



Granta EduPack White Paper

The Granta EduPack Materials Science and Engineering Package

Mike Ashby¹, Hannah Melia², Madga Figuerola², Lee Philips², Stéphane Gorse³

¹Department of Engineering, University of Cambridge

²Ansys Materials Education Division

³Bordeaux INP & Institut de Chimie de la Matière Condensée de Bordeaux,
France.

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Abstract

Experience suggests that learning is better achieved by discovery for oneself than by passive listening. The Granta EduPack Materials Science and Engineering (MS&E) Edition was designed to allow students to explore the relationships between Processing, Structure, Performance and Properties. The database includes data for the elements, data for structural, functional and biological materials, for processes for shaping, joining and finishing, tools to aid understanding of phase diagrams and resources that focus explicitly on the process-structure-property relationship. This paper showcases the details of this edition.

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1. Introduction-- what's this package and what can it do?

Experience suggests that learning is better achieved by discovery for oneself than by passive listening. The Granta EduPack Materials Science and Engineering (MS&E) Package is a set of resources that allows students to explore the relationships between Processing, Structure and Properties. They stimulate discovery and pose questions: why does this property change in that way when the material is processed? Why is this other property unchanged? The package includes data for the elements, data for structural, functional and biological materials, for processes for shaping, joining and finishing, tools to aid understanding of phase diagrams and resources that focus explicitly on the process-structure-property relation. The package includes a set of 41 micro-projects that stimulate discovery. It is visual (almost all the charts in this White Paper were made with the package) and it is backed-up with down-loadable “science notes” and teaching and learning resources from which many of the schematics shown here were exported.

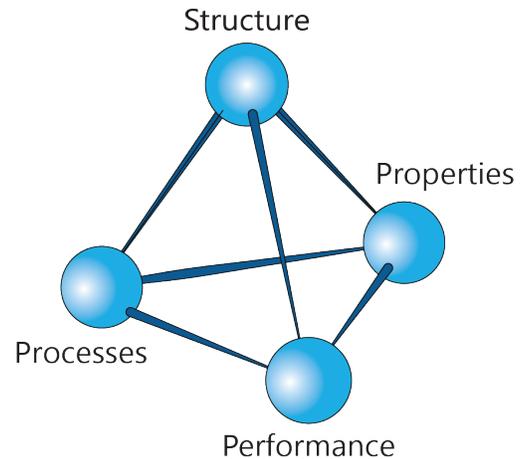


Figure 1: The Process-Structure-Properties-Performance tetrahedron

The approach adopted here flows from the unifying theme of MS&E: the relationship between **processing, structure, properties and performance** (Figure 1). It involves information and understanding that spans a vast range of scale ranging from the sub-microscopic to the massive (Figure 2). The package is designed to engage student interest and to support the teaching of MS&E both when taking a science-led, “bottom-up”, approach as in textbooks by Callister, Shackelford and others (Figure 2, read from left to right), or a design-led, “top-down”, approach typified by the more engineering-oriented texts of Dieter and Ashby et al¹ (Figure 2, right to left). The White Paper is an introduction to the package; links within it take you to other documents that explore subsections of it in greater depth.

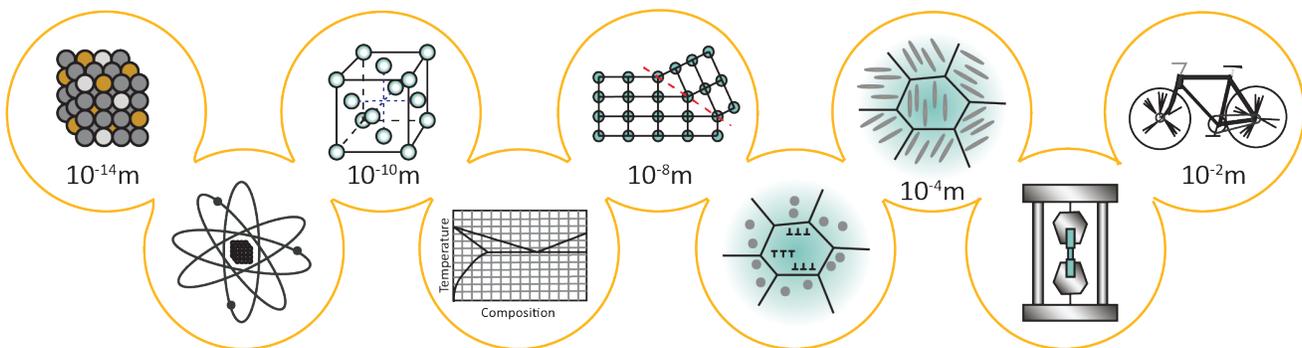


Figure 2: Length scales and the structures and properties associated with them. A bottom-up approach to teaching MS&E flows from left to right in this diagram; a top-down approach flows from right to left

1 See Section 7, references

2. What's in the Granta EduPack MS&E Package?

The package is a set of interrelated resources.

- This White Paper
- PowerPoint sets to help present it to students
- Exercises, multiple choice questions and MicroProjects that stimulate self-learning
- Interactive tools to explore phase diagrams and environmental audits
- the MS&E database itself-- more details in the paper

The **MS&E database** is a set of linked data-tables (Outer ring of Figure 3) that connect key information and concepts from the atomic to engineering scale, from processing to performance, and from science to application. Some data-tables are an expanded version of those already found in the Level 2 (intermediary) editions of the Granta EduPack; others are unique to the MS&E Package.

The **Materials** and **Processes** data-tables lie at the heart of the set. The first contains records for the properties of structural, functional and biological materials. The second gives access to records for shaping, joining and finishing processes, with schematics and images of processes. The **Elements** data-table contains records for the basic properties of the elements of the Periodic Table; they are linked, where appropriate, to records in the other tables giving one-click access to relevant fundamental atomic properties. The **Phase Diagrams** data-table contains the most-used phase diagrams and an interactive tool to illustrate how to interpret them. The **Process-Property Profiles** data-table allows the effect of processing on properties to be explored and the associated **Structure and Mechanism Notes** give insight into structural changes that are used to manipulate properties. Data-tables of **Producers and References** (not shown in Figure 3) give access to the sources of the data and commercial materials-suppliers.

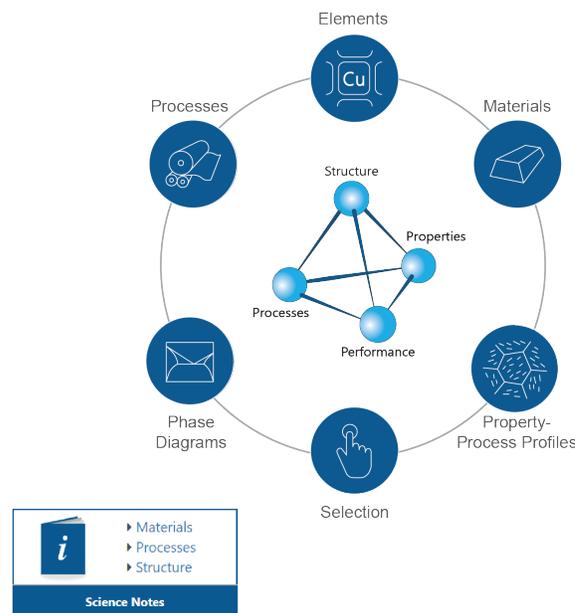


Figure 3: The data structure of the Granta EduPack MS&E database. This schematic appears as the Home Page of the database. Clicking on any of the six icons takes the user to that component of the database

The Homepage (Figure 3), acts as an interactive portal to the data-tables and the associated student resources and tools. The content, in more detail, takes the following form.

The **Elements data-table** provides fundamental data about the elements of the Periodic Table: nuclear, electronic, atomic and crystallographic data, and mechanical and thermal properties, environmental characteristics and global geo-economic and criticality standing. It is linked to the other data-tables giving direct access from their records to the relevant element-records. Like the other data-tables it is fully documented in a separate White Paper, which can be found on our resource hub.

The **Materials data-table** has the same format as the Level 2 MaterialUniverse database, with two major expansions. They are:

- Records for **functional materials**, including magnetic, magneto-caloric, piezo/pyro/ferroelectric, semiconducting and thermoelectric materials. The functional properties are described in embedded Science Notes and fully documented in a separate White Paper
- Records and data for **biological materials**, including molecular building blocks, natural fibers, tissues (both soft and mineralized), woods and wood-like materials. It too is fully documented in a separate White Paper

The **Process data-table** contains 109 shaping, joining and surface treatment processes from the Level 2 ProcessUniverse available, updated to include **additive manufacturing** and schematics and images of the process and the things they can do. A **cost model** allows the costs of alternative processes to be compared. **Links** between Materials and Processes allow selection of materials by their processing options and vice-versa.

The **Phase Diagram data-table** gives access to phase diagrams for 12 of the most widely use engineering alloys. It is further supported by an **interactive teaching tool** which works in three modes:

- the **glossary mode** explains the terminology of phase diagrams,
- the **microstructure mode** explores the microstructural development during solidification through sketches, annotations and text
- the **Lever Rule** mode helps students visualize the weight fraction of two phases, while at the same time reviewing the Lever Rule calculation.

The tool uses two common phase diagrams to illustrate features of phase diagrams: Cu-Ni for the lever rule and the Ph-Sn for eutectics. A “Teach Yourself Phase Diagrams” booklet encourages independent learning.

The **Process-Property Profiles data-table** illustrate control of properties by processing. It contains sets of records chosen to illustrate how processes such as alloying, heat treatment, mechanical working, sintering and foaming, change mechanical, thermal and electrical properties. Each set is accompanied by a folder-level record describing the underlying structural changes. Suggested mini-projects prompt students to explore significant property trajectories. Like other Granta resources, this data-table encourages “learning by discovery” and can be used for independent study or for a structured lesson. The Process-Property Profiles database and its contents are described in detail in another White Paper.

Comprehensive sets of **Science Notes** are accessed from the Home Page (Figure 3, bottom left). They give background to material properties, to processes attributes, and to the mechanism that underlie properties and the way processes change them.

With that background, we can move on and explore what the database can do.

3. What can the Granta EduPack MS&E package do?

The database and teaching resources support teaching across the great range of scales shown in Figure 2. This part of the White Paper gives some illustrations of how it can be used, covering:

- Nuclear properties
- Bonding and bond-dependent properties
- Crystal structures and related properties
- Phase diagrams
- Processing and process-dependent properties
- Natural materials and their properties
- Functional materials and their properties
- Materials selection

We distinguish groups of properties (Figure 4):

- Microstructure-insensitive properties, determined mainly by the interatomic bonding, and
- Microstructure-sensitive properties, strongly influenced by microstructure and thus by processing.

We next explore what the MS&E edition can tell us about each.

3.1 Bonding dependent properties and the Elements data-table

The Elements data-table contains data for the nuclear and atomic characteristics of the elements of the



Microstructure-insensitive properties:

- Density
- Melting point
- Modulus
- Specific heat
- Expansion coefficient
- Saturation magnetization

Microstructure-sensitive properties:

- Strength
- Toughness
- Elongation
- Thermal conductivity
- Electrical conductivity
- Coercive field, energy product

Figure 4: Properties that don't depend strongly on microstructure (left) and those that do (right)

Periodic Table (Figure 5) and the microstructure-independent properties that depend on these.

What's in it? The Elements data-table contains records for the elements of the periodic table, including

- Nuclear characteristics
- Electronic properties
- Crystal structure and parameters
- Physical, mechanical, thermal and electrical and magnetic properties
- Diffusion parameters and surface energies
- Geo-economic data (abundance, countries of origin, annual production)
- Environmental properties and
- Criticality status



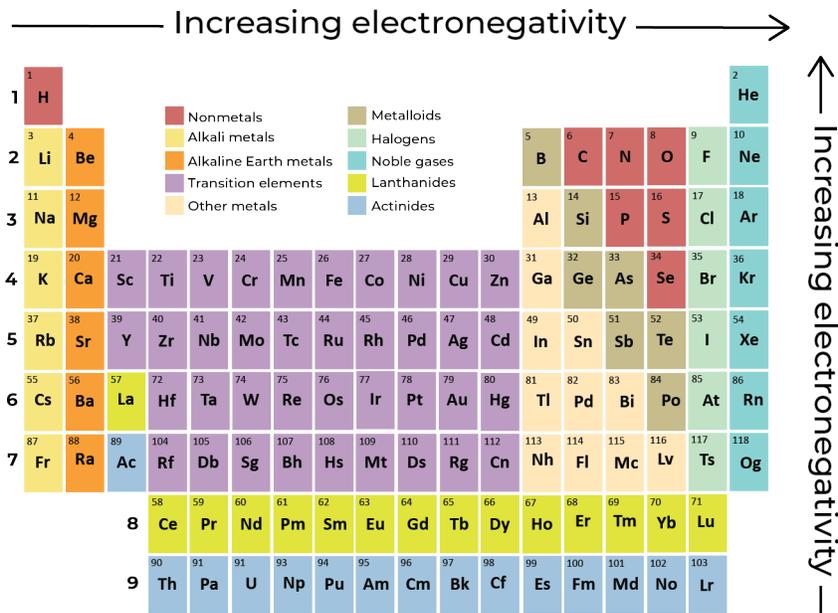


Figure 5: The Periodic Table. It acts as the home page for the Elements data-table

What can you do with it? Here are examples of how the Elements data-table can be used to explore the origins of microstructure-independent properties.

Nuclear properties. The nucleus of an atom is made up of protons and neutrons, known collectively as nucleons (Figure 6). Records in the Elements data-base contain data for the nuclear properties of the elements: the binding energy per nucleon, thermal neutron absorption cross section, thermal neutron scattering cross section, and, for fuels, the half-life. These properties are defined more fully in the Science Notes attached to the property names in the data-table. Additional records are included for isotopes of particular interest: deuterium (2), tritium (3), the four isotopes of plutonium (239, 240, 241, 242), the three isotopes of uranium (233, 235, 238), the two of thorium (232, 233) and one each of protactinium (233), samarium (149), xenon (135) and boron (10).



Figure 6: The Nuclear Core

The Granta EduPack system allows the data to be presented in ways that bring out features of interest. Figures 7 and 8 show two of these. The first is a plot of binding energy per nucleon against atomic number. The most stable nuclei (those with the greatest binding energy) cluster around iron. Elements which are above iron in atomic number can release energy by fission while those below iron can do so by fusion, and that fission releases, at most, a few hundred keV per event, whereas fusion can release many thousands.

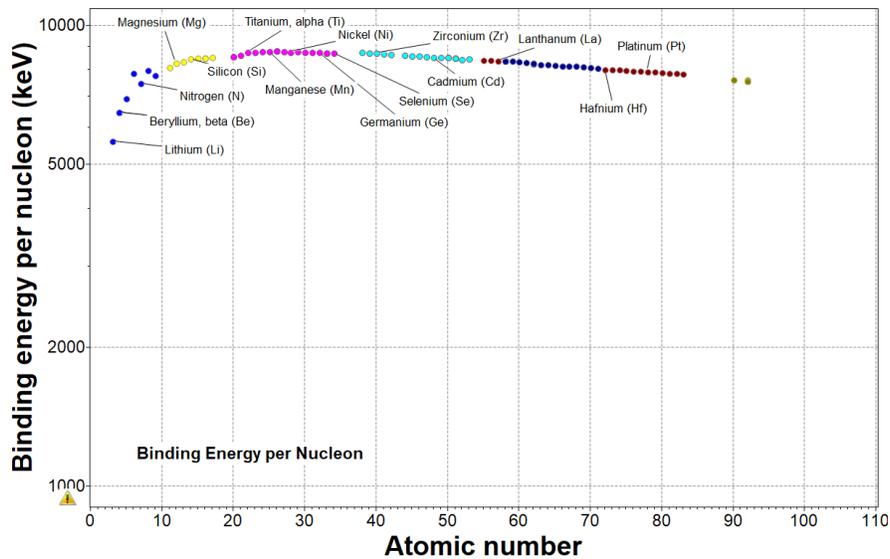


Figure 7: The binding energy per nucleon, a measure of nuclear stability.
(Made with the Elements data-table of the MS&E database)

One might expect that the most stable elements would also be the most abundant in the earth’s crust. Figure 8 shows that, broadly speaking, this is true. Silicon, aluminum, iron, calcium, sodium and magnesium and oxygen, between them, account for over 80% of the content of the crust. The high atomic number platinum group, by contrast, accounts for only 10⁻⁷% (1 part in 10⁹).

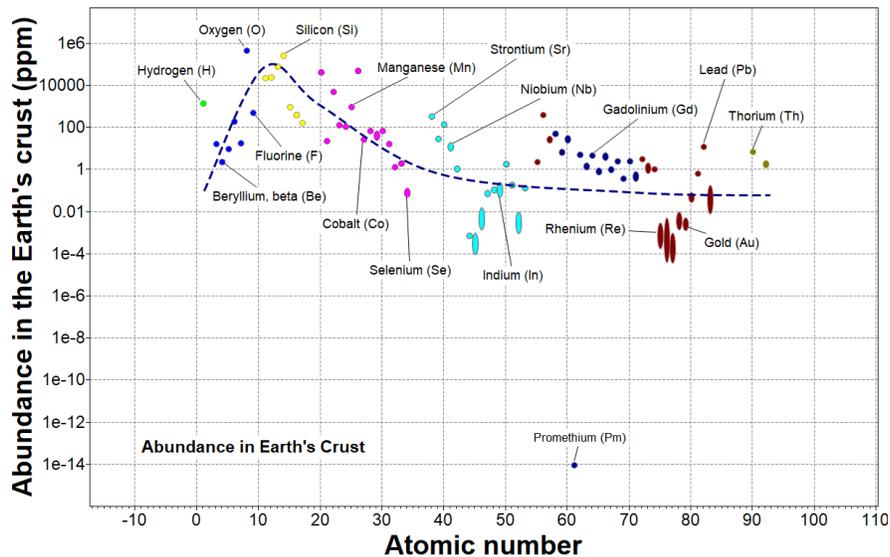


Figure 8: The abundance of the elements in the earth’s crust (ppm by mass).
(Made with the Elements data table.)

More examples of what this data-table can do are given in the “Materials for Nuclear Power Systems White Paper”.

Interatomic bonding. When atoms bond, it is because the electrons in the outermost shell of electron orbitals interact (Figure 9). The cohesive energy measures the strength of this bonding. It is defined as the energy per mol (a mol is 6.022×10^{23} atoms) required to separate the atoms of a solid completely, giving neutral atoms at infinity. Equally it is the energy released if the neutral, widely spaced atoms

are brought together to form the solid. The greater the cohesive energy, the stronger are the bonds between the atoms and the higher is the modulus and the melting temperature. Surfaces and vacancies both involved broken bonds with the consequence that the surface energy and the activation energy for diffusion scale approximately with the cohesive energy.



All these correlations can be explored using the Elements data-table of the Materials Science and Engineering package. **Figure 9: Atomic Bonding** Figure 10 is an example: the correlation between Melting Temperature T_m (here multiplied by the gas constant, R) and cohesive energy H_c . It shows the linear relationship between the two, and that the thermal energy RT_m at the melting point is about 3% of the cohesive energy.

Electronegativity is a measure of the tendency of an atom to attract a bonding pair of electrons. The Pauling electronegativity scale assigns fluorine, the most electronegative element, the value 4. The values range down to cesium and francium, the least electronegative of the elements, with the value of 0.7 (Figure 11). An atom with low electronegativity tends to lose electrons to become a positive ion; one with high electronegativity tends to gain electrons to become a negative ion.

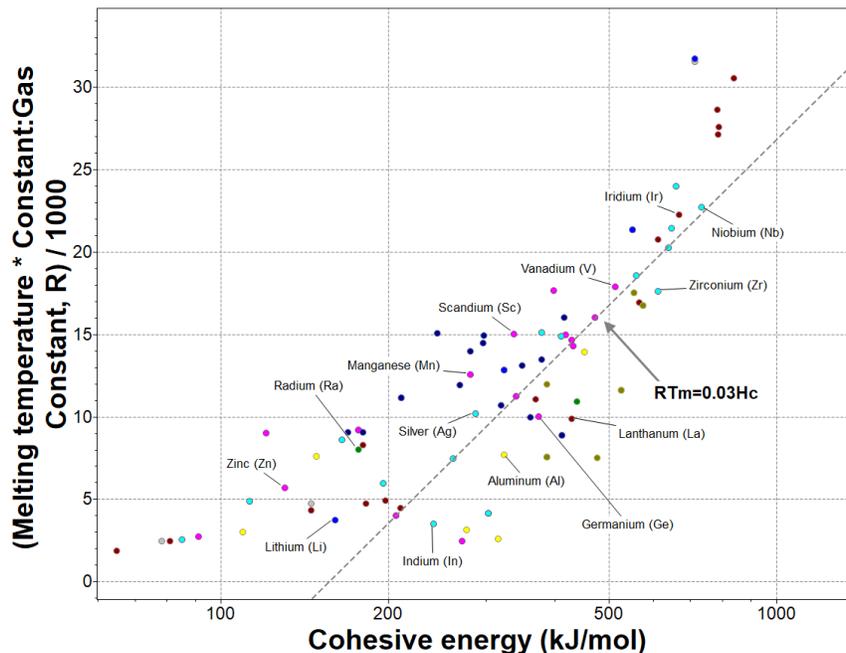


Figure 10: Melting temperature and cohesive energy of the elements. (Made with the Elements data table.)

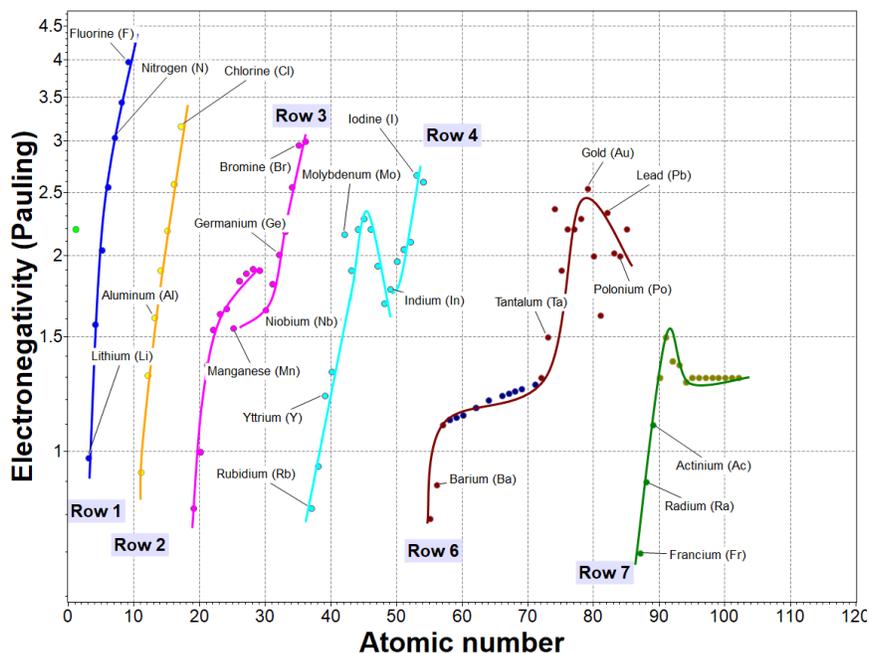


Figure 11: Electronegativity of the elements.
(Made with the Elements data table.)

Crystal structure and atom size. The Elements data-table has schematics for the crystal structures of each of the elements. Figure 12 is an example. When the element exists in more than one allotropic form there are separate records and structures for each.

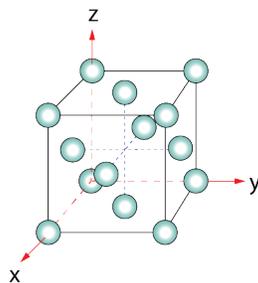


Figure 12: Face-centered cubic crystal structure

Figure 13 is an example of a chart made with the data-table. It is a plot of atomic volume across the periodic table, made with this data-table and color-coded row by row. The atomic volume depends on the packing-density of atoms in the crystal (and thus on the crystal structure), but the plot shows that the position in the row has a much greater influence: in any row, the atomic volume is a minimum in the middle. This is because the atom “size” reflects the radius of the outermost valence shell of electrons. As the atomic number increases across a row, the positive charge on the nucleus increases and this charge is incompletely screened out by the inner shells of electrons, causing the valence shell to contract. The imperfect screening is a maximum in the middle of the row, leading to the minimum in atomic volume.

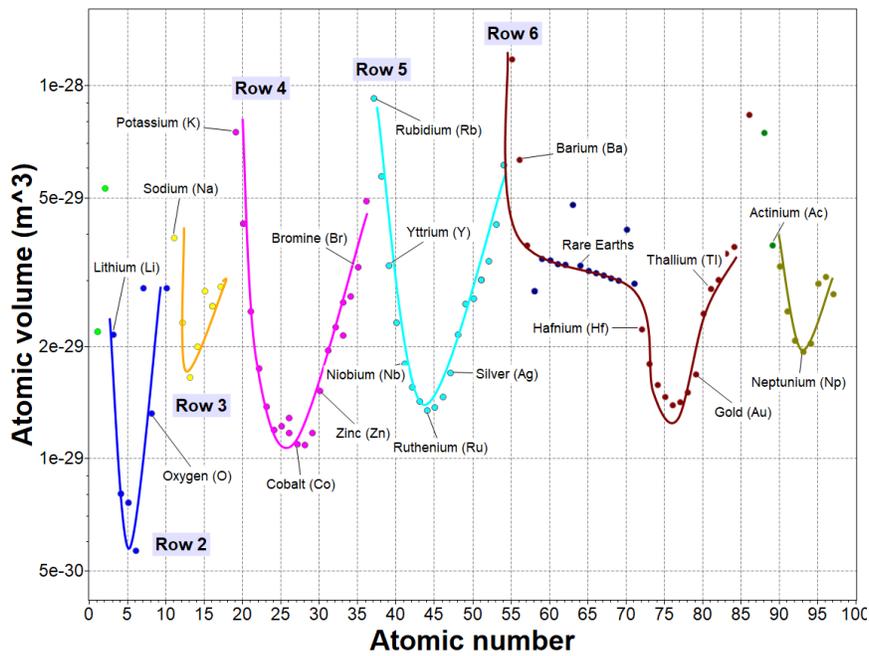


Figure 13: Variation of atomic volume across the rows of the Periodic Table (Made with the Elements data table.)

Other properties vary across the rows of the periodic table in a similar way. Figure 14 shows an example: Young's modulus, plotted against Atomic number. The modulus peaks at the center of each row, falling sharply at the end of one row and the start of the next.

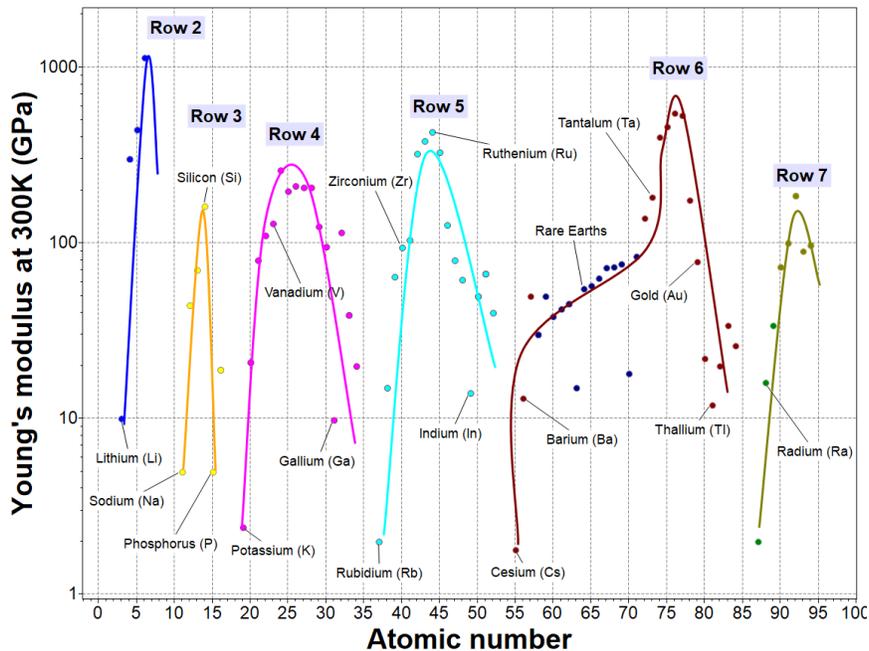


Figure 14: Variation of Young's modulus across the rows of the Periodic Table (Made with the Elements data table.)

Explore for yourself- Microstructure-insensitive properties

Explore (and then explain) the following correlations, using the Elements data-table to make charts of:

- Young's modulus E (GPa) and Cohesive energy H_c (kJ/mol)
- Activation energy for lattice diffusion Q_d (J/mol) and Cohesive energy H_c (kJ/mol)
- Surface energy γ (J/m²) and Cohesive energy H_c (kJ/mol)
- Heat of vaporization H_v (J/kg) and Cohesive energy H_c (kJ/mol)
- Specific heat capacity per unit volume C_{pp} J/m³.K (specific heat capacity C_p times density ρ) and Atomic volume V_m (m³)
- Thermal conductivity λ (W/m.K) and Melting temperature T_m (K)
- Latent heat of melting L_m (J/kg) and Specific heat C_p (J/kg.K) times Melting temperature T_m (K)
- Thermal conductivity λ (W/m.K) and Electrical resistivity ρ_e (Ω .m)
- First ionization energy and electronegativity
- Specific heat capacity per unit volume (specific heat capacity times density) and atomic volume.

3.3 Exploring microstructure-dependent properties with the Process-Property Profiles data-table



The microstructure-sensitive properties of a material are manipulated by processing. Some of the process-induced property-changes are desired (the increase in strength achieved by alloying or work-hardening, for example); others change in ways that may be less desirable (reduced elongation and toughness, for instance); still others do not change. The Granta EduPack Process-Property data-table is a do-it-yourself kit that allows students to explore how the processes it contains change the properties of selected metals, polymers and ceramics. The database stimulates discovery and it poses questions: why does the property change in that way? Why is this other property unchanged?

The Process-property profiles data-table contains seven sets of records chosen to illustrate how processes influence properties. All the records have a full Level 2 property listing allowing the effect of the process to be explored across the entire property-spectrum.

The seven sets are:

1. Alloying and working: copper alloys
2. Heat treatment: carbon steels
3. Alloying and heat treatment (1): stainless steels
4. Alloying and heat treatment (2): aluminum alloys
5. Filling and reinforcement: thermoplastic polymers
6. Powder processing: sintered ceramics
7. Foaming: polymers, metals, ceramics

The full set and what can be done with them are described in a White Paper. Here we give two examples.

Set 1. Alloying, precipitation and working: copper-nickel alloys.

Pure, annealed metals are good thermal and electrical conductors but they are soft. They can be strengthened by work-hardening (as in cold rolling, cold forging and wire drawing). They can also be

strengthened by alloying (as in brass and bronze). And they can be strengthened by precipitation hardening (as in age-hardening aluminum alloys and stainless steels) (Figure 15). All three change the properties of metals, but in different ways. This set of records illustrates the effect of work-hardening, solid-solution (alloy) hardening and precipitation hardening on the mechanical, thermal and electrical properties of copper.

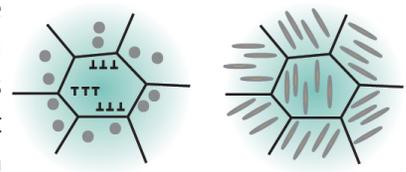


Figure 15: Aspects of structure: solute, defects, precipitates, grains.

What's in Set 1? The folder contains 19 records covering

- Pure copper, in the soft, 1/4 hard, 1/2 hard, 3/4 hard and fully hard condition, and
- Copper-nickel alloys, ranging in composition from pure copper to pure nickel
- Copper-beryllium alloys in the solution treated, worked, aged, and aged plus worked states. The symbol “w” means solution heat-treated; “wh” means solution heat-treated and work-hardened; “wp” means solution-heat treated and aged to allow precipitation; “whp” means solution heat-treated, work-hardened and aged.

What can you do with it? The record-set allows students to explore the effect of the three hardening mechanisms on properties. Figure 16 shows an example of their effect on two properties of importance for heat exchangers: strength and thermal conductivity. Increasing cold work increases the yield strength of copper dramatically but has very little effect on conductivity. Solution-hardening, by contrast, gives strength but greatly reduces conductivity. Precipitation hardening gives the most desirable combination of high strength with good conductivity.

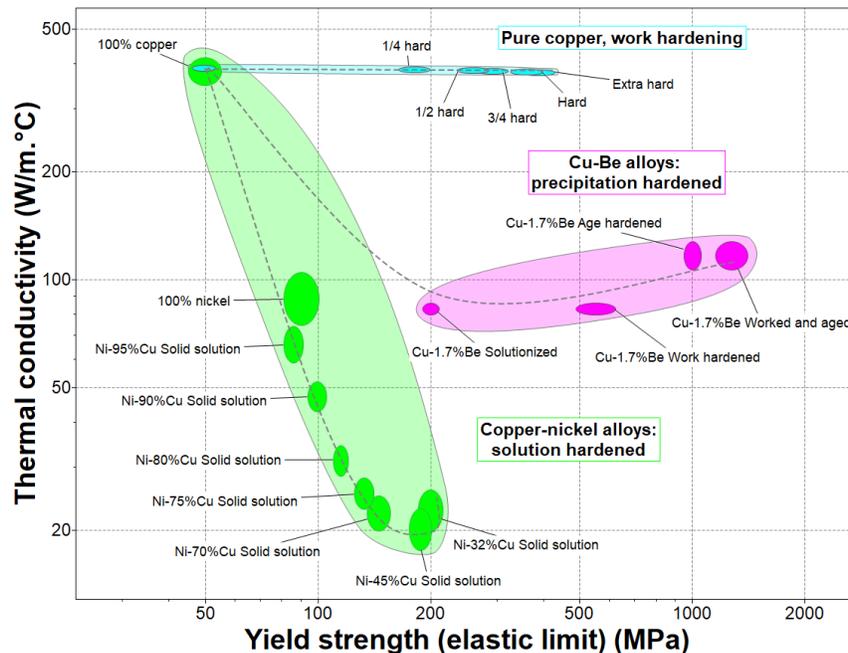


Figure 16: . The effect of processing on thermal conductivity and strength of copper. (Made with the Process Property Profiles data table.)

Explore for yourself- alloying, precipitation, and working

Use Set 1 of the Process-Property Profiles data-table to create the following charts. Read the Science notes attached to the property fields in the data-table and the Structure and Mechanism notes linked to the material records for insight into the trends you observe.

- Thermal conductivity plotted against Electrical resistivity. Is there a relationship?
- Young's modulus plotted against Yield strength. Does work-hardening change the modulus? Does solution-hardening?
- Yield strength plotted against Copper content (choose a linear, not log, scale for the copper content). At what copper content is the strength a maximum?
- Elongation plotted against Yield strength. Does work-hardening affect elongation more strongly than solution-hardening?

Set 5. Filling and reinforcement of thermoplastic polymers.

Polymers have low elastic moduli and moderate strength. They can be stiffened (raising the modulus) by blending them with fillers such as talc, calcium carbonate or other minerals; and they can be both stiffened and strengthened by reinforcing them with chopped or long fibers of glass or carbon (Figure 17). The fillers and reinforcements affect not only the stiffness and strength, but all the other properties as well. This set of records allows the effect of fillers and fibers on polymer properties to be explored.

What's in Set 5? The folder contains a record for the mechanical, thermal and electrical properties of Polypropylene (homopolymer) and for the same polypropylene filled or reinforced with a variety of fillers.

- Four weight fractions of talc (hydrated magnesium silicate, $Mg_3 Si_4 O_{10} (OH)_2$) particles
- Four weight fractions of calcium carbonate (chalk, $CaCO_3$) particles
- Six weight fractions of glass fibers, both chopped and long-fiber
- Two weight fractions of EPDM (an elastomeric ethylene propylene diene, an elastomeric terpolymer).

What can you do with it? Figure 18 shows the way in which Yield strength and Young's modulus of polypropylene homopolymer change with filler type and content. All the fillers raise the modulus; only glass fibers significantly increase the strength as well.

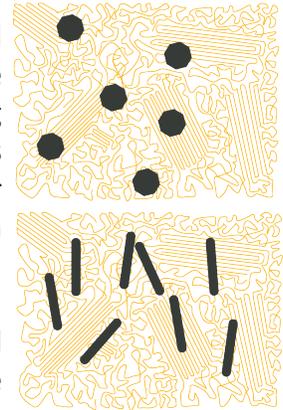


Figure 17: A polymer with particulate and fiber fillers

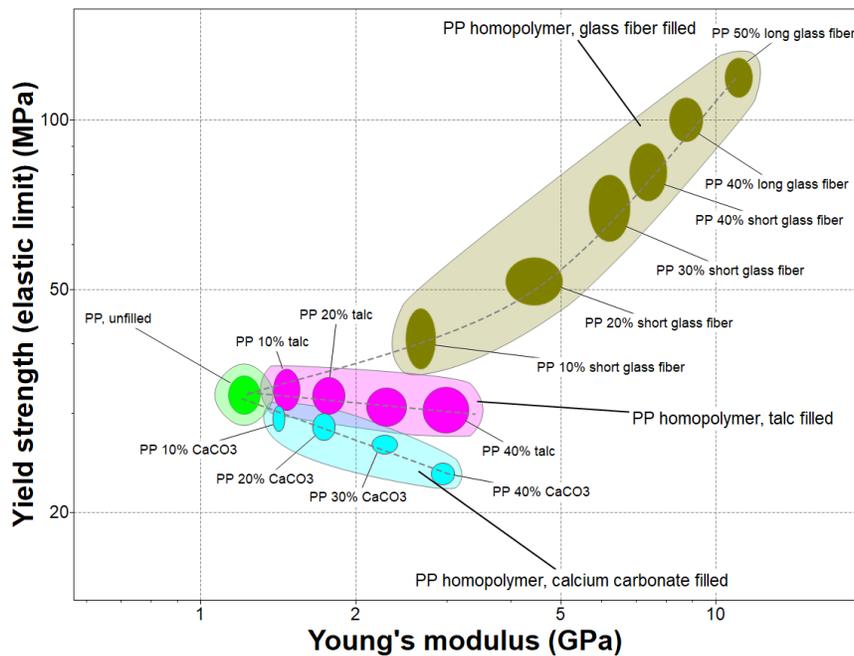


Figure 18: . Polypropylene, shown in green, with particulate and fiber fillers. (Made with the Process Property Profiles data table.)

Explore for yourself- filling and reinforcement of thermoplastic polymers

Use Set 5 of the Process-Property profile data-table to create the following charts and answer the questions. Read the Science notes attached to the property fields in the data-table and the Structure and Mechanism notes linked to the material records for insight into the trends you observe.

- Fillers increase the modulus but they also increase the density. What happens to the specific stiffness (modulus/density)? A chart of yield strength/density and Young's modulus/density reveals how these combinations of properties change with filler content.
- What do fillers do to the thermal properties of polymers? A chart of Thermal conductivity against Thermal expansion coefficient shows what happens.

3.4 Comparing natural and man-made materials using the Biological materials subset of the MaterialsUniverse data-table.



The materials of nature – wood, bone, shell, horn, for example – have properties that can compete with or exceed those of man-made materials. The Biological materials folder in the MaterialsUniverse data-table of the MS&E Package contains records for 88 of them.

What's in the Biological Materials subset? The categories of materials in the Biological materials folder are listed in Table 1. The mechanical, thermal and electrical properties in Biological materials records are the same as those in the rest of the MaterialsUniverse data-tables, allowing direct comparison of natural materials with those of engineering.

Table 1: Biological Materials (88 records)

Category	Examples
Molecular building blocks	Chitin, Collagen, Elastin, Lignin, Cellulose
Soft tissues	Artery, Cartilage, Horn, Skin, Tendon
Mineralised tissues	Antler, Bone, Coral, Egg-shell, Mollusc
Natural fibers	Cotton, Kenaf, Silk, Wool, Ramie, Silk
Woods and wood-like materials	Oak, Pine, Bamboo, Nut, Plywood, paper

What can you do with it? The ensemble enables a number of investigations. Here are a few:

- Retrieval of the properties of natural and man-made materials in a consistent framework.
- The construction of material property charts for both engineering and biological materials allowing direct comparison between them.
- Exploration of the ways in which the basic structural building blocks of the natural world (minerals, polysaccharides and proteins) combine to give exceptional performance.

Figures 19 and 20 illustrate what can be done with it. Tensile strength σ_{ts} and elastic modulus E are key properties for mechanical performance in both engineering design and in nature. The first of the two figures charts these properties for engineering materials. Each small bubble encloses the range of σ_{ts} and E for one material. Large envelopes enclose material classes: metals, polymers, elastomers, ceramics, and foams. In Figure 20 the same two properties for natural materials are plotted on the same axis-ranges. Again, the little bubbles describe single material-types while the larger envelopes enclose classes: biological materials and wood and wood-like materials.

Charts like these allow a direct comparison of the properties of natural and man-made materials. They can set the scene for discussions of bio-mimicry and for materials selection for medical applications. This pair shows that natural materials have properties that cover a range almost as large as those of the engineering materials we use today even though their chemical and structural make-up are very different. Any subset of the numeric properties in the database to be plotted and compared in this way. The quantity $U = \sigma_{ts}^2/E$ is a measure of the maximum elastic energy that the material can store –important in the design of springs and energy-absorbing structures. The contour (blue diagonal line) on Figures 19 and 20 lies at the value $U = 10 \text{ MJ/m}^3$. Materials above this line store more energy, those below, less. Among engineering materials elastomers (on the right) and high strength steels (on the left) have high values of U. Among natural materials elastin, collagen and keratin have high U; viscid spider silk is outstanding with higher U-values than any man-made material.

Mineralized tissue – bone, shell, tusk – are composites of hard, brittle minerals (calcite, aragonite, hydroxyapatite) cemented with a protein such as collagen. The resulting structural materials are remarkably tough and resistant to cracking. Resistance to crack propagation is measured, in engineering terms, by the fracture toughness K_{1c} . Toughness – ability to absorb impact – is measured by the toughness $G_{1c} = K_{1c}^2/E$. Toughness helps organisms survive the bumps and shocks of life and it has a defensive role; a tough shell is harder for a predator to penetrate than a shell that is brittle.

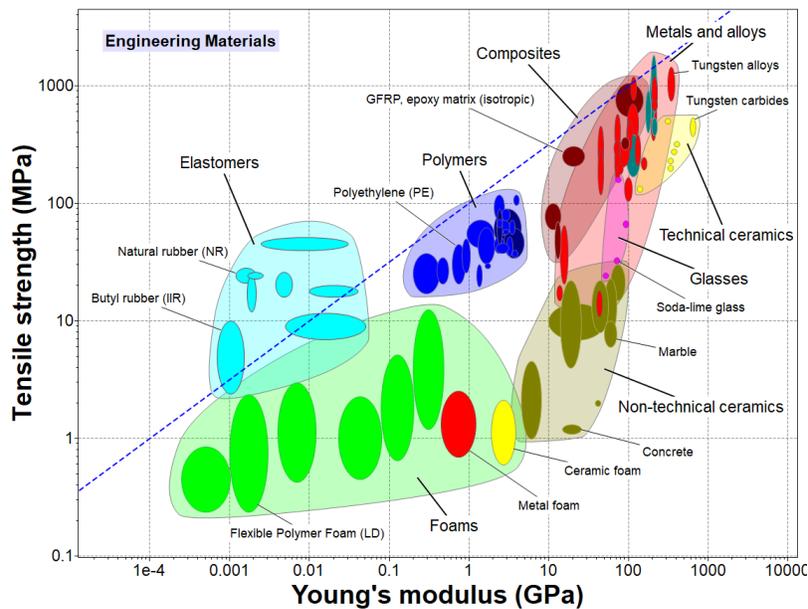


Figure 19: Strength σ_{ts} and modulus E of engineering materials, with a contour of maximum elastic energy storage, U_{max}

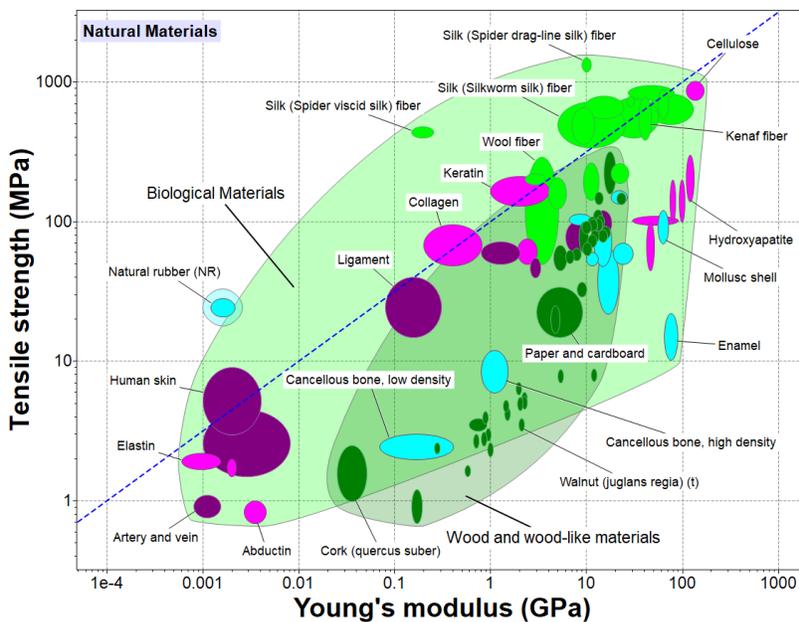


Figure 20: Strength σ_{ts} and modulus E of natural materials, with a contour of maximum elastic energy storage, U_{max}

Figure 21 is a chart with K_{1c} and E as axes for natural materials. Contours of G_{1c} plot as diagonal lines with a slope of 2 – one with a value of $G_{1c} = 0.1 \text{ kJ/m}^2$ is shown in blue. Antlers are used for fighting; a brittle antler is not a good idea. Antler, dense bone and dentine are between three and ten times more resistant to crack-propagation and ten to a hundred times tougher than the hydroxyapatite with which they are mineralized. Calcite, aragonite and hydroxyapatite lie well below the G_{1c} contour; mollusc shell, cortical bone and dentine, largely made up of these minerals, lie far above it. The gain in toughness derives from the way the mineral is deposited and configured in the tissue. More information and charts can be found

in two White Papers describing another pair of Granta EduPack databases devoted to biomaterials².

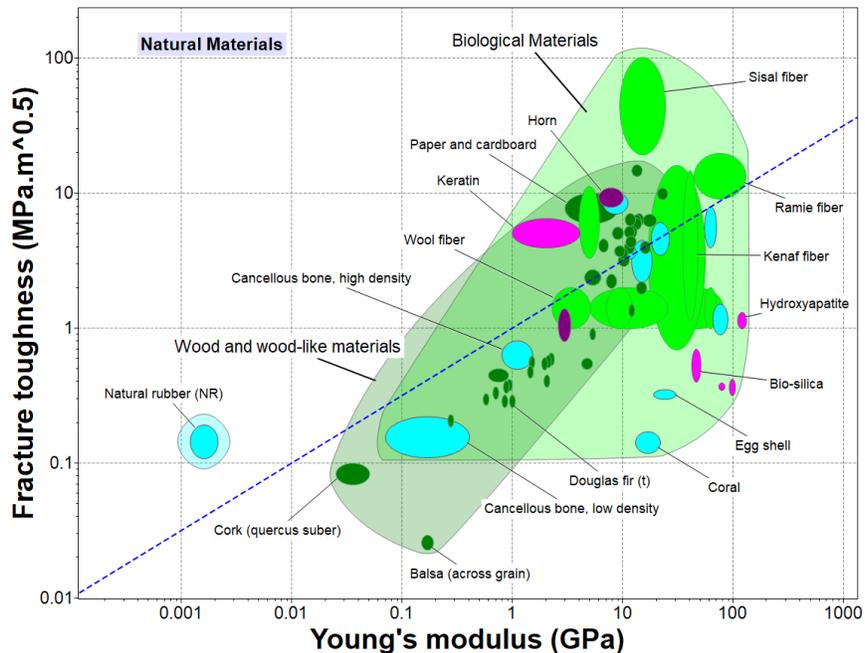


Figure 21: Fracture toughness K_{1c} and modulus E of natural materials with a contour of toughness, G_{1c}

Explore for yourself- filling and reinforcement of thermoplastic polymers

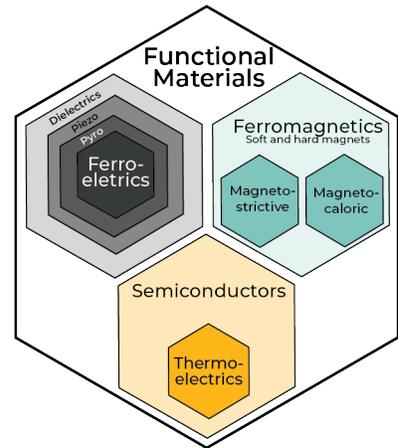
Use the MaterialsUniverse data-table to explore the following questions.

- How does the Young's modulus E for hard and soft woods depend on density ρ ? Make a chart with E on one axis and ρ on the other. Does the transverse (t) modulus – the one across the grain– depend on density in a different way from the longitudinal (l) modulus parallel to the grain? Fit a power law to each by plotting trial “display” lines onto the chart with slopes of 1 (a linear dependence), 2 (quadratic dependence) and 3 (cubic dependence) to see which best matches the data.
- It is sometimes claimed that spider drag-line silk is stronger than steel. Patented steel wire (“piano” wire) has a tensile strength σ_{ts} of 3800 MPa and a density ρ of 7900 kg/m³. Find data for these two properties from the record for drag-line silk to establish whether the claim is true. Do the claimants perhaps mean “stronger per unit weight” (σ_{ts}/ρ) rather than just “stronger” (σ_{ts})?
- Badly broken bones are often repaired with stainless steel implants. Ideally an implant should have properties that match those of bone as closely as possible. Compare the strength σ_{ts} and modulus E of stainless steel and cortical (dense) bone, drawing data from the database. Is there a good match? Can you suggest a better one?
- In nature, as in engineering, specific strength and stiffness (σ_{ts}/ρ and E/ρ) are more important than just strength and stiffness (σ_{ts} and E). (Here ρ is the density.) Make a pair of charts like those of Figures 19 and 20 for specific strength and stiffness and examine how natural and manmade materials now compare.
- Imagine yourself to be a 12th century Viking seeking light, tough materials to make shields to protect yourself while you pillage and plunder. “Tough” means high $G_{1c} = K_{1c}^2/E$, where K_{1c} is the fracture toughness and E is Young's modulus. “Light” means low density, ρ . Use the “Advanced” facility to make a chart of bio-materials with G_{1c} on the y-axis and ρ on the x-axis. Apply a selection line with a slope of 1 describing light, tough materials (G_{1c}/ρ) and use it to find the two best natural materials for shields. Then do a quick web-search to find out if these two materials were ever, in the past, used in this way.

²“The CES EduPack Bio Engineering Database. Part 1: Introduction to Biological and Bio-medical materials”, Mike Ashby, Ana G. Pereira-Medrano Granta Design, Cambridge (2015) and “The CES EduPack Bio Engineering Database. Part 2: Bio-derived materials and example applications”, Ana G. Pereira-Medrano, Mike Ashby and Harriet Crawford, Granta Design, Cambridge (2015)

3.5 Exploring functional properties with the Functional materials subset of the MaterialsUniverse data-table.

Although there is no standard definition of functional materials, it is commonly taken to mean materials with “interesting” properties that allow them to do more than simply support loads or conduct heat or electricity. Functional materials respond to applied stimuli in non-intuitive ways, for example generating a voltage when strained, or cooling on application of a magnetic field. Records for functional materials contain fields for properties that do not appear in the other records in the MaterialUniverse to capture these unusual characteristics.



What’s in the Functional Materials subset? Figure 22 lists the classes of functional materials that appear in it. The subset contains 46 records.

Figure 22: Classes of functional materials

What can you do with it? Here we give two examples of its use. Selecting magnetic materials. Two key characteristics of a magnetic material are its remanent induction, B_r , and its coercive field H_c (Figure 23). Soft magnetic materials have low coercive fields and narrow hysteresis loops. Hard magnetic materials have high remanence (making them powerful magnets) and high coercive fields (making them resistant to demagnetization).

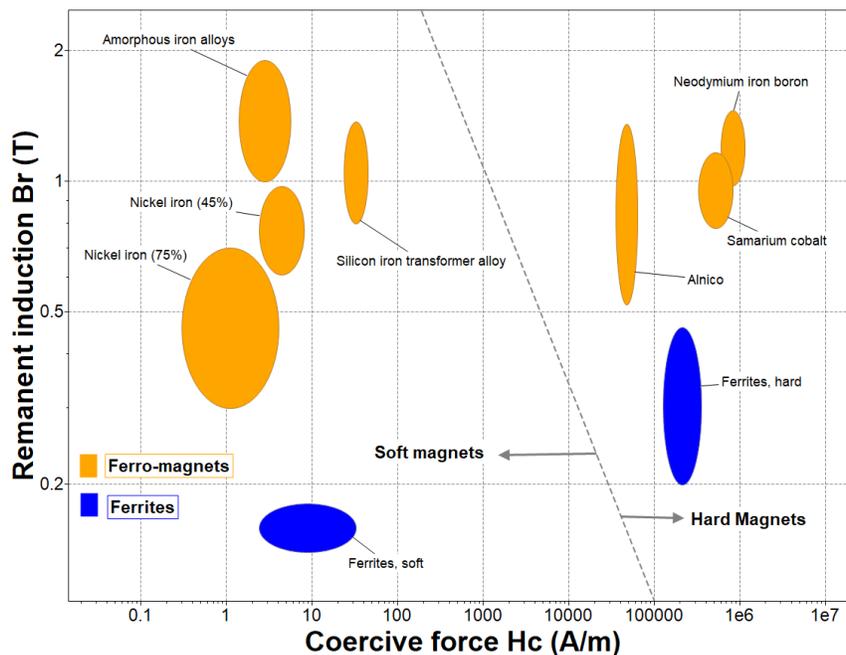


Figure 23: Remanent induction and coercive force for common magnetic materials. Soft magnetic materials lie on the left of the chart, hard magnetic materials on the right. (Made with the Functional materials subset of the MaterialUniverse data-table.)

Neodymium-iron-boron alloys have the best combination of hard (permanent) magnetic properties, followed by Samarium-cobalt, and, significantly less good, the Alnicos. Soft magnetic materials are used for transformer cores and electromagnets, where they are used to trap and guide magnetic flux. Materials

for these applications are chosen to have a large permeability, giving large inductance for a given applied magnetic field— amorphous iron alloys and silicon-iron are particularly good. Eddy currents induced in the core by the magnetic field cause energy loss through resistive heating. Eddy currents, are reduced by high resistivity. Here the ferrites, in blue on Figure 23, are a good choice.

Thermo-electric materials. To provide power a thermoelectric material must have a high Seebeck coefficient S to generate a voltage, a high electrical conductivity κ_e to reduce resistive losses and a low thermal conductivity λ to maintain a steep temperature gradient between the hot and cold side of the generator. This combination is captured by the figure of merit, zT :

$$zT = \frac{S^2 \kappa_e}{\lambda} T$$

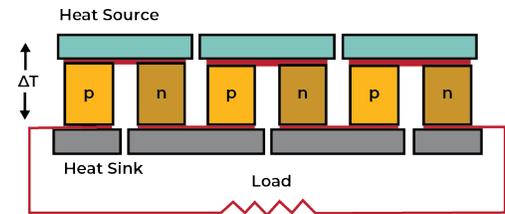


Figure 24: Schematic multicouple thermoelectric generator

where T is the mean temperature at which the device operates. Good materials for thermoelectric applications combine a large Seebeck coefficient with high electrical conductivity and low thermal conductivity – a combination not easily achieved. All the material properties in this expression for zT depend on temperature, so the best choice of material depends on the temperature of the heat source. Figure 25 shows two properties of these properties – λ and κ_e – for common materials. Metals lie along a straight line of slope 1 (the Wiedemann-Franz law). Good thermoelectrics, shown in purple, lie at the lower right. More examples of the use of the Functional materials data can be found in the White paper.

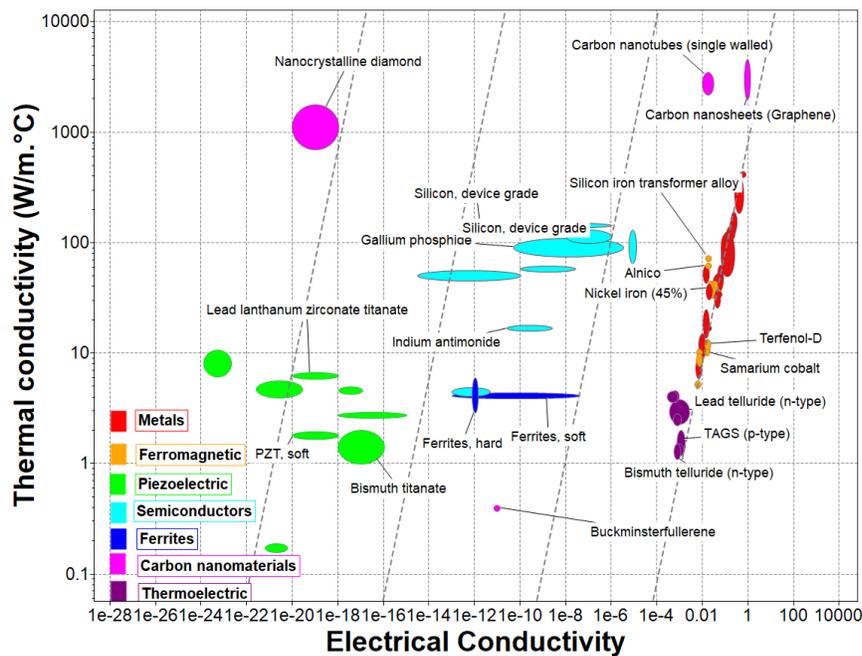


Figure 25: Thermal and electrical conductivity. The line of slope 1 marks the Wiedemann-Franz law. Good thermoelectric materials (in purple) lie at the lower right. (Made with the MaterialUniverse data-table.)

Explore for yourself- exploring functional materials

Use the MaterialsUniverse data-table to explore the following questions.

- What are magnetostrictive materials and what are they used for? Use the Search facility to extract records for magnetostrictive materials to find out.
- What are magnetocaloric materials and what are they used for? Select the MaterialUniverse data-table, open a Limit stage and click on “Magnetocaloric” under the heading “Functional materials” to find out.
- What are pyroelectric materials and what are they used for? Use the Search facility to extract records for pyroelectric materials to find out.
- Efficient transformers and electric motors rely on soft magnets with high saturation magnetisation and high permeability. What are the best choices for these applications? Make a chart with saturation magnetisation on the y-axis and maximum permeability on the x-axis to find out.
- The figure of merit for thermoelectric materials takes the form Thus good thermoelectrics combine a high

$$zT = \frac{S^2 \kappa_e}{\lambda} T$$

Seebeck coefficient S with a high conductivity ratio κ_e/λ . Make a chart with S on the y-axis and κ_e/λ on the x-axis to identify and rank good thermoelectric materials.

4. The Phase Diagram data-table, Interactive tools and Teach Yourself Unit

Clicking on the Phase Diagram icon on the home page gives access to a set of interactive resources that illustrates their use:



- A library of most-used phase diagrams
- A glossary tool that explains the meaning of terms that appear on phase diagrams
- A tool illustrating phase structure at the atomic level
- A tool tracking the evolution of microstructure down chosen cooling paths
- A tool illustrating the Lever Rule.

A phase (α -brass, for instance) is a chemically and physically uniform part of a system. It is made up of one or more components – distinct chemical species (copper, Cu, and zinc, Zn, for example). Distinct phases meet at phase boundaries where there is a discontinuity in composition or structure or both.

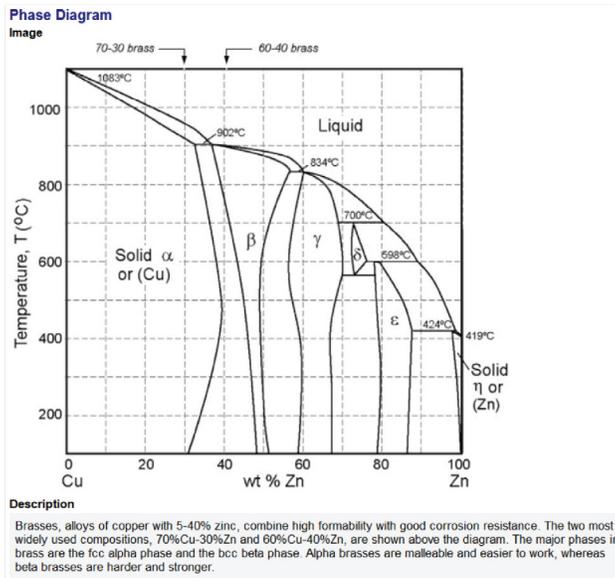


Figure 26: Granta EduPack Phase Diagram for the copper zinc system.

A phase diagram is a map in composition-temperature space of the regions of stability of the phases that co-exist in equilibrium for a system made up of two or more components. The Granta EduPack MS&E package contains records for 12 common phase diagrams, typifying the most important features. Figure 26 is an example, here for the Cu-Zn system that includes common brasses. Each diagram is linked to the records for its constituents in the Elements data-table (here, Copper and Zinc) and to the records for prominent alloys that appear on it in the Level 2 MaterialsUniverse (here, Brass). The diagrams can be copied and used for educational purposes.

Structure at the atomic level is illustrated by three interactive diagrams (Cu-Ni, Ph-Sn and Fe-C) with schematics that appear when the user clicks on a phase-field (Figure 27). The evolution of microstructure down selected cooling paths on the same three diagrams appears as the user drags the cursor down the path (Figure 28). An interactive Lever Rule tool calculates the composition of the liquid and solid phases on a cooling path of a schematic A-B phase diagram; boxes on the diagram list the composition and weight-fraction of each phase, updating as the point on the cooling path is changed (Figure 29).

Teach Yourself Phase Diagrams. Learning how to read and interpret phase diagrams is best achieved through practice. The Granta EduPack includes a comprehensive on-line Teach Yourself unit on Phase Diagrams and Phase Transformations³. This can be reached from within the Granta EduPack software via the Learn button on the main toolbar.

The unit has eight parts (Figure 30). The first four progress from an introduction to the terminology (“Component”, “Phase”, “Liquidus” etc.) to simple diagrams (Cu-Ni, Pb-Sn), the Lever rule, intermediate phases (Al-Cu) and the Iron-Carbon and other more complex systems. The remaining four introduce ideas of phase transformations: nucleation and growth in the liquid and solid state, the eutectic and eutectoid reactions, deviations from equilibrium and TTT diagrams. Each part ends with exercises with worked solutions. The unit can be copied and distributed for educational purposes.³

³ Also available in Materials: Engineering, Science, Processing and Design, 3rd edition, Butterworth-Heinemann, Oxford, UK. ISBN-13: 978-0-08-097773-7, North American Edition: ISBN-13: 978-1-85617-743-6, Ashby, M. Shercliff, H. and Cebon, D. (2014)

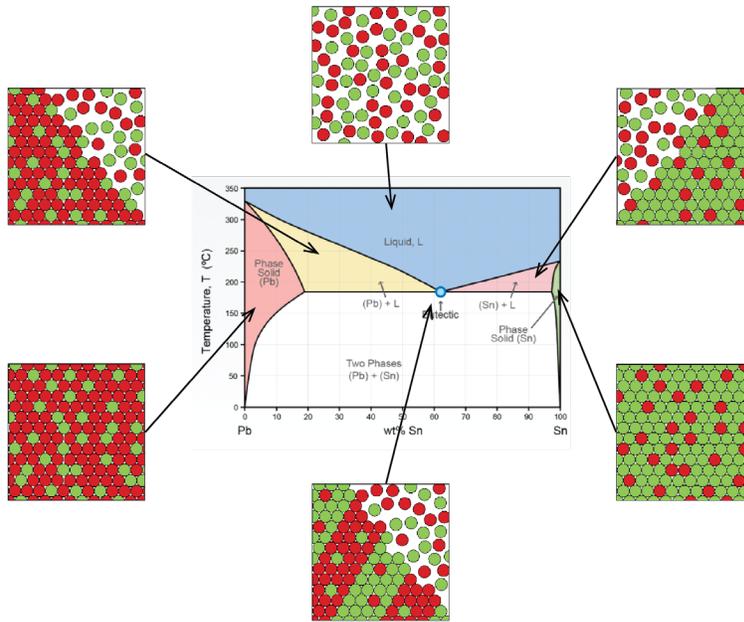


Figure 27: Interactive tool suggesting structure at atomic level

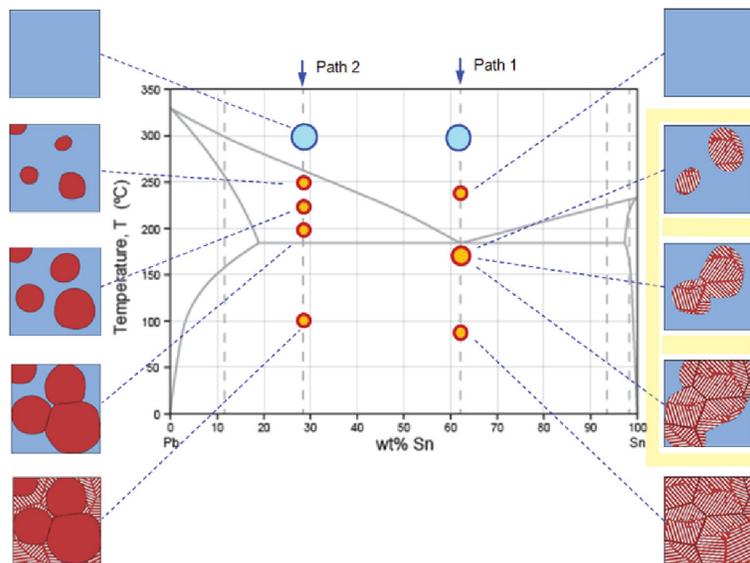


Figure 28: Interactive tool suggesting microstructure evolution on a series of cooling paths

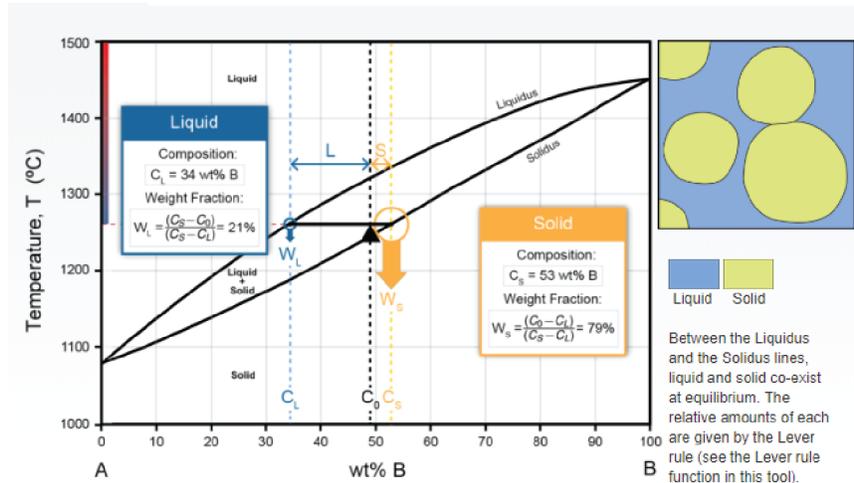
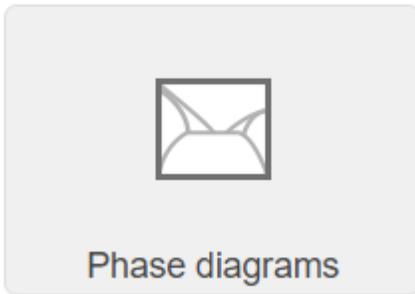


Figure 29: Interactive tool illustrating the Lever rule

Contents



- Part 1: Key terminology
- Part 2: Simple phase diagrams, and how to read them
- Part 3: The iron-carbon diagram
- Part 4: Interpreting more complex phase diagrams
- Part 5: Phase transformations and microstructural evolution
- Part 6: Equilibrium solidification
- Part 7: Equilibrium solid-state phase changes
- Part 8: Non-equilibrium solid-state phase changes

Figure 30: The contents of the Teach Yourself Phase Diagram Unit

5. Additional resources – Science notes

The links on the lower left of the Home page (Figure 3) give access to three sets of Science Notes. These are text files with illustrative schematics explaining the meaning and physical background of attributes in the Database.

Material Science notes define the properties that appear in the records of the Materials data-table with descriptions of their physical origins. That for “Young’s modulus”, for example, explains what it is, how it is measured and how it relates to interatomic bonding.

Process Science notes explain the meaning of the process attributes that appear in the Process data-table. That for “Material compatibility”, for instance, explains why some processes work well with some materials but not with others; that for “Cost modeling” explains how the cost model in the data-table works.

Structure Science notes are a little different. As the tetrahedron of Figure 1 suggests, processing, microstructure and properties are closely linked. The microstructure-sensitive properties described in Section 3.3, particularly, are manipulated by control of structure through processing. But what do we mean by “microstructure”? And what is the underlying mechanism that links it to “properties”? The Structure Science notes are a set of eight 2-page portraits of microstructural features and the mechanisms that link them to properties. They cover

- Solid solution strengthening
- Strain hardening
- Precipitation and dispersion strengthening
- Grain-size strengthening
- Toughening
- Electron scattering
- Phonon scattering
- Domain-wall pinning

Each set gives background about the mechanism, a schematic explains its structural features and, where appropriate, a microstructure of a material that exploits it.

6. Summary and Conclusions

The macroscopic properties of materials derive from their structure at the nuclear, atomic, micron and millimeter levels. The Granta EduPack Materials Science and Engineering Package is an assembly of resources to support University-level teaching about materials across this wide range of structural scales and about the ways in which material properties are controlled by processing. The central component of the Package is a set of linked data-tables (so called to distinguish them from the database as a whole), with the following features.

- **The Elements data-table** provides data for the elements of the Periodic Table at the nuclear and atomic levels, including electronic structure and electronegativity, crystal structure, physical, mechanical, thermal and electrical properties and environmental data.
- **The Materials data-table** focuses on engineering materials, characterizing 158 of the most widely used alloys, polymers, elastomers, ceramics, glasses and biological materials. Each record is linked to those for the element of which it is composed, allowing fast downward access to underlying basics at the atomic scale. The records themselves list typical applications of the material with images of products that contain it, giving upward connections to the macroscopic scale.
- **The Process data-table** introduces student to processing methods via records for 116 shaping, joining and finishing processes. These, too, are illustrated with schematics and images of the process or products made by using it. The process records are linked in turn to the engineering materials to which they can be applied.
- **The Process-Property Profile data-table** illustrates control of properties through processing. It contains sets of records for a single material-type in different processed states, chosen because they illustrate how alloying, heat-treatment, mechanical working and – in the case of polymers – blending and reinforcement influence properties. They illustrate the need for trade-offs: a process that raises strength, for instance, may cause a decrease in toughness, a loss of ductility and a decline in thermal and electrical conductivity.
- **The Phase Diagram data-table** contains a set of the most commonly encountered phase diagrams. It is supported by a simple interactive Phase Diagram tool that illustrates through schematics the equilibrium structures associated with different points on a simple phase diagram and introduces the user to the Lever rule.

Each part of the package is further supported with linked **Science notes** that provide scientific underpinning for the material properties and process attributes that appear in it.

This **White Paper** introduces the Granta EduPack Materials Science and Engineering Package and illustrates what it can do. It can do a great deal. The White Paper contains links to 10 more specialized White Papers that provide greater depth, more detailed illustrations and worked Case Studies than can be included here.

7. References

Materials Science texts

Ashby, M. Shercliff, H. and Cebon, D. (2014), *Materials: Engineering, Science, Processing and Design*, 3rd edition, Butterworth-Heinemann, Oxford, UK. ISBN-13: 978-0-08-097773-7, North American Edition: ISBN-13: 978-1-85617-743-6. (An introductory text taking a top-down approach to teaching MS&E.)

Askeland, D.R., Phulé, P.P. and Wright W.J. (2010) *The Science and Engineering of Materials*, 6th edition, Thomson, Toronto, Canada. ISBN 9780495296027. (A well-established materials text that deals well with the science of engineering materials.)

Budinski, K.G. and Budinski, M.K. (2010) “*Engineering materials, properties and selection*”, 9th edition, Prentice Hall, NY, USA. ISBN 978-0-13-712842-6. (Like Askeland, this is a well-established materials text that deals well with both material properties and processes.)

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Shackelford, J.F. (2014) “*Introduction to materials science for engineers*”, 8th edition, Prentice Hall, NJ, USA. ISBN 978-0133789713 . (A well-established materials text with a material and a design slant.)

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ANSYS, Inc.
Southpointe
2600 Ansys Drive
Canonsburg, PA 15317
U.S.A.
724.746.3304
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