The Elements database:

Properties, relationships and resources

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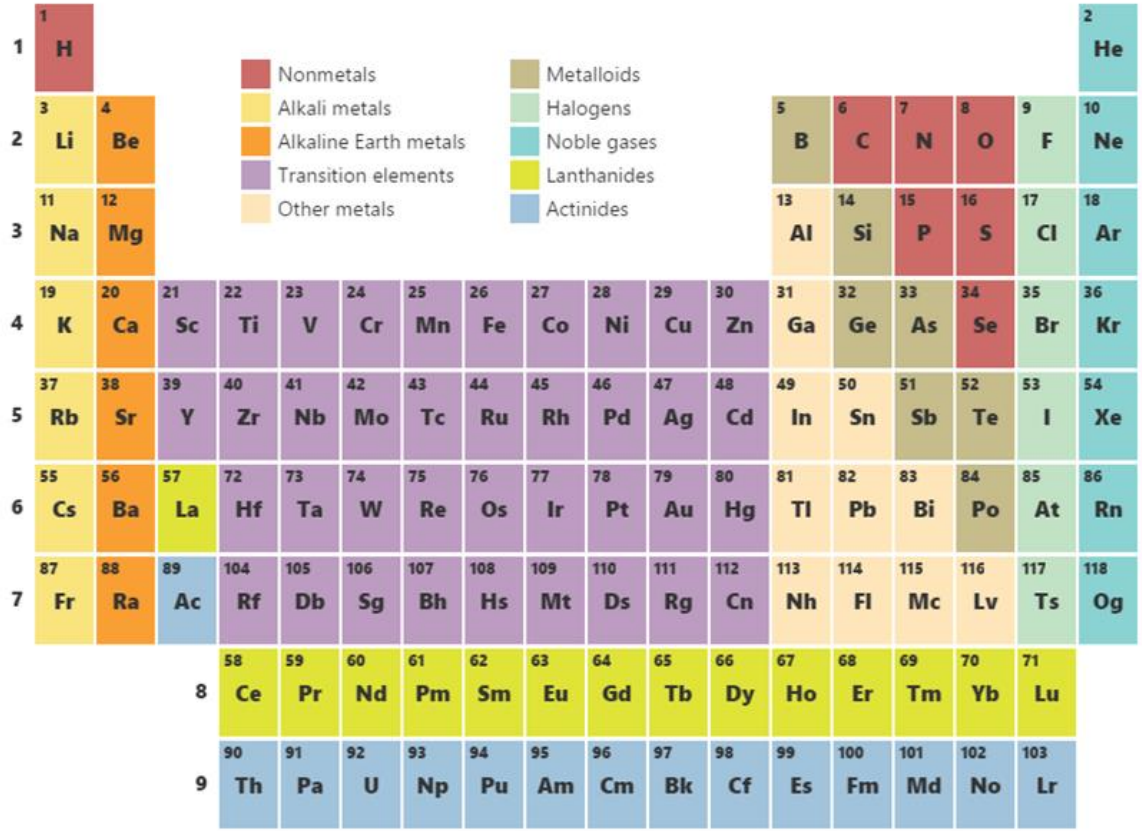


Learning objectives for this lecture unit

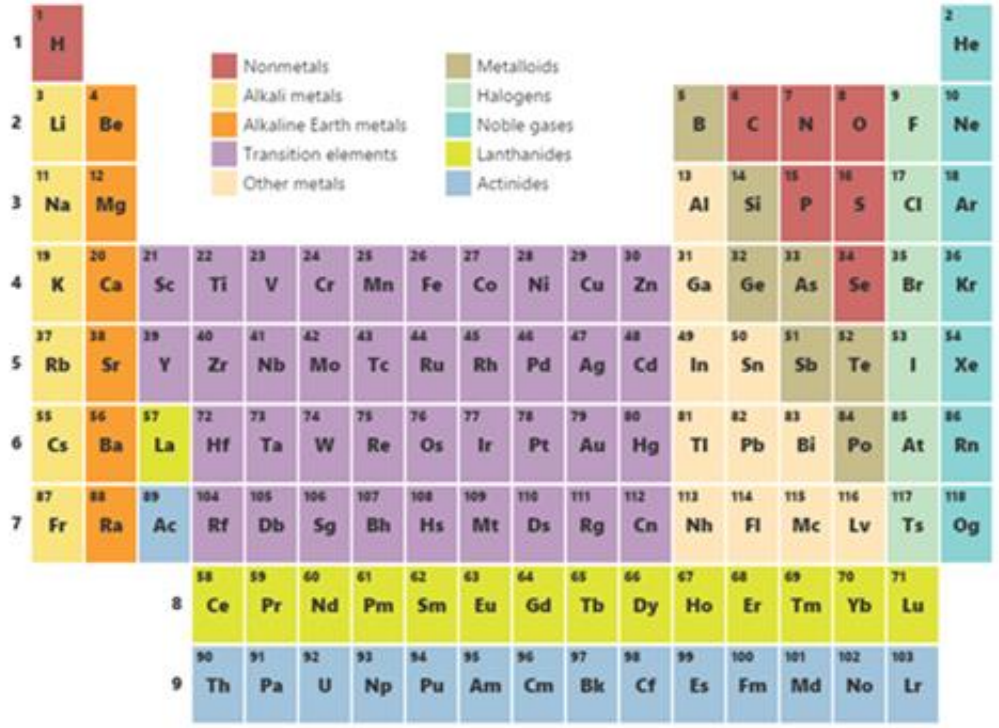
Ansys software mentioned	• Ansys Granta EduPack™, a teaching software for materials education

Intended Learning Outcomes	
Knowledge and Understanding	Knowledge of the Periodic Table and understanding of underlying principles
Skills and Abilities	Ability to explore fundamental scientific relationships using the elements
Values and Attitudes	Insight into the ways elements influence material properties, *e.g.* bond type

Resources

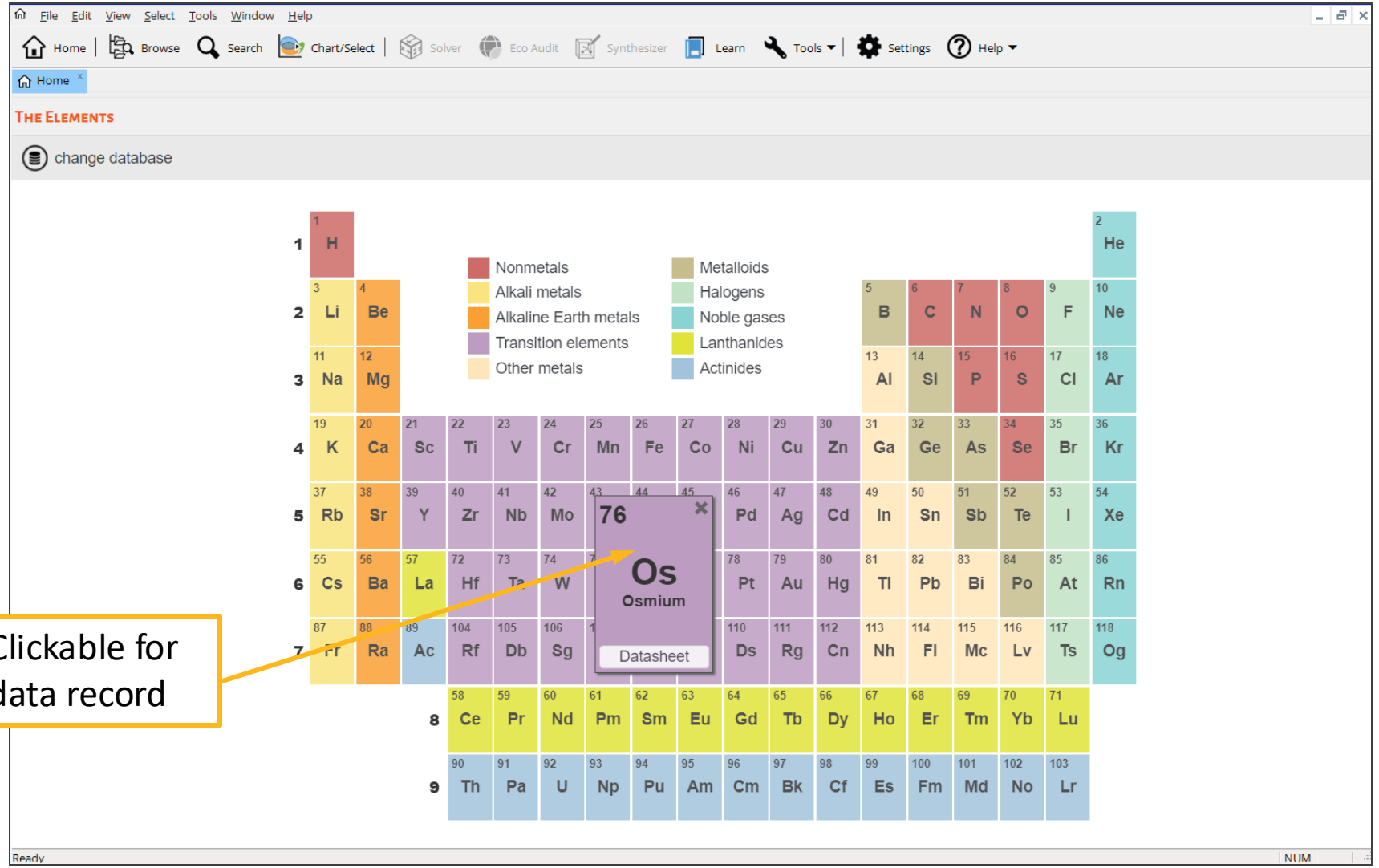
- White Papers: Paper: the Elements Database and Paper: Materials for Nuclear Power Systems

Lecture Outline



- **The Periodic Table**
- **Database features**
- **Relationship charts**
- **Magnetic and Nuclear properties**
- **Resource aspects and Sustainability**

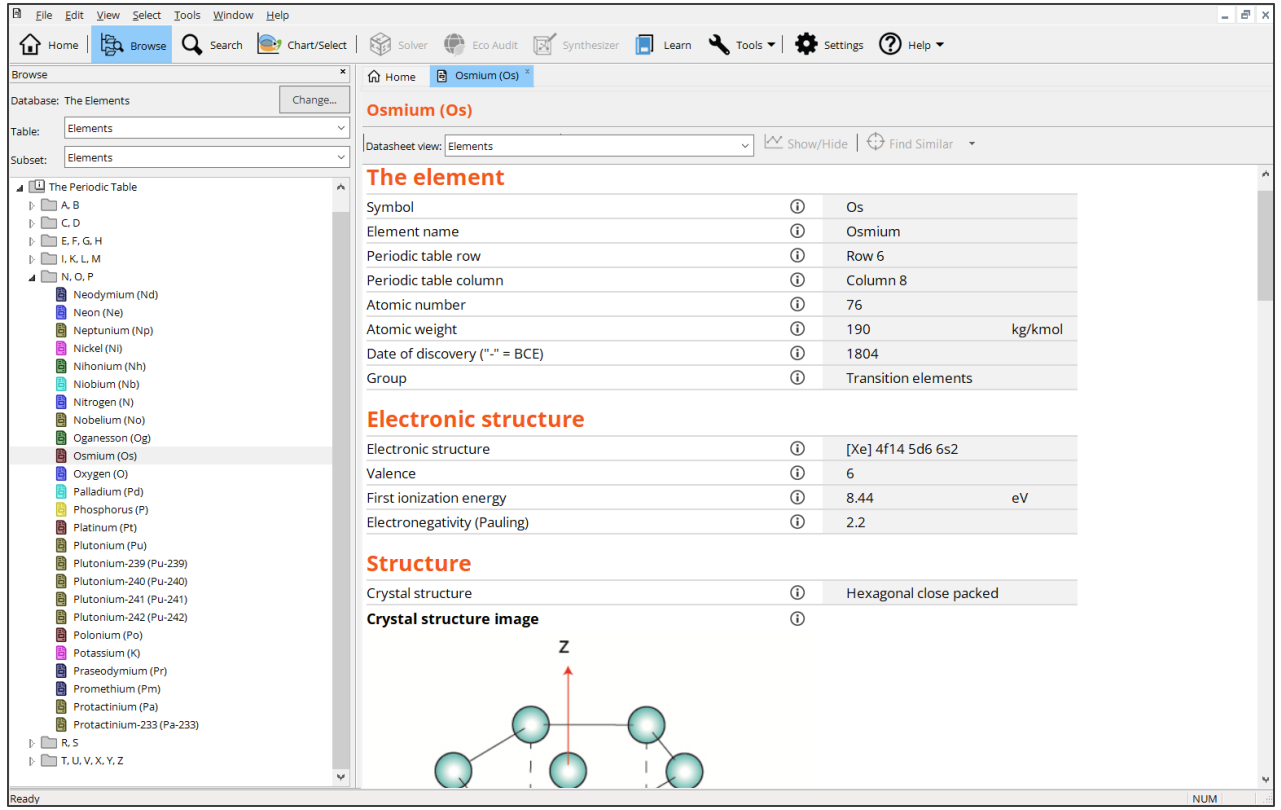
Interactive periodic table interface



The Elements database

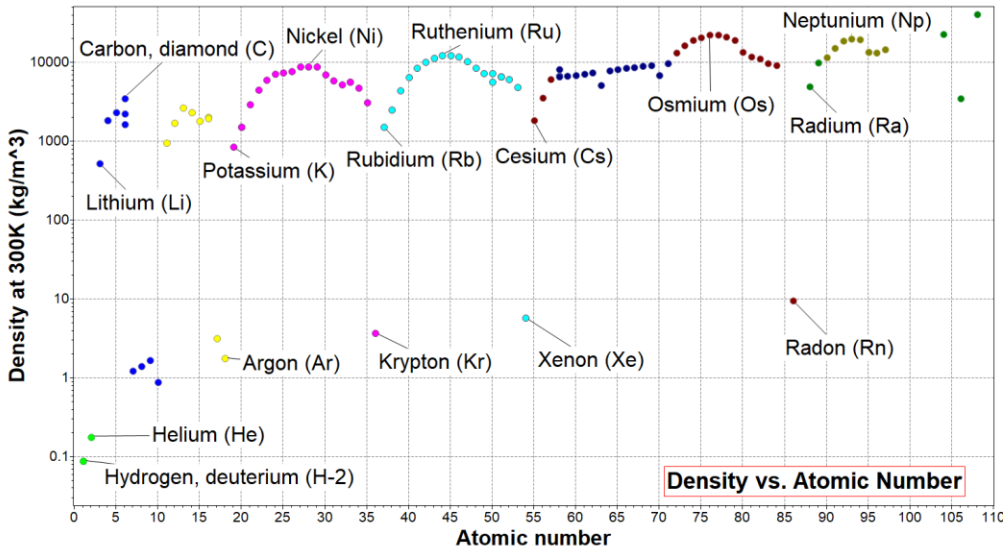
Elements

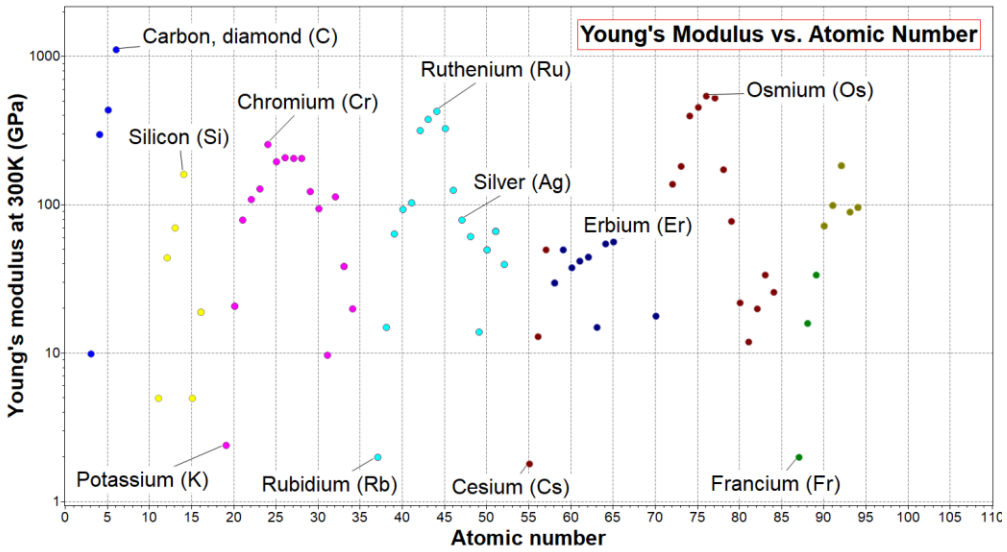
- 149 records for 118 elements
- Periodic table properties
- Electronic structure data
- Crystal structure properties
- Mechanical properties
- Thermal properties
- Surface energy
- Electrical and superconducting properties
- Magnetic properties
- Nuclear properties
- Geo-economic data
- Eco properties
- Critical materials info
- Principal uses and substitutes



Using the Elements database

- Explore how properties change across the Periodic Table
- The Elements provide an excellent range of all properties





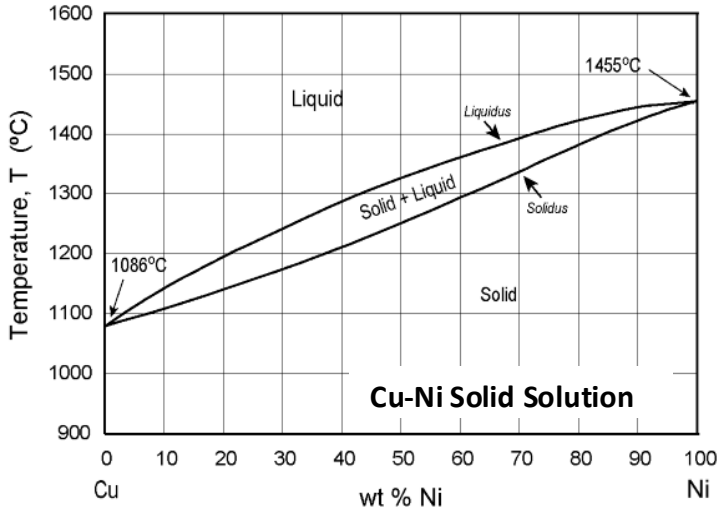
Electronic structure data

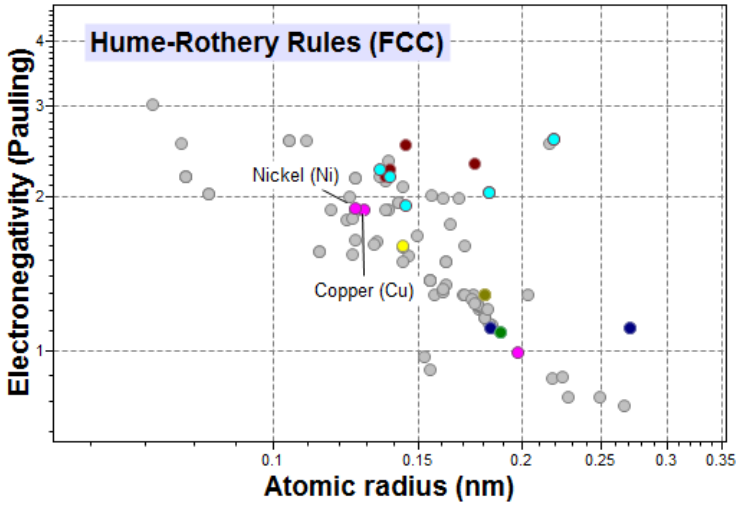
Electronic structure			
Electronic structure	ⓘ	[Ar] 3d10 4s1	
Valence	ⓘ	2	
First ionization energy	ⓘ	7.73	eV
Second ionization energy	ⓘ	20.3	eV
Electronegativity (Pauling)	ⓘ	1.9	

In Elements database

Hume-Rothery: extensive substitutional solid solution when

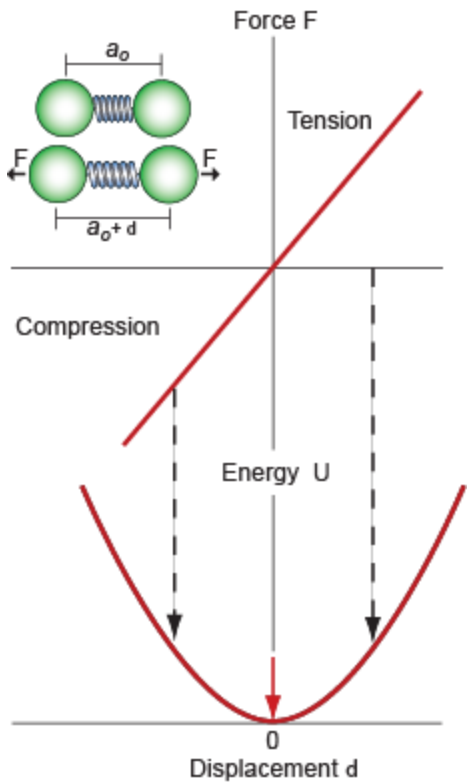
- Atomic radii differs by less than 15%
- Electronegativity differs by less than 0.075
- Same crystal structure and valence

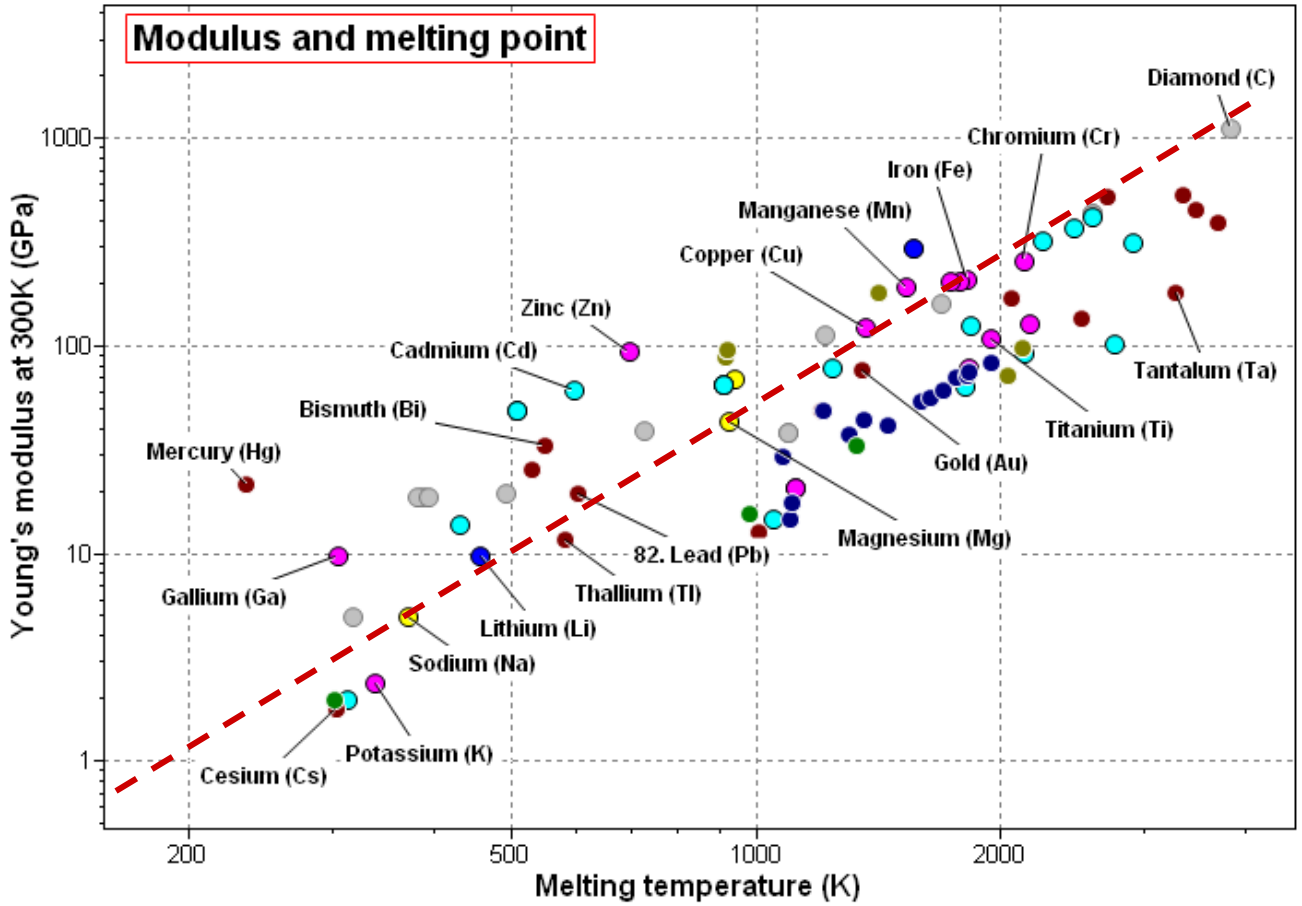




Relationships between properties (1)

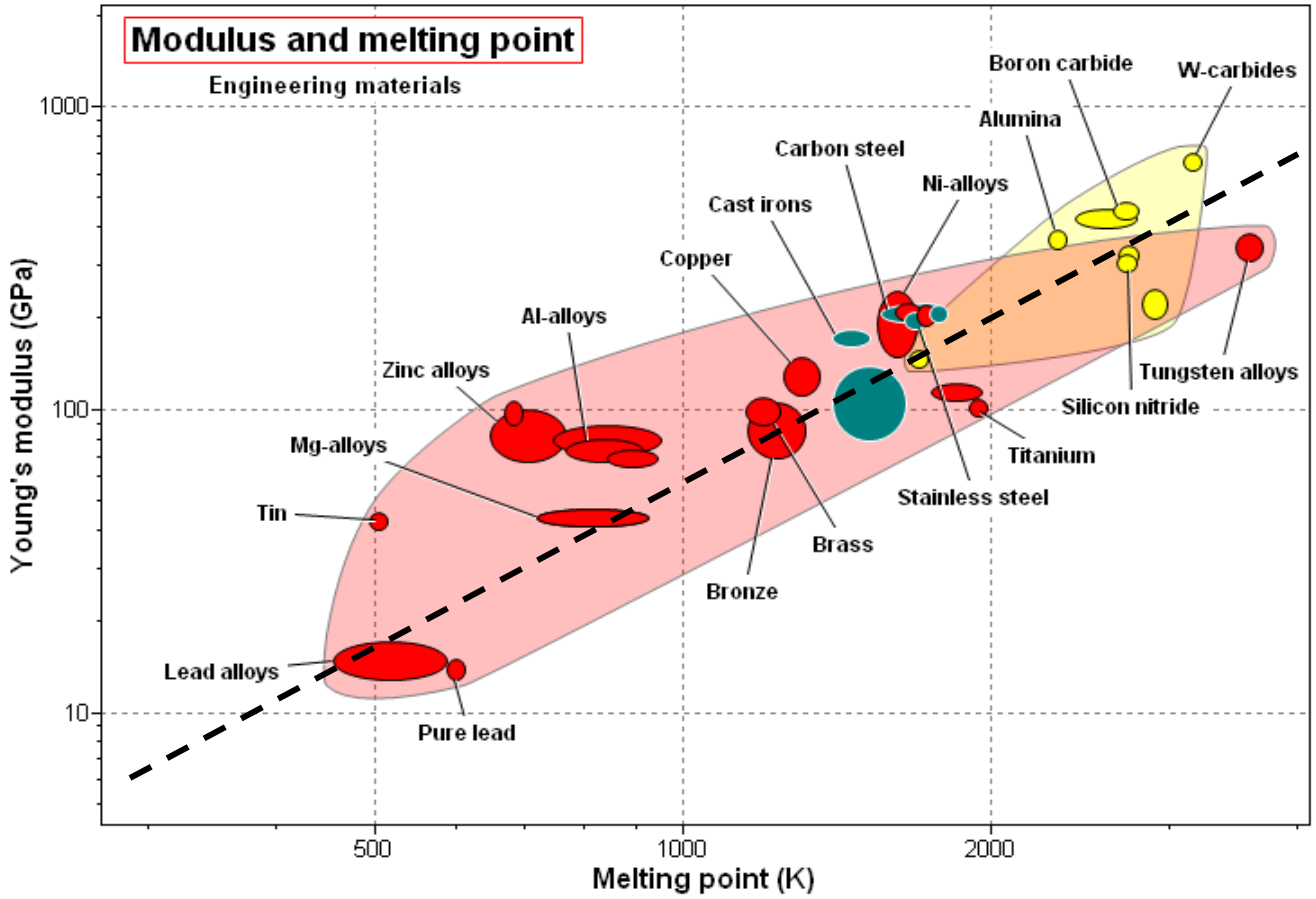
- Modulus and melting point both reflect bond strength between element atoms





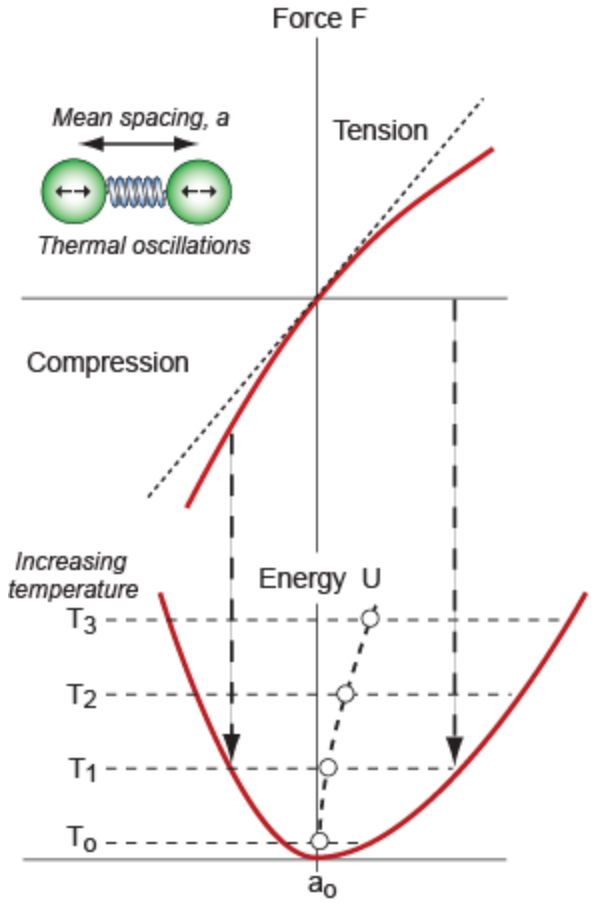
Engineering materials – a similar trend

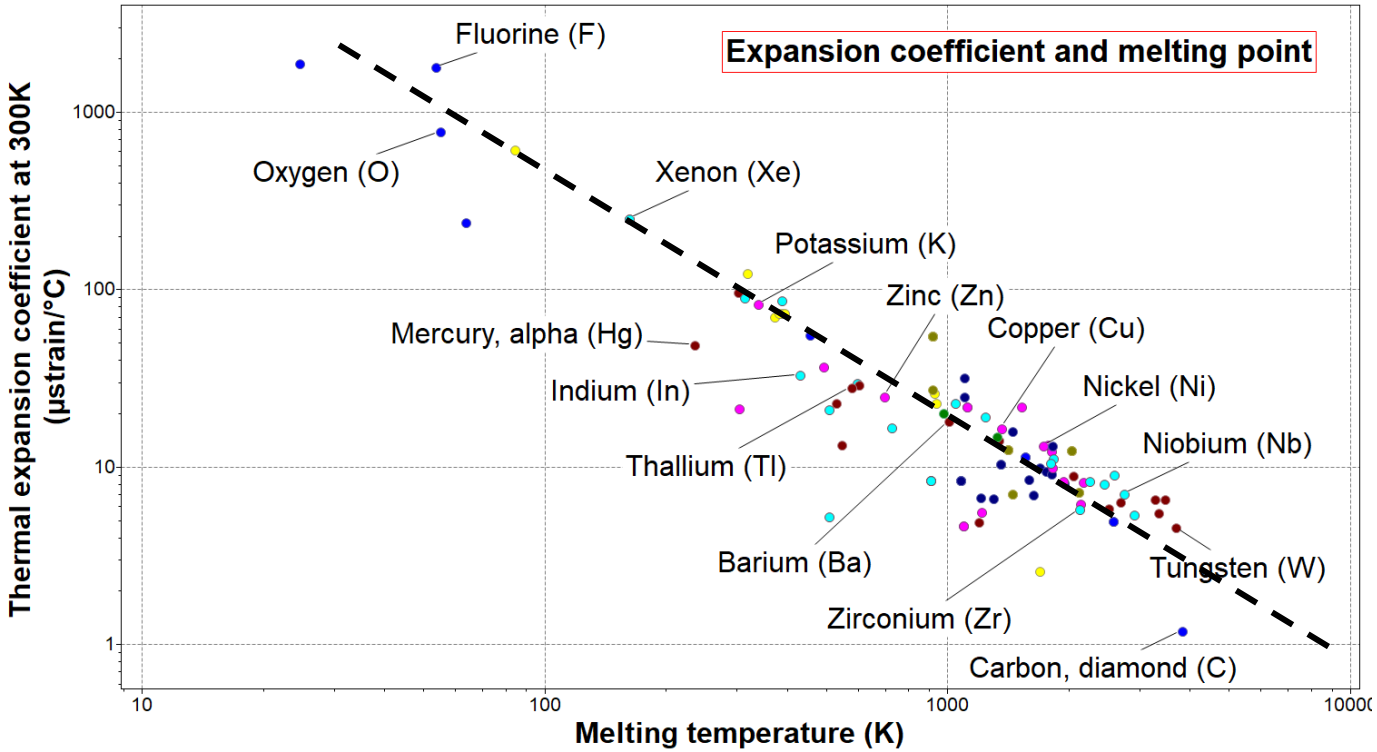
- Modulus and melting point both reflect bond strength in engineering materials



Relationships between properties (2)

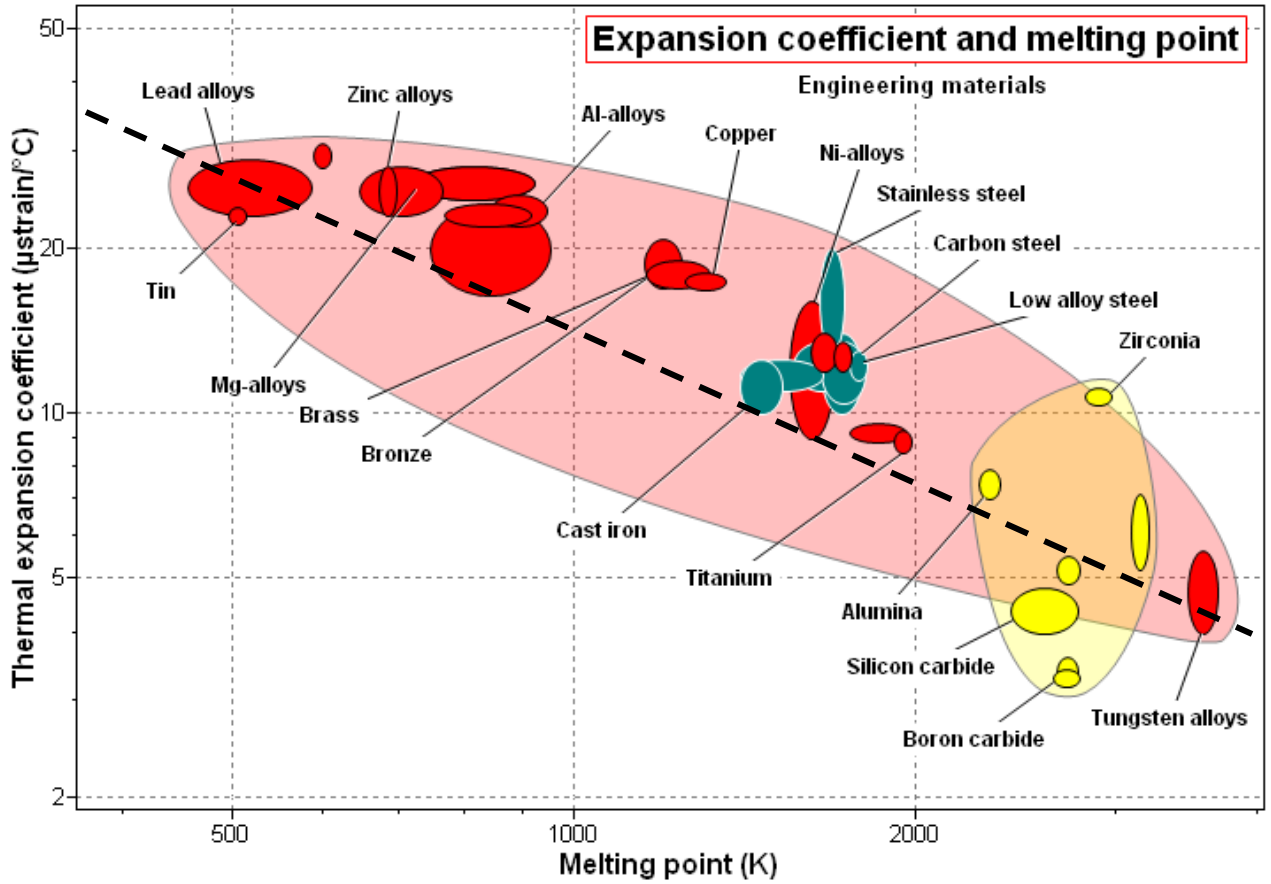
- Expansion coefficient and melting point both relate to depth and shape of the “potential well”





Engineering materials – a similar trend

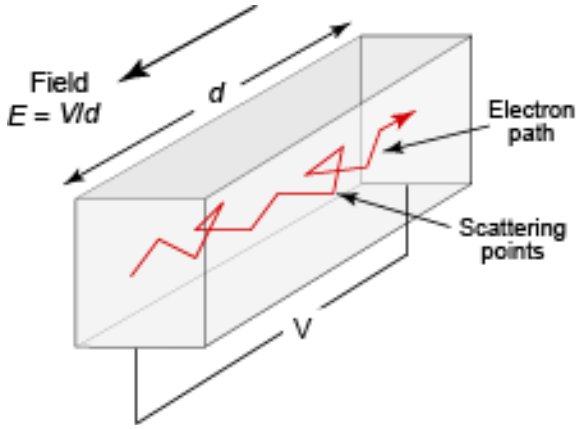
- Expansion coefficient and melting point both relate to depth and shape of the “potential well”

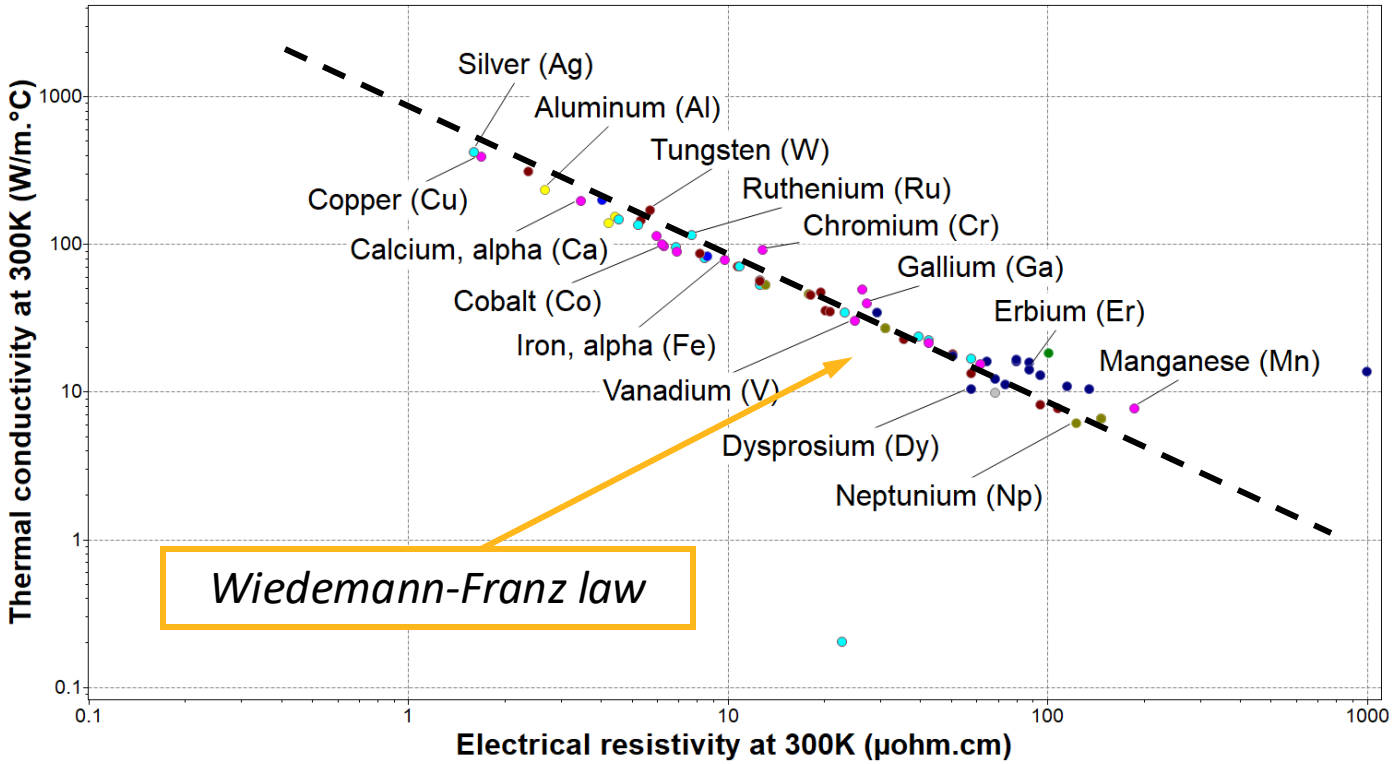


Relationships between properties (3)

- The empirical relationship between thermal conductivity and electrical resistivity can be used to determine the proportionality constant in the Wiedemann-Franz law

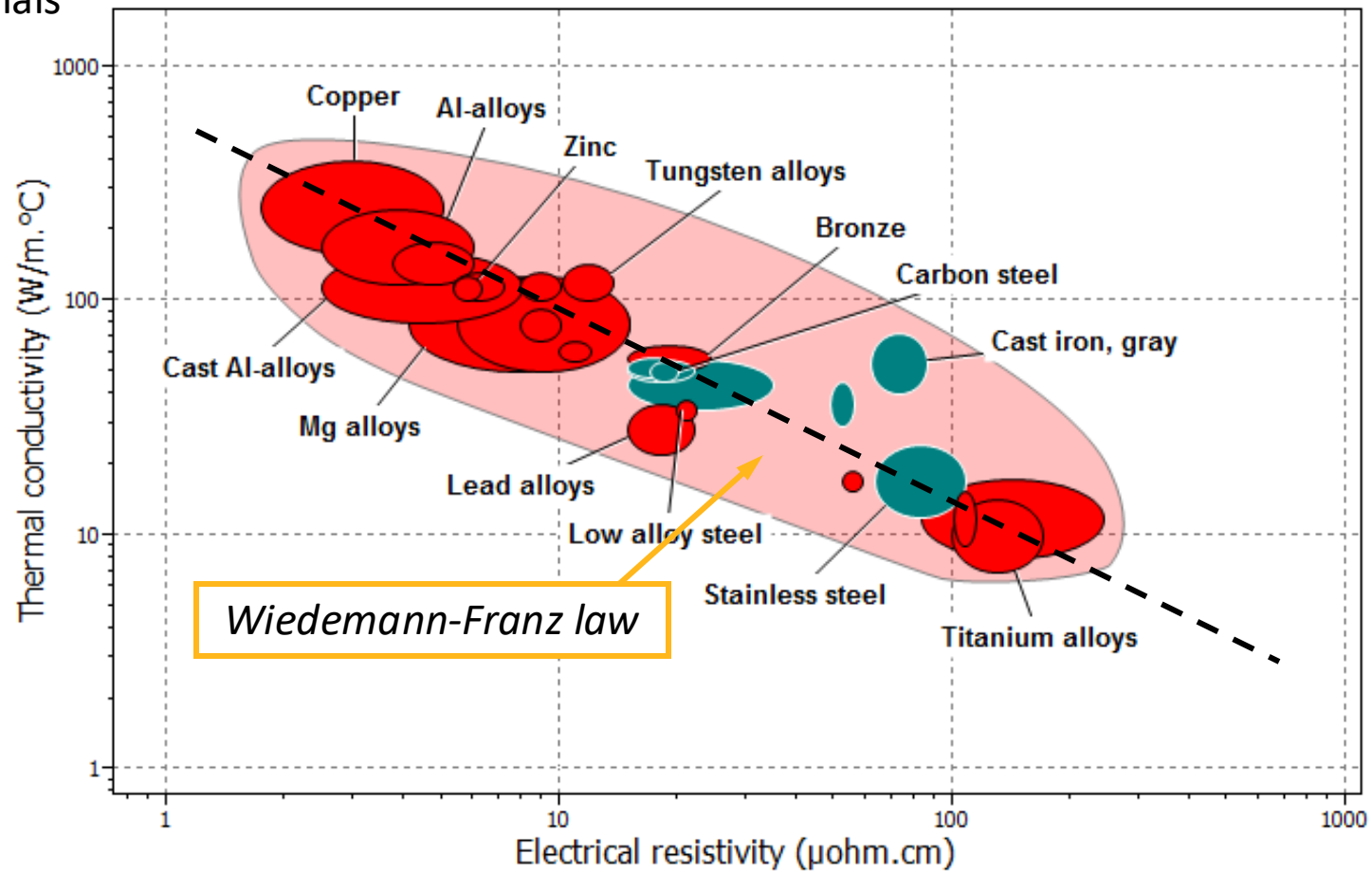
Electrical and thermal conduction





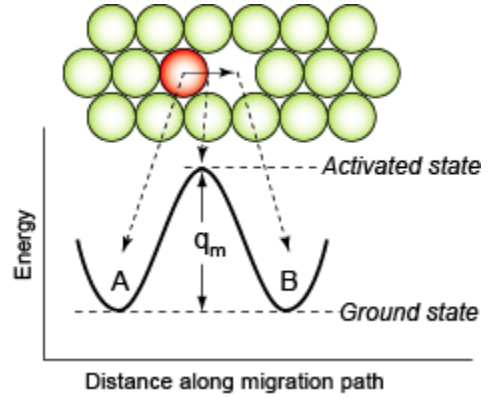
Engineering materials – a similar trend

- The empirical relationship between thermal conductivity and electrical resistivity in the Wiedemann-Franz law is in agreement with data from Ansys Granta EduPack software level 1 materials

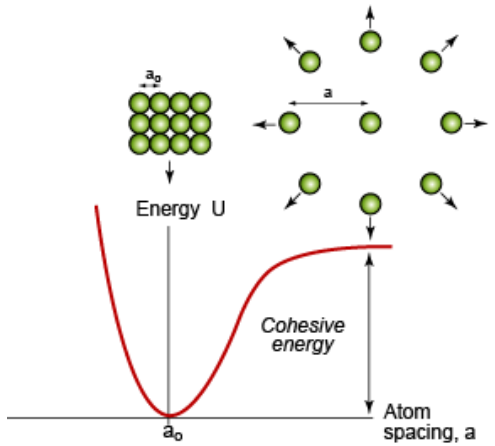


Relationships between properties (4)

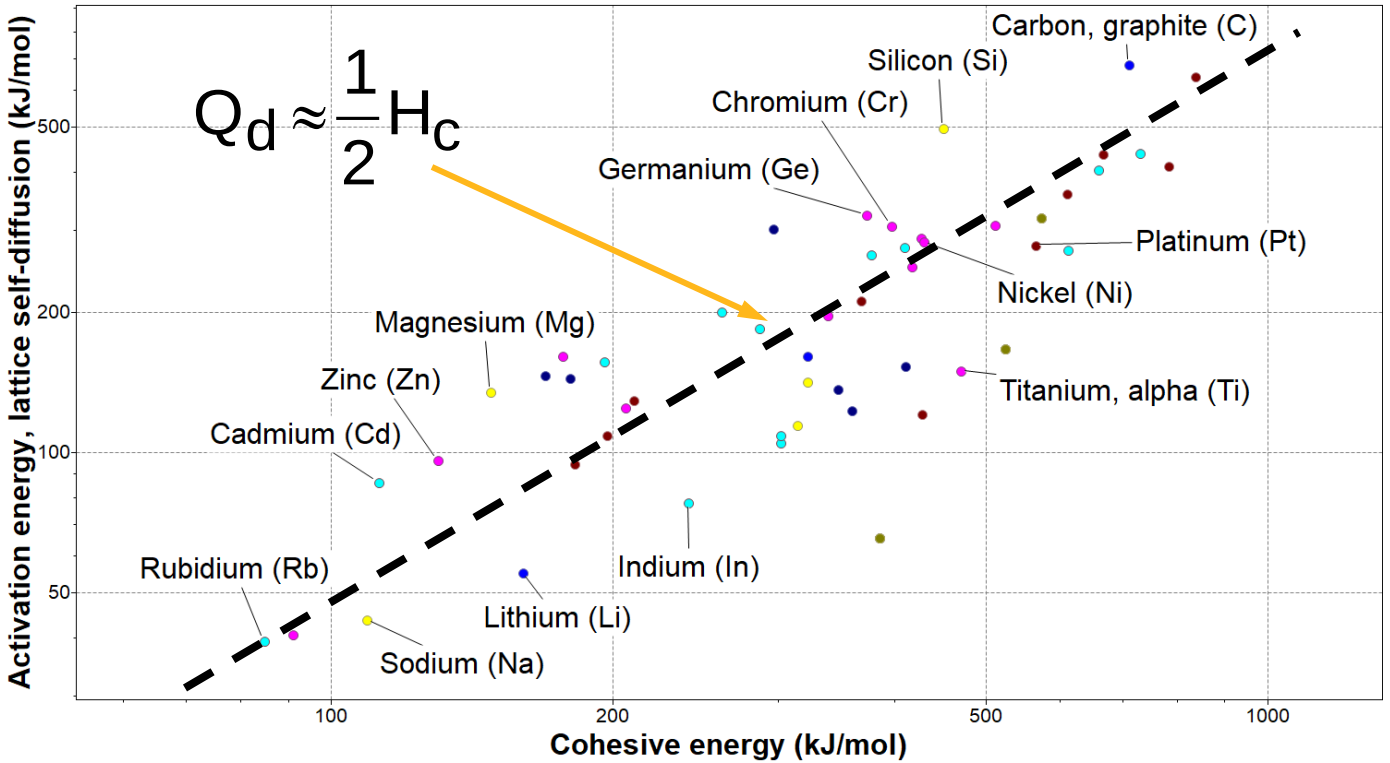
Activation energy for diffusion



Cohesive energy

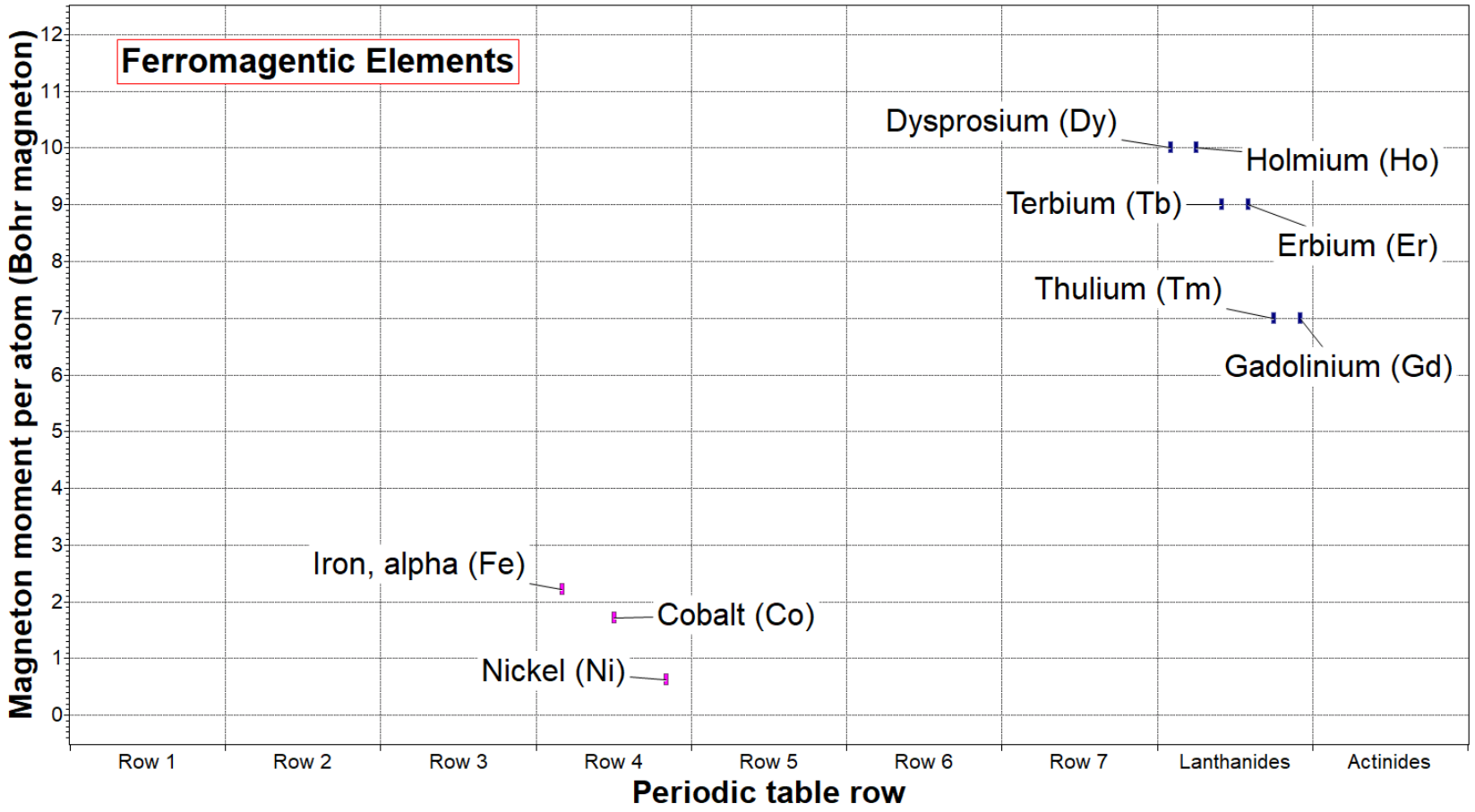


- Activation energy for diffusion and cohesive energy



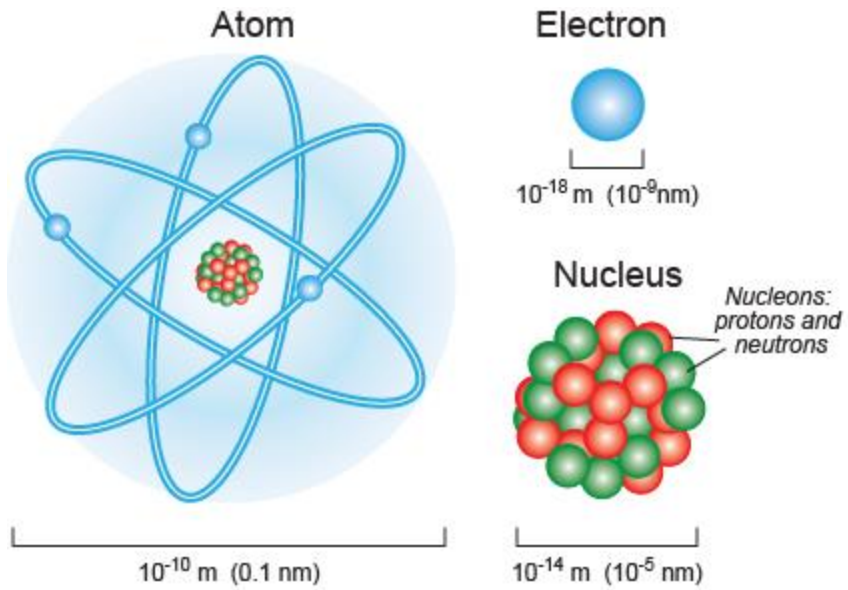
Magnetic properties

- Grouping of ferromagnetic elements into two distinct areas of the chart, due to electron configuration



Nuclear properties of the elements

- Nuclear properties of the elements added to the Elements database



- Binding energy per nucleon

  Relevant for fuels for fission and fusion

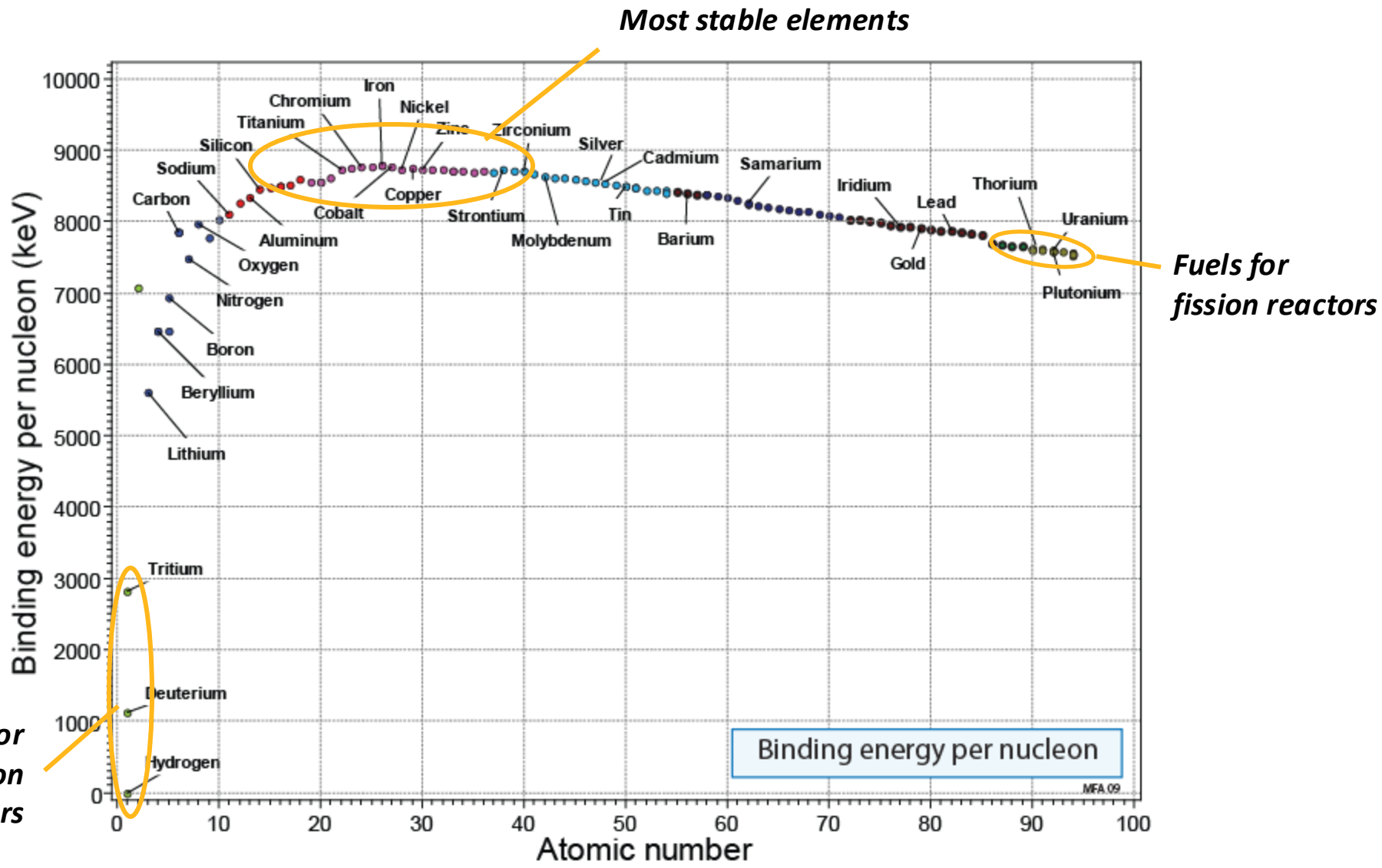
- Neutron absorption and scattering X-sections

  Relevant moderator, reflector and control rod materials

- Half-lives of selected isotopes

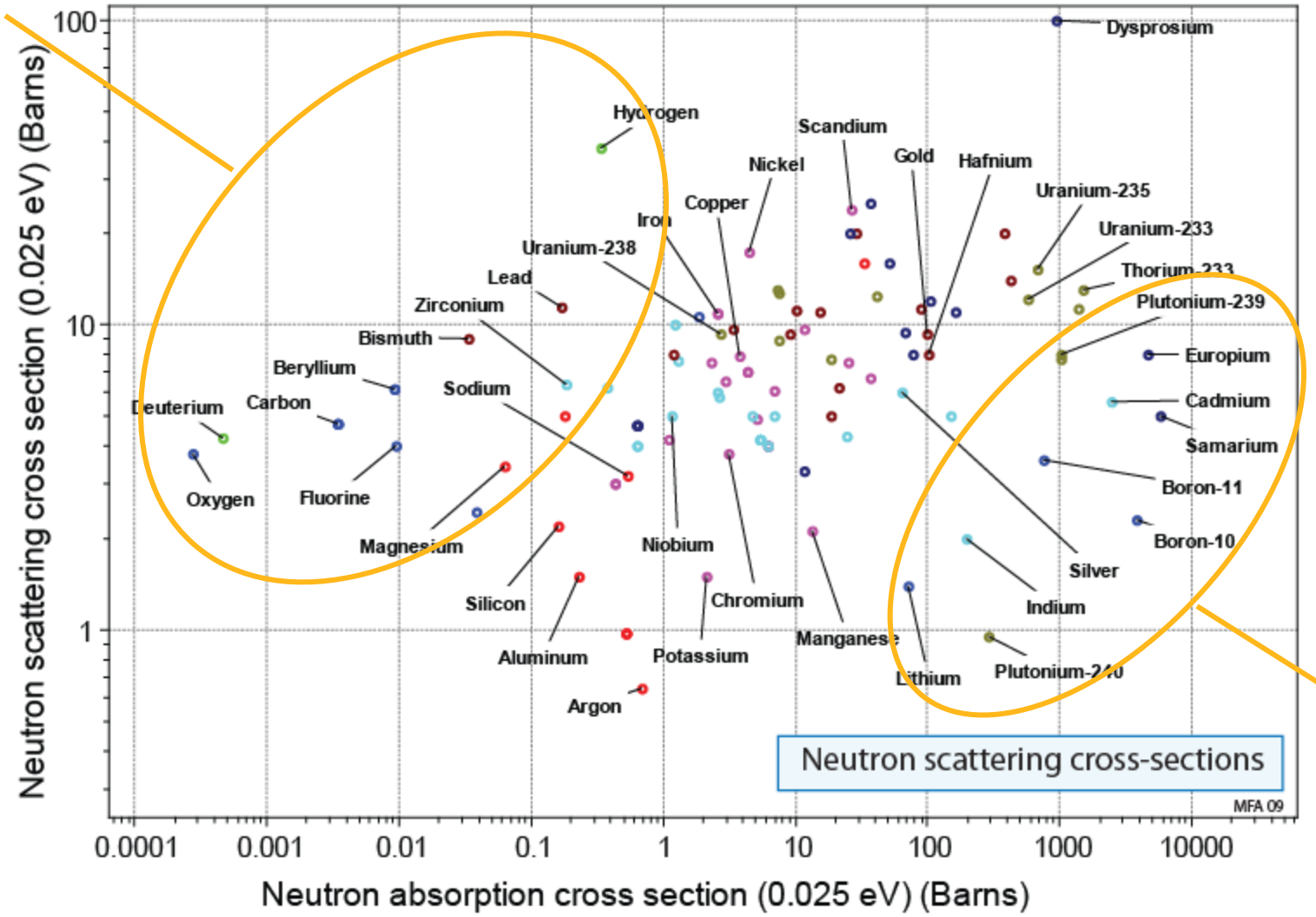
  Relevant for spent fuel and system decommissioning

Binding energy per nucleon



Absorption and scattering cross-sections

Moderator materials
High scattering, low absorption



Control rod materials
High absorption, low scattering

The Elements resource aspects

Resource-related properties in Elements data records

- Eco properties (Climate Change, Embodied energy, Water usage)
- Geo-economic data

Geo-economic data					
Typical exploited ore grade	ⓘ	0.096	-	0.106	%
Minimum economic ore grade	ⓘ	0.002	-	0.2	%
Abundance in the Earth's crust	ⓘ	0.8	-	1.5	ppm
Abundance in seawater	ⓘ	0.01			ppm
Annual world production	ⓘ	2.67e5			tonne/yr
World reserves	ⓘ	1.63e7			tonne

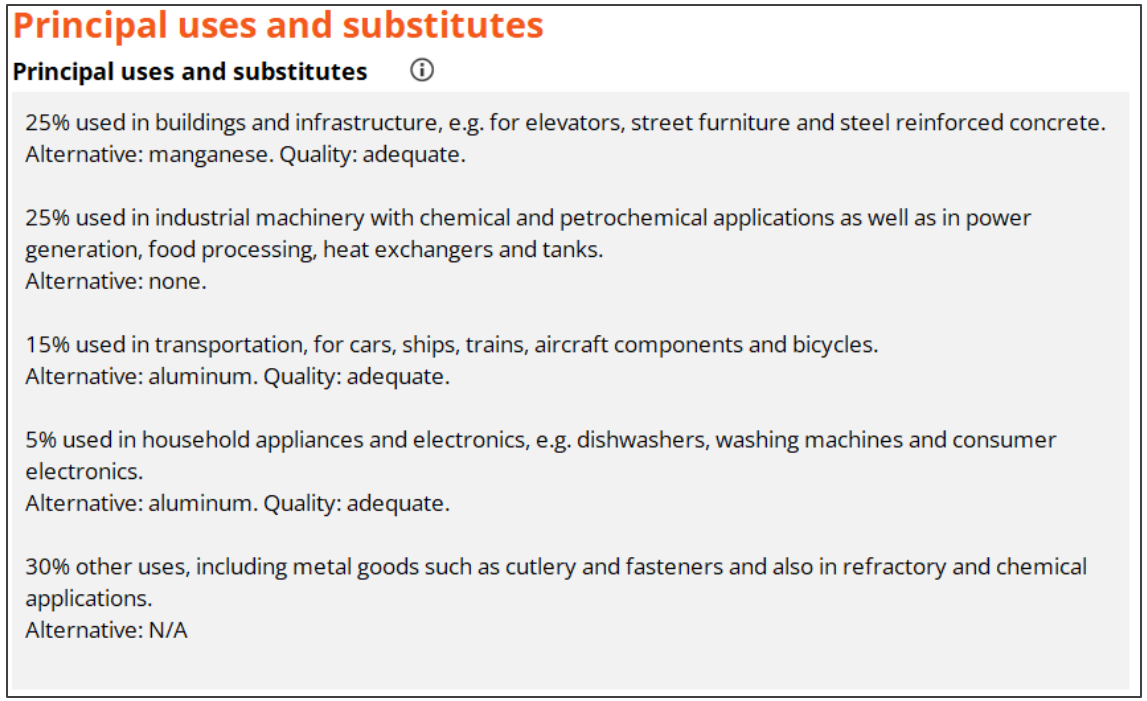
- Critical materials info

Critical materials information			
In EU Critical list?	ⓘ	✓	
In US Critical list?	ⓘ	✗	
Abundance risk level	ⓘ	Medium	
Environmental country risk Herfindahl-Hirschman Index, HHI	ⓘ	1.54	
Environmental country risk level	ⓘ	Low	
Sourcing and geopolitical risk Herfindahl-Hirschman Index, HHI	ⓘ	1.2	
Sourcing and geopolitical risk level	ⓘ	Low	
Price volatility	ⓘ	89.9	%
Price volatility risk	ⓘ	Very low	

The Elements resource aspects

Resource-related properties in Elements data records

- Eco properties (Climate Change, Embodied energy, Water usage)
- Geo-economic data
- Critical materials info
- Principal uses and substitutes for relevant elements (e.g., Chromium)



Principal uses and substitutes

Principal uses and substitutes

25% used in buildings and infrastructure, e.g. for elevators, street furniture and steel reinforced concrete.
Alternative: manganese. Quality: adequate.

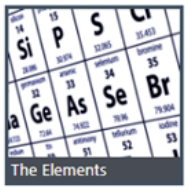
25% used in industrial machinery with chemical and petrochemical applications as well as in power generation, food processing, heat exchangers and tanks.
Alternative: none.

15% used in transportation, for cars, ships, trains, aircraft components and bicycles.
Alternative: aluminum. Quality: adequate.

5% used in household appliances and electronics, e.g. dishwashers, washing machines and consumer electronics.
Alternative: aluminum. Quality: adequate.

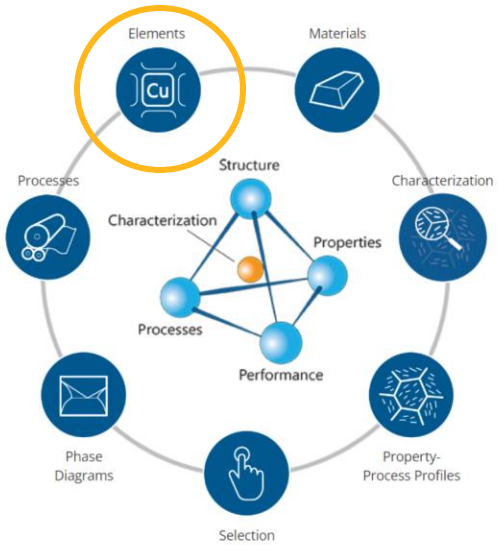
30% other uses, including metal goods such as cutlery and fasteners and also in refractory and chemical applications.
Alternative: N/A

Elements data table of the different databases



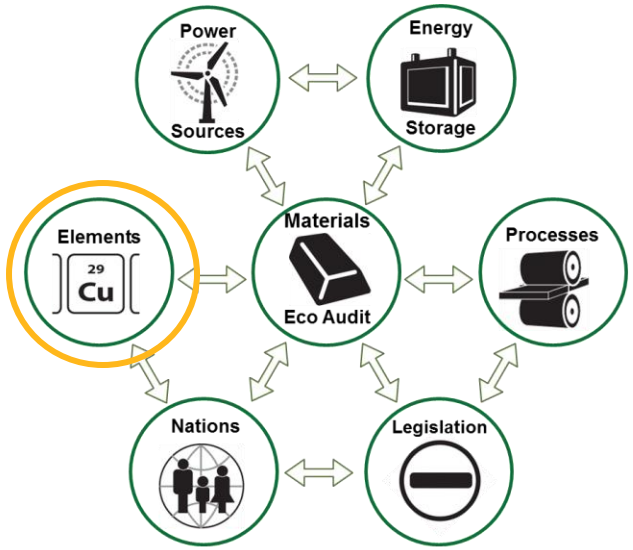
- Same content as Elements database
- Linked to materials records via composition

Materials Science and Engineering



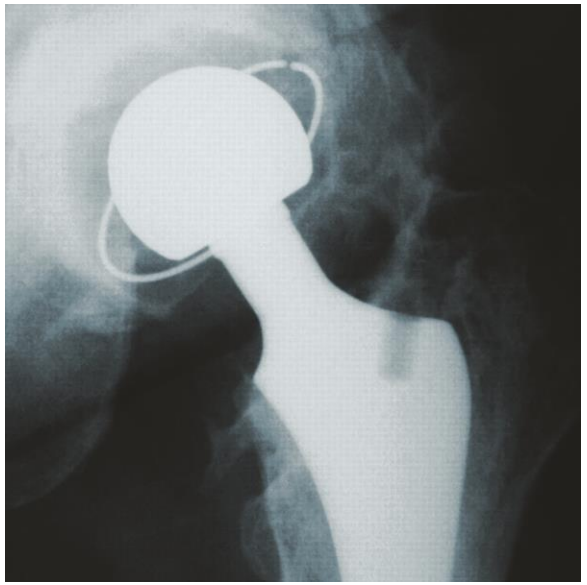
- Linked to Property-Process profiles
- Linked to ProcessUniverse

Sustainability



- Linked geographically via mining areas to Nations of the world data table
- Traceable eco-data

Level 2 Bioengineering



- Linked to MaterialUniverse, including biomedical materials.

Summary

- **Contains properties of the elements of the Periodic Table**
- **You can explore:**
  - **variation in properties with atomic number**
  - **correlations between properties**
  - **nuclear properties**
- **Also covers resource-related properties of the elements**
- **Direct link to Elements data table in the Material Science and Engineering, Sustainability, and Level 2 Bioengineering databases.**

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