The Elements Database: A White Paper

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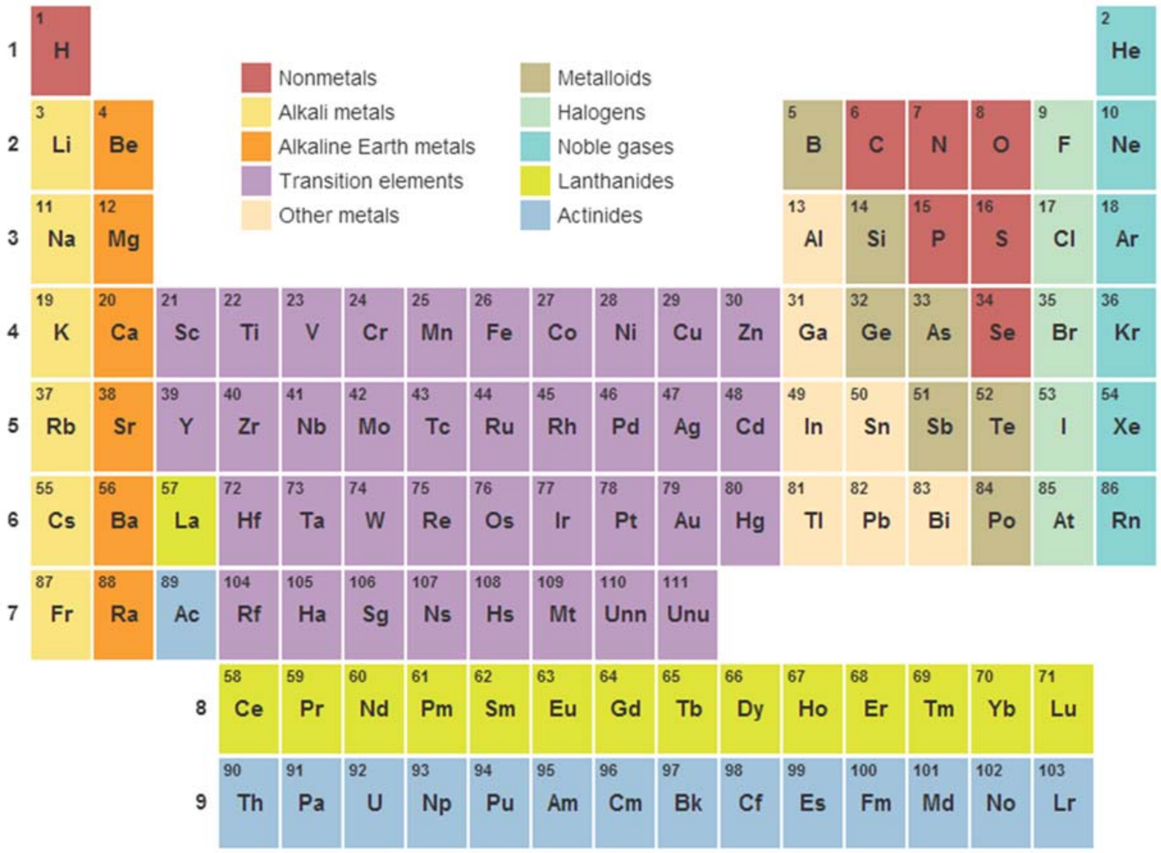

1	1 H																	2 He
2	3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
3	11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
4	19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
5	37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
6	55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
7	87 Fr	88 Ra	89 Ac	104 Rf	105 Ha	106 Sg	107 Ns	108 Hs	109 Mt	110 Unn	111 Unu							
8				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	
9				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	

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1. Introduction

The periodic table of elements is fundamental to the understanding of material properties. It consists of the basic building blocks of all materials, the atoms, organized in an ingenious way. Knowledge of the elements and how they relate to each other is relevant at most levels of education, from pupils at school to advanced students of Chemistry, Physics, Materials Science, or Engineering. In this paper, a number of examples of how CES EduPack and, in particular, the Elements database can support materials-related teaching are described.

The elements of the Periodic Table are arranged into rows in a periodic manner, according to electron shell occupancy, and ordered by increasing number of protons, *i.e.*, atomic number. They are also ordered in columns referred to as groups, each reflecting chemical properties that depend on the electron configuration of the atom. This revealing organization was first proposed in 1869 by Dimitri Mendeleev, who is usually credited as the originator of the modern Periodic Table [1].

Interestingly, not all the elements had been discovered or isolated at that time, which left several gaps in the Table. As it happens, this is one of the many features that can be investigated using the Elements database of CES EduPack, since it contains information on *Date of Discovery* for each element. Moreover, many material properties can be rationalized from the basic atomic characteristics in the database. The Elements database could thus be useful as background or starting point for materials-related courses.

Most elements, except notably the Noble gases, form chemical bonds with each other and cluster into molecules or aggregates of atoms. Minerals formed of a single chemical element can in some cases (such as carbon, sulfur, copper, or gold) be found in nature. They are then called native elements. The vast majority of elements in the Periodic Table, both native and man-made, are metals that form crystals. Structural data from the Elements database, such as crystal structure, lattice parameters, and atomic radii/volume can be used to facilitate students learning crystallographic concepts. In this context, one of the many Teaching Resources associated with CES EduPack deserves to be mentioned. It is the *Teach Yourself Crystallography* guide [2], which allows students to explore crystal structures at greater depth.

Although nearly all common materials are compounds, or mixtures of atoms, knowledge of the fundamental atomic characteristics of these elements—the atomic number and mass, the crystal structure, the cohesive energy, chemical bond stiffness, the nuclear stability *etc*.—influence the properties that are essential for understanding and selecting materials in real applications.

The material properties of pure elements also remain important as an educational tool. In subsequent sections of this paper, we demonstrate how many thermal and mechanical properties of metals can be understood more easily using the visual support of property charts. The wide range of values represented by the elements within each property allow trends and relationships to be displayed clearly to students. The Elements database of CES EduPack is aimed primarily at 1st and 2nd year university courses, introducing the elements alongside materials of Engineering, Materials Science, or Design. It may, however, be used both at higher and lower levels of education.

2. The Elements database

The Elements database described in this paper is available with most CES EduPack Editions [3] and includes comprehensive cover of the elements of the Periodic table. A total of 142 records are available from 111 different elements, including some common isotopes and allotropes. The records are ordered by atomic number and are divided into folders corresponding to the rows of the Periodic Table. Each record contains data for the crystal structure, physical, mechanical, thermal, diffusion, surface energy, electrical, magnetic, nuclear properties, and cost. The properties contained in the database are listed in Table 1.

Each attribute is linked to a *Science note* that provides a definition and other useful information, see Figure 1. Thus, the database provides not only data that can be plotted, compared, combined, and displayed as property charts [4-5], but also the underlying background to the property and its relationship to other properties, as illustrated below. Further links to relevant *references* are also provided in the record.

Table 1. Attributes of the Elements database in CES EduPack

Properties of the Elements

The element
Symbol
Periodic table row
Periodic table column
Atomic number
Atomic weight
Date of discovery

Structure
Crystal structure
Space group
Lattice parameter, a
Atomic radius
Atomic volume
Molar volume
State at 300K (Metal / Non-metal)
Phase at 300K (Solid / Liquid / Gas)

Physical properties
Density at 300K

Relative cost
Approx. relative cost, pure element (Fe=1)

Mechanical properties
Young's modulus at 300K
Shear modulus at 300K
Bulk modulus at 300K
Poisson's ratio
T- dependence of modulus

Thermal properties
Melting temperature
Boiling point
Heat of fusion
Heat of vaporization
Cohesive energy
Thermal expansion coefficient at 300K
Specific heat capacity
Debye temperature
Thermal conductivity at 300K

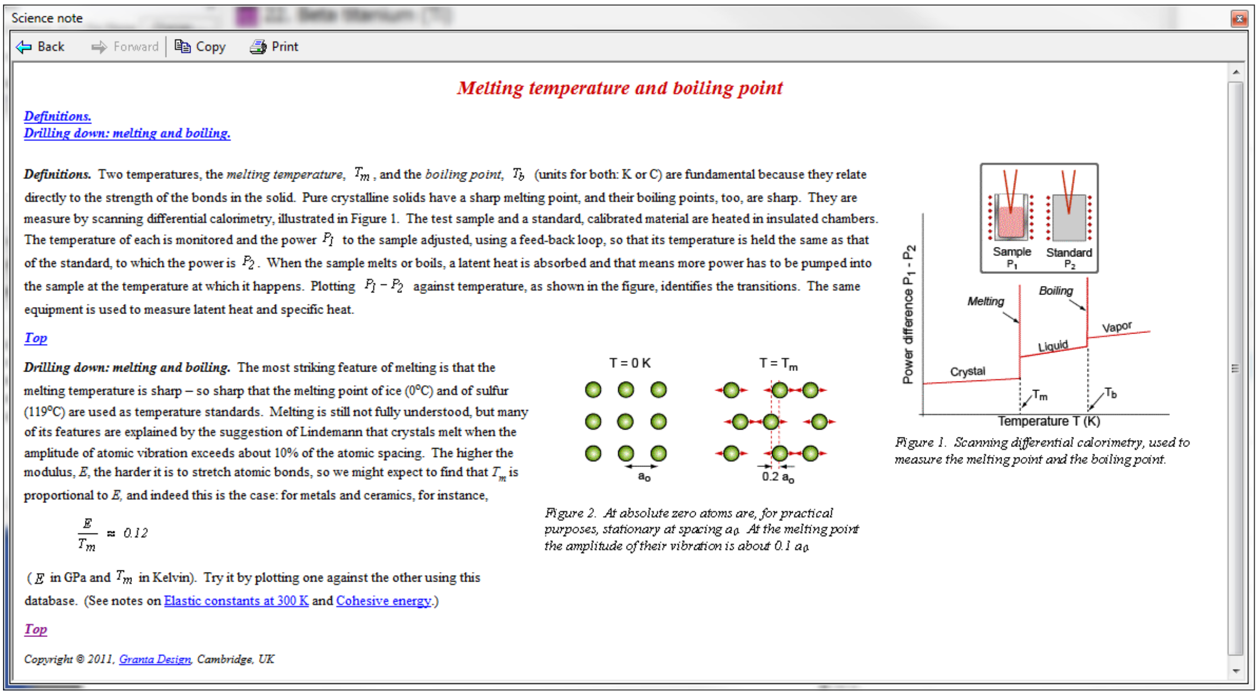
Diffusion data
Pre-exponential, lattice self-diffusion
Activation energy, lattice self-diffusion
Pre-exponential, g-boundary diffusion
Activation energy, g-boundary diffusion

Surface energies
Surface energy, solid
Surface energy, liquid

Electrical and superconducting properties
Electrical resistivity at 300K
T - dependence of resistivity
Free electron concentration
Electron mobility
Hall coefficient, RH
Work function
Superconducting transition temperature Tc
Critical superconduction magnetic field
Standard electrode potential

Magnetic properties
Magnetic classification
Magnetic susceptibility

Nuclear properties
Neutron absorption cross section (0.025 eV)
Neutron scattering cross section (0.025 eV)
Binding energy per nucleon



Melting temperature and boiling point

Definitions.
Drilling down: melting and boiling.

Definitions. Two temperatures, the *melting temperature*, T_m, and the *boiling point*, T_b (units for both: K or C) are fundamental because they relate directly to the strength of the bonds in the solid. Pure crystalline solids have a sharp melting point, and their boiling points, too, are sharp. They are measure by scanning differential calorimetry, illustrated in Figure 1. The test sample and a standard, calibrated material are heated in insulated chambers. The temperature of each is monitored and the power P_1 to the sample adjusted, using a feed-back loop, so that its temperature is held the same as that of the standard, to which the power is P_2. When the sample melts or boils, a latent heat is absorbed and that means more power has to be pumped into the sample at the temperature at which it happens. Plotting $P_1 - P_2$ against temperature, as shown in the figure, identifies the transitions. The same equipment is used to measure latent heat and specific heat.

Figure 1. Scanning differential calorimetry, used to measure the melting point and the boiling point.

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Drilling down: melting and boiling. The most striking feature of melting is that the melting temperature is sharp – so sharp that the melting point of ice (0°C) and of sulfur (119°C) are used as temperature standards. Melting is still not fully understood, but many of its features are explained by the suggestion of Lindemann that crystals melt when the amplitude of atomic vibration exceeds about 10% of the atomic spacing. The higher the modulus, E, the harder it is to stretch atomic bonds, so we might expect to find that T_m is proportional to E, and indeed this is the case: for metals and ceramics, for instance,

$$\frac{E}{T_m} \approx 0.12$$

(E in GPa and T_m in Kelvin). Try it by plotting one against the other using this database. (See notes on Elastic constants at 300 K and Cohesive energy.)

Figure 2. At absolute zero atoms are, for practical purposes, stationary at spacing a_0. At the melting point the amplitude of their vibration is about 0.1 a_0

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Figure 1. Example of additional information provided by a science note, regarding the material properties of a record

3. Chemical and physical properties

The material property graphs used by CES EduPack can be powerful visual tools. Starting even at high school level, they can be used to show fundamental features of the elements. The color coding and graphical family envelopes can be used to highlight properties associated with rows. As a simple but colorful example of how the Elements database of CES EduPack might be used, atomic weight can be plotted against the atomic number for the elements, as shown in Figure 1. It can be seen that the atomic weight rises almost linearly with increasing atomic number. Since the atomic number is defined as the number of protons of the element, and the atomic weight includes both protons and neutrons, we can conclude from the chart that the proportion of neutrons to protons in the elements remain relatively fixed throughout almost the entire periodic table.

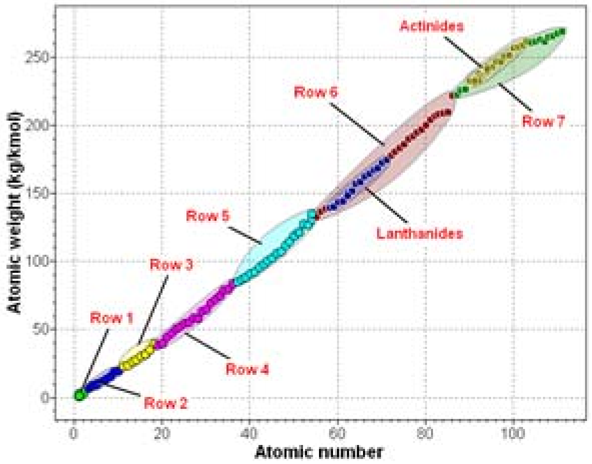

Figure 2. Atomic weight plotted against atomic number, color-coded by row and with family envelopes shown

Many basic properties of the elements can easily be displayed as they vary with atomic number. For instance, density generally increases the further down the rows of the periodic table you go. However, it does not increase linearly with the atomic number within each row, as can be seen in Figure 3. The density within one row is normally at its maximum somewhere in the middle of that row due to effects from the packing of the atoms. Again, the color coding facilitates the interpretation of the information contained in the chart.

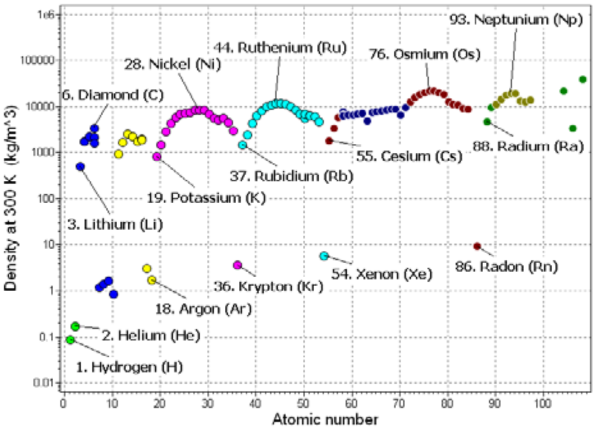

Figure 3. Density plotted against atomic number, showing a general increasing trend but with distinct mid-row peaks

For courses within Mechanical Engineering or Materials Science, for example, it can also be interesting to see that a similar pattern can be found in a charts of stiffness against atomic number (not shown here). The maximum stiffness found in a specific row occurs for elements around the middle of that row.

Charts created using the Elements database can also be used to highlight trends in the groups (columns) of the Periodic Table. One example where this is suitable is for showing the evolution of the work function for the alkali and alkali earth metals, the leftmost groups of the Table. These elements can be used for the purposes of doping or as contact materials for certain semiconductor devices. The work function of the metal reflects the energy of the valence electrons at the Fermi level of the metal (similar to the ionization potential often used for molecular materials), see Figure 4.

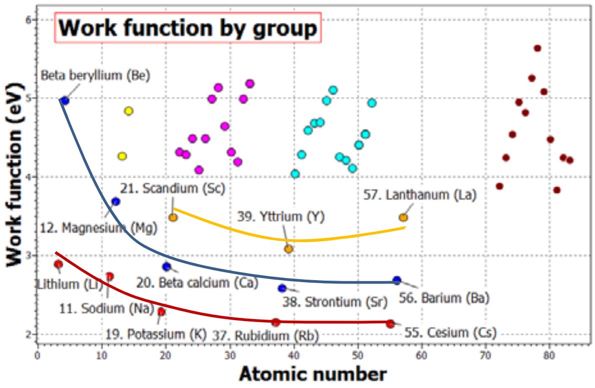

Figure 4. Work function plotted against atomic number, showing a property organized by group, as indicated

The alkali metal group clearly shows up in the lower part of the chart. CES EduPack enables you to color code data points according to specific needs. In this case, the leftmost group of the Periodic Table has been highlighted in red, the second group from the left, blue, and the third group yellow. In the context of organic semiconductors, the alkali metals (red) are known as electron donors, forming charge transfer complexes with such molecular materials. Alkali earth metals (blue), such as calcium and magnesium, have been used for electron-injecting contacts. The work function of the element in relation to the energies of the bandgap and the defect electronic states are essential to determine their performance.

4. Thermal and mechanical properties

For students of Materials Science and Mechanical Engineering, in particular, thermal and mechanical properties are of key interest. In this area, many interesting properties arise from the diatomic potential energy curve. Starting with the energy aspects of this curve, shown in Figure 5, the cohesive energy is defined as the energy gained per mol (a mol is 6.022 x 10^{23} atoms) if completely separated atoms are brought together to equilibrium distance in a solid (crystal). It arises from valence electrons rearranging around atoms to form bonds.

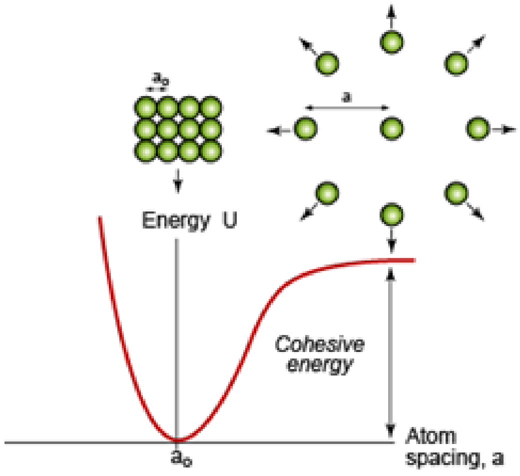

Figure 5. Potential energy of atoms plotted against atomic spacing, with equilibrium bond length denoted a_0 *[5]*

The cohesive energy is a measure of the strength of the bonds between atoms. It is therefore related to many materials properties, such as melting temperature, scratch and abrasion hardness (Woodell wear resistance for hard materials), activation energy for lattice diffusion, or surface energy [5-6]. The greater the cohesive energy, the stronger the bonds between the atoms and the higher the melting temperature *etc*.

As you might expect, the cohesive energy is also closely related to the energy required to break bonds and separate the atoms into a gas. If this is done at constant temperature, it is called latent heat of vaporization. Both the cohesive energy and the latent heat of vaporization are available attributes in the Elements database and can be used to demonstrate how the energy change going down the potential energy curve (cohesive energy) and going up (latent heat of vaporization) indeed match quite well. This can be seen through the near linear relationship between these properties in Figure 6.

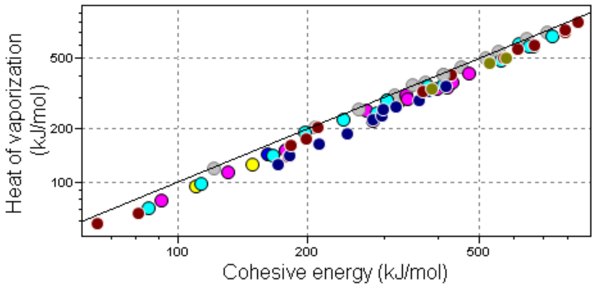

Figure 6. Heat of vaporization plotted against cohesive energy for a wide range of elements

Since the melting temperature of a material is found to be proportional to its cohesive energy [7], this parameter can also be used as a measure of the bond strength. The melting temperature is perhaps more familiar to the students and easier to use than cohesive energy.

To explore the link between the thermal and mechanical properties, we now consider the force aspect of the potential energy curve, which corresponds to its first derivative, or slope. In a simple model, bonds can be thought of as springs, where the restoring force increases linearly with displacement from the equilibrium (see Figure 7).

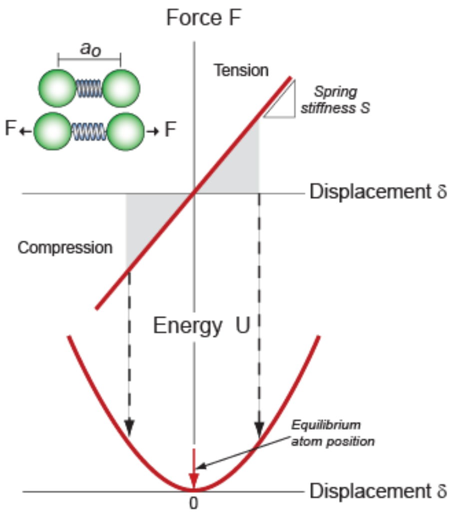

Figure 7. Forces between atoms arising from the bond depend on the shape of the potential energy curve [5]

Whereas the cohesive energy, or the depth of the potential energy curve, corresponds to the bond strength, the shape (narrowness) of the curve near the bottom will determine how stiff the bonds are. The stiffness of the bonds are then reflected in material properties, primarily in the Young's modulus. A deep potential energy curve implies steep slopes of the curve, which corresponds to a high Young's modulus. This correlation trend can be argued with the help of a chart using the Elements database (see Figure 8) with Young's modulus plotted against melting temperature.

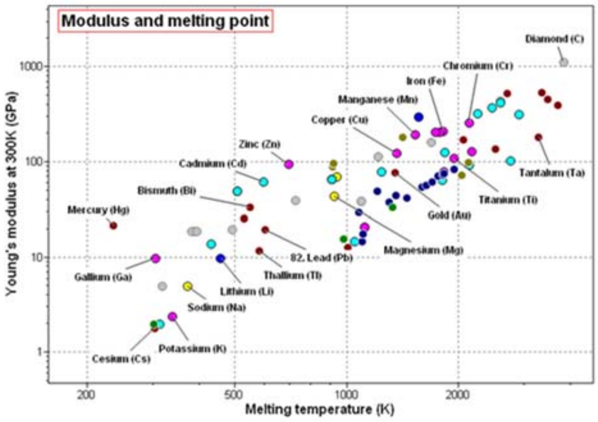

Figure 8. Correlation trend between thermal and mechanical properties for the Elements

The same trend seen for elements in the relationship between thermal and mechanical properties can also be found in non-elemental metal alloys and ceramics, as illustrated in Figure 9. This supports our claim that the properties and correlations found using the Elements database are also relevant for actual Engineering materials.

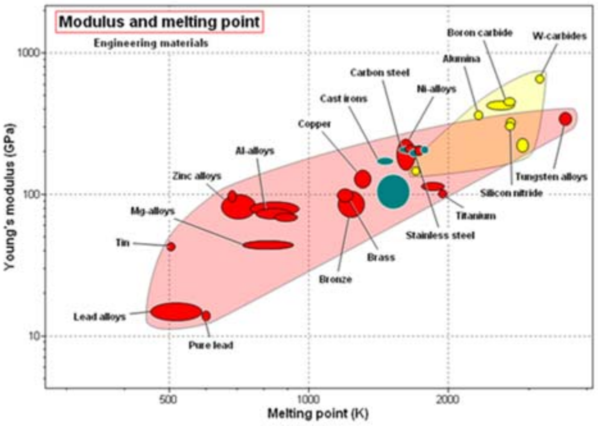

Figure 9. Correlation trend between thermal properties and mechanical for alloys and ceramics

As another example of how to use the Elements database in Materials Science and Mechanical Engineering, we consider the origins of thermal expansion, elaborating from the simple spring model for bonds. Thermal expansion arises from the asymmetric shape of the potential energy curve (Figure 5). As the atoms acquire kinetic energy when heated, their movement around the equilibrium atomic distances will increase. This is shown in Figure 10, as elevated energies at temperatures T1-T3. Since the potential energy curve is asymmetric, there is a displacement of the average atomic distance towards larger values, hence the expansion.

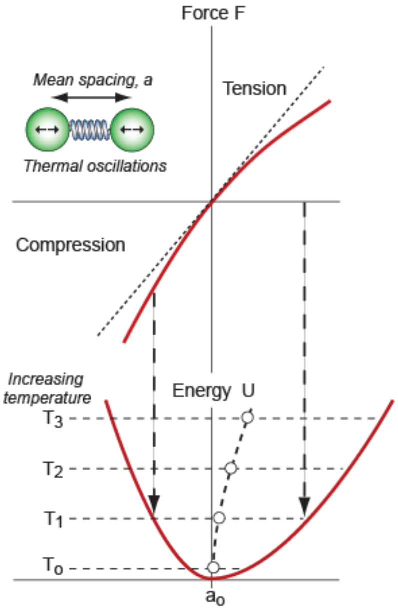

Figure 10. The mechanism of thermal expansion [5]

Having established that the melting temperature is proportional to the cohesive energy, and thus the depth of the potential energy curve, we can argue that this depth should affect the shape of the curve. The deeper the curve, the more narrow and symmetric the curve at the bottom, and hence the smaller the thermal expansion coefficient. Exactly this trend is demonstrated in Figure 11, below.

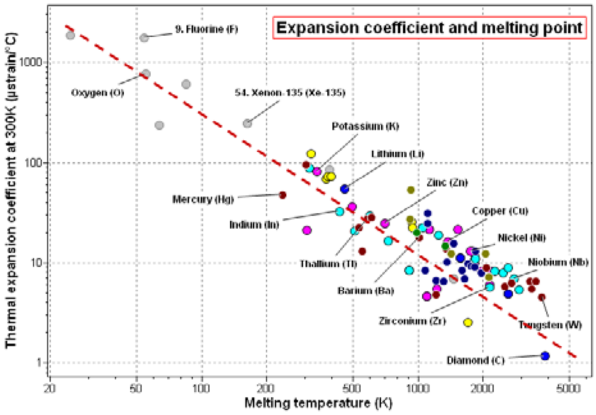

Figure 11. Support for the argument that high melting temperatures give low thermal expansion

This makes sense, since we have just seen (Figure 8) that the higher the melting temperature, which means deeper and more narrow potential energy curve, the stiffer the bonds.

We might add that since the Elements database offers a wide range of values for each material property throughout the Periodic Table, trends and correlations between properties, such as those illustrated in Figures 8 and 11, become clearer.

5. Magnetic and electrical properties

Visualization using the Elements database is a generic technique that can be used in many areas of education. It is possible to use the Elements, e.*g.*, to help introduce magnetic properties for atoms of the Periodic Table. For instance, a chart of ferromagnetic elements can be used to discuss different types of magnetism, see Figure 12. Ferromagnetism is found in materials that manifest very large and permanent magnetic moments without external magnetic fields. This permanent magnetic moment of the atom arise from unpaired electron spins. Specifically for ferromagnetic materials, coupling interactions between atoms then cause the electron magnetic moments to align in each grain.

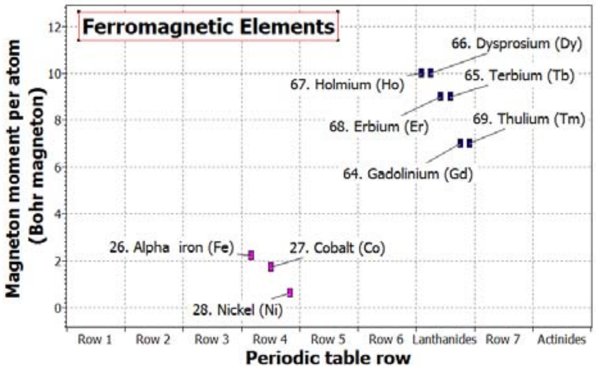

Figure 12. Grouping of ferromagnetic elements into two distinct areas of the chart, due to electron configuration

There are only nine elements characterized as ferromagnetic. These fall into two groups depending on electronic configuration, as can be seen in Figure 12. Iron, Cobalt, and Nickel (from the transition elements) have partially filled 3d orbitals whereas Gadolinium through Thulium (from the Lanthanides) all have partially filled 5d orbitals. The origins of ferromagnetism in these atoms, in terms of electron configuration, can then be elaborated on to cover other more complex materials, such as oxides of Iron. This chart also shows that the highest values of magnetic moments per atom are found for Dysprosium and Holmium, both around ten Bohr magnetons (1 Bohr magneton=9.3×10^{-24} A/m^2).

Electrical properties are explored in the next example. In this case, the Wiedemann-Franz law (see Eq.1) can be investigated using charts of the near linear correlation between thermal conductivity, λ [W/m.K] and electrical conductivity, K [S/m] (or, equivalently, the inverse of the resistivity $1/\rho$).

$$\text{Wiedemann-Franz law: } \lambda=c.1/\rho \quad \text{[Eq 1]}$$

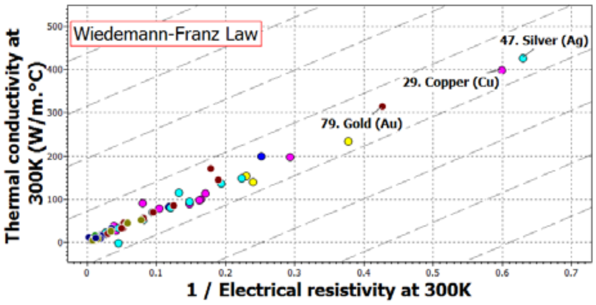

Figure 13. Empirical relationship between thermal conductivity and electrical resistivity, used to determine the proportionality constant in the Wiedemann-Franz law

Using the limit stage of the software, only the metallic elements are displayed in a property chart, see Figure 13. Linear axes are used to facilitate the interpretation. Using the Elements database, an empirical determination of the proportionality constant can be made (here at 300K).

For Silver, this gives, numerically: λ=429 W/mK and K=0.629 ($\mu\Omega$.cm)$^{-1}$, which yields:

$$c=429/0.629=\underline{682}\ W/\mu\Omega.cm.mK$$

The *Guidelines tool* is used to show the slope c in Figure 13 to aid this conclusion.

The reason for the correlation between electrical and thermal conductivity is that both properties depend on the mean free path of the electrons involved in the conduction mechanisms. In metals, the conduction electrons are free to move through the solid, until they are scattered by some impurity or imperfections in the material, which contributes to resistivity, see Figure 14. The greater the number of scattering points, the shorter the mean free path of the electrons between collisions and the slower, on average, they move. Heat can be transmitted through materials in several ways but, in metals, the main mechanism is via the movement of free electrons. Thus, the thermal conduction by electrons is governed by the mean free path in the same way as electrical conduction, as demonstrated by the chart above.

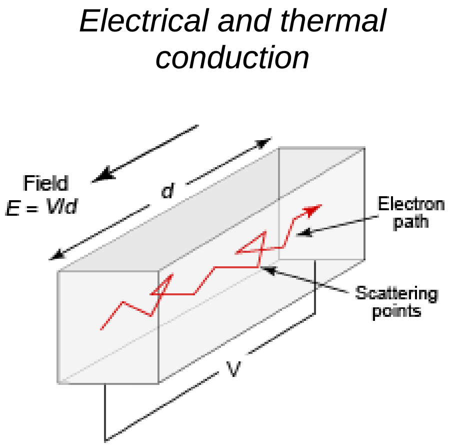

Figure 14. Electrical and thermal conduction in metals operate through common free electron mechanisms [5]

6. Nuclear properties

The Elements database contains data on atomic properties, but has also been extended to include some nuclear properties. For example, binding energy per nucleon, which is relevant for fission and fusion of nuclear fuels, and neutron absorption/scattering cross-sections, which are relevant for moderators and control rods and techniques like neutron spectroscopy [8]. There is also half-life data for selected materials.

The nuclear stability of an element is measured by the binding energy per nucleon. This property is plotted against atomic number in Figure 15. The most stable nuclei (those with the greatest binding energy) cluster around iron. It is clear from this plot that elements of the actinide group will be the most favorable fuels for fission whilst the hydrogen isotopes are favorable for fusion. When the binding energy per nucleon is increased, the energy difference is transferred to kinetic energy and radiation.

Fission releases, at most, a few hundred keV per event, whereas fusion can release many thousands. It is known that the total mass of individual protons and neutrons in a nucleus is larger than the mass derived from the atomic weight. This mass difference, m, can be calculated by students using the binding energy per nucleon and Einstein's celebrated equation (where c≈3.0x10^8 m/s):

$$E = mc^2 \qquad [Eq\ 2]$$

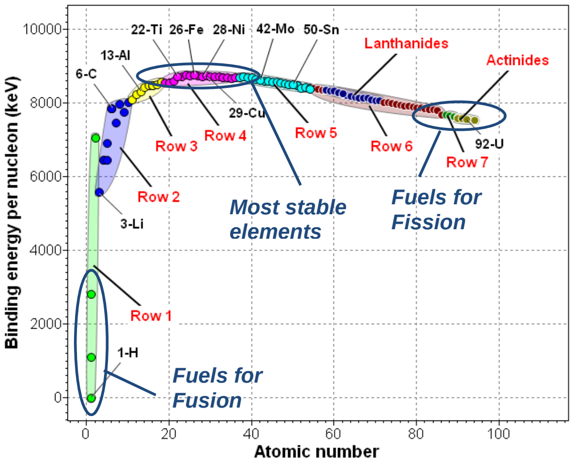

Figure 15. Binding energy per nucleon plotted against atomic number

Moderators are materials that slow neutrons by scattering them, converting their kinetic energy into heat. Neutron absorption is undesirable because it causes transmutations into possibly radio-active species. So one criterion for selecting moderator materials is that they should have a high scattering cross-section and a low absorption cross section. Control rods, on the other hand, quench the chain reaction by absorbing neutrons. Materials for control rods need high absorption cross-section but low scattering cross-section (to stop overheating). The suitable candidates for these applications are shown in Figure 16. Indeed, several of these identified materials are also used in real processes.

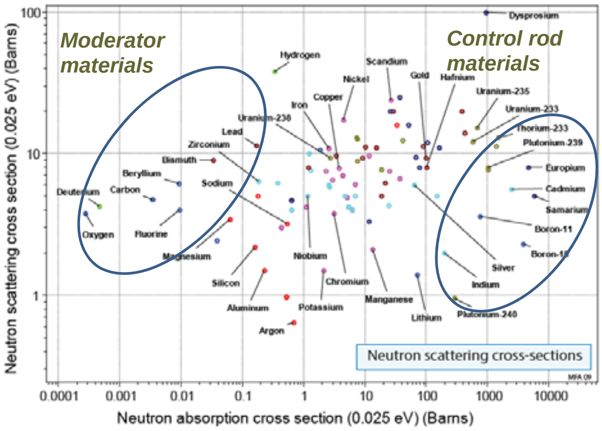

Figure 16. Neutron scattering plotted against absorption cross-sections

7. Summary and Conclusions

The periodic table of elements is fundamental to the understanding of material properties. Knowledge of the elements and how they relate to each other is relevant at most levels of education. In this paper, a number of examples of how CES EduPack and, in particular, the Elements database can support materials-related teaching have been described.

In this paper, we have demonstrated how the understanding of thermal and mechanical properties, as well as their relationship to each other, can be enhanced using the elements database. The material property graphs used by CES EduPack can be powerful visual tools to show fundamental features of the elements. Many basic properties of the elements can easily be displayed as they vary with atomic number. We have also shown examples of how magnetic and electrical properties can be discussed in teaching using visualization in combination with the elements database.

Finally, the Elements database has also been extended to include some nuclear properties. This can be used to explore, for instance, Neutron scattering and absorption cross sections for elements. It is then possible for educators to demonstrate in class how to select materials in nuclear power applications. Actual moderator materials and control rod materials can be justified from properties clearly displayed in charts made using CES EduPack.

To sum up: the Elements database is a resource to support teaching of both Materials Science and Materials Engineering. It is a source of basic data that reveals fundamental relationships and it underpins the understanding of materials at most levels and for many applications.

8. Acknowledgements

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9. Further reading

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