Granta EduPack MicroProjects + Solutions

Materials Science and Engineering

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These ***MicroProjects*** are short investigations that can be completed in less than an hour. Each poses a set of questions that can be answered using the Granta EduPack Material Science and Engineering (MS&E) database. The database needed for each project will be highlighted at the top. All start at a level that is readily accessible, using the SEARCH function to find records, creating charts using the CHART/SELECT function, and extracting relevant data from a Record and its linked SCIENCE NOTES. Hints in gray help with any difficult step.

Each MicroProject has an attached Discussion Point – a challenge to go further – highlighted in red and separated from the MicroProject by this separator:

The Discussion Point poses a question linked to or arising from the MicroProject. Responding to the Discussion point requires independent thought and research, takes longer, but is rewarding if followed. It is an add-on for more advanced study.

Each MicroProject and its Discussion point has a fully worked Sample Response, available to the instructor. The charts shown in the responses are reproduced here exactly as produced by Granta EduPack.

Example Use: In-class activities, homework assignments, activity to introduce students to functionalities of Granta EduPack

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MS&E MicroProject #1

Zirconia, a ceramic that thinks it's a metal

Database: MS&E

- What is Zirconia? (Use the Search facility to find the record. To copy and reuse text and images from a record: right click on the opened record, select Copy, then open WORD and Paste. The entire record is pasted into WORD. You can then copy and re-paste the bits you want for a report.)

- What makes it special among ceramics? (Explore the record to find out.)

- What is the value of its Fracture toughness?

- How does this compare with the Fracture toughness of other ceramics? Make a bar-chart of Fracture toughness for Technical ceramics to find out. (When you open the "Materials" data-table of the MS&E DB, a set of panels, each labeled with a sub-set of materials, appears on the right. One panel says "Technical Ceramics". Clicking on that limits the selection and charts to technical ceramics.)

- Reset the scale from log to linear and adjust its range to run from 0 to 10. (To make the changes, double click on the axis name to re-open the Axis Settings box, select "Linear" and adjust the range.)

- What does "Fracture toughness" measure? (Try the information ("i") link next to the property name on any materials record to access Science notes.)

Discussion Point

What gives Zirconia its unusual Fracture toughness?

Specimen Response

What is Zirconia? (information from the Zirconia record)

Zirconia is a technical ceramic, zirconium dioxide, ZrO_2, usually with additions of Y_2O_3, MgO and other oxides to increase toughness.

In makes it special among ceramics? (From the Zirconia record)

Zirconia, ZrO_2, is a ceramic with an exceptionally high melting point -- 2760ºC when pure. It has the highest useful strength and toughness at room temperature of all the readily available ceramics.

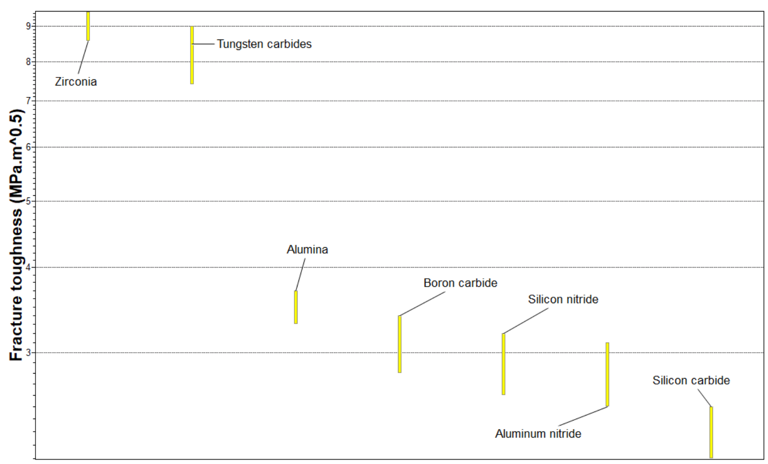
What is its Fracture toughness?

The fracture toughness of zirconia is 6 – 8 $MPa.m^{1/2}$.

How does this compare with the Fracture toughness of other ceramics?

The chart shows that Zirconia has the highest fracture toughness of all technical ceramics.

What does "Fracture toughness" measure? (From the Science note for Fracture toughness.)



The fracture toughness, K_{1c} (units: MPa $m^{1/2}$ or $MN/m^{1/2}$) measures the resistance of a material to the propagation of a crack.

Discussion point: What gives Zirconia its unusual Fracture toughness?

(1) From the Granta EduPack record for Zirconia. The exceptional toughness is imparted by transformation toughening: a change in crystal structure from tetragonal to monoclinic, with an associated change in volume of the ZrO2 crystals when subjected to stress at a crack tip. The volume expansion squeezes the crack shut, impeding crack growth.

(2) Paraphrased from a web search on "What makes zirconia tough?".
Zirconia is monoclinic at room temperature, then tetragonal and finally cubic at high temperature. When stabilized with yttria, Y2O3, the cubic phase is retained to room temperature; if partially stabilized, some reverts to tetragonal. The stress field of an approaching crack makes the tetragonal phase revert to monoclinic with a volume expansion of about 4%, clamping the crack shut.
http://www.ceramcoceramics.com/materials/zirconia/zirconia.php

MS&E MicroProject #2

Are biopolymers really greener than oil-based plastics?

Database: MS&E

- What is PLA? (Use the Search facility to find the record for PLA. You can copy text and images from the record. To do so, open the record, right-click and copy – the entire record is copied – then paste into WORD – the whole record appears. Select and copy the bits you want to paste into a report.)

- What is PLA made from if it isn't oil? (Explore the record to find out.)

- What is PLA used for? (Explore the record to find out.)

- Are there other commercial biopolymers? (Use the Search facility to find records containing the word Biopolymer.)

- Are all biopolymers bio-degradable? (Open a Limit stage, go to "Material recycling: energy, CO2 and Recycle fraction" (right at the bottom of the list) and click on Biodegrade. Add a Tree stage to limit the selection to Polymers and Elastomers. Which biopolymers pass?)

- Are the CO2 footprints for primary production of biopolymers less than that of polystyrene, with which they compete for packaging? To find out, make a bar-chart of "CO2 footprint, primary production" with biopolymers and polystyrene on it. Use a linear scale for CO2 footprint. (You can limit the bar chart to the materials you want to study by clicking on Chart/Select – Select from: "Custom – Define your own subset", then selecting the materials you want on the chart. To change to a linear scale: double click on the axis label to expose the Axis Settings, and select Linear.)

- Are biopolymers cheaper than polystyrene? Make a bar chart of Price per kg for the same subset of materials. Use a linear scale for Price.

Discussion Point

The projected production of PLA is expected to rise to 1 million tonnes per year by 2020. If 7.5 m2 of fertile land are needed to provide feedstock for 1 kg of PLA, what area (in km2) will be required to support the 2020 production? How does that compare with the area of country or State in which you live?

Specimen Response

What is PLA?

PLA is Polylactide, a thermoplastic biopolymer. It is biodegradable (not all biopolymers are) and has properties that resemble those of polystyrene (PS).

What is PLA made from if it isn't oil?

In the US, PLA is made from corn, maize or milk; in Brazil it is made from sugar cane; in Asia it is made from tapioca. All require fertile agricultural land for their growth.

What is PLA used for?

The record lists: Food packaging, plastic bags, plant pots, diapers, bottles, cold drink cups, sheet and film.

Other commercial biopolymers?

A search on "Biopolymer" gives the following list.

- Starch-based thermoplastics (TPS)
- Cellulose acetate (CA)
- Natural rubber (NR)
- Lignin
- Polylactide (PLA)
- Polyhydroxyalkanoates (PHA, PHB)

Are they all biopolymers bio-degradable?

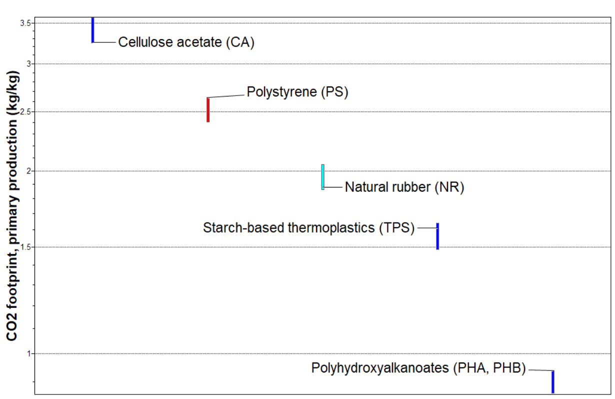
No. Three out of the five biopolymers in the database are biodegradable. Two – Cellulose acetate (CA) and Natural rubber (NR) – are not.

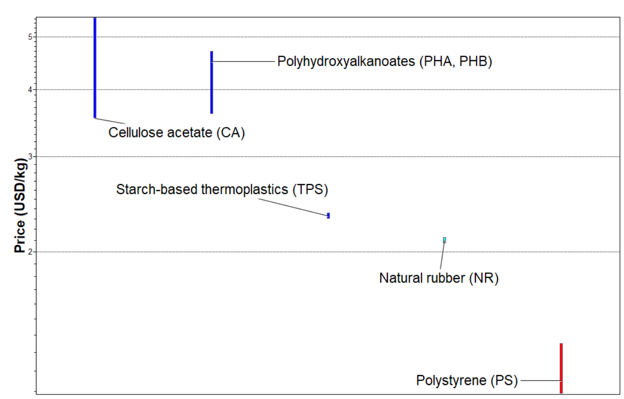
Are the carbon footprints of biopolymers less than that of polystyrene?

CA has the highest CO_2 footprint, followed by polystyrene and natural rubber. Natural rubber (NR) and Starch-based thermoplastics (TPS) have a lower CO2 footprint bar chart Polystyrene.

Are biopolymers cheaper than polystyrene?

The bar chart shows that Polystyrene is less expensive that almost all the biopolymers





Discussion point: Land-area to provide feedstock for PLA

1 million tonnes (109 kg) of PLA requires a land area of (7.5 x 109/106) = 7,500 km2. For comparison, the area of the Netherlands is 41,000 km2, and that of the State of Connecticut is 14,000 km2. Biopolymers based on crops thus use a great deal of land that could be used for crops or livestock. Efforts are underway to make biopolymers from food waste rather than from cultivated crops.

Points for further discussion.

- The "food-versus-fuel" discussion, centered on biofuels, is equally relevant for biopolymers.

- The "biodegrade-versus-recycle" discussion: biodegrading destroys the material, recycling conserves it, so it's better to recycle. See particularly http://www.rsc.org/Education/Teachers/Resources/Inspirational/resources/6.1.3.pdf

- The distinction between true biopolymers (the molecule is biological in origin) and drop-in bioplastics (the biological material is fermented to ethanol or methanol, which is then used feedstock for polyethylene, polypropylene or PET.

- PLA can be used for Additive manufacture (3-D printing) – see Micro-project 8.

MS&E MicroProject #3

Nichrome - the glowing heart of dryers and toasters

Database: MS&E

- What is Nichrome? What is its composition? What, typically, is it used for? (Use the Search facility to find the record. To copy text or images from the record, open it, right-click and copy – the entire record is copied – paste into WORD, then select and copy what you want to paste into a report)

- What is its Maximum Service Temperature range?

- What does "Maximum service temperature" measure? (Try the information ("i") link next to the property name on any materials record to access Science notes.)

- How does the Maximum service temperature of Nichrome compare with that of other metals? Make a bar-chart of this property, limiting it to metals. (When you open the "Materials" data-table of the on the Home page and click on Chart/Select you are prompted to Select a subset. Choose "Custom: Define your own subset", then use the panel that appears to select just "Metals and Alloys").

- Compare the prices of the three metals with the highest maximum service temperatures. (Price per kg appears in the record for each material. To choose the currency, go to Settings – Units – Preferred currency.)

Discussion Point

Which alloying elements impart high temperature oxidation resistance? How do they do it?

Specimen Response

Nichrome (information from the record for Nickel-chromium alloys)

Nichrome is a trade name for an alloy of nickel and chromium, sometimes with some iron, typically Ni + 10 to 30% Cr + 0 to 10% Fe. Typical uses of Nichrome include heating elements and furnace windings, bi-metallic strips, thermocouples, springs, food processing equipment, chemical engineering equipment.

Maximum service temperature range

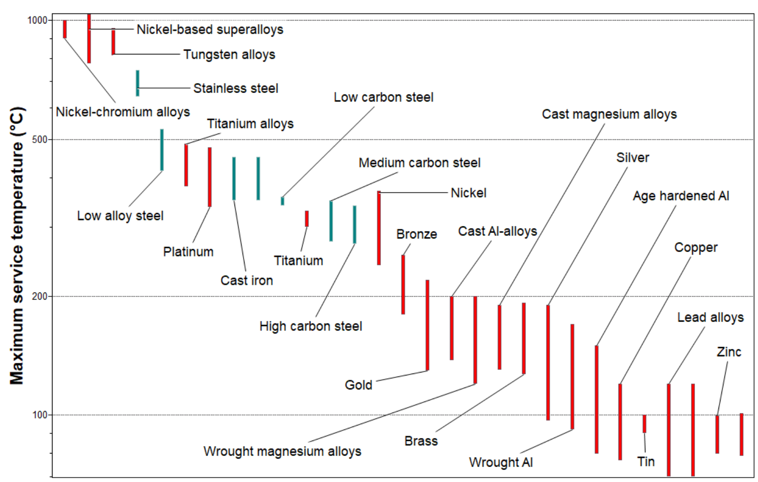
The maximum service temperature of Nichrome is 900 – 1000ºC

What does "Maximum service temperature" measure?

The maximum service temperature is the highest temperature at which the material can reasonably be used without oxidation, chemical change or excessive deflection or "creep" becoming a problem.

Maximum service temperature of Nichrome compared with other metals

The bar chart looks like this. Nickel-chromium alloys (Nichromes) have maximum service temperatures that are higher than almost all other metals, accounting for their use as heating elements.



Prices per kg of the three materials with highest maximum service temperature (retrieved from their records)

- Nichrome $13.30-16.80 per kg
- Nickel-based super alloys $15.60-18.70 per kg
- Tungsten alloys $62.10-68.70 per kg

Nichrome is the cheapest.

Nichrome resist oxidation in air at high temperatures?

The chromium provides resistance to corrosion and oxidation by creating a surface film of Cr_20_3, the same film that makes stainless steel stainless.

Discussion point: Imparting oxidation resistance

(1) Cut and pasted from a web search on “Alloying for oxidation resistance”.
“Increased contents of chromium (Cr), silicon (Si) and aluminum (Al) increase the resistance to oxidation. The addition of rare earth metals and reactive elements such as titanium (Ti), zirconium (Zr) and yttrium (Y) has a highly positive effect on oxidation resistance.”
http://smt.sandvik.com/en/materials-center/corrosion/high-temperature-corrosion/oxidation/

(2) To get further you have to go to text books. Here is an abstract from “Materials: Engineering, Science, Processing and Design” Chapter 17, section 17.4. ISBN 978-0-08-097773-7.
“The oxides chromium (Cr_2O_3), of aluminum (Al_2O_3), of titanium (TiO_2) and of silicon (SiO_2) have high melting points, so the diffusion of either the metal or oxygen through them is slow. The result: the oxide stops growing when it is a few molecules thick. If enough chromium, aluminum, titanium or silicon can be dissolved in a metal like iron or nickel – ‘enough’ means 18 to 20% – a similar protective oxide grows on the alloy. If the oxide is damaged, more of the alloying element immediately oxidizes, repairing the damage. Stainless steels (typical composition Fe–18% Cr–8% Ni), widely used for high-temperature equipment, and Nichromes (nickel with 10 to 30% chromium), used for heating elements, get their oxidation resistance in this way; so too do the aluminum bronzes (copper with 10% aluminum), and high-silicon cast irons (iron with 16–18% silicon).

MS&E MicroProject #4

Is spider silk really stronger than steel?

Database: MS&E

- Spider silk is a natural fiber. Spiders webs use strong, relatively stiff silk for the radial "drag-line" strands and a more compliant, resilient "viscid" silk for the circumferential strands. It is sometimes claimed that spider drag-line silk is stronger than steel. To get an overview of the strength and modulus of natural and man-made fibers, make a chart with Tensile strength on the y-axis and Young's Modulus E on the x-axis. (Use a Tree stage to isolate "Natural fibers" and "Man-made fibers", removing all other materials from the chart. Create the chart and add envelopes for Natural and Man-made fibers by clicking on Show family envelopes in the tool-bar across the top of the chart.)

- Label the materials on the chart. "Patented" steel wire (Piano wire) and Spider drag-line silk appear on it. Recolor the steel red to distinguish it from all the others. Is drag-line silk stronger than steel? Is it stiffer, meaning a higher Young's modulus? (To recolor: Right click on the record name on the chart and select "Record Color".)

- Is it possible that the more accurate statement is that spider silk is stronger than steel per unit weight σ_{ts}/ρ("Specific strength") where ρ is the density? Make a new chart with σ_{ts}/ρ on the y-axis and E/ρ on the x-axis. Does drag-line silk have higher specific strength than steel piano wire? (Use the Advanced option in the Axis choice window to create the functions of properties.)

- Which fiber has the highest specific strength? What is it used for?

Discussion Point

Parachutes are made of strong, light fibers. Long ago they were made of cotton, then silk-worm silk, then nylon, then Terylene, now Kevlar* or even Zylon, a polyoxazole.

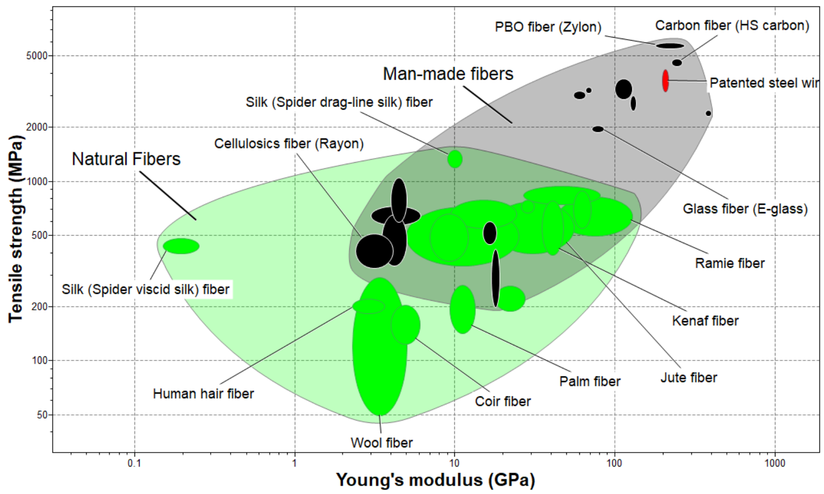
Color all the parachute materials purple in your specific strength plot. What commentary can you make about their evolution over time?

https://www.azom.com/article.aspx?ArticleID=10429

Specimen Response

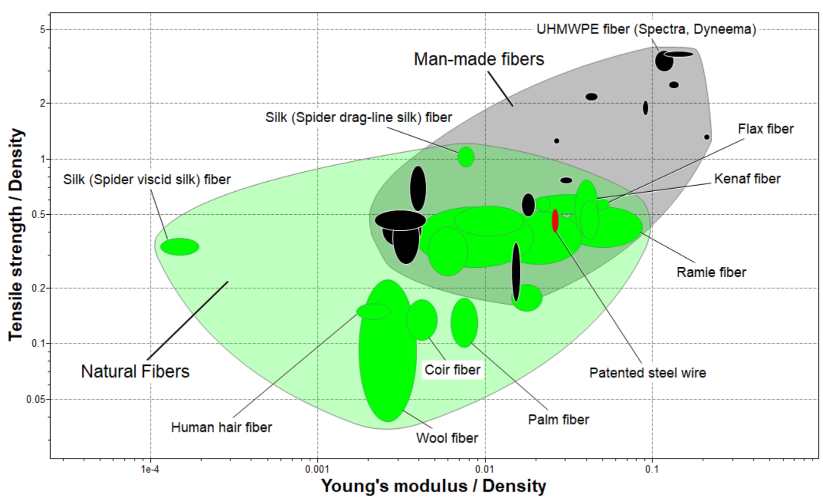
Tensile strength and modulus chart for fibers

The Tensile strength - Modulus chart looks like this. Spider drag-line is the strongest of the natural fibers but the steel wire is twice as strong and twenty times stiffer.



Should it be Strength per unit weight?

A chart of specific strength σ_{ts}/ρ and specific modulus E/ρ (strength per unit weight and modulus per unit weight) looks like this. Now the picture has changed. Drag-line silk, and even flax fibers, are stronger per unit weight than the strongest steel.

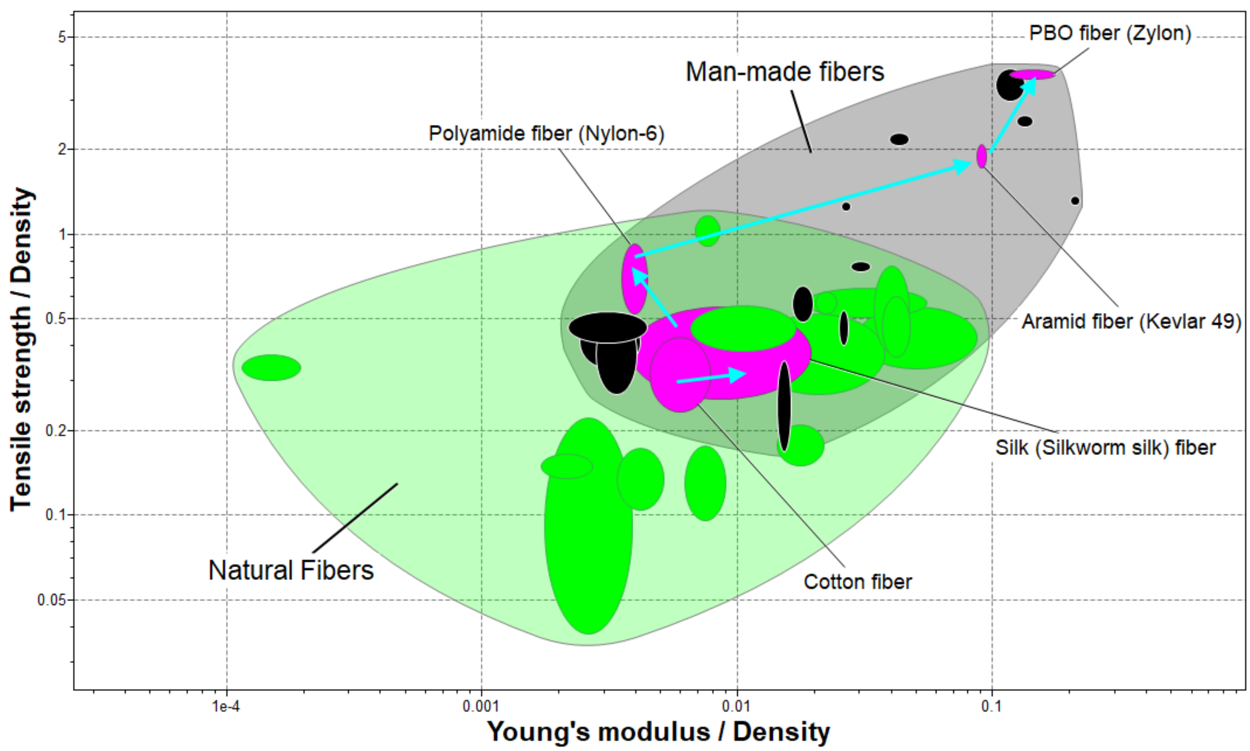


The fiber with the highest specific strength

The fiber with the highest specific strength is Spectra (high strength, gel-spun polyethylene). Its applications are listed as: Ballistic vests; Helmets; Armored vehicles; Sailcloth; Fishing lines; Marine cordage and lifting slings; and Cut-resistant gloves and safety apparel.

Discussion point. Parachute materials.

The chart shows the progressive improvement of the properties of parachute fibers with Nylon, Terylene and Zylon added. The parachute materials are colored purple and the arrows show the progression over time.



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MS&E MicroProject #5

What's special about egg shell?

Database: MS&E

- What is the shell of an egg made of? (Use the Search facility to find the record. You can copy text and images from the record. To do so, open the record, right-click and copy – the entire record is copied – then paste into WORD – the whole record appears. Select and copy the bits you want to paste into a report.)

- What is the fracture toughness of egg shell? What is its Young's modulus? (Open the Materials data-table and locate the Biological Materials folder. You will find "Egg shell" in the folder for "Tissue, Mineralized".)

- How does the fracture toughness of egg shell compare with that of other mineralized tissues? Make a bar-chart of fracture toughness for mineralized tissues and to find out. (Use a Tree stage to isolate "Tissue, Mineralized" in the Biological Materials folder, removing all other materials from the chart. Convert the default logarithmic scale for Fracture toughness to a linear one by double clicking on the axis name and selecting "Linear".)

- Make the same comparison for Young's Modulus.

- Why might fracture toughness and modulus be relevant property for the shell of an egg?

Discussion Point

Measuring the mechanical properties of thin, curved shells is not easy. How has the fracture toughness of eggshell been measured? What was the experimental set up? How do you apply controlled loads to the shell without destroying it?

Specimen Response

What is the shell of an egg made of? (copied from the record)

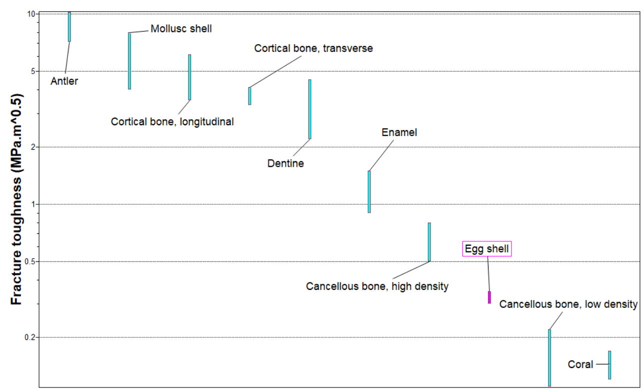
Egg shell is calcite, calcium carbonate. It is porous to allow air to reach the developing bird. Egg shell is composed of four layers. From inside out, these are the cone, the plaisade, the vertical crystal layer and the cuticle. The crystal layer is a thin layer just beneath the cuticle, a protein. The main structural layer is the plaisade, made of calcium carbonate.

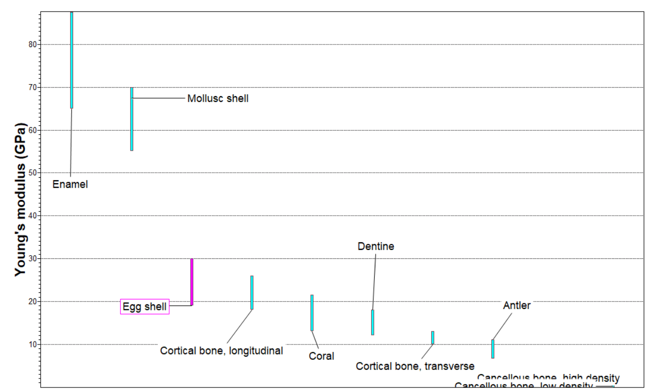
What is the fracture toughness of egg shell?

The fracture toughness of egg shell = 0.3 – 0.35 MPa.m$^{1/2}$. Its Young's modulus is 19 – 30 GPa.

The fracture toughness of egg shell compared to other mineralized tissues

The bar-chart is shown on the left. Egg shell has a very low fracture toughness compared to dense (cortical) bone, shell, tooth (dentine, enamel) or antler





The Young's modulus of egg shell compared to other mineralized tissues

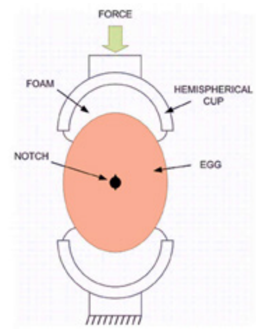
The bar-chart is shown on the right. Egg shell has a relatively high Young's modulus.

Why might fracture toughness and modulus be relevant property for the shell of an egg?

The fracture toughness of egg shell must be low to allow the chick to break its way out when it hatches. The modulus determines the stiffness of the shell – its relatively high stiffness allows the shell to retain its shape when loaded by a sitting hen.

Discussion point. Measuring the fracture toughness of eggshell

Taylor (1,2) and Meyers (3) report an experimental method for measuring the fracture toughness of egg shell. A small hole is drilled into the egg at its equator. A starter-crack is cut at the north and south poles of the hole with a scalpel. The egg is loaded with hemispherical cups (Taylor used wooden egg cups) lined with plastic foam to distribute the load evenly.



When a thin spherical (or nearly spherical) shell is loaded in this way, the stress state at the equator parallel to the loading direction is compressive, and that at right angles to the loading direction is tensile. If you know the thickness of the shell, you can calculate the stress. In the test, the egg is loaded until the starter-crack at the hole suddenly extends. The fracture toughness is calculated from this critical load.

"The fracture toughness of eggshell" Taylor, D., Walsh, M., Cullen, A. and O'Reilly, P., Acta Biomaterialia, Vol 37, (2016) 21-27.

(1) https://www.researchgate.net/publication/301643291_The_Fracture_Toughness_of_Eggshell

(2) https://www.researchgate.net/publication/305623802_Fracture_Mechanics_in_Biology_and_Medicine

(3) http://meyersgroup.ucsd.edu/papers/journals/Meyers%20426.pdf

MS&E MicroProject #6

Materials for acoustic guitars

Database: MS&E

There are two types of acoustic guitars: the classical guitar and the folk guitar. Both have wooden bodies. The classical guitar has nylon strings, but the folk guitar is different – it has metal strings.

- Which wood for the body? SEARCH on “Guitar” to find out. Why does the same wood appear twice in the search results?

- The modulus and the mechanical loss coefficient are key property for the bodies of musical instruments. Modulus affects natural vibration frequencies, and thus resonance and harmonics. Mechanical loss coefficient measures acoustic damping: too little damping and the tone is tinny, too much and it is dull. Make bar-charts for these two properties for Softwoods. What does do they suggest about the guitar-wood? (To limit the Soft woods, click on Chart/Select – Select from: (choose Custom Define your own subset) – deselect all, then select Biological materials - Woods – Softwoods)

- Which metal for strings? Try a search on guitar string or piano string. What is the material that the search brings up?

- The pitch (first harmonic) f of a string with a length l and mass per unit length m_l=$A\rho$ carrying a

$$f = \frac{1}{2L}\sqrt{\frac{T}{m_l}} = \frac{1}{2L}\sqrt{\frac{T}{A\rho}} = \frac{1}{2L}\sqrt{\frac{\sigma}{\rho}}$$

  tension T is:

Here A is the cross-section area, ρ is the density, and σ=T/A is the stress in the string. The maximum stress a string support is limited to its tensile strength σ_{ts}. The strings on a guitar are all about the same length, so highest pitch that a string can reach $\sqrt{\sigma_{ts}/\rho}$ scales as .

Make a bar chart of this quantity with three materials on it: nylon (PA), high carbon steel and Piano wire. Which allows the highest frequencies? (https://en.wikipedia.org/wiki/String_vibration)

- The three strings of a classical guitar with the lowest frequencies are made of nylon, but are wound with a metal. Why?

Discussion Point

What is the history of piano wire? Why does it need to have such a high strength?
(https://en.wikipedia.org/wiki/Piano_wire is informative.)

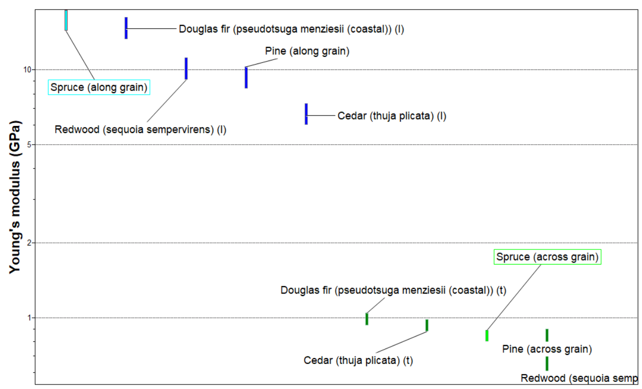
Specimen Response

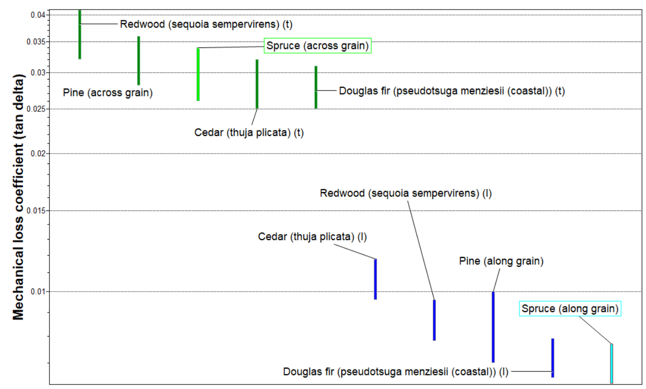
Which wood?

A search on "Guitar" brings up two woods: Spruce (along grain) and Spruce (across grain). The same wood appears in two records because the properties along the grain and across the grain differ greatly, requiring two separate records.

Modulus and Mechanical loss coefficient.

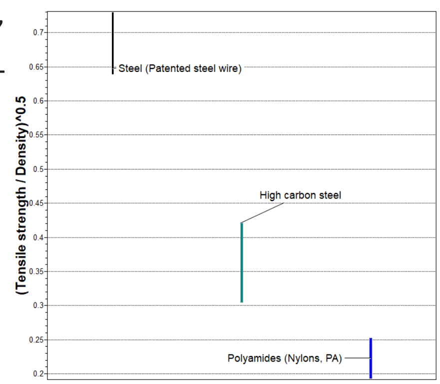
The bar-charts looks like this. Among softwoods, Spruce has an unusually high modulus and low damping coefficient. The tone of the instrument depends on this.





Which metal for guitar strings?

The search guitar string brings up "Steel (Patented steel wire)" also known as Piano wire. It is a heavily drawn high-carbon steel – used for the higher-pitched metal strings of pianos and violins.



The relative pitch chart.

The maximum pitch scales as $\sqrt{\sigma_{ts}/\rho}$, plotted here as a bar-chart. There is little to choose between Nylon and High carbon steel. Piano wire (which is heavily drawn and thus work-hardened high carbon steel) allows 3-fold higher pitch than the other two.

Why metal-wound strings?

$$f = \frac{1}{2L}\sqrt{\frac{T}{m_l}}$$

The pitch is determined by the tension T and the mass m_l per unit length of the string. Winding the nylon string with a metal wire increases m_l and lowers the pitch.

Discussion point: the history of piano wire.

Piano strings are among the most demanding of applications of steel. They are under high tension, they are subject to repeated blows, they are stretched and slackened during tuning and are still expected to last for decades. Similar challenges arise in plucked instruments like guitars, along with the additional demand of being bent when plucked.

The oldest record of wire being made for musical instruments is from Augsburg in 1351. Piano wire, or "music wire", is made from tempered high-carbon steel, which replaced iron as the material starting in 1834.

MS&E MicroProject #7

Shields for Viking invaders

Database: MS&E

Imagine yourself to be a 12th century Viking seeking a light, tough materials to make shields to protect yourself while you pillage and plunder. The only materials available to you are those that occur naturally, derived from plants or animals.

- “Light” means low density, ρ. What does “Tough” mean? (Fracture toughness, K_{1c}, and Toughness, G_{1c}, differ. The first is in the database, the second is not but can be circulated from the properties that are.)

- How is the property “Toughness” defined in term of the properties that are in the database? (The science note (i) for Fracture Toughness may help here.)

- Make a bar chart of the Toughness of natural materials. Which three have the highest toughness? (First apply a Tree stage to limit the selection to Biological materials – woods, soft and hard tissue. Then use the Advanced option in the axis-choice panel to create *G1c*)

- That deals with toughness, but what about lightness? Add Density ρ to the x-axis. Apply a selection line with a slope of 1 describing light, tough materials (G_{1c}/ρ) and move it upwards to find the two best natural materials for shields. What are they?

Discussion Point

Which of the materials that you have identified really been used for shields in the past? Use the Internet to research materials for shields. What do you find?

Specimen Response

What does "Tough" mean?

"Tough" means that the propagation of a crack dissipates a lot of energy. It is measured by the property G_{1c}, with units of Joules per square meter.

How is toughness related to other properties?

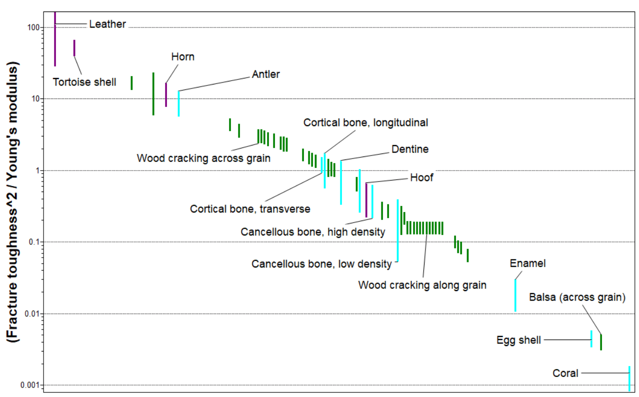
From the science note("i") for Fracture toughness we find that Toughness is related to the other properties by $G_{1c}=K_{1c}^2/E$, where K_{1c} is the Fracture toughness and E is Young's modulus.

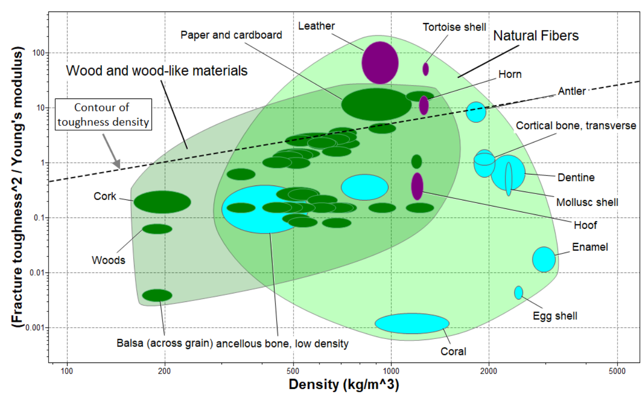
Bar chart of the Toughness of natural materials.

The bar chart appears on the left. The three natural materials with the greatest toughness are tortoise Leather, Tortoise shell and Paper (try tearing a phone directory in half).

Chart of Toughness and Density.

The chart appears on the right. Two materials stand out as having high toughness at low weight: leather and tortoise shell





Discussion point: materials used for shields[1,2]

There are many web entries on shields. Both tortoise shell and leather shields were used in medieval times and are still used today, as these pictures below indicate.

Tortoise shell shield from the Sudan, about 1950

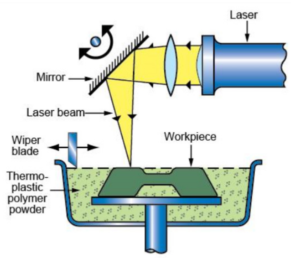
Maasai shield from Kenya, made of cattle hide

1 Tortoise shell shield: http://www.oriental-arms.com/item.php?id=2417

2 Leather shield: http://www.hamillgallery.com/MAASAI/MaasaiShields2/MaasaiShield25.html

Are materials made by additive manufacture any good? (1-polymers)

Database: MS&E



Selective laser sintering (polymers)

Additive Manufacture (AM) or 3D printing is seen as part of the ongoing "4th Industrial Revolution" (following the revolutions of steam, electricity and information technology). AM technologies use computer-controlled deposition to build shapes layer-by-layer. All can create shapes of great complexity without the need for dies or molds. But is the material made in this way as good as that made by conventional methods such as injection molding?

- Which polymers can be shaped by AM? (Open the record for the process shown in the figure and copy the materials to which it is linked from the tab at the bottom of the record.)

- Explore the properties of conventional Acrylonitrile butadiene styrene (ABS), for which there is a record in the MS&E DB, by making a chart with Tensile Strength (MPa) on the y-axis and Elongation (%) on the x-axis. (Use the "Define your own subset" option or use a Tree stage to isolate ABS. Just one big bubble appears on the chart.)

- ABS samples made using four different AM machines give the data listed in the table

AM method	Tensile strength (MPa)	Elongation (%)
PLATCure ABS	50 - 54	4 - 8
ABfled ABS	26 - 30	12 - 15
Accura ABS	40 - 44	10 - 14
DWS Systems ABS	34 - 37	7 - 10

Add these materials to the MS&E database. (Adding a new record: Right-click on a chart. Select "Add record". Enter a name: PLATCure ABS. Enter the data. Return to the chart – PLATCure ABS now appears on it).

- Add a title to the chart, reset both axes from log to linear to give a fair comparison and adjust the range of both to give a well-proportioned chart. How do the properties of ABS made by AM compare to those of conventionally molded ABS? (To adjust an axis, double click on the axis name, then make the changes in the Axis settings box.)

Discussion Point

The precision and surface quality of AM products are limited, and the process is slow (typically 1 to 20 hours per part). The range of materials that are compatible with AM methods is limited and – as the project showed, the properties may not be as good as those of conventionally processed materials. Who would want to use it? What's the business case for AM?

Specimen Response

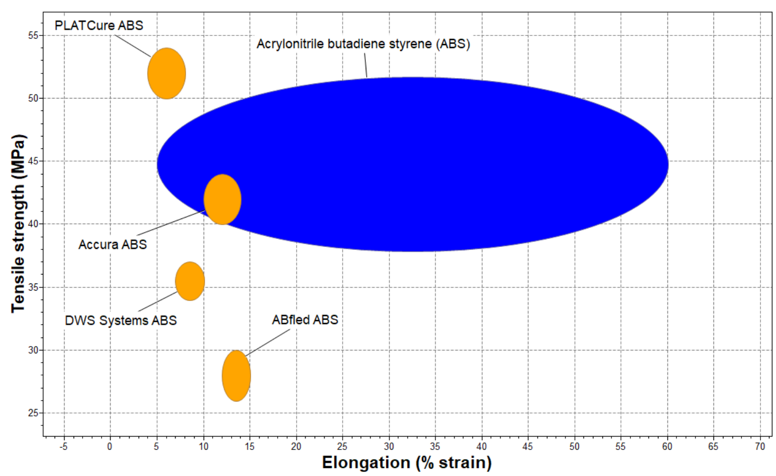
Which polymers can be shaped by AM?

The "Materials" link in the record for Selective Laser Sintering (polymers) gives the following list:

- Acrylonitrile butadiene styrene (ABS)
- Polyamides (Nylons, PA)
- Polycarbonate (PC)
- Polymethyl methacrylate (Acrylic, PMMA)
- Polystyrene (PS)
- Polytetrafluoroethylene (Teflon, PTFE)

Strength and elongation of conventional ABS

Conventionally-molded ABS appears as a large blue bubble on axes of Tensile Strength and Elongation. (Both have a wide range of values because the single record for ABS encompasses a number of different grades. These grades have separate records in the Granta EduPack Level 3 database.)



Adding records for AM ABS

When the data for the four AM materials are added, they appear on the chart as orange bubbles, shown here. The axes have been set to linear and the ranges adjusted in the ways suggested in the question.

Property comparison

AM processes differ so greatly from conventional molding methods that one might expect the resulting properties to differ also. The chart shows that the strengths of the AM samples span the same range as those that are conventionally molded but the elongations of the AM samples are low. It also shows the properties depend strongly on the details of the AM process: the reported strength of the PLATCure ABS is almost twice that of the ABfled ABS.

These observations should be treated with caution. Additive manufacturing fabrication and post-processing techniques are evolving rapidly. Standards for AM processing have not yet been established, characterization of AM materials is in its infancy and reproducibility is largely untested. But that will change: this is a rapidly evolving field.

Discussion point: The business case for AM.

A search on Business case for additive manufacture generates many leads; some are listed below. They make the following points.

- AM (3D printing) can make parts with simple and complex geometries with equal ease, allowing part-integration.
- It can be cheaper for custom, one-off or low volume, production than conventional manufacturing methods because no expensive dies are needed.
- Since all the manufacturing information is held in a CAD file, it is easily shared, it allows on-site manufacture of replacement parts on demand and it reduces the need for inventories of spares, warehousing and transport over long distances.

These are features that are attractive in four sectors: aerospace, automotive, medical engineering and defense.

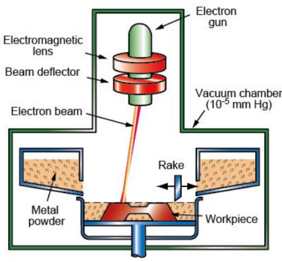
- Aerospace because volumes are low, shapes often complex, and the materials involved (titanium alloys, stainless steels, nickel-based super alloys) lend themselves to laser and electron-beam sintering methods.
- Automotive because AM is a cost-effective way to make tooling, jigs and fixtures, and to build concept models and functional prototypes.
- Medical engineering because repair to the skull, teeth, esophagus and other hard and soft tissue requires one-off production of parts that reproduce the unique geometry of the patient.
- Defense, because of the difficult logistics of holding large central banks of replacement parts for equipment and the delivery of these, when needed, to a conflict zone. It simpler to make the parts on demand where they are needed.

Sources of information on AM methods, materials, opportunities and constraints.
https://3dprintingindustry.com/3d-printing-basics-free-beginners-guide#05-materials
https://medium.com/am-on-the-cusp/making-the-business-case-for-additive-manufacturing-a-manager-s-guide-2ce592096d97
http://scw3dprints.weebly.com/the-positive-and-negative-effects-of-3d-printing.html
https://www2.deloitte.com/insights/us/en/deloitte-review/issue-15/additive-manufacturing-business-case.html

MS&E MicroProject #9

Are materials made by additive manufacture any good? (2-metals)

Database: MS&E



electron beam melting

Additive Manufacture (AM) technologies use computer-controlled deposition to build shapes layer-by-layer. All can create shapes of great complexity without the need for dies or molds. The precision and surface roughness, at present, are limited to ±0.1mm at best and the process is slow (typically 1 to 20 hours per part) but the freedom of choice of shape is enormous. What about the properties of metals shaped in this way: are they as good as those of materials made by conventional methods such as casting or forging?

- Which metals can be shaped by AM? (Open the record for the process shown in the figure and copy the materials to which it is linked from the tab at the bottom of the record.)

- Explore the properties of conventional Titanium alloys, for which there is a record in the MS&E DB, by making a chart with Tensile Strength (MPa) on the y-axis and Elongation (%) on the x-axis. (Use the "Define your own subset" option or use a Tree stage to isolate Titanium alloys. Just one big bubble appears on the chart.)

- AM methods are new – there are not yet many measurements of the properties of AM materials. The alloy Ti-6Al-4V is one of the most studied. The table lists data from five independent tests.

AM method	Tensile strength (MPa)	Elongation (%)
Renishaw Ti-6-4 (annealed 750 C)	1120 - 1150	6 – 8.5
Renishaw Ti-6-4 (annealed 850 C)	1030 - 1070	6.5 - 10
SLM Solutions Ti-6-4 (annealed)	965 - 985	9 – 10.5
Optomec Ti-6-4 (no post processing)	1060 - 1080	10 - 12
ARCAM Ti-6-4 (hot-isostatic pressed)	960 - 985	13.5 - 16

Add these materials to the MS&E database. (Adding a new record: Right-click on a chart. Select "Add record". Enter a name: Renishaw Ti-6-4. Enter the data. Return to the chart – Renishaw Ti-6-4 now appears on it).

- Add a title to the chart, reset both axes from log to linear to give a fair comparison and adjust the range of both to give a well-proportioned chart. How do the properties of Ti-6Al-4V made by AM compare to those of conventionally cast Ti-6-4? (To adjust an axis, double click on the axis name, then make the changes in the Axis settings box.)

Discussion Point

AM is seen as a component of the evolving "4th Industrial Revolution" (following the revolutions of steam, electricity and information technology). The spectrum of materials that can be shaped successfully by additive manufacture is increasing rapidly. Carry out a survey of reports on materials for additive manufacture, linking them to the industrial sector to which they contribute.

Specimen Response

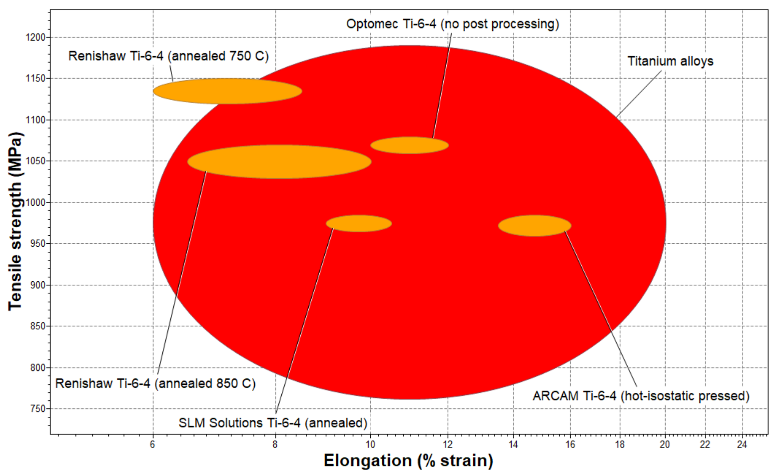
Which metals can be shaped by AM?

The “Materials” link in the record for Electron Beam Melting gives the following list:

- Commercially pure titanium
- Titanium alloys (basically Ti-6AL-4V)
- Medium carbon steel

Strength and elongation of conventional ABS

Conventionally cast Ti-6-4 appears as a large red bubble on axes of Tensile Strength and Elongation. (Both have a wide range of values because the single record for Ti-6-4 encompasses a number of different variants and heat treatments. These grades have separate records in the Granta EduPack Level 3 database.)



Adding records for AM Titanium 6Al 4V

When the data for the three AM materials are added, they appear on the chart as orange bubbles, shown here. The axes have been set to linear and the ranges adjusted in the ways suggested in the question.

Property comparison

AM processes differ so greatly from conventional casting methods that one might expect the resulting properties to differ also. The chart shows that the reported strengths of the AM samples span the same range as those that are conventionally cast, but that the elongations of the AM samples have a wide spread and depend on both the primary AM process and the subsequent post-processing.

The scatter in the properties plotted in the chart reflect the present immaturity of additive manufacturing methods, that the characterization of AM materials is in its infancy and that reproducibility is largely untested. That will change: this is a rapidly evolving field.

Discussion point: Material that can be shaped by Additive Manufacture.

A search on "Materials for additive manufacture" generates many leads; some are listed below. A survey gives the following industrial sectors and materials.

Early AM used easily-formed materials – polymers and waxes – focusing on shape, not properties. Today's rapidly expanding AM technologies focus on markets. The materials that are now commercially available reflect the business opportunities in aerospace, medical engineering and defense.

Sector	Materials
Aerospace, Transport, Defense	Titanium alloys: CP titanium, Ti-6Al-4V
	Aluminum alloys: Al-Si-Mg alloys; 6061
	Stainless steels: 316, 420, PH 17-4
	Superalloys: IN625, Stellite
	Tool steels: H13
	Ceramics: Alumina
Medical and Dental	Titanium
	Nylon, ABS, PP, PLA, proprietary plastics and elastomers
	Calcium phosphate
	Cartilage and other living tissue
Other	Paper
	Food: chocolate, sugar, pasta, meat
	Art, Design, Jewelery: gold, silver, plastics, glass
	Archaeology, Construction: stone

https://www.azom.com/article.aspx?ArticleID=8132
http://www.spilasers.com/application-additive-manufacturing/additive-manufacturing-materials/

MS&E MicroProject #10

Why don't things stick to Teflon?

Database: MS&E

- What is Teflon? (Use the Search facility to find the record.)
- What makes it special among polymers?
- Limit the selection that follows to Polymers only. (To limit the selection to Polymers. To do this, click on Chart/Select, then Select from: Custom – Define your own subset. Clear the Subset, then choose Polymers.)
- What is its Maximum Service Temperature of Teflon? How does this compare with the values for other polymers? Make a bar chart of Maximum Service Temperature to find out.
- Use a linear, not a logarithmic, scale and set the ranges to start from zero. (To adjust axes, double click on the axis name to re-open the Axis Settings box, select "Linear" and adjust the range.)
- What is the Dielectric constant of Teflon? How does this compare with the Dielectric constants of other polymers? Make a bar-chart of Dielectric constant for Polymers to find out. Use a linear, not a logarithmic, scale and set the ranges to start from zero.
- What do "Dielectric constant" measure and "Maximum Service Temperature" measure? What bearing might they have on the non-stick question? (Try the information ("i") link next to the property name on any materials record to access Science notes.)

Discussion Point

The coating on non-stick saucepans is Teflon. Why does nothing stick to Teflon? And if Teflon is non-stick, how does it stick to the saucepan?

Specimen Response

What is Teflon?

Polytetrafluoroethylene (PTFE) with the chemical formula (CF2-CF2)n

What makes it special among polymers?

PTFE has exceptionally low friction, is water repellent, and extremely stable.

What is its Maximum Service Temperature?

The Maximum Service Temperature of PTFE is 250 – 271ºC

How does this compare with the Maximum Service Temperatures of other polymers?

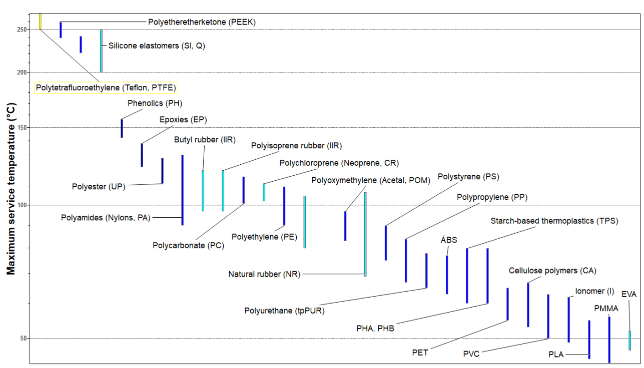
The bar-chart shows that PTFE has the highest Maximum Service Temperature of all polymers.

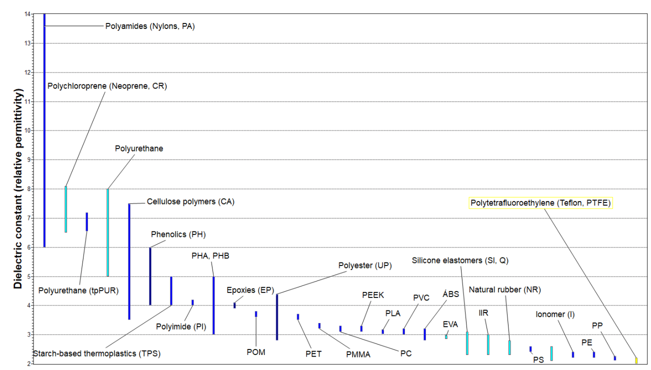
What is its Dielectric constant?

The Dielectric constant of PTFE is 2-2.2

How does this compare with the Dielectric constants of other polymers?

The bar-chart shows that PTFE has the lowest Dielectric constant of all polymers.





What do "Maximum Service Temperature" and "Dielectric constant" measure?

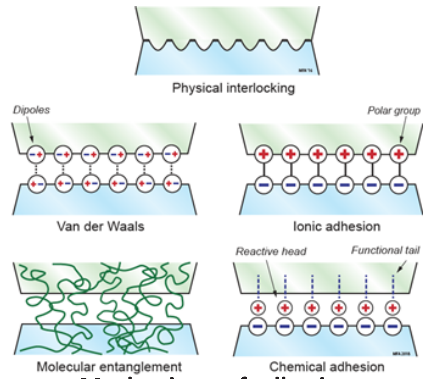
The Maximum Service Temperature is the maximum temperature at which a material can be used without decomposition or severe softening. It is a measure of the stability and bond-strength of the material.

The dielectric constant measures the extent to which a material polarizes when in an electric field. Equivalently, it is the ratio of the capacitance of a capacitor with the material between its electrodes and that of the same capacitor with air or vacuum between its electrodes. Being a ratio, it is dimensionless. Its value for empty space and, for practical purposes, for most gases, is 1. Most dielectrics have values between 2 and 20, although some ("Ferroelectrics") have values as high as 20,000.

"Sticking" means forming a chemical or physical bond, and that means exchanging or sharing electrons, or polarizing sufficiently to induce polarization in neighboring molecules. The stability of the Teflon molecule means that forming a chemical bond is not possible, and the low dielectric constant means that polar-bonding is inhibited.

Discussion point: How does Teflon stick to saucepans?

To get anywhere with this you have to explore the Mechanisms of adhesion. The figure illustrates the basic mechanisms.



Mechanisms of adhesion

(Ashby, M.F. "Materials Selection in Mechanical Design" 5th edition, Elsevier (2017)).

There are five general mechanisms for getting two bodies to stick together; the same mechanisms are responsible for the bonding of paint and other coatings to a surface.

- Surface roughening by sand blasting or chemical etching creates cavities into which an adhesive, paint or coating cures and sets, giving mechanical interlocking.
- Van der Waals adhesion relies on the attractive interaction between dipoles in non-metallic surfaces giving a weak but reversible bond (it's how flies walk on ceilings).
- Ionic adhesion occurs between surfaces with polar groups.
- Molecular entanglement works well for coatings or adhesives on amorphous plastics such as polycarbonate (PC), ABS and PVC but is less effective with semi-crystalline thermoplastics.
- Chemical adhesion is the formation of chemical bonds between the surfaces, stimulated by a chemical adhesion promoter. The reactive "head" of the promoter forms a strong chemical bond with one surface, while its functional "tail" interacts and bonds to the other.

Sticking Teflon to pans. Teflon is non-polar (exceptionally low dielectric constant), chemically inert (the C-F bond very strong and can't bond to a metal by entanglement). That leaves just the first mechanism – physical interlocking – as the way to get non-stick coatings to stick.

MS&E MicroProject #11

What do Processes do to Properties?

Database: MS&E

The Process-Property Profile (PPP) data-table in the MS&E database allows charting of the effect of processing on properties. This project uses the PPP facility to explore solid-solutions.

- Open the PPP data-table from the home page and isolate Copper-Nickel alloys for exploration. (Chart/Select – Select from: Custom Define your own subset – Deselect all then open 1. Alloying and work hardening: copper alloys – select Copper-Nickel alloys)

- Make a chart with Young's modulus on the y-axis and Copper content on the x-axis. Use linear scales for both. Set the axis range for Copper content (%) to run from 0 to 100. (To choose linear scales and set axis ranges first make the chart then double click on the axis name on the chart to bring up Axis settings. Click on "Linear" and use "Set" to adjust range.)

- Add a title using the Text label function (T) and draw a curve through the data using the Curve function (C) above the chart. Your modulus chart should now look like this.

- Now step through the mechanical, thermal and electrical properties in the same way, copying and pasting the charts into WORD to allow comparison. Follow the order

1. Yield strength,
2. Fracture toughness
3. Thermal conductivity
4. Thermal expansion
5. Heat capacity
6. Electrical resistivity

- Some properties (like Young's modulus) vary with composition in an almost linear way. Which behave like this?

- Some, by contrast, show a much stronger dependence, with a maximum or minimum in the middle of the composition range – which are these?

Discussion Point

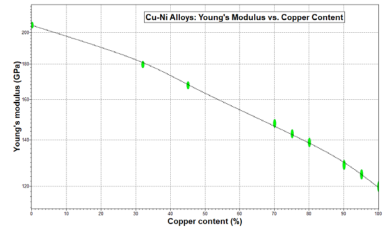
Why does the Yield strength vary with solute concentration in the way shown in Chart 1? Got to the Home page, locate Science Notes, open Structure Science notes and open "Solid-solution strengthening" to find out.

Why does the Electrical resistivity vary with solute concentration in the way shown in Chart 6? Open the Structure Science note "Electron scattering" to find out. (Text and images can be copied from these Science notes by highlighting, copying and pasting into WORD.)

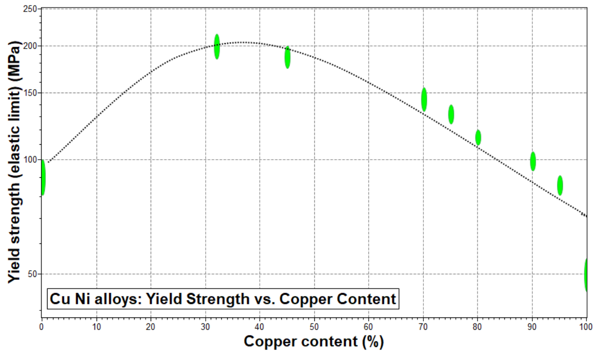
Specimen Response

Mechanical properties

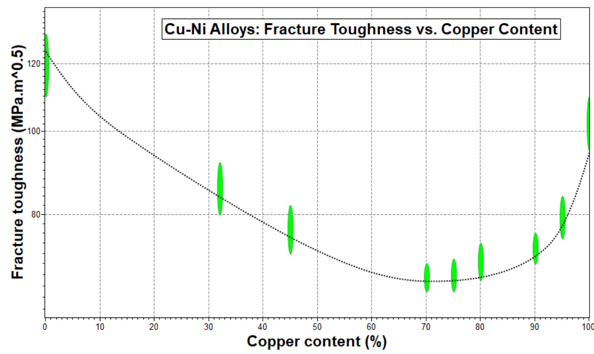
The Modulus, as shown here, varies almost linearly with composition. By contrast, Yield strength, Fracture toughness show a strongly non-linear behavior with a peak or trough towards the middle of the composition range.



(1)



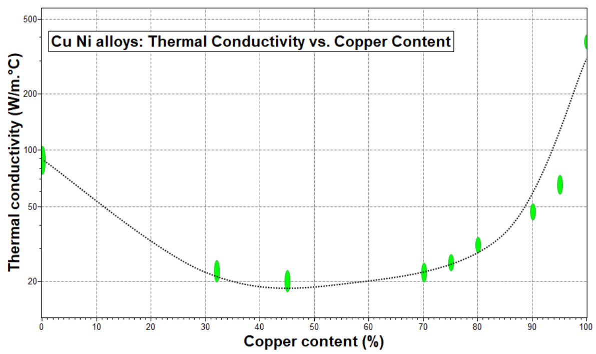
(2)



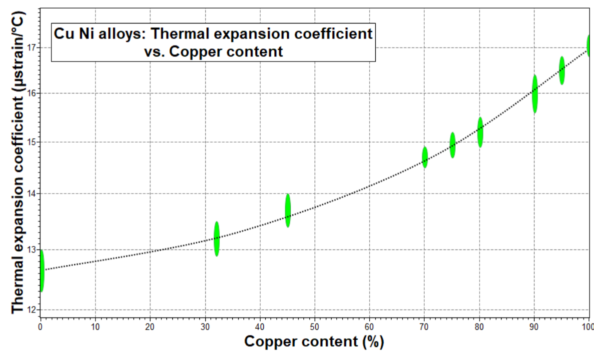
Thermal and Electrical properties

Thermal expansion coefficient and Heat capacity vary almost linearly with composition. Thermal conductivity and Electrical resistivity vary in a strongly non-linear way.

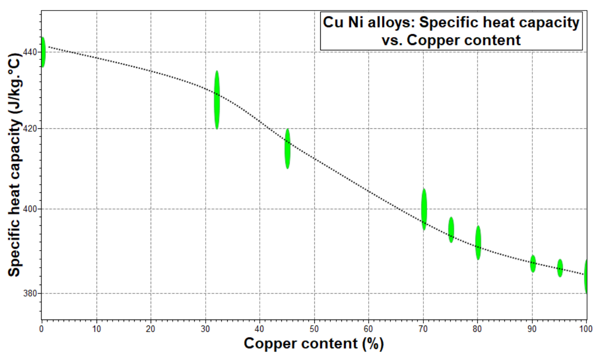
(3)



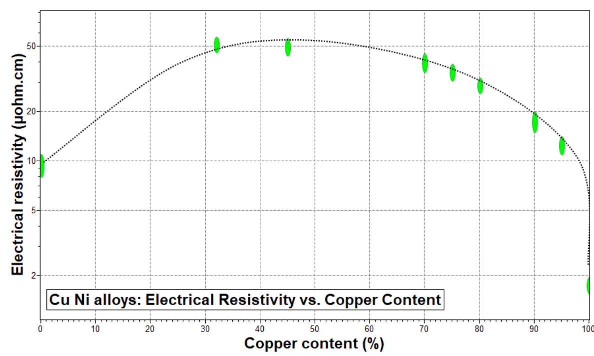
(4)



(5)



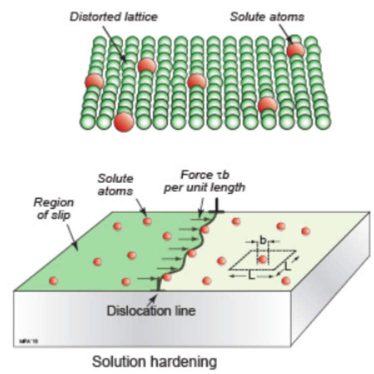
(6)



Discussion point: The underlying mechanisms.

Why does the Yield strength vary with solute concentration in the way shown in Chart (1)? The Structure Science note gives the following insight.

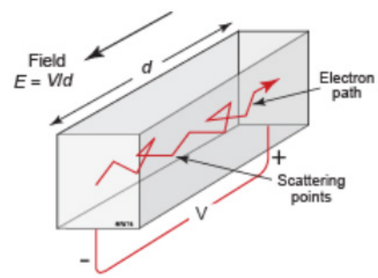
Solute atoms differ in size from those of the host, roughening the planes on which dislocations move, and thus obstructing their motion. The number of such obstacles increases with solute concentration, c, leading to a parabolic (c1/2) dependence of yield strength on concentration. This dependence is evident in Chart 1, which shows a roughly parabolic rise starting from 0% Ni or from 0% Cu.



Solid-solution strengthening

Why does the Electrical resistivity vary with solute concentration in the way shown in Chart (6)? The Structure Science note for Electron Scattering gives the following insight.

Electrical conduction in a metal is by the movement of "free" electrons in response to the field V/d caused by the potential difference V. Impurity or solute atoms act as scattering centers, limiting the mean free path of the electrons, which is why alloys always have a higher resistivity than pure metals.

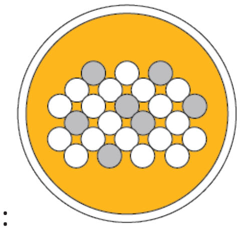


Electron scattering

MS&E MicroProject #12

Which elements form extensive solid-solutions with Cu?

Database: MS&E



The Hume-Rothery rules set out criteria for the formation of extensive solid-solution:

1. Atom size difference less than 15%
2. Electronegativity difference less than 0.2

Strong influence

3. The components have the same crystal structure
4. The components have the same valence within

Less strong influence

The Elements data-table of the MS&E database contains data for all of these. Which elements would you expect to form an extensive solid -solution with copper?

- Select the ELEMENTS data-table from the Home page. Make a chart with atomic radius difference from copper (Atomic radius – Atomic radius of copper) on one axis and electronegativity difference from copper (Electronegativity – Electronegativity of copper) to find elements that are close to copper. (First look up the atomic radius and electronegativity of copper in the Copper record, then use the Advanced axis facility to make the functions in brackets above. Chose linear scales for both axes – double click on the axis name and select "linear" instead of "log".)

- Apply a selection box centered on Copper with a width that is 15% of the atomic radius of copper on either side and differs from copper by an electronegativity of 0.075 above and below. List the elements appearing in the Results window. These meet the first two H-R criteria and will form extensive solid-solutions with copper.

- Complete solid-solubility across the entire composition range from 0 to 100% requires that the remaining two conditions are also met. Which of the elements in your list fulfill these additional requirements?

- The Phase Diagram data-table has diagrams for three copper alloys: Cu-Ni, Cu-Zn and Cu-Sn. What is the maximum solid solubility at the copper-rich side of each diagram? Are they consistent with the Hume-Rothery rules?

Discussion Point

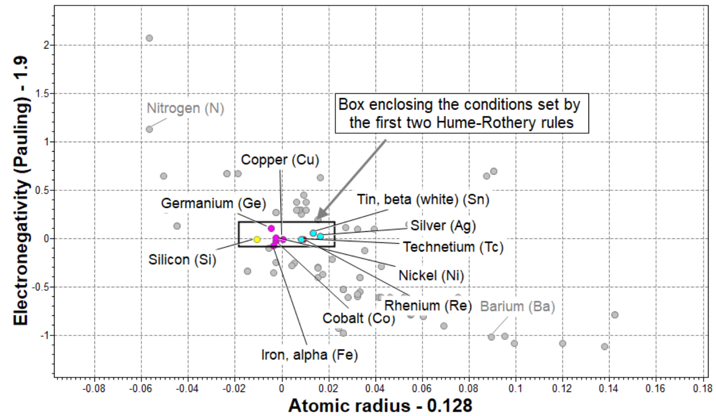
What is the entropy of mixing? What is its value for a mole of an alloy with a concentration c of atoms A and (1-c) of atoms B?

Specimen Response

Satisfying the first two Hume-Rothery criteria

Copper has an atomic radius of 0.128 nm and an electronegativity of 1.9 on the Pauling scale. The chart showing the difference between the radius and electronegativity of copper and the other elements looks like this. Copper is at the point (0,0). The blue selection box encloses the conditions set by the first two of the Hume Rothery rules. The elements captured in the box are listed below.

- Cobalt (Co)
- Germanium (Ge)
- Silicon (Si)
- Technetium (Tc)
- Silver (Ag)
- Iron, alpha (Fe)
- Nickel (Ni)
- Rhenium (Re)



Which elements should form complete solid-solutions with copper?

Of the elements in the list above, only two have the same valence and crystal structure: nickel and silver. Both do form full solid-solutions with copper.

Maximum solid solubility for Cu-Ni, Cu-Zn and Cu-Sn

Phase diagram	Max solid solubility	Comment
Cu-Ni	100 wt%	All four H-R criteria are met
Cu-Zn	39 wt%	Three criteria satisfied; crystal structures differ
Cu-Sn	15 wt%	First two criteria satisfied; crystal structure and valence differ

Discussion point: What is the entropy of mixing?

When n atoms of element A are mixed with N-n atoms of element B on a mole N (6.02 x 1023) of atomic sites, there is an increase in the entropy of A + B due to the numerous ways in which the two kinds of atoms can be arranged among each other. The total number of ways of doing this is $\dfrac{N!}{n!\,(N-n)!}$

The entropy associated with the mixing is $S = -k \ln\left[\dfrac{N!}{n!\,(N-n)!}\right]$

where k is Boltzmann constant (1.38 x 10-23 J/K). This simplifies, using the Stirling approximation to

$$S = -Nk[c\ln(c) + (1-c)\ln(1-c)]$$

here c = n/N and (1-c) = (N-n)/N. The entropy of mixing reduces the free energy of an alloy, increasing it stability; it is this that keeps the alloy mixed and acts against it separating out into two distinct phases. When c = 1 or 0, S = 0 (no entropy of mixing). When c = (1-c) = 0.5, S = 5.7 J/mol.K

MS&E MicroProject #13

Designing high-entropy alloys

Database: MS&E

High entropy alloys are solid-solutions with five or more components each with concentrations above 5%. The cumulative entropy of mixing reduces the free energy of the alloy, stabilizing it and enhancing mechanical properties. The Hume-Rothery rules give guidance in selecting components that will form extensive solid-solutions:

1. Atom size difference less than 15%
2. Electronegativity difference less than 0.2

Strong influence

3. The components have the same crystal structure
4. The components have the same valence within

Less strong influence

The Elements data-table of the MS&E database contains data for all of these. Make a chart for selecting promising component-sets for high-entropy alloys.

- Make a chart for selecting promising component-sets for high-entropy alloys. Plot Electronegativity on the y-axis and Atomic radius on the x-axis. Use a linear scale for Electronegativity but retain the default Log scale for Atomic radius. (To change an axis from log to linear, double click on the axis name, then click on "linear" in the Axis settings box.)

- Recolor the elements to identify their crystal structure. (The best way to do this is to use a limit stage to select all the elements with a "Cubic, face centered" structure, highlight the resulting list, right click and select Record color, chose color, then repeat for the other structures.)

- Create a selection box with a width that corresponds to 15% change in atomic radius and a height that corresponds to a difference of 0.075 in electronegativity. Use this box to track across the array of elements on the chart, placing it over clusters to identify promising components. (Feel free to relax the constraints a little – we are only looking for a solubility greater than 5%, not total solid solubility.)

- Enclose each cluster with a line using the Curve tool in the tool-bar across the top of the chart. Label the encircled clusters, listing the elements they contain, using the Text label tool in the same tool-bar. How many promising clusters do you find?

Discussion Point

High-entropy alloys are a new and currently-active field of research. Research "High-entropy alloys" on the world-wide web. What are their characteristics, properties and potential applications?

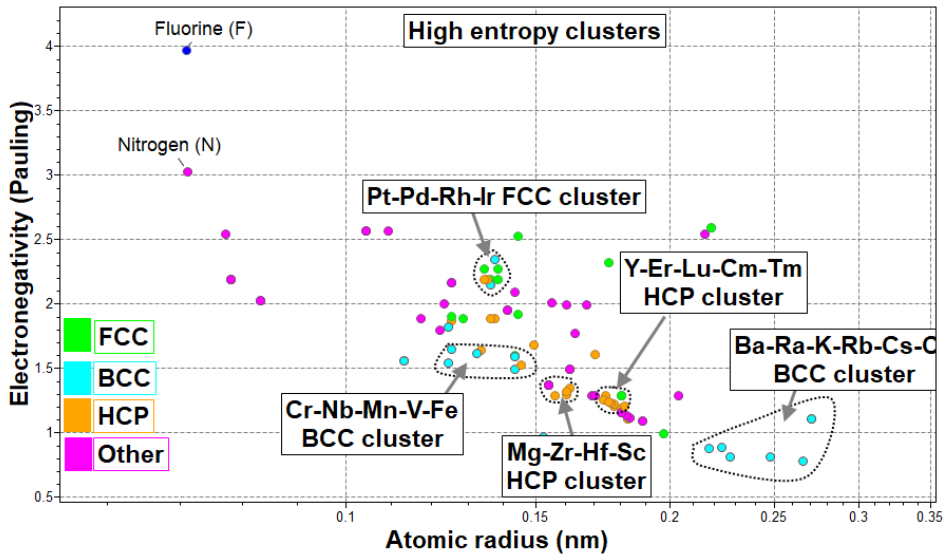
Specimen Response

Create and recolor the chart.

The chart is shown here. The elements have been recolored to identify crystal structure following the color code shown at the lower right.

Create a H-R selection box.

The blue bars at the lower left show the dimensions of a selection box that meets the first two Hume-Rothery criteria.



Identify the most promising groups.

Clusters of elements that meet the first three of Hume-Rothery's rules are labeled. Experience suggest that the Hume-Rothery rules are relaxed somewhat in multi-component systems. The rule that solvent and solute elements have the same crystal structure, for instance, does not seem to apply – a Fe-Ni-Cr-Co-Mn alloy, for example, forms a single FCC solid-solution even though the components have four different crystal structures. In a scoping exercise, the crystal-structure rule can be relaxed and the selection box widened a little to suggest a wider range of compatible components.

Discussion point. Characteristics and properties of high entropy alloys

There is a great deal of information about high entropy alloys on the web1, 2. The following information is paraphrased from them.

High Entropy Alloys (HEAs) are a new class of metallic materials. They do not have a principal component, but are instead based on near equi-atomic mixtures of five or more elements. You might expect the microstructure of these materials to contain a number of intermetallic phases but most don't; instead they have single phase microstructure with simple crystal structures, such as FCC or BCC.

The Gibbs free energy of an alloy is G = H – TS (where H is enthalpy, T is temperature, and S is entropy). The high entropy of mixing when five or more components are dissolved together reduces G, stabilizing the solid-solution

Diffusion and phase transformation kinetics in HEAs are slower than those in their conventional counterparts. First, the difference in local atomic configuration leads to different bonding and therefore different local energies for each site; atoms in low-energy sites are trapped, unable to jump. Second, the diffusion rate of each element in a HEA is different. Elements with high melting points have lower success rates for jumping into vacancies and it is these that influence the overall diffusion rate.

HEAs have promising properties, including high strength, good wear characteristics and excellent corrosion resistance, making them industrially relevant.

Potential applications for HEAs are as hydrogen storage materials, radiation resistant materials, diffusion barriers for electronics, precision resistors, electromagnetic shielding materials, soft magnetic materials, and thermoelectric materials. This exciting new field awaits further exploration.

(1) "High-entropy alloys" Rolls Royce UTC (2017) https://www.rrutc.msm.cam.ac.uk/research-themes/high-entropy-alloys
(2) "High-entropy alloys, a critical review" (2014) Ming-Hung Tsaia and Jien-Wei Yeh , Mater. Res. Lett., 2014 Vol. 2, No. 3, 107–123, http://www.tandfonline.com/doi/pdf/10.1080/21663831.2014.912690

MS&E MicroProject #14

Harvesting waste energy without regulatory risk

Database: MS&E

A maker of small sensors to be embedded in products that may not have access to electrical power hopes to power them by harvesting waste energy – thermal, using thermoelectric materials, or kinetic, using piezo-electrics. The maker is risk-averse: materials containing “Restricted” elements or elements that appear on the “Critical” lists in Europe or the US are to be avoided. You are asked to do a survey of available materials and report back, flagging those to be avoided.

The Materials data-table of the MS&E database has records for thermo-electric and piezo-electric materials, including their composition. Draft a report that meets the makers remit. Before you start, make sure you know what is being asked.

- What are “critical” materials? Why would the sensor-maker wish to avoid them? (The records for Elements list “Critical materials information” and indicate if the element is on the EU or US Critical list. The science note (i) for these entries explain what “Critical” means.)

- What does “restricted” mean? Use the Internet to find elements listed under the Restriction of Hazardous Substances (RoHS) Directive. (Other nations have very similar restrictions).

- Why might the sensor-maker wish to avoid Critical or Restricted materials?

- Open the Materials data-table on the Home page and Browse to Functional materials – Semiconductors and thermoelectrics – Thermoelectrics to make a list of thermoelectric materials.

- Do the same for Piezo-electric material

- Annotate the two lists, indicating which materials are free from Critical or Restricted materials. (The links from the materials in the lists to the Elements data-table gives direct access to these elements. Their records report whether or not they appear on the US or EU Critical Lists.)

Discussion Point

What is the WEEE directive? Would knowledge of this Directive be important to the sensor-maker?

Specimen Response

Critical elements

Elements for which the supply chain is at risk and are of particular importance to the Economy or National Security are flagged as “Critical”. Put another way, a critical element is one you need but may not be able to get.

Restricted substances.

The full name of the RoHS Directive is “The Restriction of the Use of Certain Hazardous Substances in Electrical and Electronic equipment”. This Directive bans the placing on the EU market of new electrical and electronic equipment containing more than agreed levels of: lead, cadmium, mercury, hexavalent chromium and biphenyls and phthalates used in pigments, paints, flame-retardants and plasticizers.

Why does the maker of sensors want to avoid critical or restricted elements?

Dependence on an element with a risky supply chain exposes the maker to loss of business if supply fails. Toxic elements that are “restricted” must be reported when used and may be totally banned. Dependence on these is again a business threat.

The annotated list of thermo-electric materials

Thermo-electric material and elements	Acceptability	
Antimony telluride Sb-Bi-Te	X	Antimony on EU and US “Critical”lists
Bismuth telluride Bi-Te-Se	X	Bismuth on EU and US “Critical”lists
Lead telluride Pb-Te-Na	X	Lead on “Restricted” and “Critical” lists
Magnesium silicide Mg2(Si,Sn)	X	Magnesium on EU and US lists, Silicon on EU list, Tin on US list
Silicon germanium Si-Ge	X	Silicon on EU list, Germanium on EU and US list
TAGS (GeTe)x(AgSbTe2)1-x	X	Germanium, Antimony, and Tellurium on Critical lists

The annotated list of piezo-electric materials

Piezo-electric material and elements	Acceptability	
Barium titanate Ba-Ti-O	X	Titanium added to US critical list 2018
Bismuth titanate Bi-Ti-O	X	Titanium added to US critical list 2018
Lead lanthanum zirconate titanate Pb-La-Zr-Ti-O	X	Titanium added to US critical list 2018, Lead restricted
Lithium niobate Li-Nb-O	X	Lithium and Niobium on critical list
Lithium tantalate Li-Ta-O	X	Lithium on critical lists
Polyvinylidene fluoride (PVDF) C-H-F	OK	
Lead zirconium titanate (PZT) Pb-Zr-Ti-O	X	Lead, Zirconium, and Titanium on critical lists
Quartz, device grade Si-O	X	Silicon on EU list

Discussion point: Regulation - the WEEE Directive

The WEEE Directive (EC 2002/96 and 2003/108) sets collection, recycling and recovery targets for electrical goods. It is part of a legislative initiative to solve the problem of toxic waste arising from electronic products. It requires that producers finance the collection, recovery and safe disposal of their products and meet certain recycling targets. Products failing to meet the requirement must be marked with a “no disposal” mark (a crossed out wheeled bin).

This is yet another concern for the makers of electronic equipment, who are subjected to ever more demanding responsibilities for their products.

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