



The Elements database: Properties, relationships and resources

Mike Ashby

Department of Engineering,
University of Cambridge

Legend:

- Nonmetals (Red)
- Alkali metals (Yellow)
- Alkaline Earth metals (Orange)
- Transition elements (Purple)
- Other metals (Light Orange)
- Metalloids (Brown)
- Halogens (Light Green)
- Noble gases (Light Blue)
- Lanthanides (Yellow-Green)
- Actinides (Blue)

1																	2			
1	H																	He		
2	3	4													5	6	7	8	9	10
	Li	Be													B	C	N	O	F	Ne
3	11	12													13	14	15	16	17	18
	Na	Mg													Al	Si	P	S	Cl	Ar
4	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36		
	K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr		
5	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54		
	Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe		
6	55	56	57	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86		
	Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn		
7	87	88	89	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118		
	Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og		
8			58	59	60	61	62	63	64	65	66	67	68	69	70	71				
			Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu				
9			90	91	92	93	94	95	96	97	98	99	100	101	102	103				
			Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr				

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, <i>e.g.</i> bond type

Resources

- White Papers: [Paper: the Elements Database](#) and [Paper: Materials for Nuclear Power Systems](#)

Lecture Outline

The periodic table is color-coded by groups. The legend is as follows:

- Nonmetals (Red)
- Alkali metals (Yellow)
- Alkaline Earth metals (Orange)
- Transition elements (Purple)
- Other metals (Light Orange)
- Metalloids (Light Green)
- Halogens (Teal)
- Noble gases (Light Blue)
- Lanthanides (Yellow-Green)
- Actinides (Blue)

1	2																	3	4	5	6	7	8	9	10		
H																	B	C	N	O	F	Ne					
3	4																	13	14	15	16	17	18				
Li	Be																	Al	Si	P	S	Cl	Ar				
11	12																	31	32	33	34	35	36				
Na	Mg	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr										
19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36										
K	Ca	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe										
37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54										
Rb	Sr	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn										
55	56	57	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86										
Cs	Ba	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Nh	Fl	Mc	Lv	Ts	Og										
87	88	89	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118										
Fr	Ra																	119	120	121	122	123	124	125	126	127	128
		8	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu											
		9	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	No	Lr											

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

Interactive periodic table interface

File Edit View Select Tools Window Help

Home Browse Search Chart/Select Solver Eco Audit Synthesizer Learn Tools Settings Help

Home x

THE ELEMENTS

change database

1 H

2 He

3 Li 4 Be

5 B 6 C 7 N 8 O 9 F 10 Ne

11 Na 12 Mg

13 Al 14 Si 15 P 16 S 17 Cl 18 Ar

19 K 20 Ca 21 Sc 22 Ti 23 V 24 Cr 25 Mn 26 Fe 27 Co 28 Ni 29 Cu 30 Zn 31 Ga 32 Ge 33 As 34 Se 35 Br 36 Kr

37 Rb 38 Sr 39 Y 40 Zr 41 Nb 42 Mo 43 Tc 44 Ru 45 Rh 46 Pd 47 Ag 48 Cd 49 In 50 Sn 51 Sb 52 Te 53 I 54 Xe

55 Cs 56 Ba 57 La 58 Ce 59 Pr 60 Nd 61 Pm 62 Sm 63 Eu 64 Gd 65 Tb 66 Dy 67 Ho 68 Er 69 Tm 70 Yb 71 Lu

76 Os Osmium

78 Pt 79 Au 80 Hg 81 Tl 82 Pb 83 Bi 84 Po 85 At 86 Rn

87 Fr 88 Ra 89 Ac 90 Th 91 Pa 92 U 93 Np 94 Pu 95 Am 96 Cm 97 Bk 98 Cf 99 Es 100 Fm 101 Md 102 No 103 Lr

104 Rf 105 Db 106 Sg 107 Bh 108 Hs 109 Mt 110 Ds 111 Rg 112 Cn 113 Nh 114 Fl 115 Mc 116 Lv 117 Ts 118 Og

8 Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb Lu

9 Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No Lr

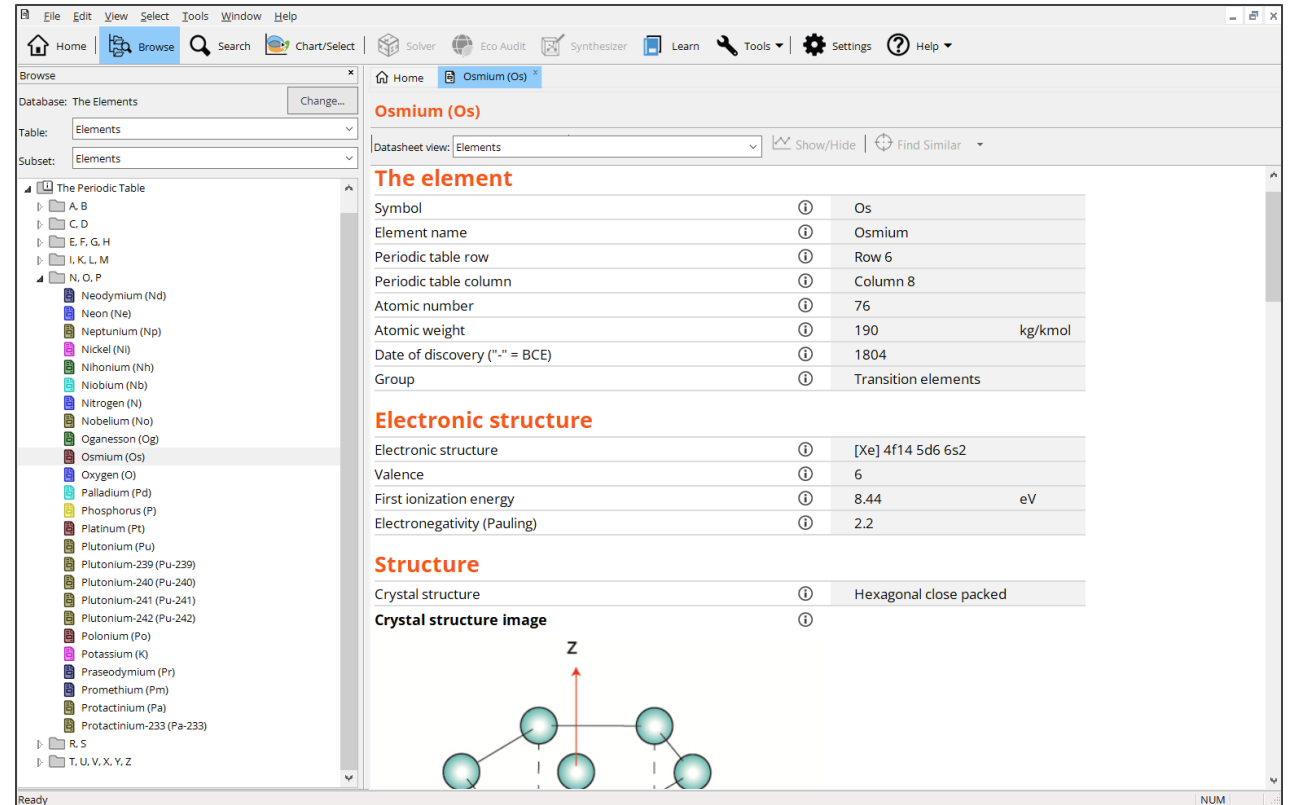
Ready NUM

Clickable for data record

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



The screenshot displays the Ansys Granta EduPack interface for the Elements database. The left sidebar shows a tree view of the periodic table, with Osmium (Os) selected. The main window displays the following information for Osmium (Os):

Osmium (Os)

Dataset view: Elements

The element

Symbol	Os
Element name	Osmium
Periodic table row	Row 6
Periodic table column	Column 8
Atomic number	76
Atomic weight	190 kg/kmol
Date of discovery ("-" = BCE)	1804
Group	Transition elements

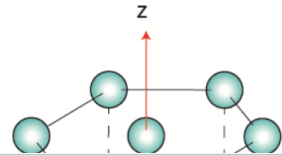
Electronic structure

Electronic structure	[Xe] 4f14 5d6 6s2
Valence	6
First ionization energy	8.44 eV
Electronegativity (Pauling)	2.2

Structure

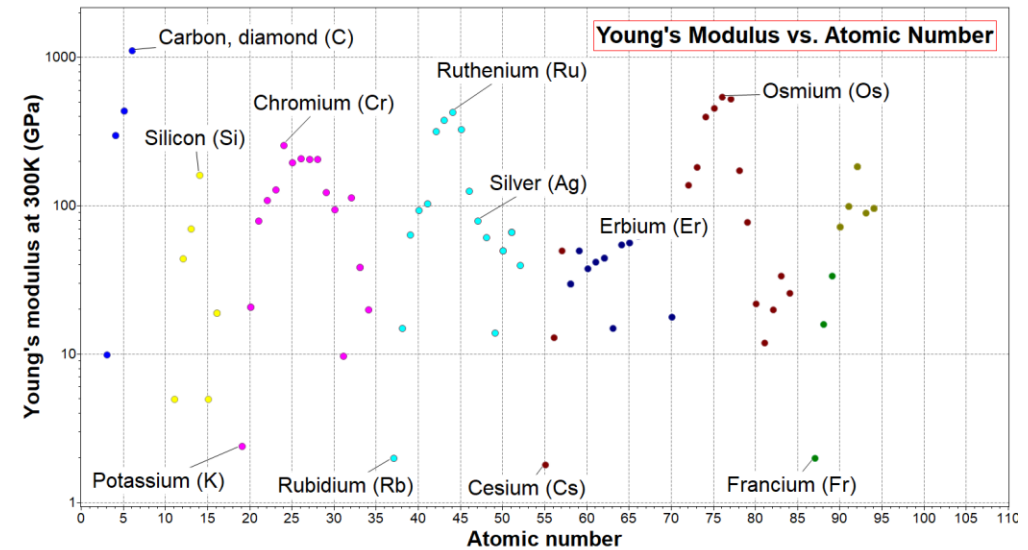
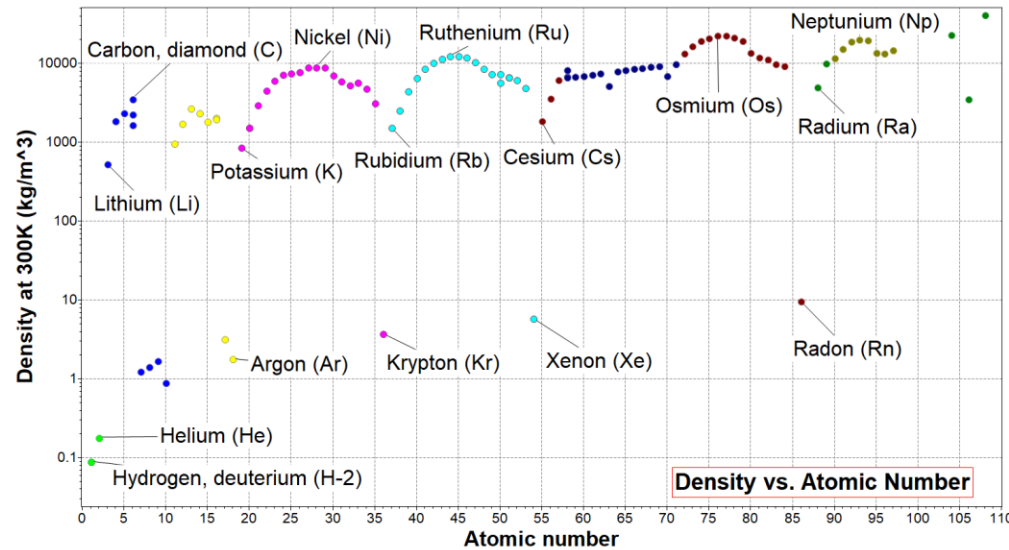
Crystal structure	Hexagonal close packed
-------------------	------------------------

Crystal structure image



Using the Elements database

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



Electronic structure data

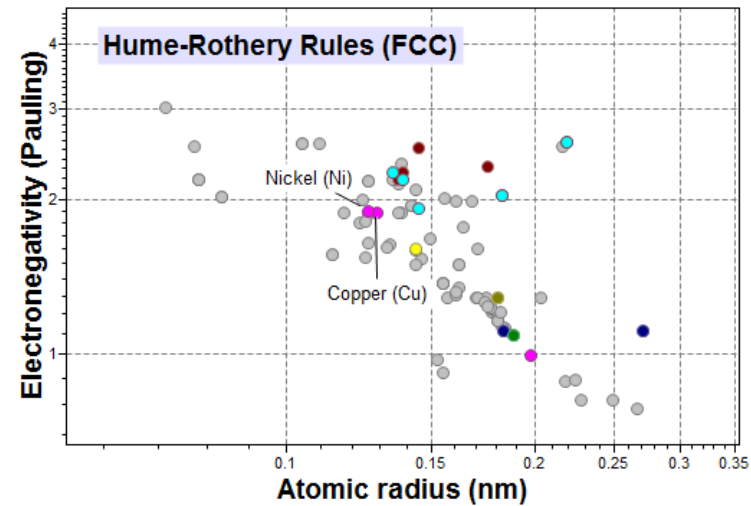
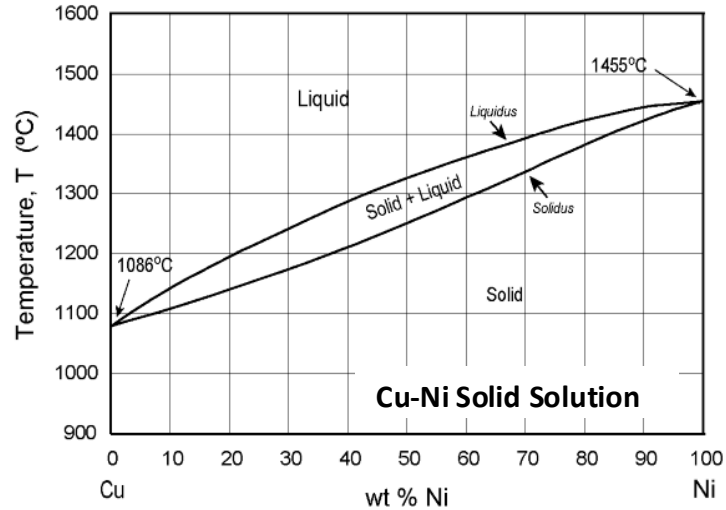
Electronic structure

Electronic structure	(i)	[Ar] 3d ¹⁰ 4s ¹
Valence	(i)	2
First ionization energy	(i)	7.73 eV
Second ionization energy	(i)	20.3 eV
Electronegativity (Pauling)	(i)	1.9

In Elements
database

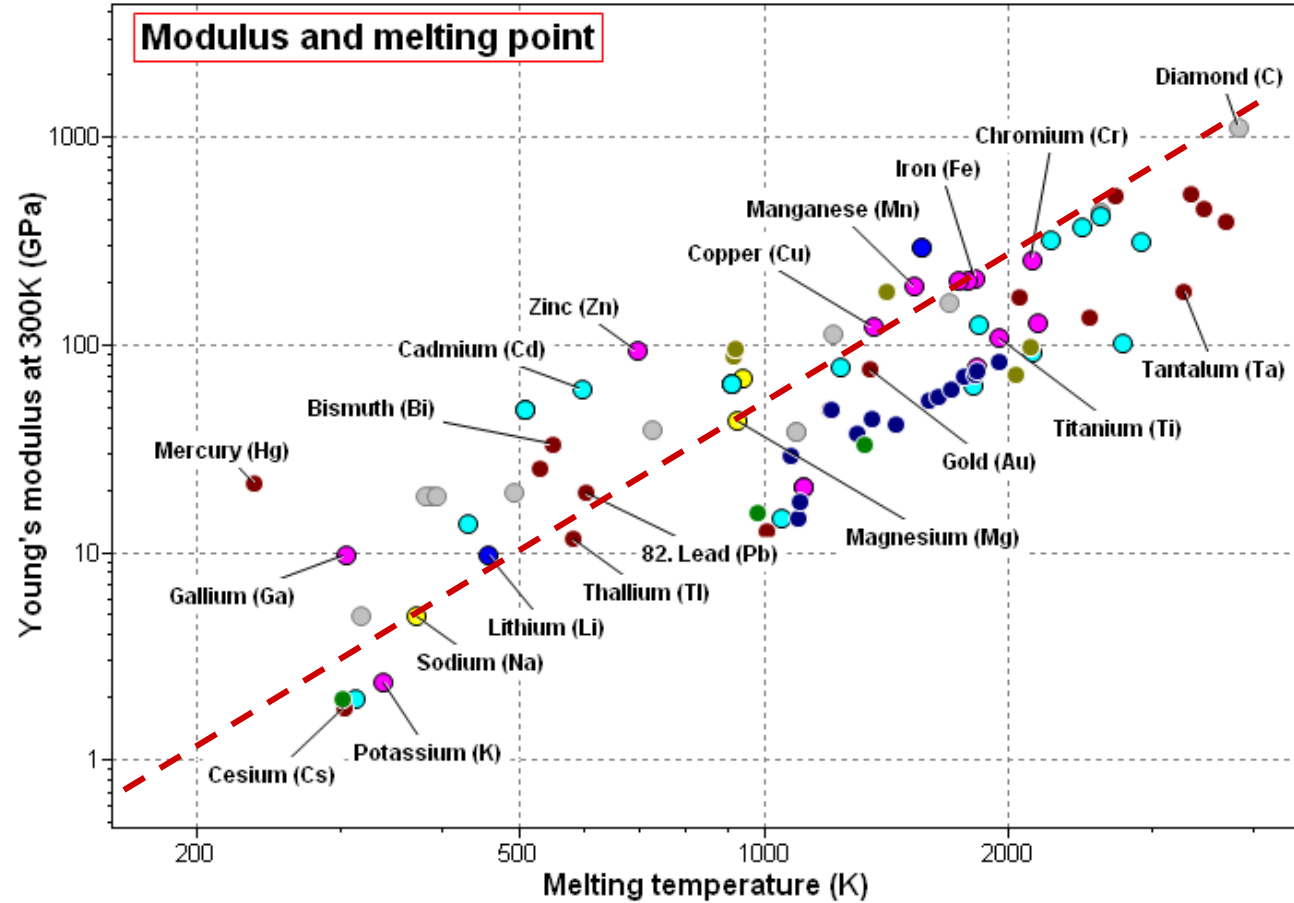
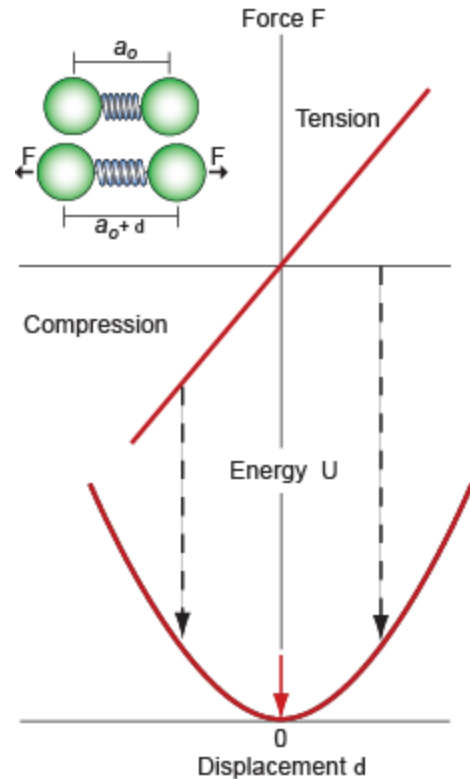
Hume-Rothery: extensive substitutional solid solution when

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



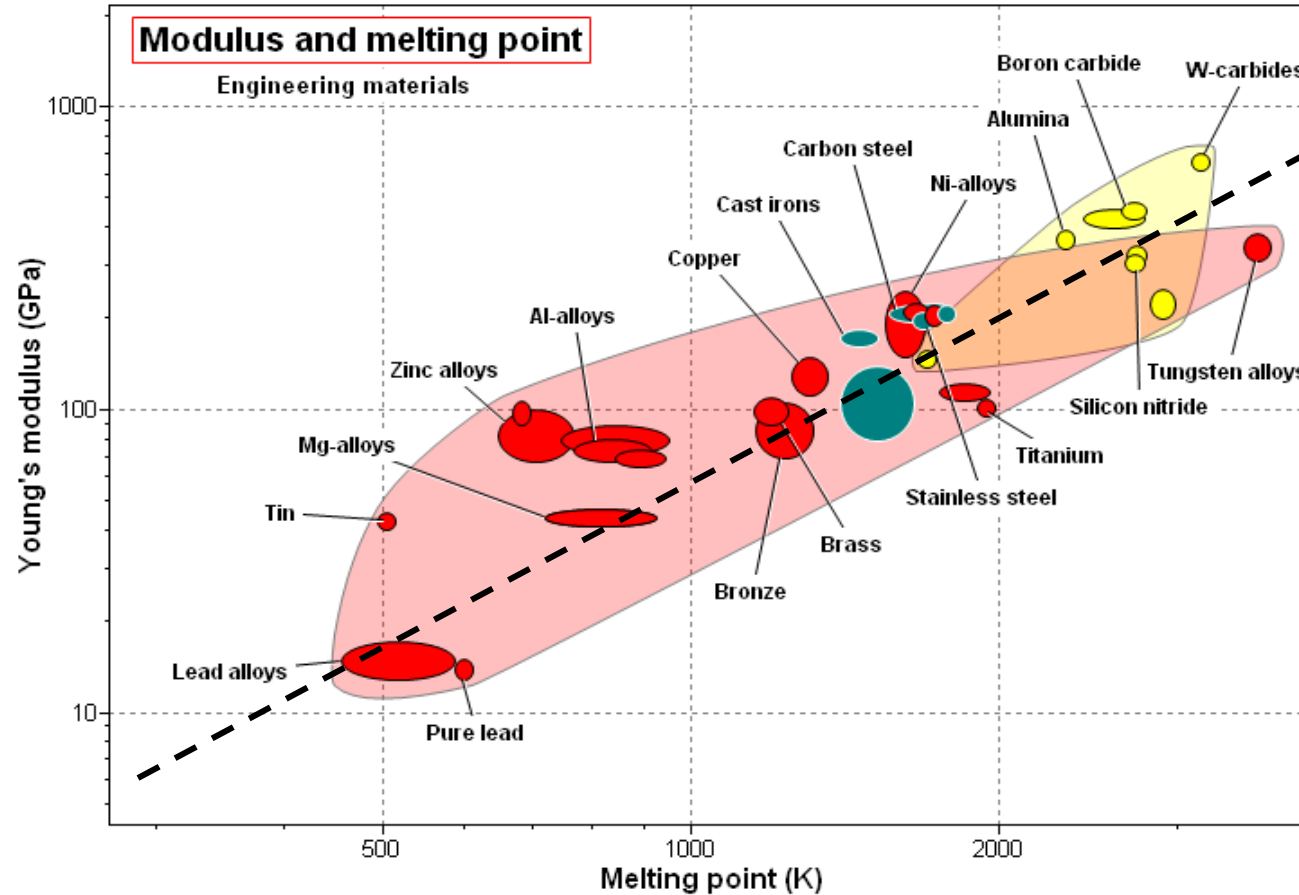
Relationships between properties (1)

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



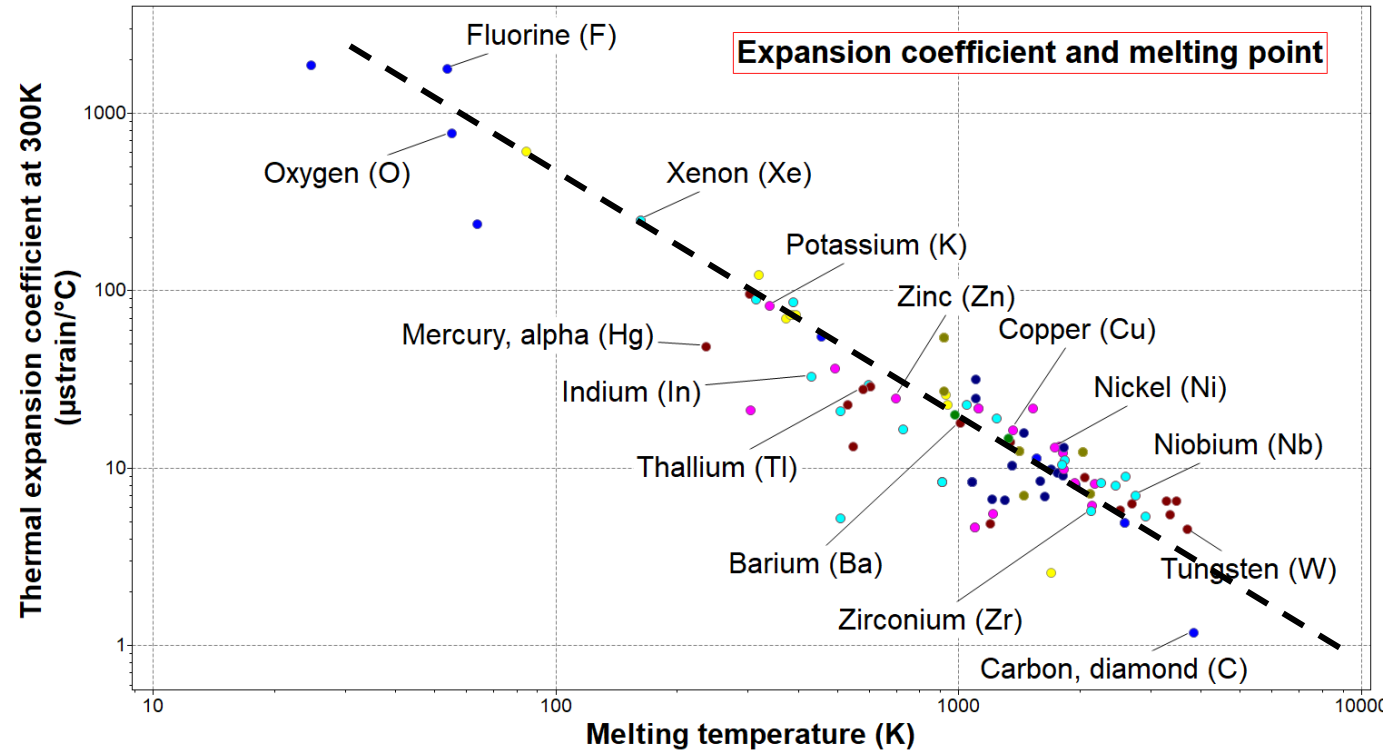
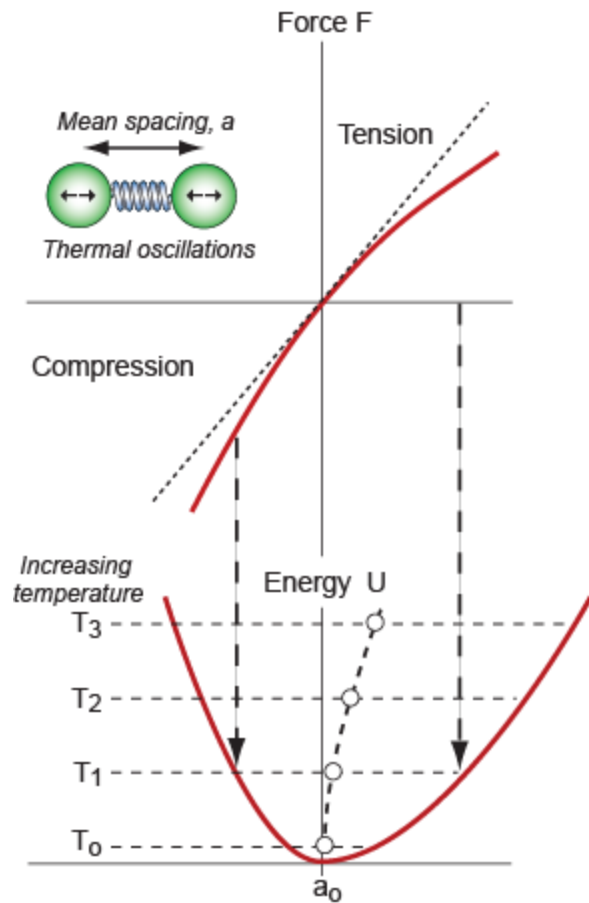
Engineering materials – a similar trend

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



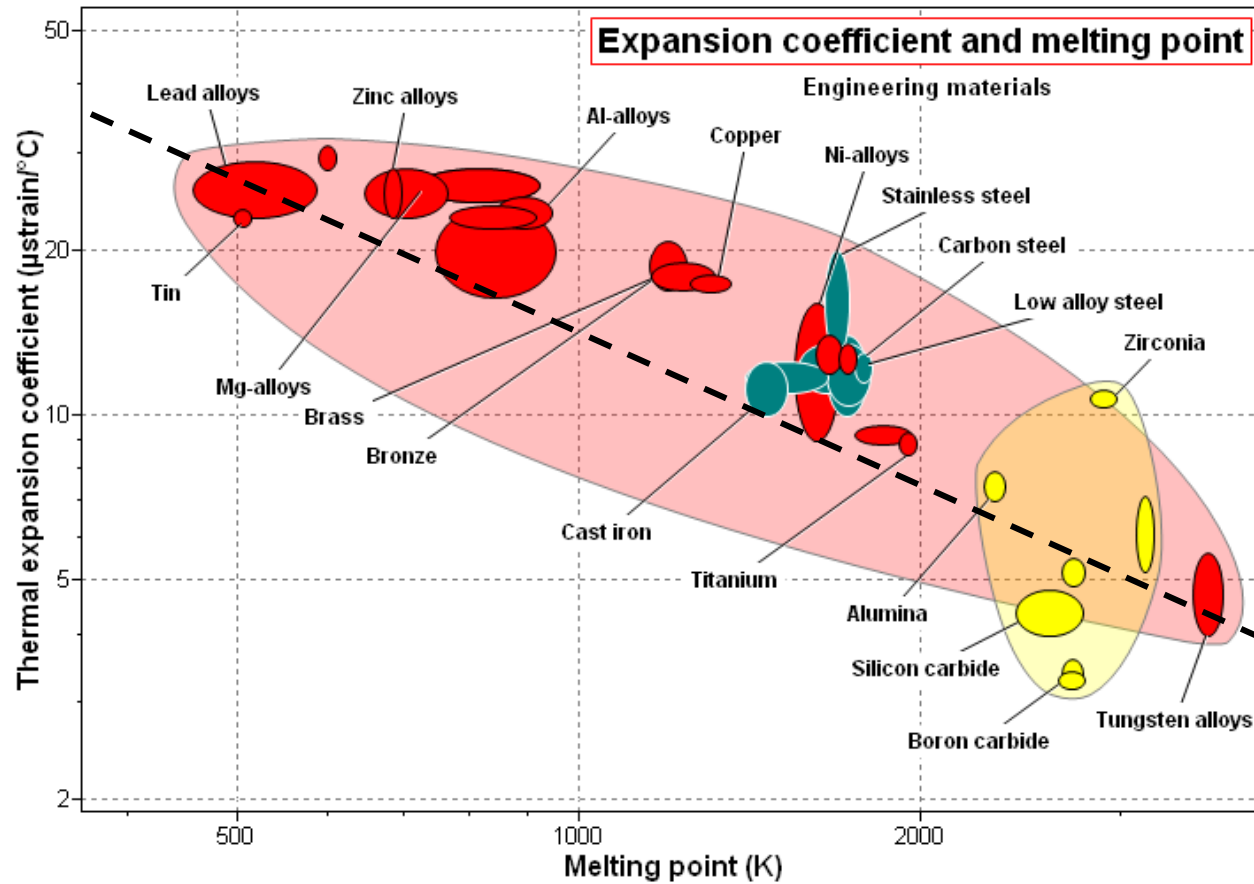
Relationships between properties (2)

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



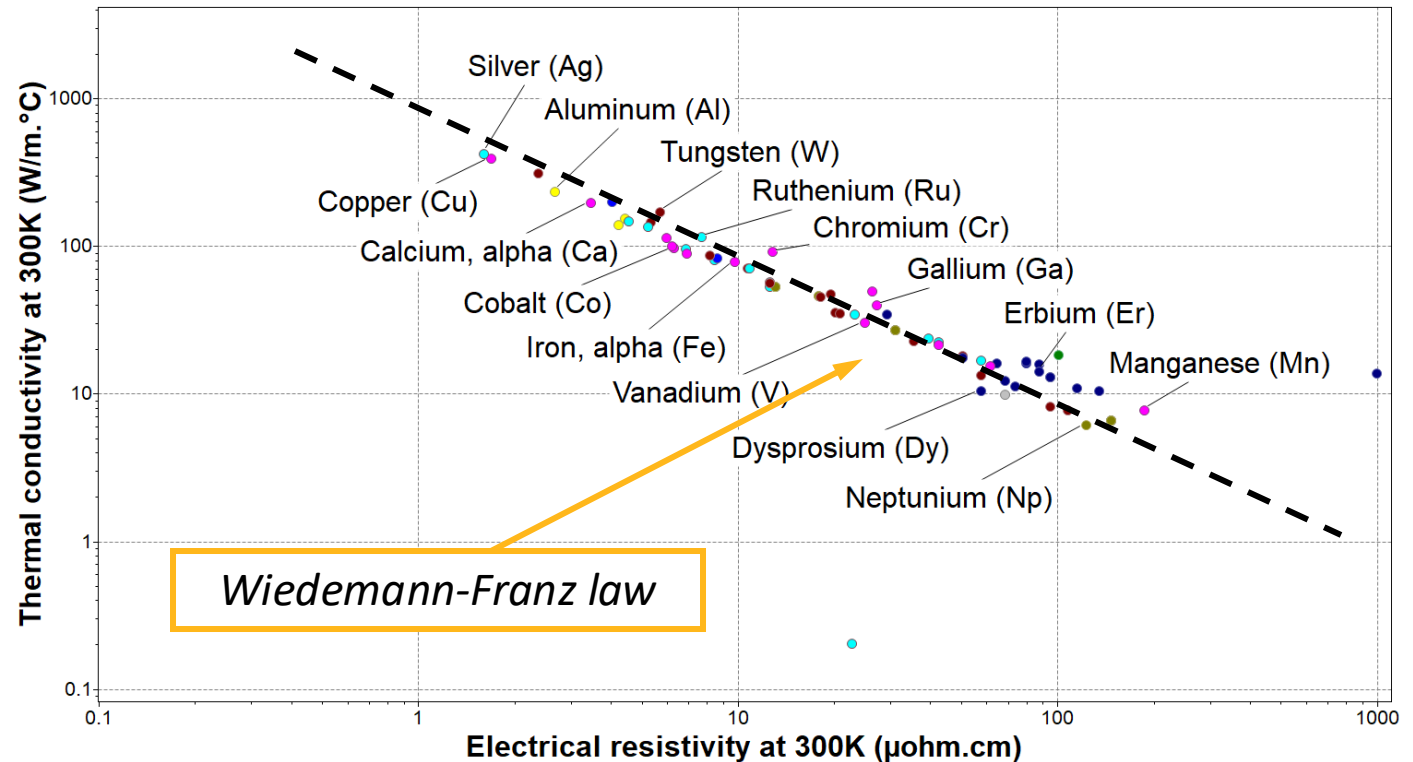
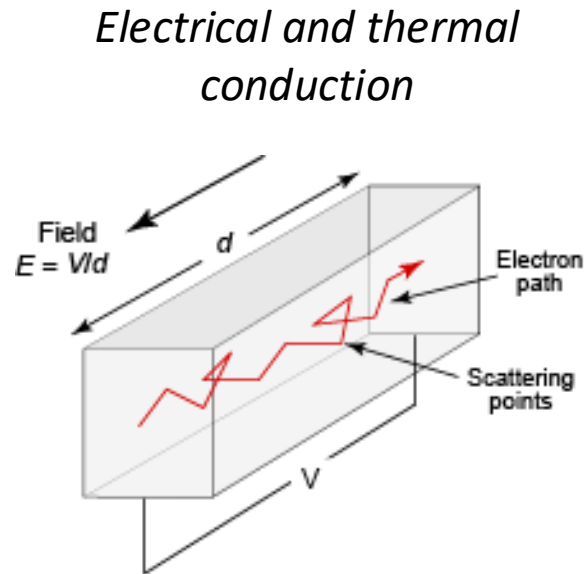
Engineering materials – a similar trend

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



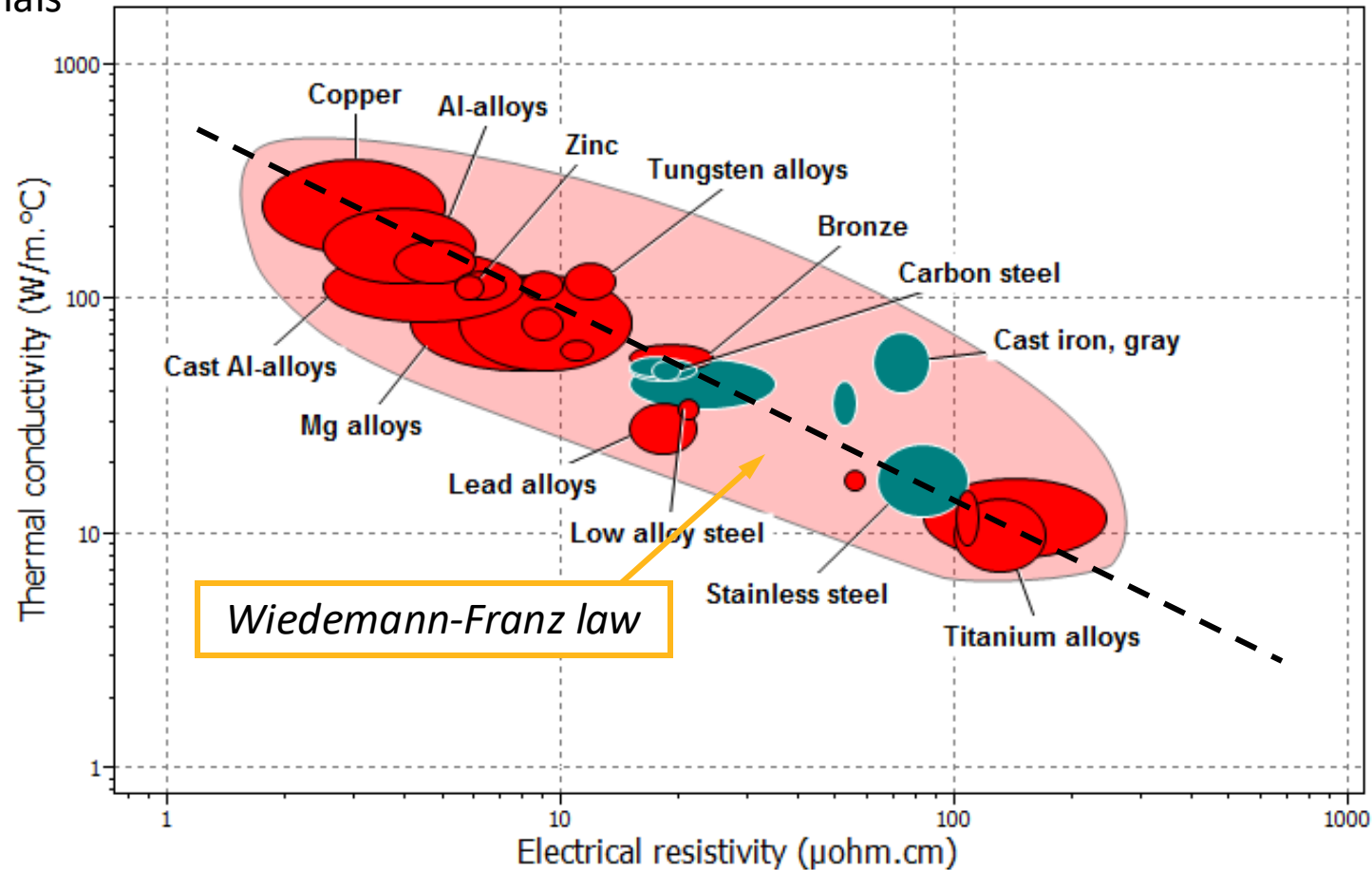
Relationships between properties (3)

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



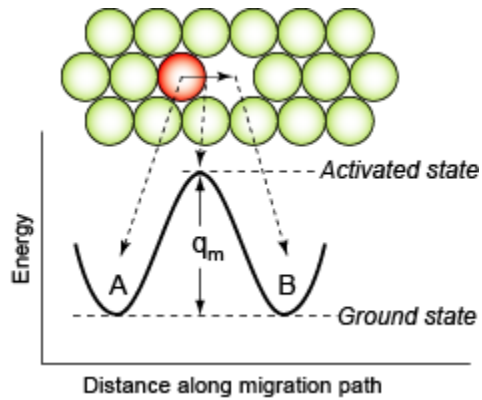
Engineering materials – a similar trend

- 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

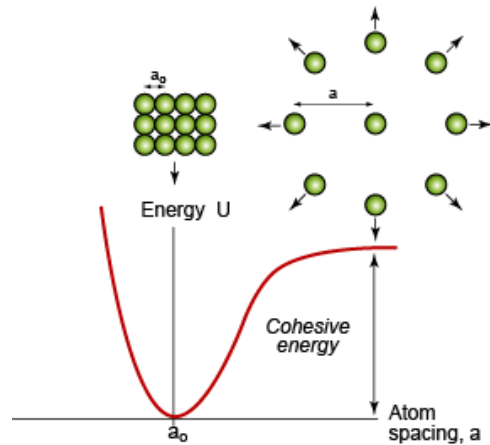


Relationships between properties (4)

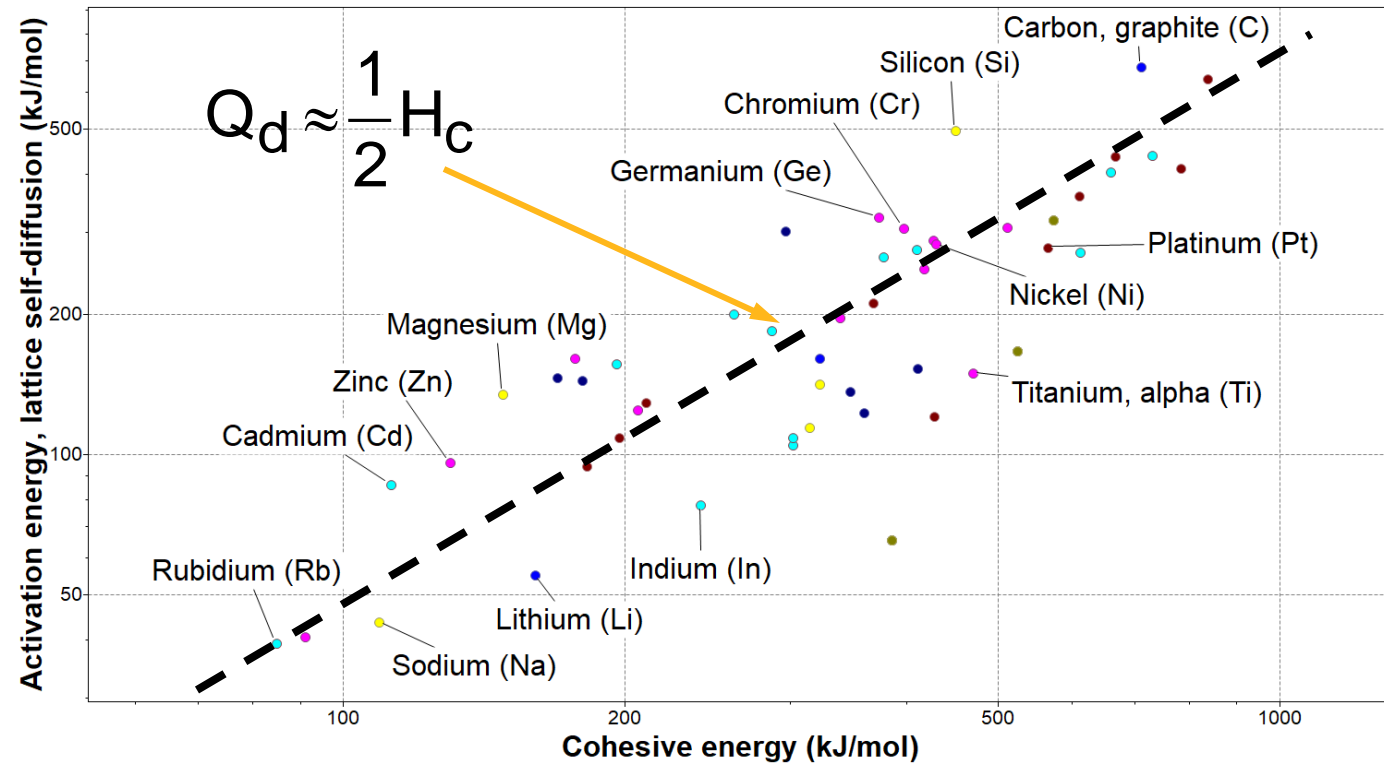
Activation energy for diffusion



Cohesive energy

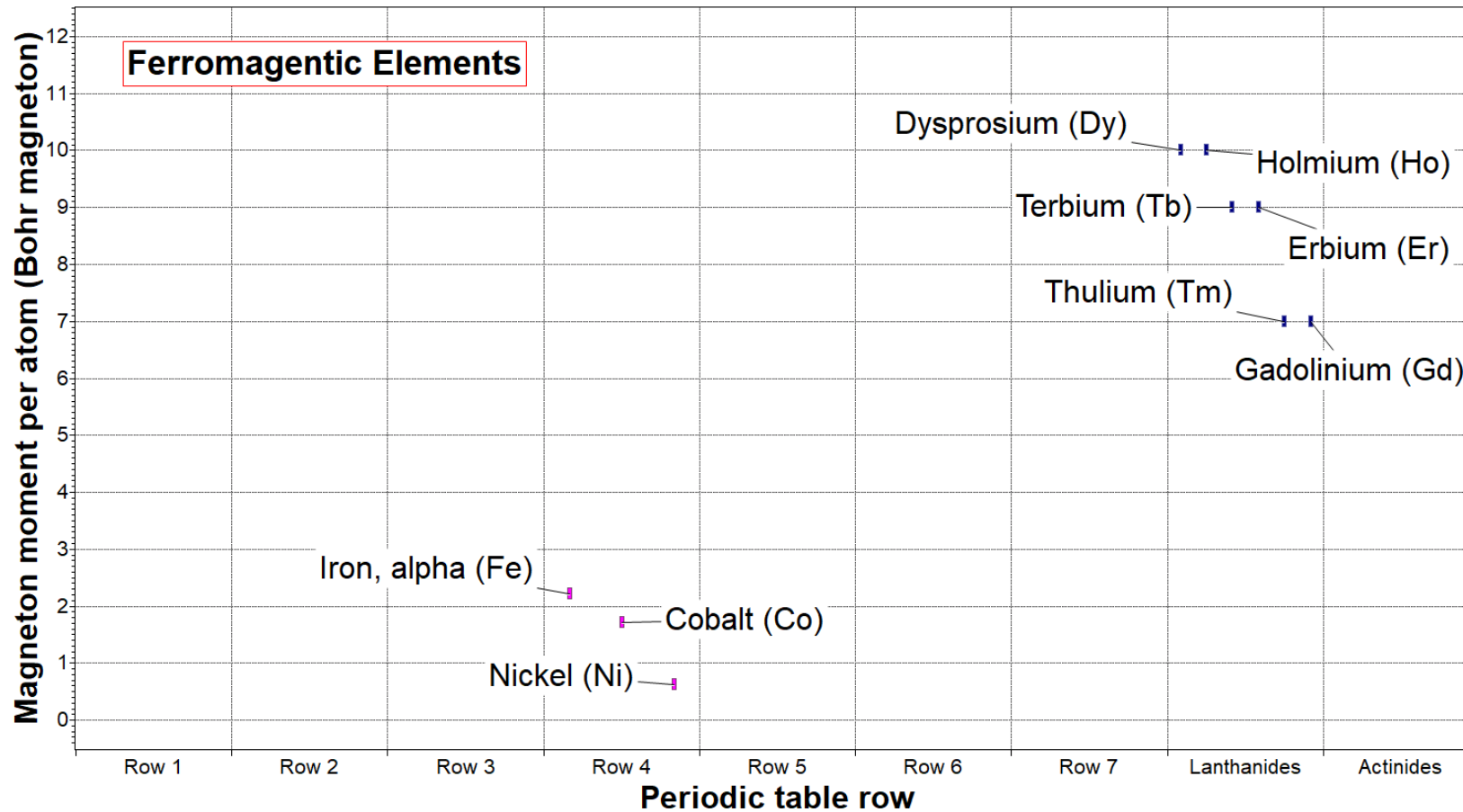


- Activation energy for diffusion and cohesive energy



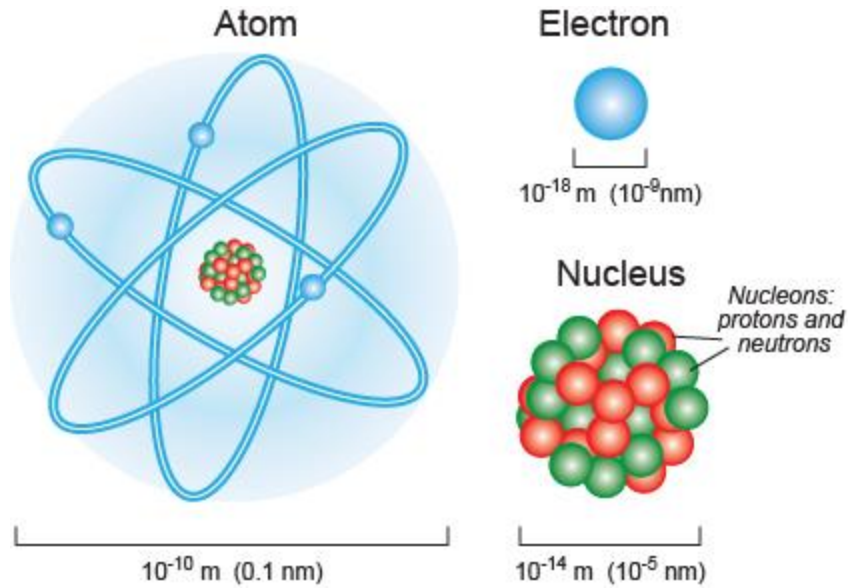
Magnetic properties

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



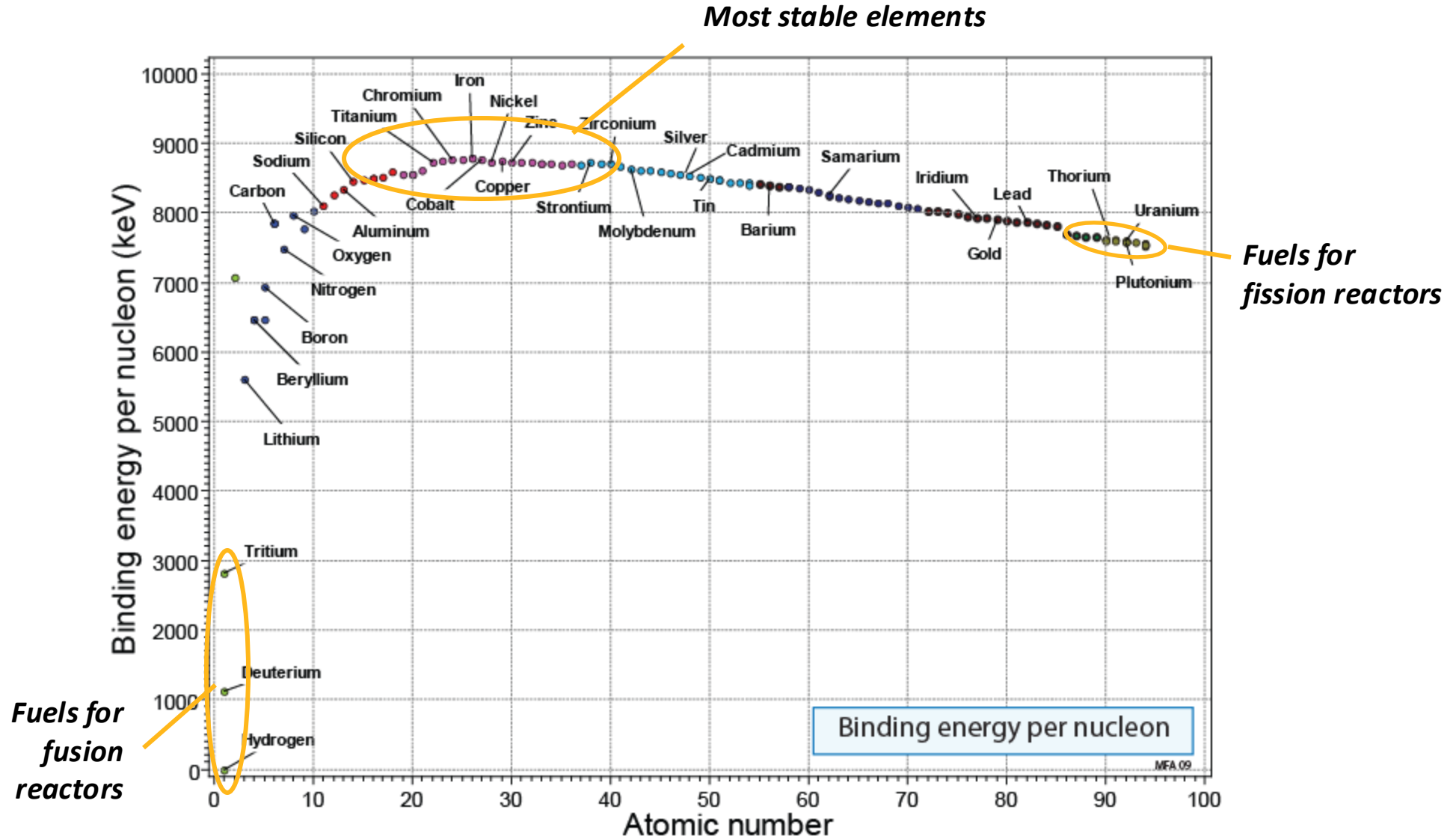
Nuclear properties of the elements

- Nuclear properties of the elements added to the Elements database



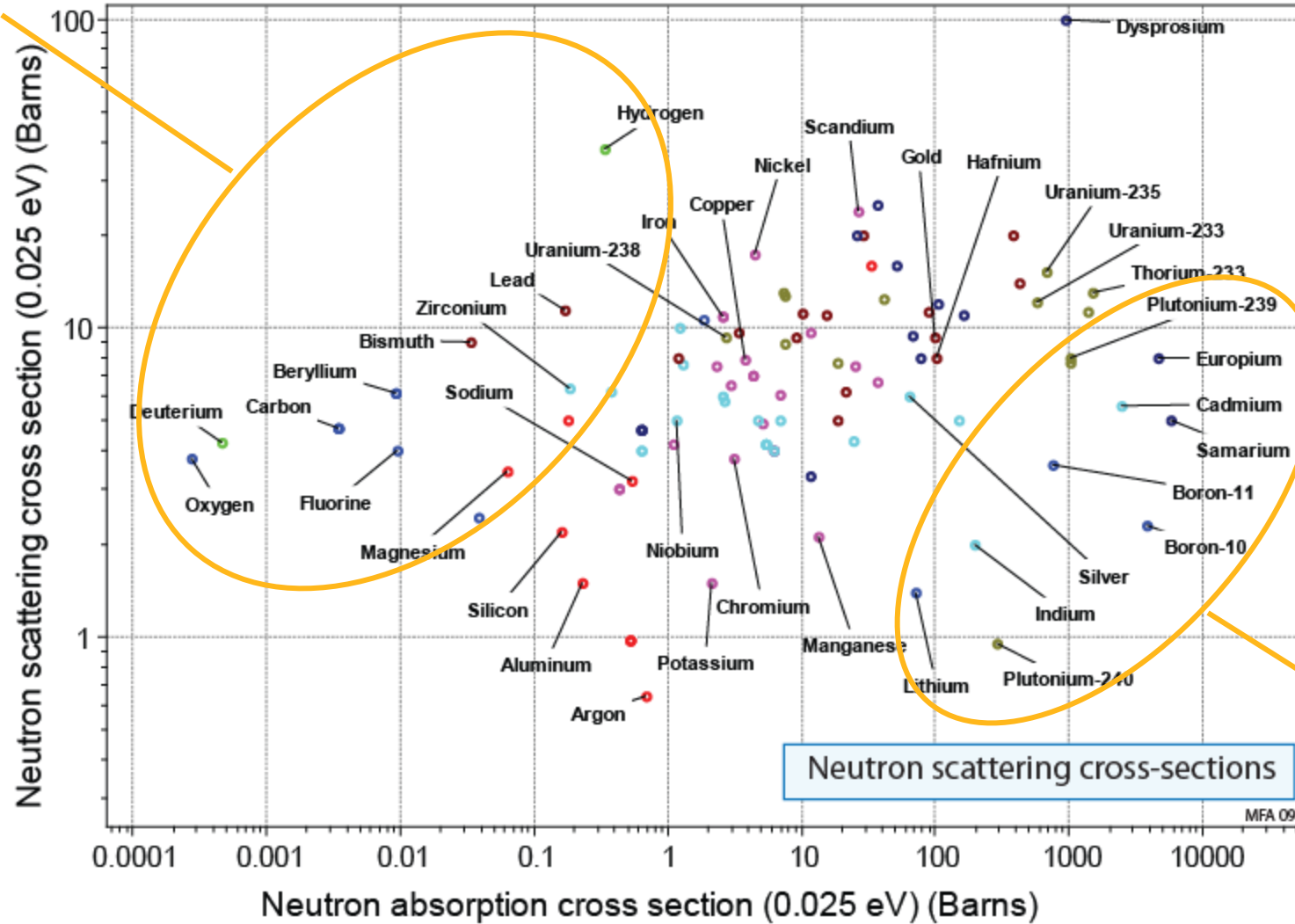
- Binding energy per nucleon
Relevant for fuels for fission and fusion
- Neutron absorption and scattering X-sections
Relevant moderator, reflector and control rod materials
- Half-lives of selected isotopes
Relevant for spent fuel and system decommissioning

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.

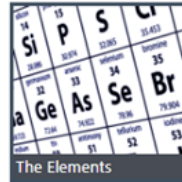
25% used in industrial machinery with chemical and petrochemical applications as well as in power generation, food processing, heat exchangers and tanks.
Alternative: none.

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.

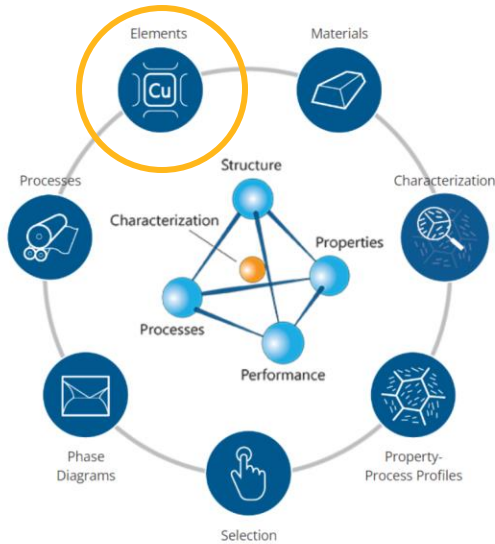
30% other uses, including metal goods such as cutlery and fasteners and also in refractory and chemical applications.
Alternative: N/A

Elements data table of the different databases



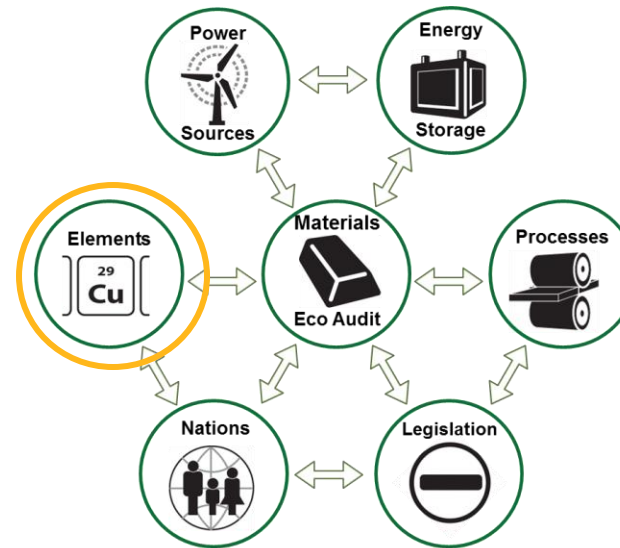
- Same content as Elements database
- Linked to materials records via composition

Materials Science and Engineering



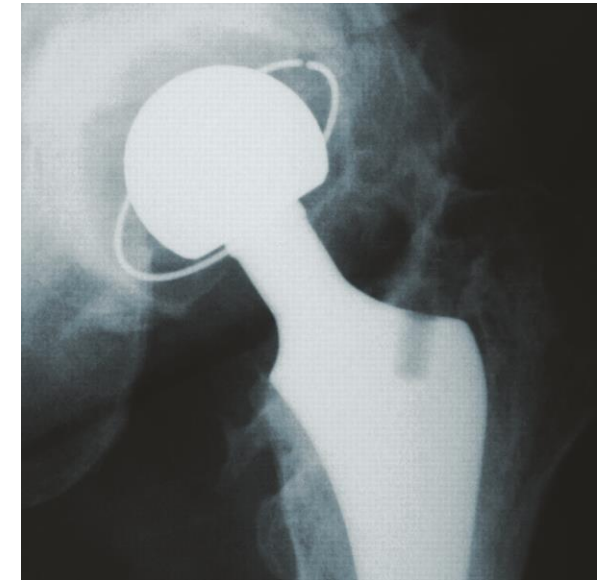
- Linked to Property-Process profiles
- Linked to ProcessUniverse

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.**

Ansys Education Resources Feedback Survey

Here at Ansys, we rely on your feedback to ensure the educational content we create is up-to-date and fits your teaching needs.

Please click the link below to fill out a short survey (~7 minutes) to help us continue to support academics around the world utilizing Ansys tools in the classroom.

[Feedback Survey Link](#)

© 2025 ANSYS, Inc. All rights reserved.

© 2018 Mike Ashby

Use and Reproduction

The content used in this resource may only be used or reproduced for teaching purposes; and any commercial use is strictly prohibited.

Document Information

This lecture unit is part of a set of teaching resources to help introduce students to materials, processes and rational selections.

Ansys Education Resources

To access more undergraduate education resources, including lecture presentations with notes, exercises with worked solutions, microprojects, real life examples and more, visit www.ansys.com/education-resources.