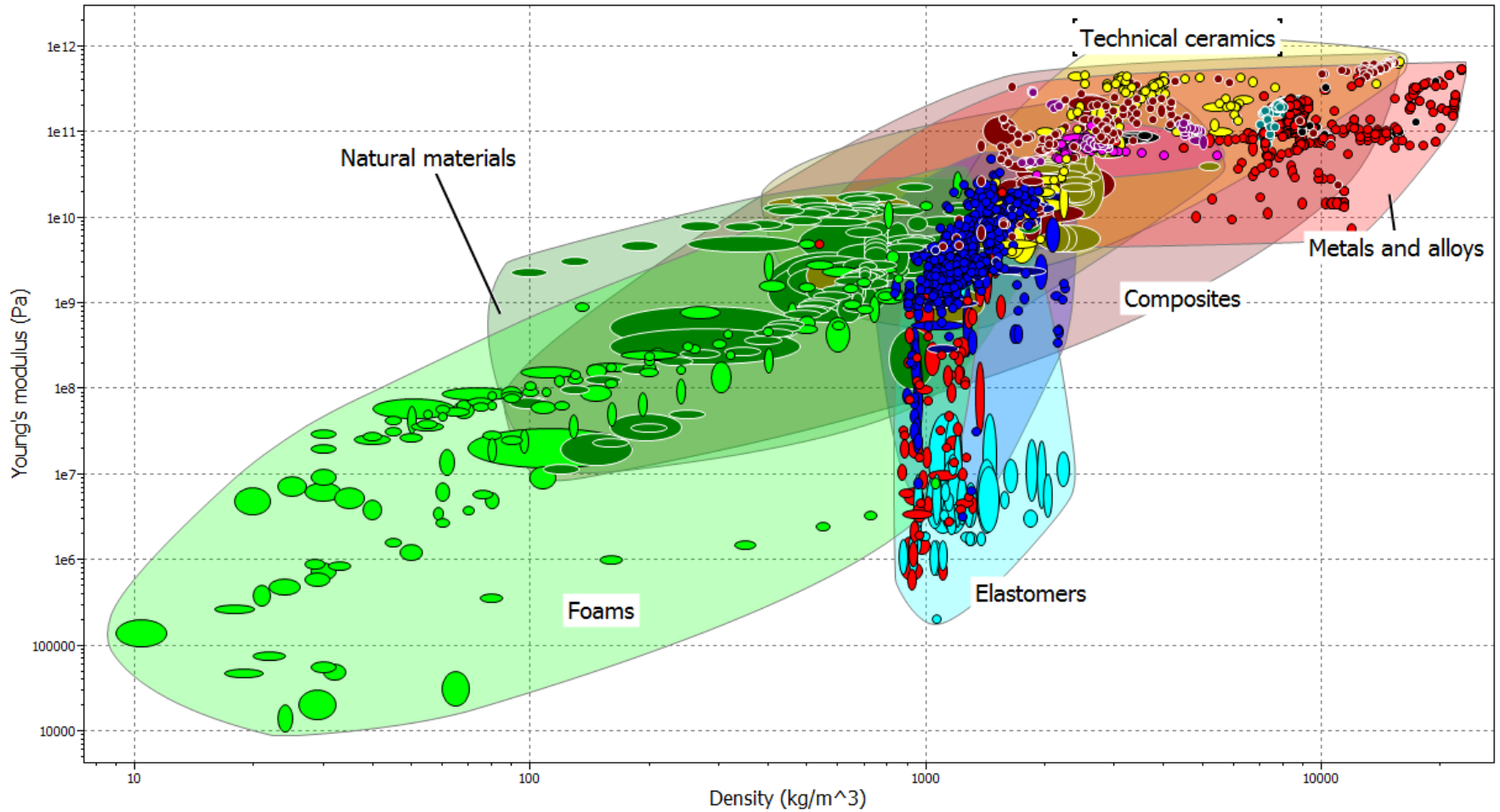
Example of single property graph



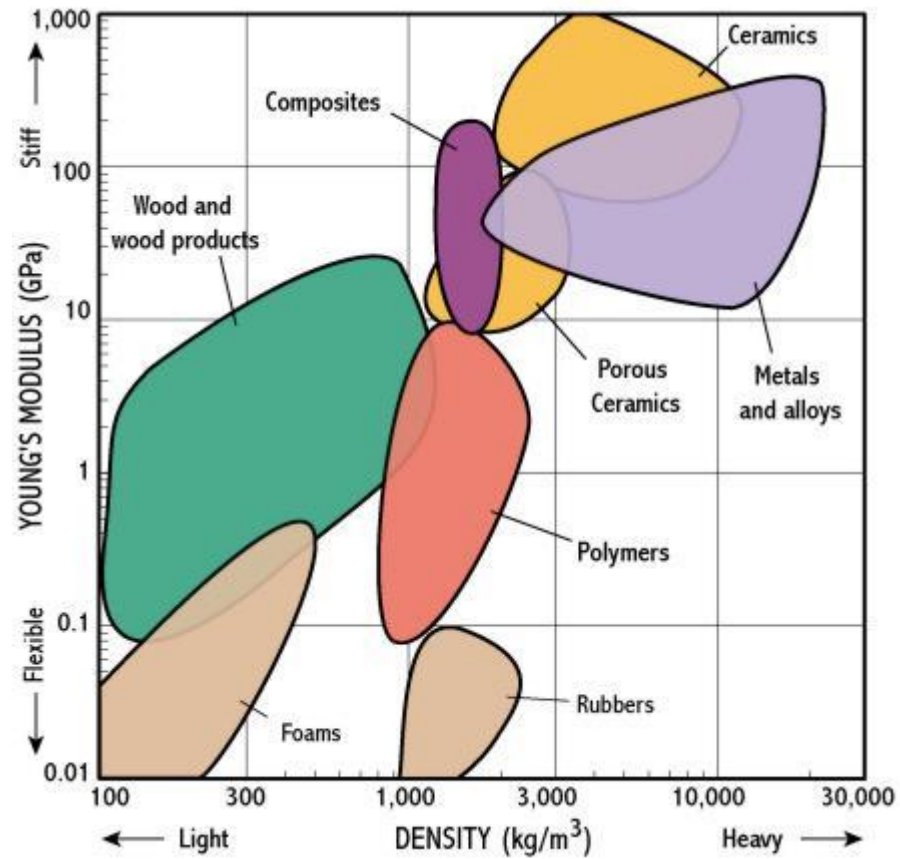
See CES

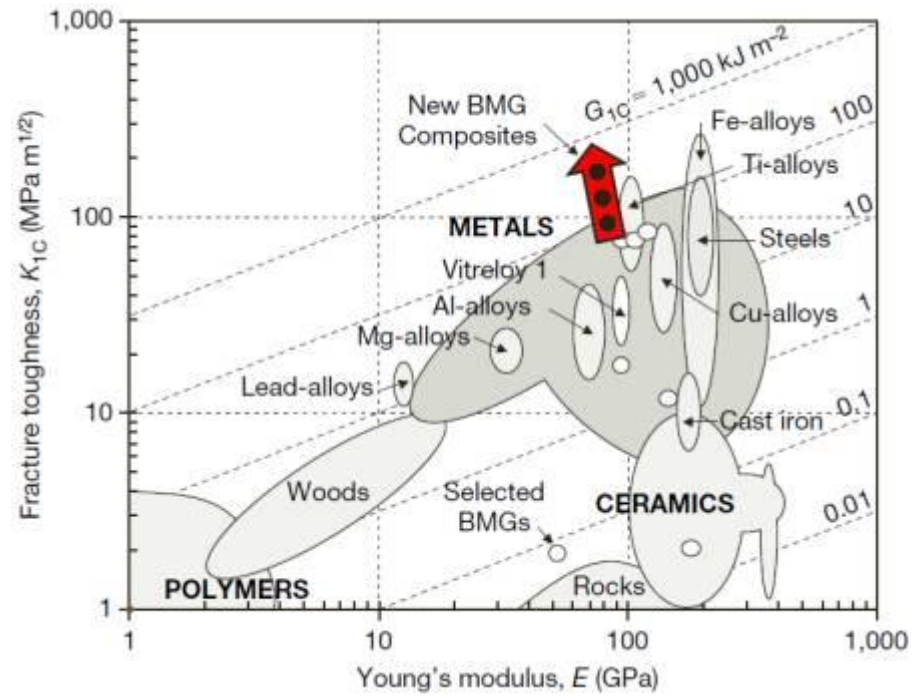
Materials Data

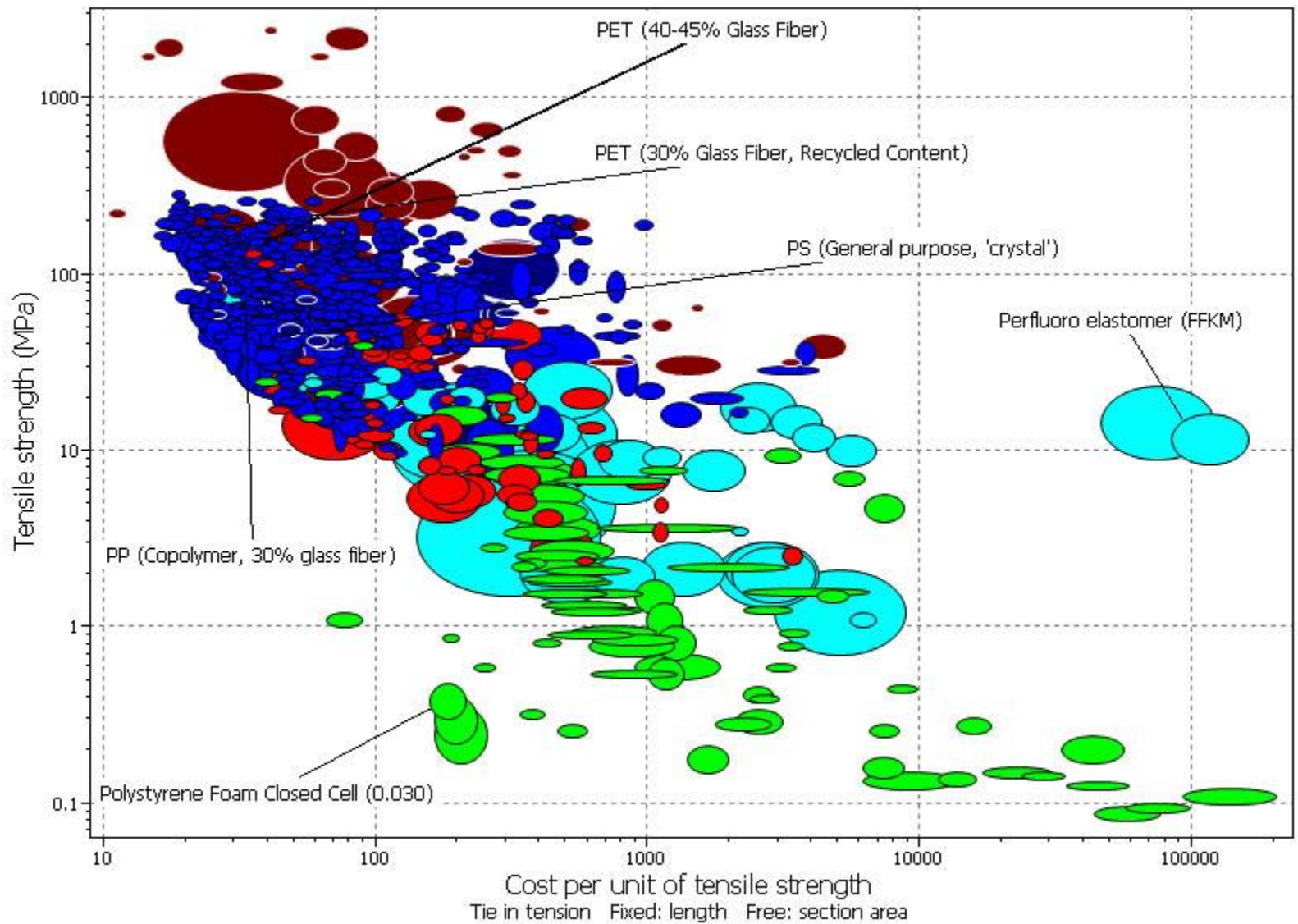
Examples of two-property graph

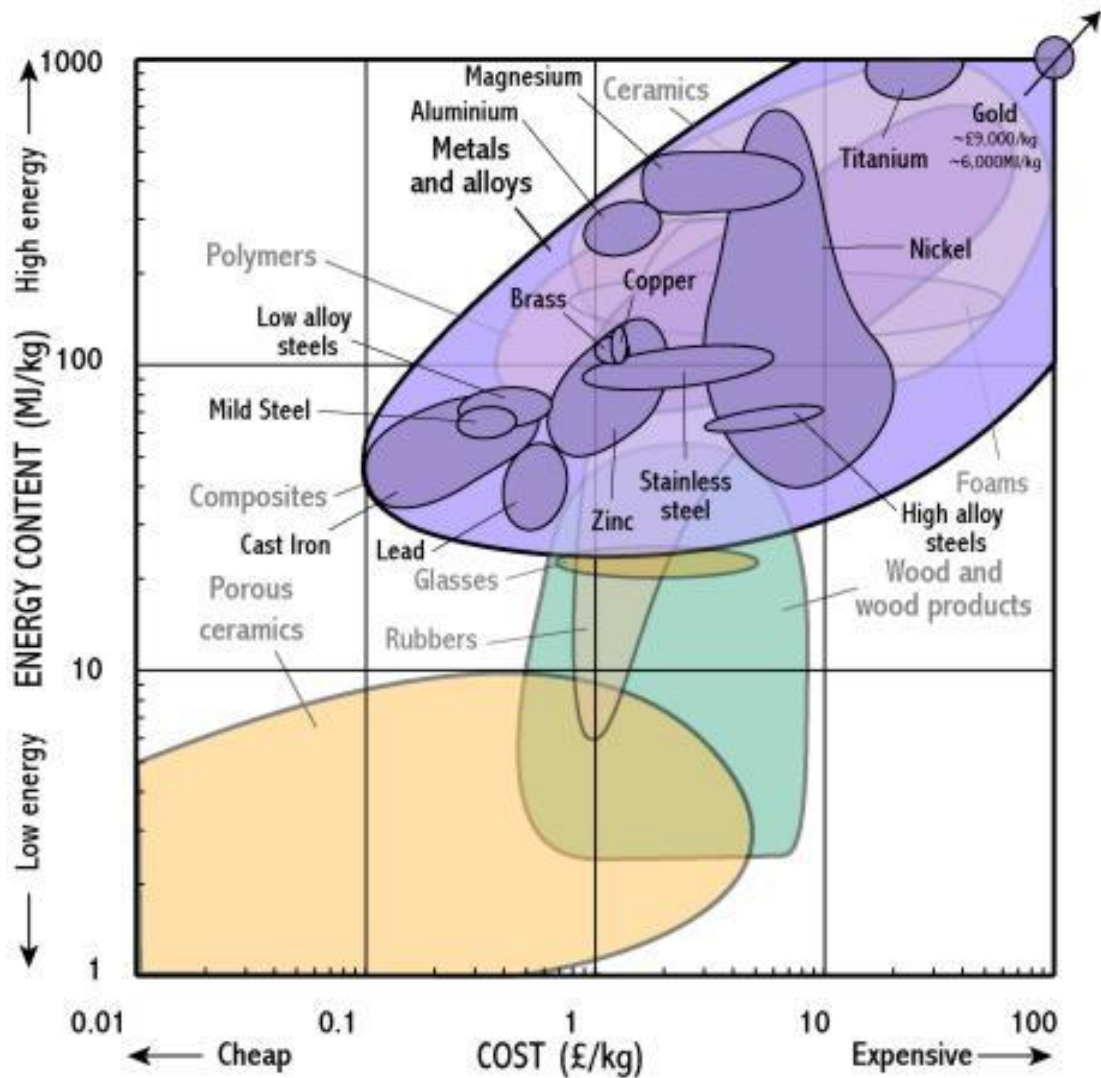


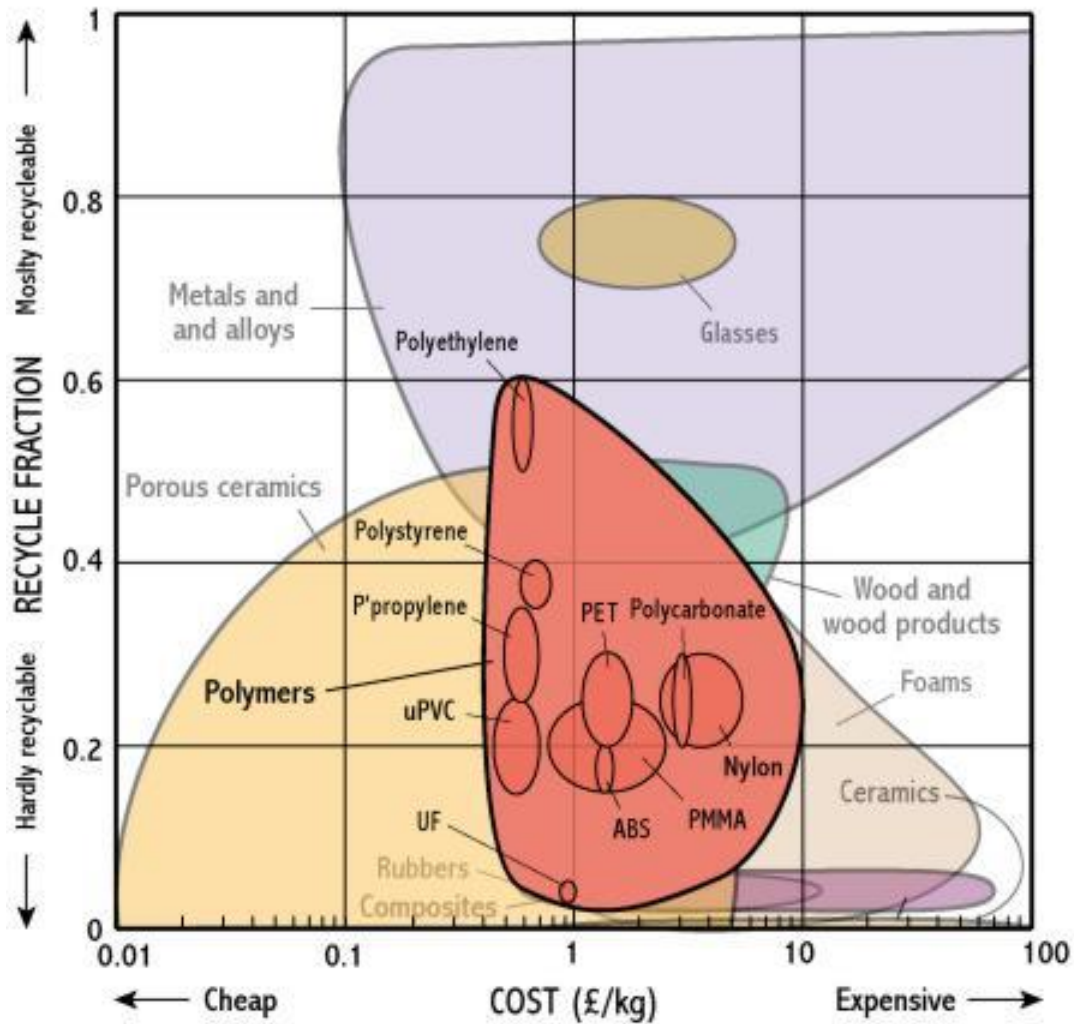
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Selection tools

Example of comparison table

Comparison - MaterialUniverse

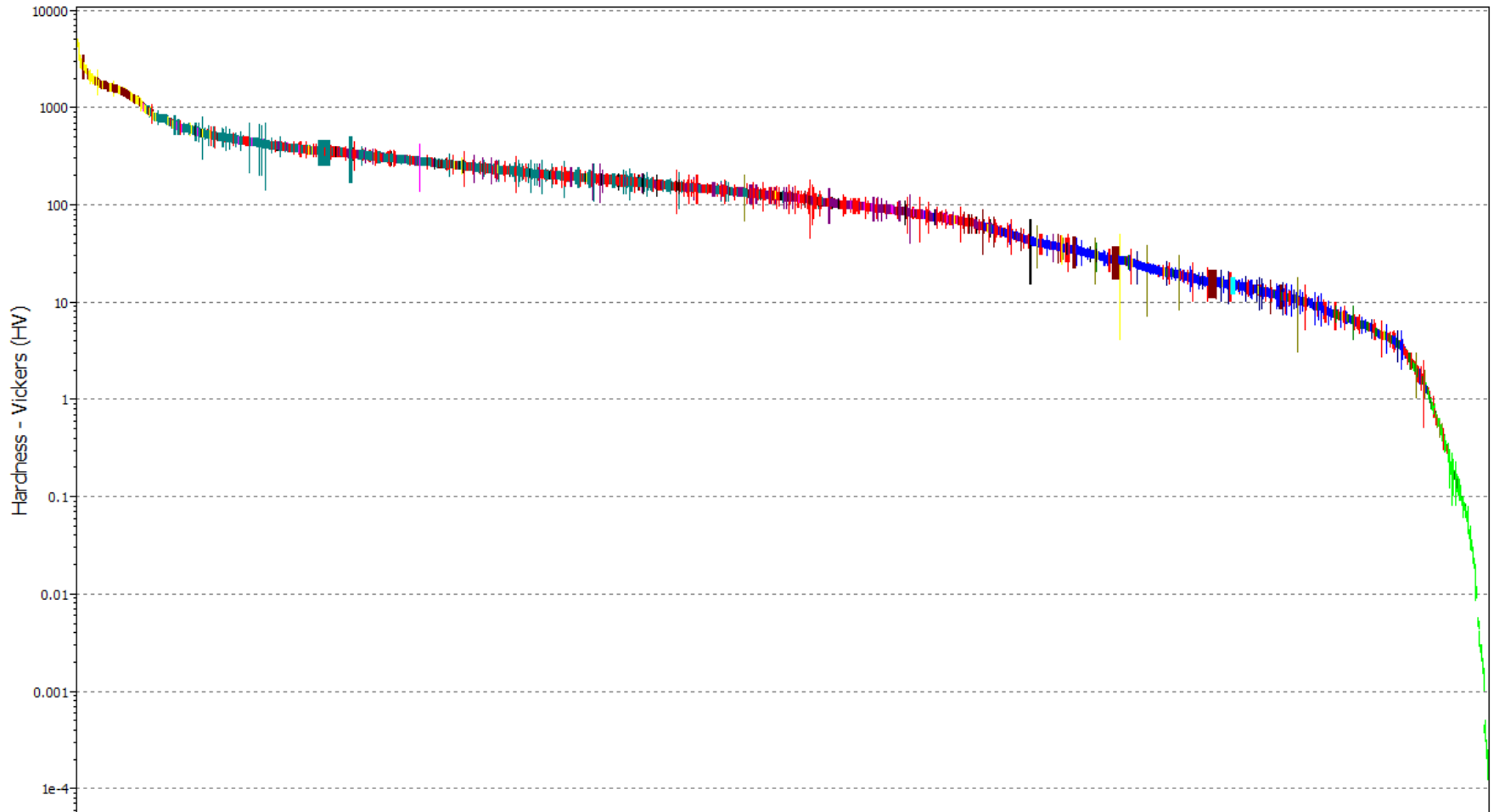
All Data Project Data Ranges Averages #. Values % Change Highlight % Change > 10 Apply

	Concrete (normal (Portland cement))	High density concrete	Aerated concrete	Concrete (high performance)
General properties				
Density (kg/m ³)	2200 - 2600	4900 - 5500 ↑	400 - 900 ↓	2200 - 2600
Porosity (closed) (%)	0	0	0	0
Porosity (open) (%)	0.1 - 0.15	0.1 - 0.15	0.53 - 0.85 ↑	0 - 0.03 ↓
Price (EUR/kg)	0,0291 - 0,0436	0,182 - 0,225 ↑	0,0436 - 0,0582	0,0582 - 0,124 ↑
Composition overview				
Base	Other	Other	Other	Other
Composition detail (metals, ceramics and glasses)				
Al ₂ O ₃ (alumina) (%)	0.59	0.36 ↓	0.81 ↑	0.94 ↑
C (carbon) (%)	0	0.15 ↑	0	0
CaO (calcia) (%)	8.55	5.17 ↓	11.6 ↑	13.6 ↑
Fe (iron) (%)	0	50.3 ↑	0	0
Fe ₂ O ₃ (ferric oxide) (%)	0.43	0.26 ↓	0.58 ↑	0.68 ↑
H ₂ O (water) (%)	7.9	4.61 ↓	10.7 ↑	5.65 ↓
MgO (magnesia) (%)	0.33	0.2 ↓	0.44 ↑	0.52 ↑
Mn (manganese) (%)	0	0.38 ↑	0	0
P (phosphorus) (%)	0	0.01 ↑	0	0
S (sulfur) (%)	0	0.01 ↑	0	0
SiO ₂ (silica) (%)	81.7	38.2 ↓	75.2 ↓	77.9 ↓
Other oxide (%)	0.49	0.29 ↓	0.67 ↑	0.78 ↑
Bio-data				
RoHS (EU) compliant grades?	✓	✓	✓	✓
Toxicity rating	Non-toxic	Non-toxic	Non-toxic	Non-toxic
Mechanical properties				
Young's modulus (GPa)	15 - 25	40.2 - 41.6 ↑	12 - 18	32 - 43 ↑
Flexural modulus (GPa)	15 - 25	40.2 - 41.6 ↑	12 - 18	32 - 43 ↑
Shear modulus (GPa)	6.5 - 10.9	16.5 - 17 ↑	5.1 - 7.6	13.9 - 18.7 ↑
Bulk modulus (GPa)	7.1 - 11.9	23.9 - 24.8 ↑	6.3 - 9.5	15.2 - 20.5 ↑
Poisson's ratio	0.1 - 0.2	0.2 - 0.24	0.17 - 0.2	0.1 - 0.2
Shape factor	3	3	3	3
Yield strength (elastic limit) (MPa)	1 - 1.2	3.1 - 3.7 ↑	0.6 - 1.1	5.3 - 9.3 ↑
Tensile strength (MPa)	1.1 - 1.3	3.1 - 3.7 ↑	0.6 - 1.1	5.3 - 9.3 ↑
Compressive strength (MPa)	13.3 - 30	30.6 - 36.6 ↑	1.2 - 1.87 ↓	53.3 - 93.3 ↑
Flexural strength (modulus of rupture) (MPa)	1.7 - 2.4	2.7 - 4.4 ↑	0.7 - 1.2 ↓	6.4 - 11.2 ↑

See CES

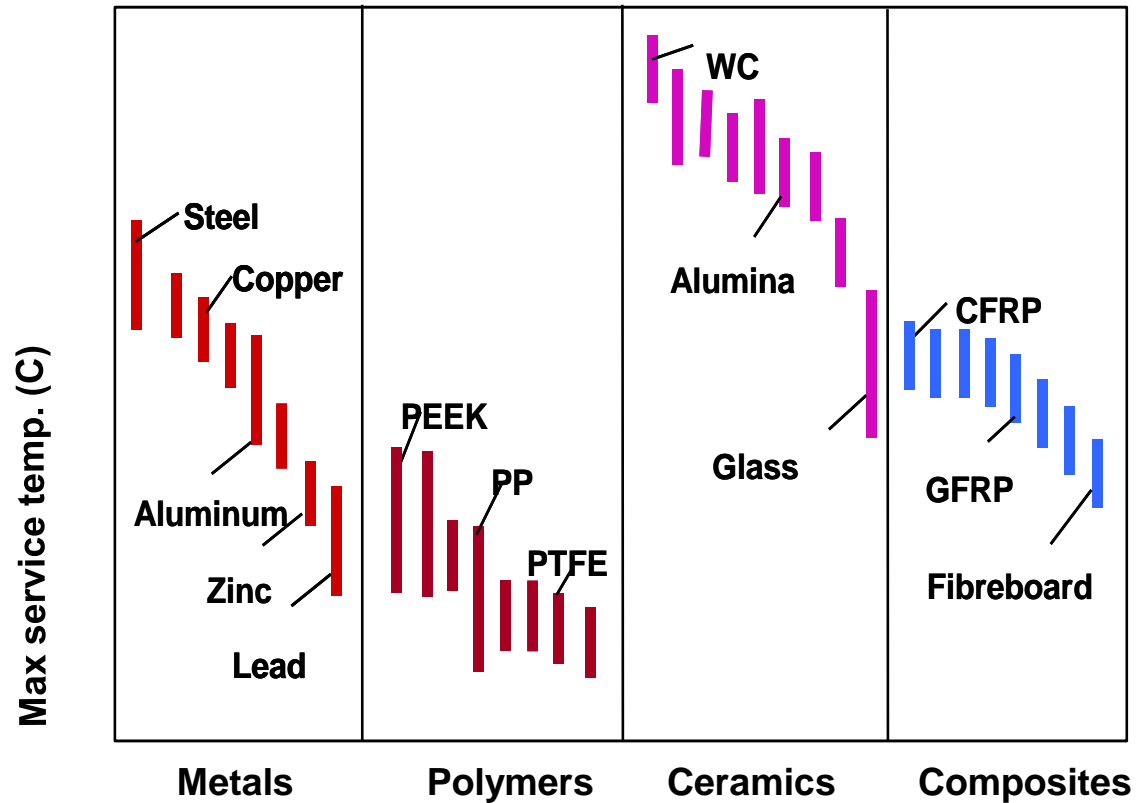
Selection tools

Using 1D graphs – 1 constraint



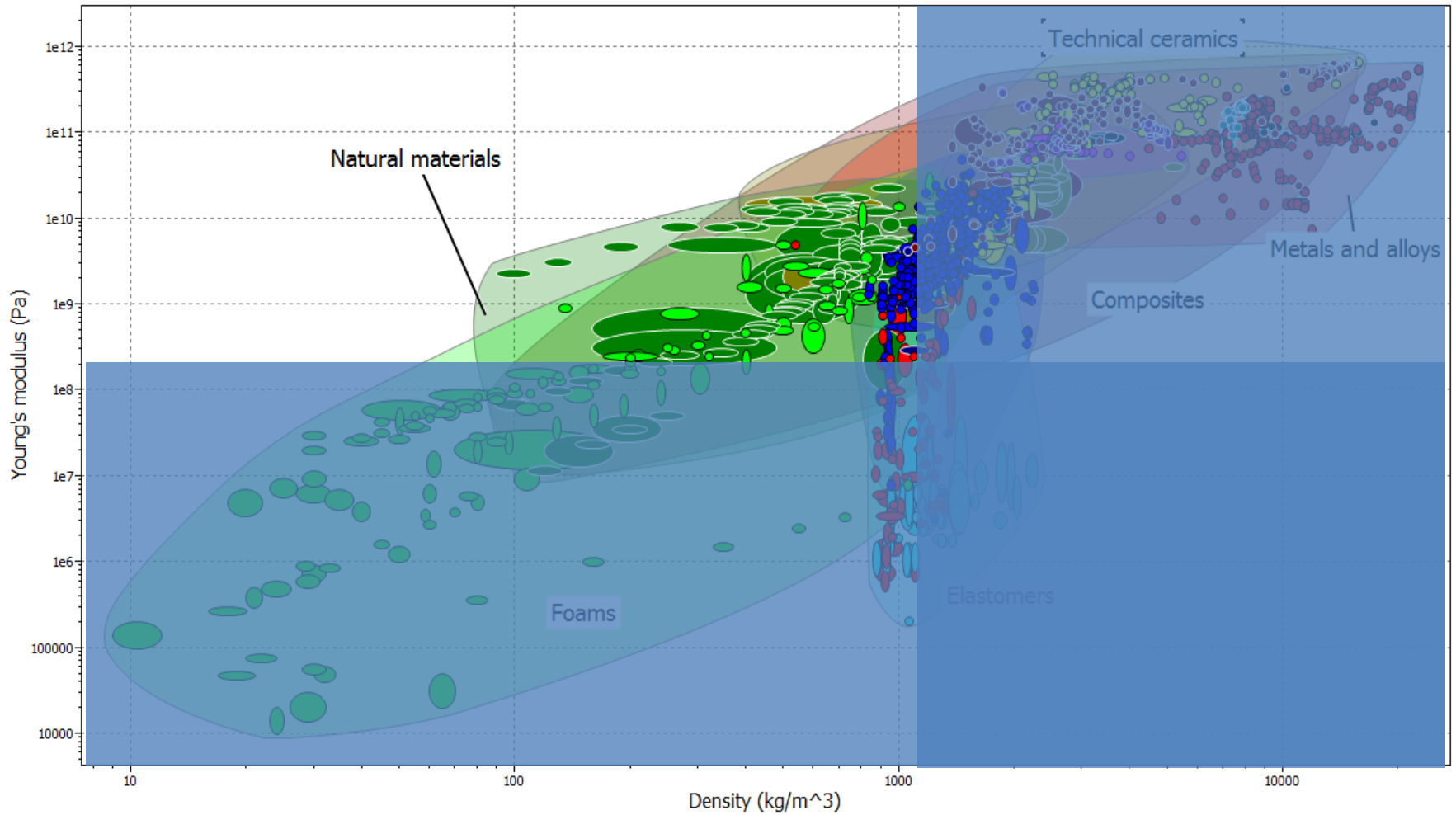
Selection tools

Using 1D graphs – 1 constraint



Selection tools

Using 2D graphs – 2 constraints



See CES

Selection tools

Using software – multiple constraints

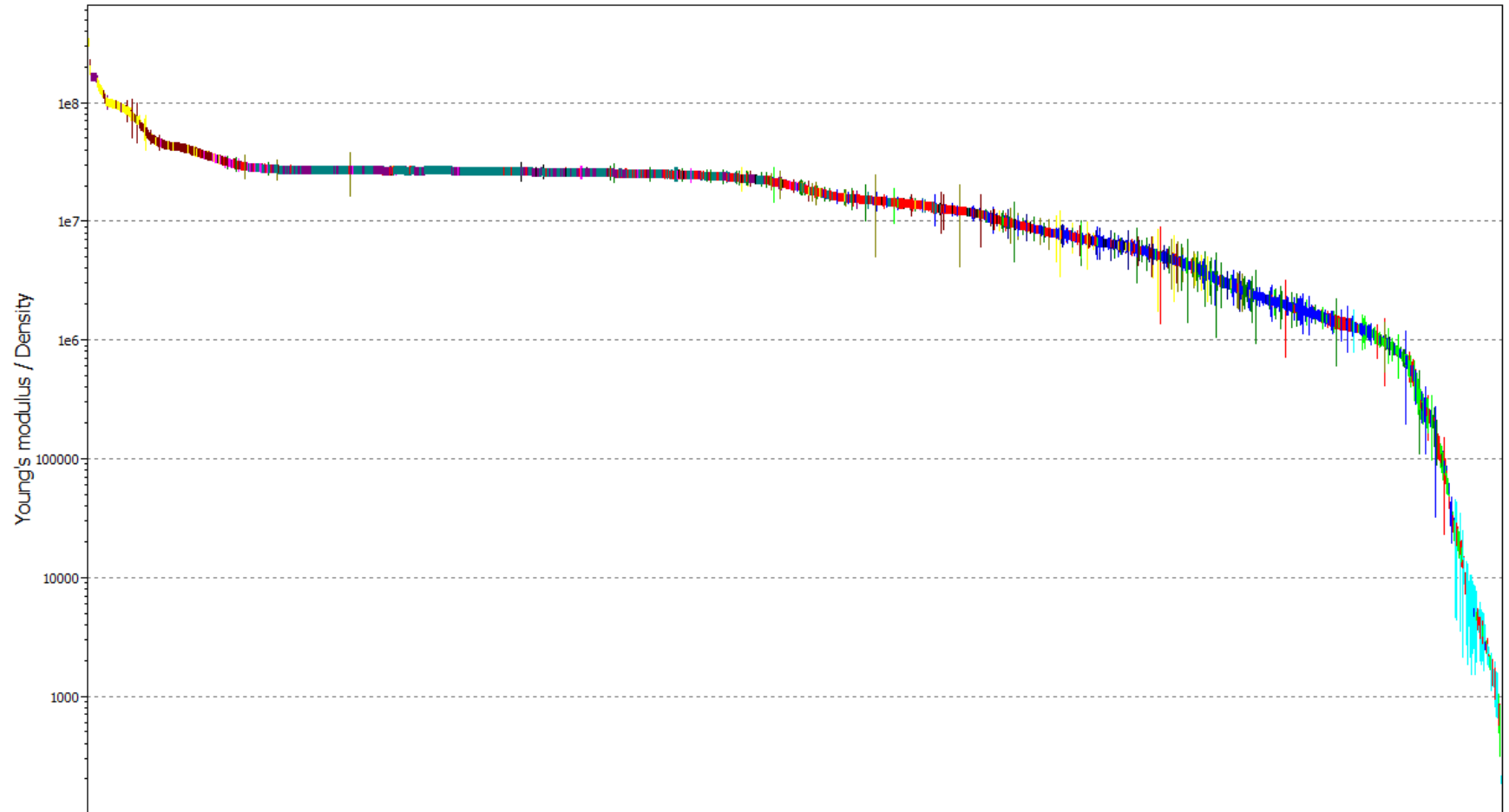
The screenshot displays the 'Limit' software interface. At the top, there are buttons for 'Properties', 'Apply', and 'Clear'. Below this, a section titled 'Click on the headings to show/hide selection criteria' contains a dropdown menu for 'General properties'. Under 'General properties', there are input fields for 'Density' (kg/m³) and 'Price' (EUR/kg), with a 'Minimum' and 'Maximum' column for each. A list of material types is shown, including Unidirectional composite, Biaxial composite, Quasi-isotropic composite, and Short fiber composite. Below this, there are sections for 'Composition overview', 'Composition detail (metals, ceramics and glasses)', 'Composition detail (polymers and natural materials)', 'Bio-data', and 'Mechanical properties'. The 'Mechanical properties' section has input fields for Young's modulus, Flexural modulus, Shear modulus, Bulk modulus, Poisson's ratio, Shape factor, Yield strength (elastic limit), Tensile strength, Compressive strength, and Flexural strength (modulus of rupture), each with 'Minimum' and 'Maximum' columns and units in Pa.

The 'Limit Bar' chart shows the distribution of Young's modulus (Pa) for various material classes. The x-axis is logarithmic, ranging from 10,000 Pa (Flexible) to 1E+12 Pa (Stiff). The data is as follows:

Material Class	Approximate Young's Modulus Range (Pa)
Glasses	1E+10 to 1E+12
Non-technical ceramics	1E+09 to 1E+11
Technical ceramics	1E+08 to 1E+10
Composites	1E+07 to 1E+09
Foams	1E+04 to 1E+06
Natural materials	1E+06 to 1E+08
Metals and alloys	1E+08 to 1E+10
Elastomers	1E+05 to 1E+07
Plastics	1E+06 to 1E+08

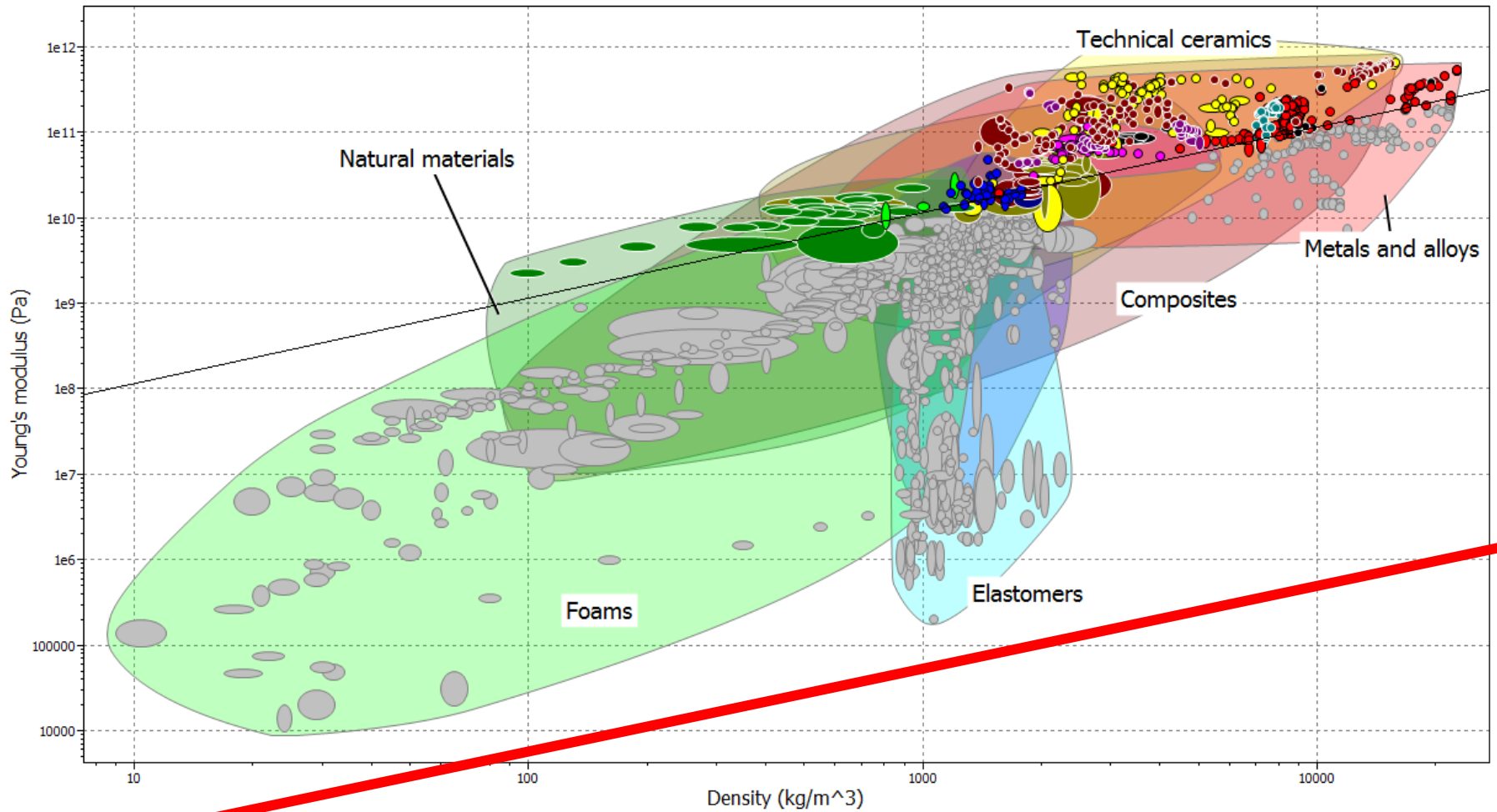
Selection tools

Using 1D graphs - multiproperty



Selection tools

Using 2D graphs - multiproperty



See CES