Materials Science Data

July 8, 2019

Outline : The data questions

- What is materials science ---- the challenge of spanning length scales
- Where do we start --- the periodic table
- Categories of material properties --- what are the relevant descriptors
- How do we measure these properties
- Why are these properties important

- Materials Science : describes how characteristics at different length scales

- From picometer (1 / 1,000,000,000,000 meters) to larger than meters

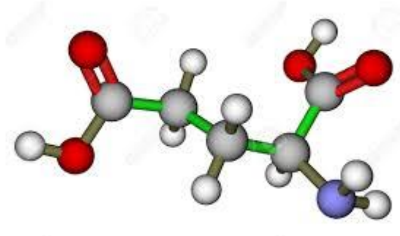
- Relate to properties….. We will discuss some of these relevant properties here

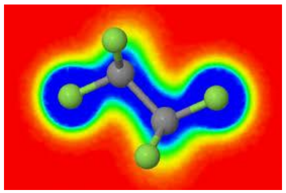
- Includes materials as diverse as electronics, ceramics, metals, rubbers, etc.)

Length Scales

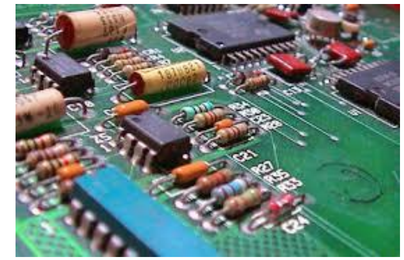
Electron

Atom

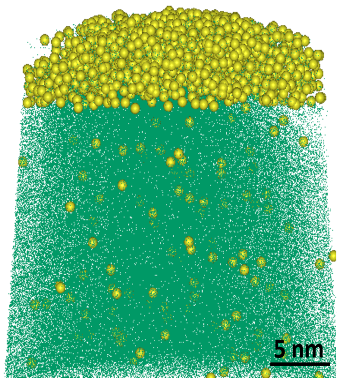




Molecule

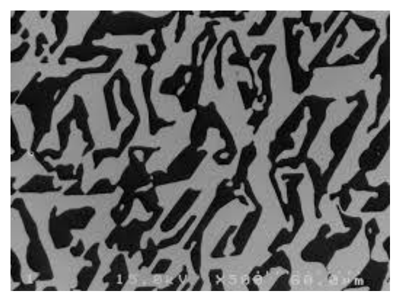


Microstructure

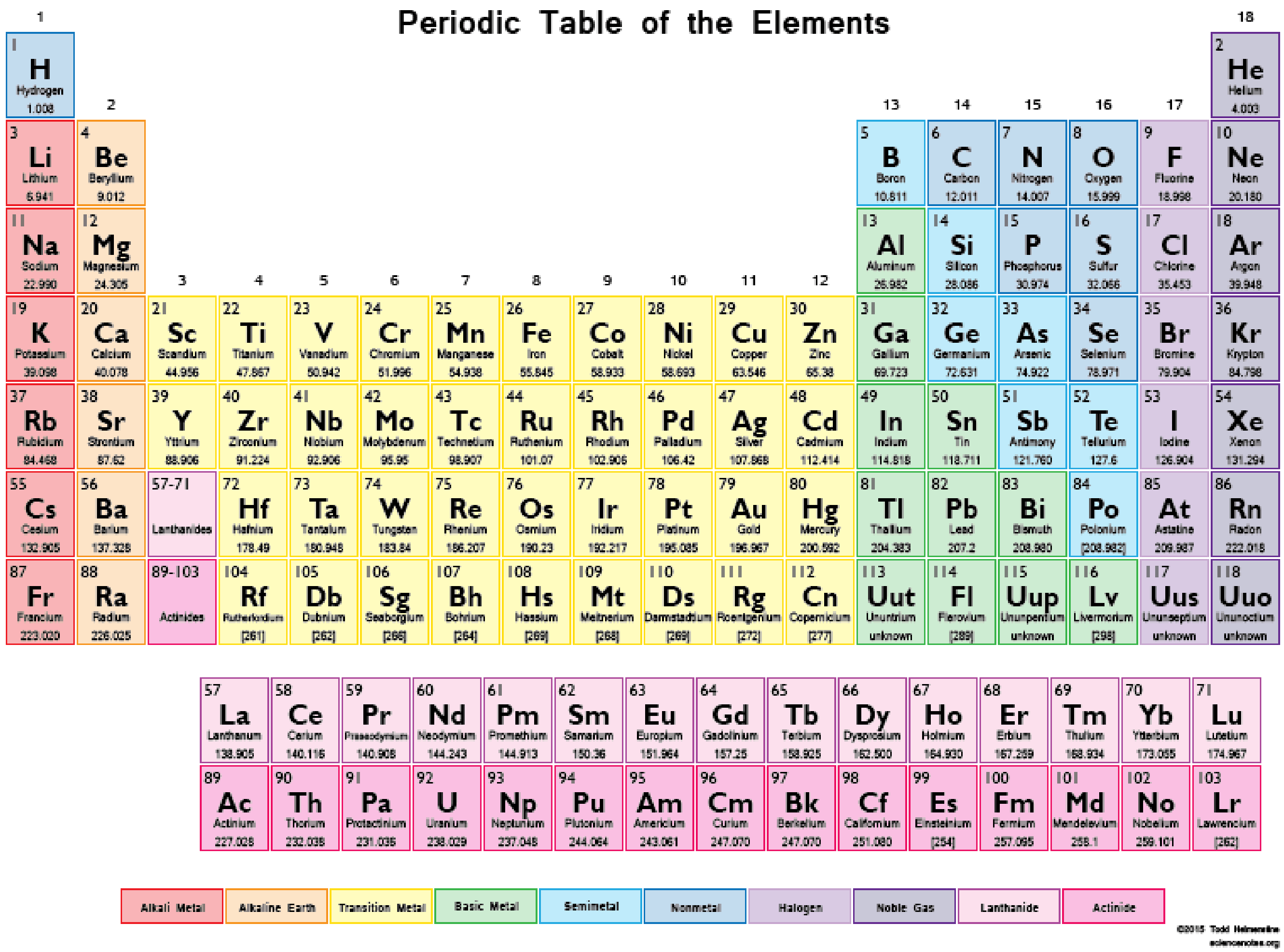


Device

Structure



The question materials science asks is : how does a change at the electronic or atomic level impact the property of the final material ?



The periodic table defines the number of electrons for each element

The Periodic Table as a Data Table

Symbol	Atomic Number	Atomic Weight	Atomic Radius	Covalent Radius	Valence Electrons	Density	Electronegativity	Melting Point	Boiling Point	Toxic	Heat Capacity	Specific Heat
H	1	1.00794	0.78	0.3	1	8.99E-05	2.2	14.01	20.28	FALSE	28.836	14.304
He	2	4.002602	1.28	0.93	2	0.000179		0.95	4.216	FALSE	20.786	5.193
Li	3	6.941	1.52	1.23	1	0.534	0.98	453.69	1620	FALSE	24.86	3.6
Be	4	9.012182	1.13	0.89	2	1.8477	1.57	1551	3243	TRUE	16.443	1.82
B	5	10.811	0.83	0.88	3	2.34	2.04	2573	3931	FALSE	11.087	1.02
C	6	12.011		0.77	4	3.513	2.55	3820		FALSE		0.71
N	7	14.00674	0.71	0.75	5	0.001251	3.04	63.29	77.4	FALSE	29.124	1.04
O	8	15.9994		0.66	6	0.001429	3.44	54.8	90.188	FALSE	29.378	0.92
F	9	18.9984	0.709	0.58	7	0.001696	3.98	53.53	85.01	FALSE	31.304	0.82
Ne	10	20.1797		0.71	8	0.0009		24.48	27.1	FALSE	20.786	0.904
Na	11	22.98977	1.54	1.54	1	0.971	0.93	370.96	1156.1	FALSE	28.23	1.23
Mg	12	24.305	1.6	1.36	2	1.738	1.31	922	1363	FALSE	24.869	1.02
Al	13	26.98154	1.43	1.25	3	2.698	1.61	933.52	2740	FALSE	24.2	0.9
Si	14	28.0855	1.17	1.11	4	2.329	1.9	1683	2628	FALSE	19.789	0.71
P	15	30.97376		1.1	5	1.82	2.19	317.3	553	FALSE	23.824	0.77
S	16	32.066	1.04	1.04	6	2.07	2.58	386	717.824	FALSE	22.75	0.71

Combines qualitative (ie. True / False) data as well as quantitative data, with a wide range of values and scales.

Assessing the Properties of the Elements

	Average Value	Standard Deviation
Atomic Number	56.00	32.19
Atomic Weight	136.80	83.59
Atomic Radius	1.58	0.38
Covalent Radius	1.37	0.35
Valence Electrons	4.99	2.90
Density	8.09	6.93
Electronegativity	1.72	0.63
Melting Point	1280.91	907.94
Boiling Point	2518.12	1629.34
Heat Capacity	26.03	3.77
Specific Heat	0.60	1.59
Heat of Fusion	12582.36	10731.84
Heat of Vaporization	258257.38	213142.15
Thermal Conductivity	0.62	1.19
Electrical Conductivity	0.09	0.12
First Ionization Potential	7.94	3.35
Bulk Modulus	91.93	108.84
Shear Modulus	0.52	0.71
Price	60387.95	447439.30

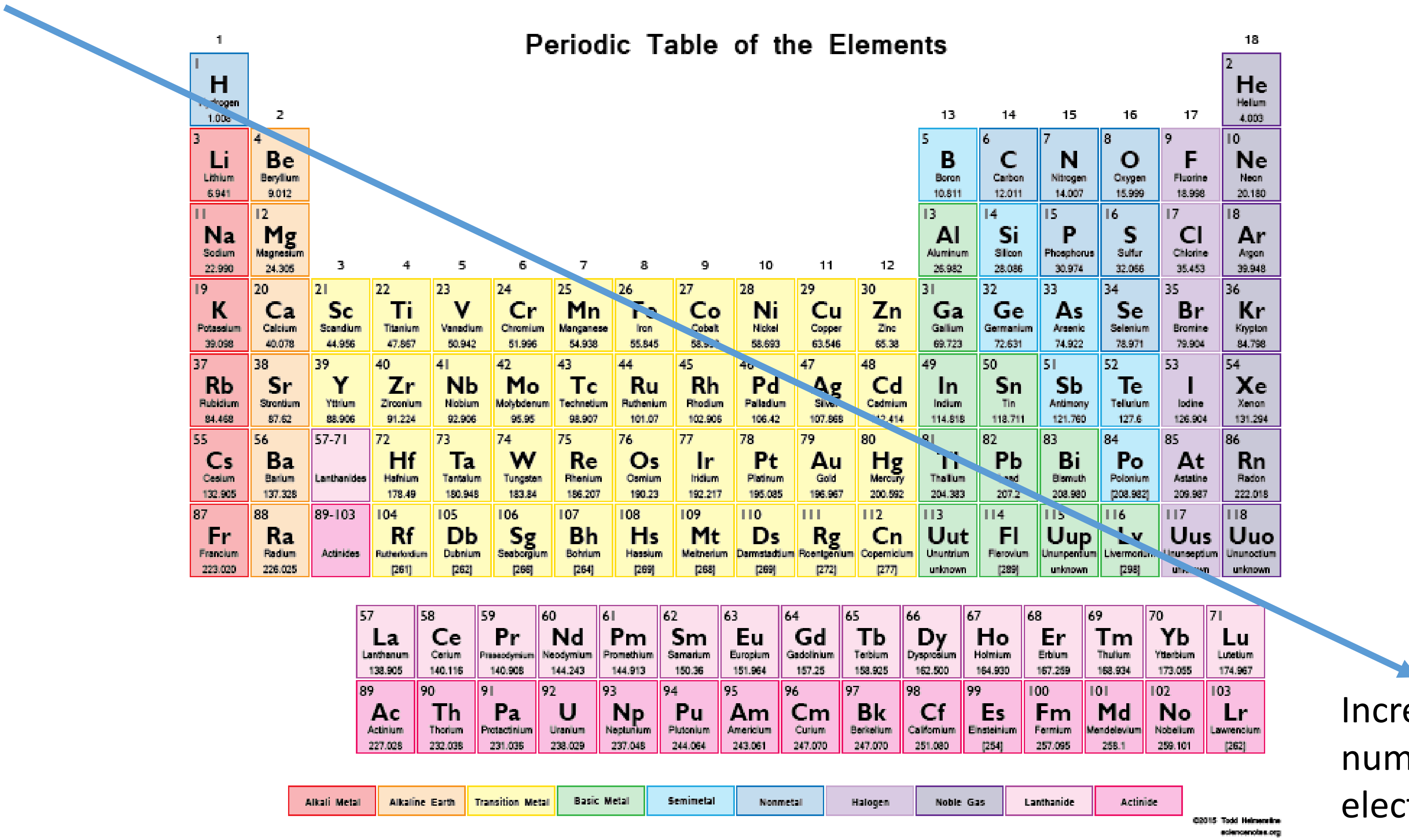
Some data is on the scale of 10^{-2} while other data is on the scale of 10^{5}

Considering range of standard deviations

--- For heat capacity, the standard deviation is only 14% of the average value – small fluctuation in value across the periodic table.

--- For price, the standard deviation is 700% the average value – large fluctuation

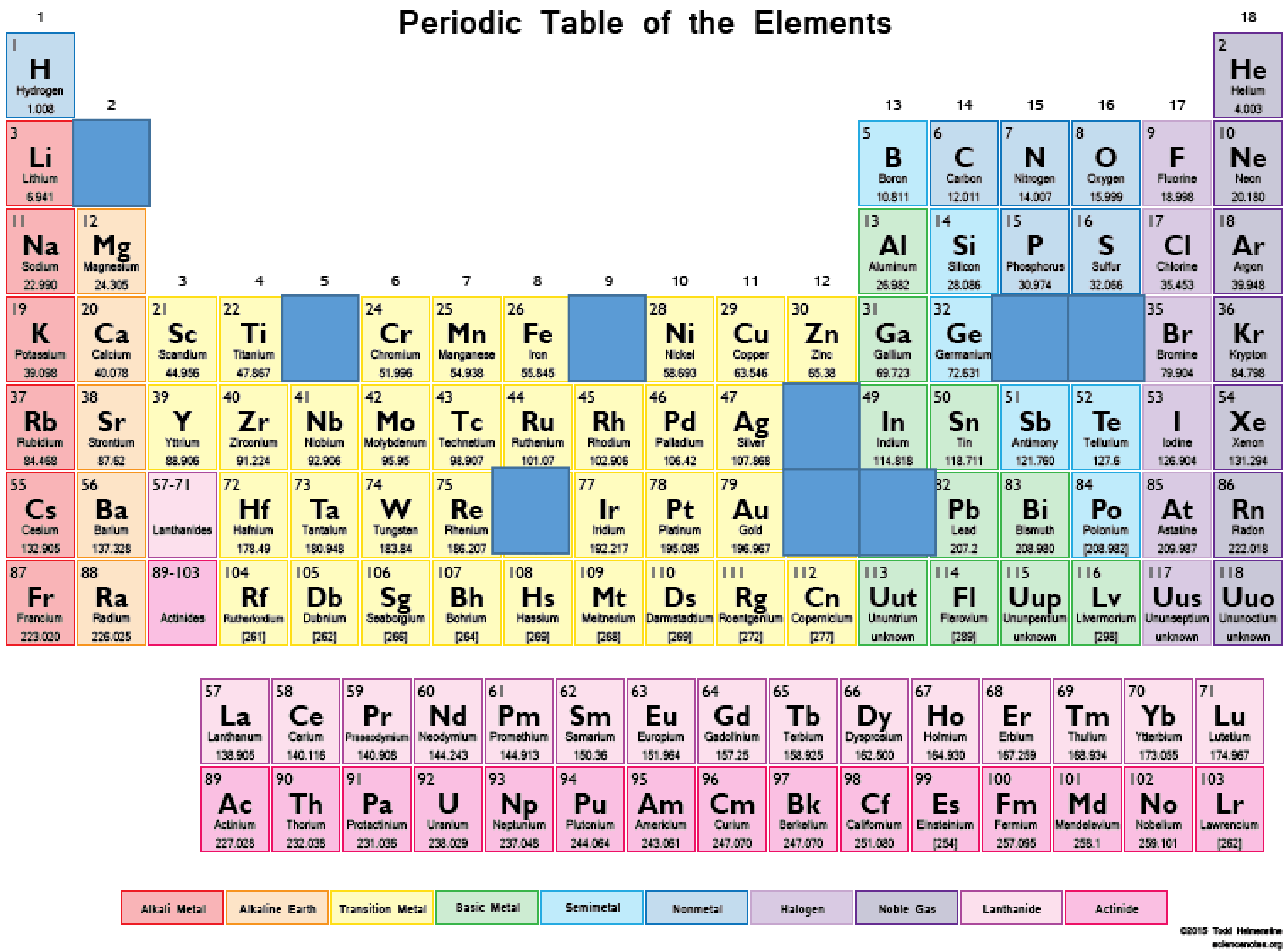
Where to Begin



Increasing number of electrons

The periodic table defines the number of electrons for each element

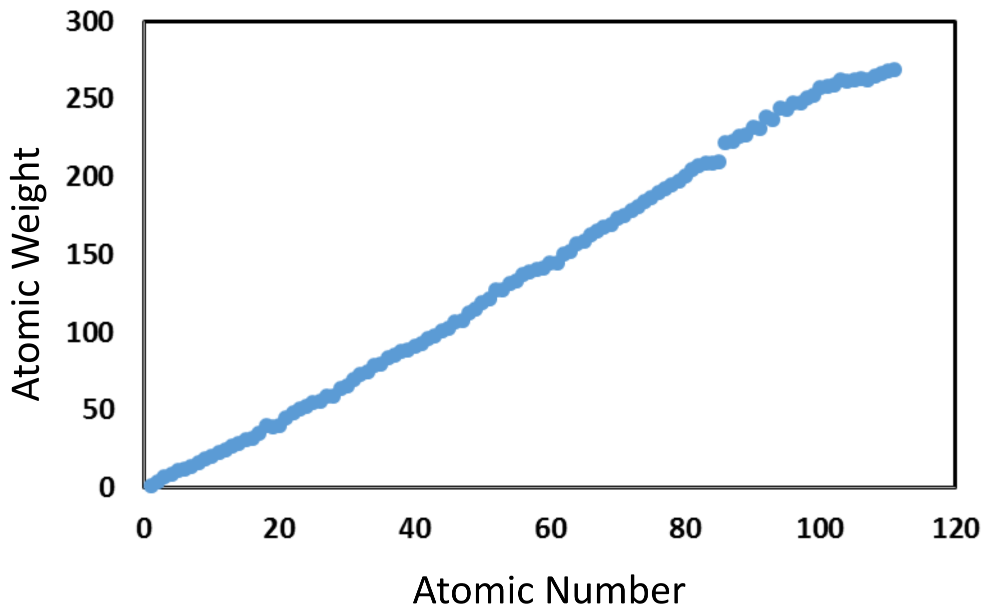
The Periodic Table -- toxicity

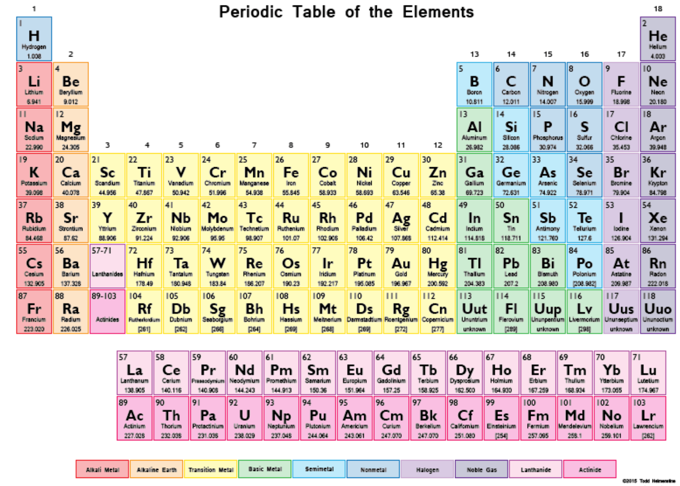


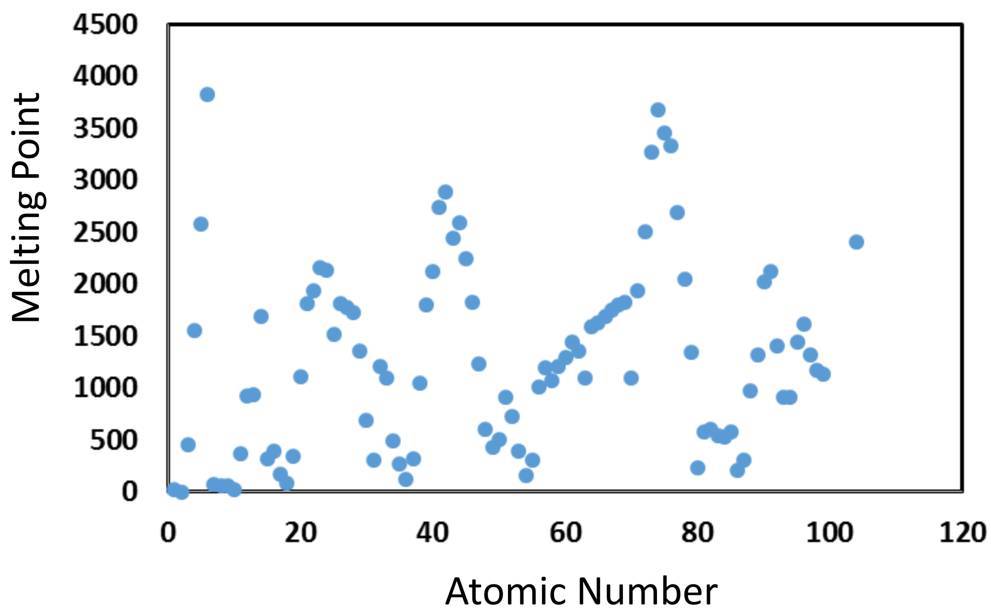
How to use the periodic table for design : Binary description of elements :

-- This figure : is the element toxic : yes / no --- blue boxes are for yes --- **<u>no obvious pattern</u>**

The Periodic Table







In some cases, the trends reflected in the periodic table are clear ; other times they are not obvious

-- atomic weight increases as we move along the table ; the temperature at which the element melts does not follow a clear pattern

Example Properties / Categories from the Periodic Table

Thermal Properties	Size Properties	Electronic Properties	Engineering Property	Environmental Property
Boiling Point	Atomic Weight	Valence Electrons	Bulk Modulus	Toxic
Heat Capacity	Atomic Radius	Density	Shear Modulus	Radioactive
Melting Point	Covalent Radius	Electronegativity		Price
Specific Heat		First Ionization Potential		
Heat of Fusion		Metal Classification		
Heat of Vaporization		Electrical Conductivity		
Thermal Conductivity				

- While properties address specific aspects, they can also be broken up into larger categories, as shown for example here :

- Thermal properties : how does the element behave as temperature changes
- Size properties : how do we describe the change in size
- Electronic properties : what does the electron impact on the element
- Engineering properties : mechanical description, eg. Strength, toughness, etc.
- Environmental property : health and availability

Importance of Remembering Units

“NASA lost a $125 million Mars orbiter because a Lockheed Martin engineering team used English units of measurement while the agency's team used the more conventional metric system for a key spacecraft operation, according to a review finding released Thursday.

“The units mismatch prevented navigation information from transferring between the Mars Climate Orbiter spacecraft team in at Lockheed Martin in Denver and the flight team at NASA's Jet Propulsion Laboratory in Pasadena, California.”

…….

“That probably stopped the engine from completing its burn, so Climate Orbiter likely plowed through the atmosphere, continued out beyond Mars and now could be orbiting the sun.”

From CNN : September 30, 1999

Example Units

Temperature (eg. Melting point, boiling point) often reported in units of degrees Kelvin (defined so that the lowest possible temperature = 0 K). As opposed to Celsius which is defined so that water freezes at 0 and boils at 100, and Fahrenheit where 0 and 100 are based on salt water mixtures

Kelvin = 273 + Celsius = 241 + 1.8*Fahrenheit

Size / Length vary in reported unit depending on the length scale. Atoms measured in angstroms (10^{-10} m) ; Electronic circuits often measured in microns (10^{-6} m) ; Objects measured in meters (m)

nm = 10^{-9} m ; um = 10^{-6} m ; mm = 10^{-3} m ; cm = 10^{-2} m

Going From the Element to the Material

The complexity is the material is greater than just summing the elemental properties :

eg. melting point of material AB does not likely scale with melting point of A + melting point of B

Multiple issues to consider : for example <u>bonding</u> and <u>charge</u>

Types of bonds (example materials):

Metallic (metals),
Ionic (salt),
Covalent (diamond),
Molecular (wax)

Obviously, this plays a major role in the properties of the material

Going From the Element to the Material

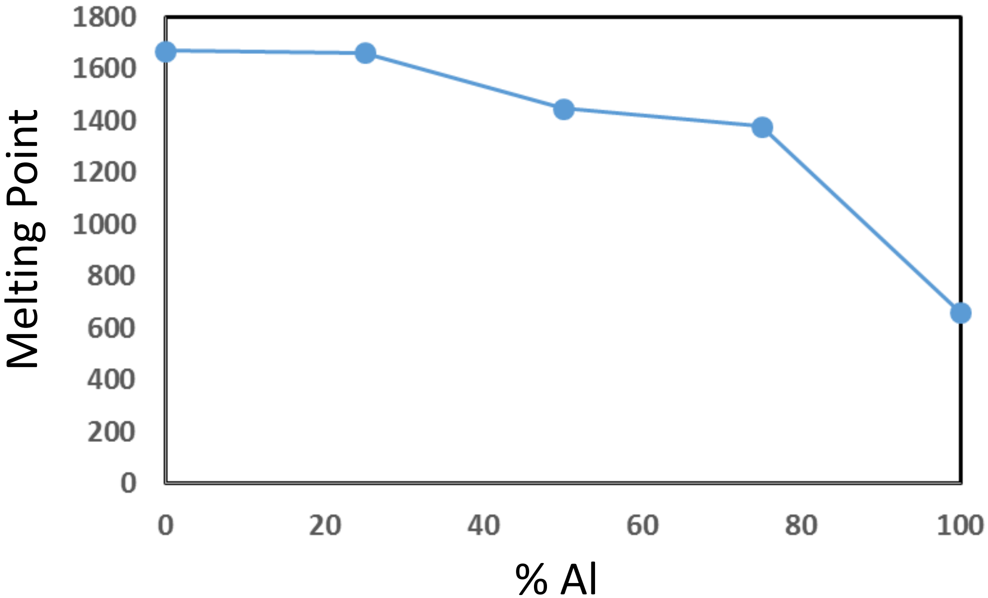
100% Ti Melting point (MP) = 1670 ° C

100% Al MP= 660 °C

25% Al – 75% Ti MP = 1663 °C

50% Al – 50% Ti MP = 1447 ° C

75% Al – 25% Ti MP = 1378 ° C



Complexity of materials prevents us from just averaging the values of elemental properties.

Correlations / trends clearly exist, but this defines the difficulty in design.

Desired Properties of Materials

Metals : want strong and tough metals for structural applications : eg. Cars, buildings, etc. Want them to be lighter – use less gas

Batteries : want to provide large amounts of current and for long time periods

Nanoparticles : Want them to have good properties for the application, but do not want them to be toxic

Magnets : Want high magnetization values, while also being able to operate them at high temperature (eg. Hard disk drives)

While the exact design specifications for each material depends on specific applications, some characteristics are common :

Want it to be cheap, want it to have elements which are available, and want it to not be toxic or environmentally harmful

Data challenges

- **Small dataset**
- **High dimensional dataset**
- **Multicollinearity**

Data of Metals

Metals : want strong and tough metals for structural applications : eg. Cars, buildings, etc. Want them to be lighter – use less gas

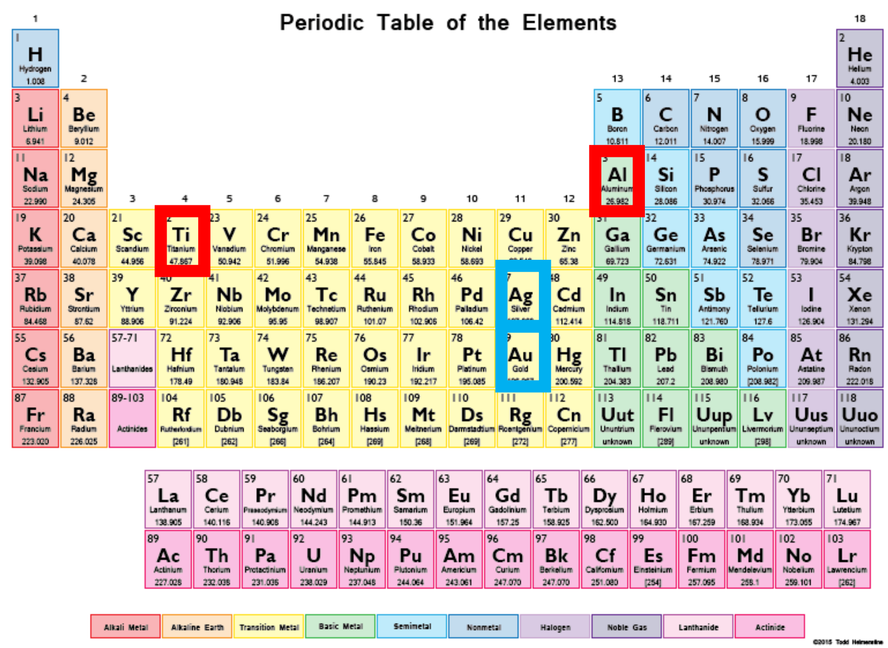
X	Alloy Strength	Alloy Toughness	Alloy Density
Ag	114.63	1.91	3.66
Au	118.89	1.89	3.67
Cd	111.94	1.81	3.73
Co	112.83	1.94	3.45
Cr	119.18	1.79	3.39
Cu	115.92	1.96	3.45
Fe	114.02	1.8	3.38
Hf	113.03	1.74	3.86
Hg	115.12	1.78	3.97
Ir	125.63	2.03	3.59

Popular metal currently is titanium-aluminum alloys (alloy is a metal containing multiple elements)

What is studied is how does the material change when another element X is added : Ti-Al-X

For example, for X = Ag, strength is worse but toughness is better than for X = Au.

Often trade-offs must be considered in design



Data of Metals

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Au	118.89	1.89	3.67
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Cr	119.18	1.79	3.39
Cu	115.92	1.96	3.45
Fe	114.02	1.8	3.38
Hf	113.03	1.74	3.86
Hg	115.12	1.78	3.97
Ir	125.63	2.03	3.59

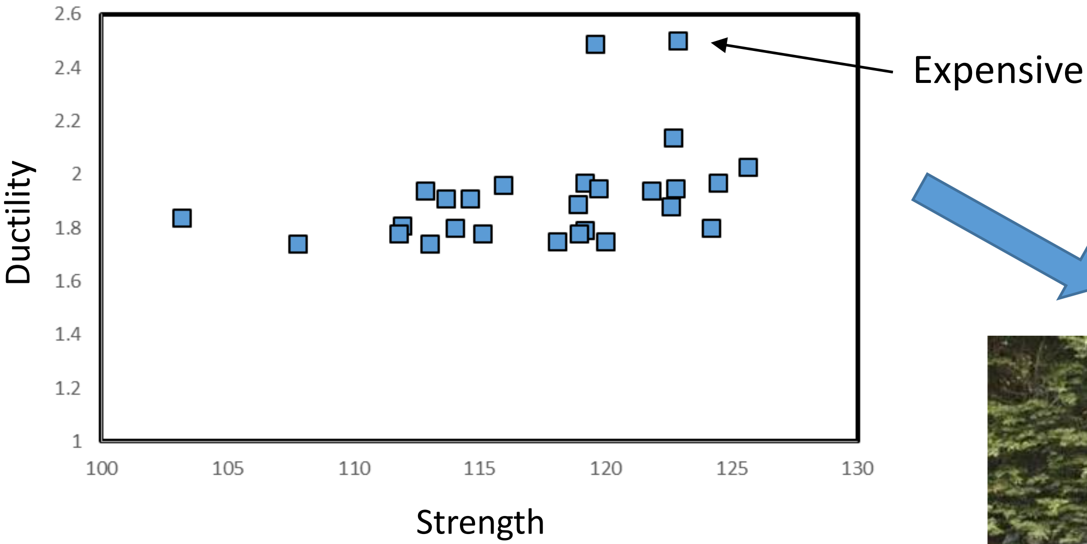
Strength is a measure of how well a material can resist being deformed from its original shape

Toughness is the ability of a material to absorb energy and plastically deform without fracturing

Density is the mass / volume. Therefore, assuming a uniform volume, density is correlated to the mass. Can be measured by weighing the material and measuring the volume.

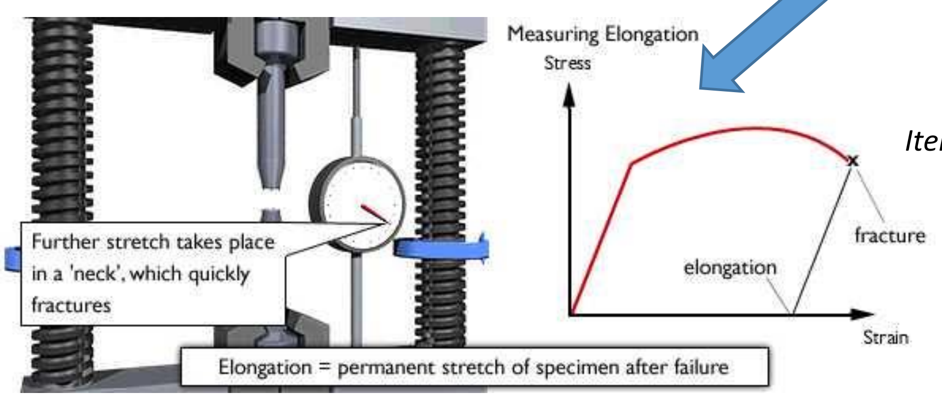
In general, we want a material which is strong, tough, and has low density --- ie. you can hit the material with a large force without damage and the material is light

Data of Metals : Design Loop



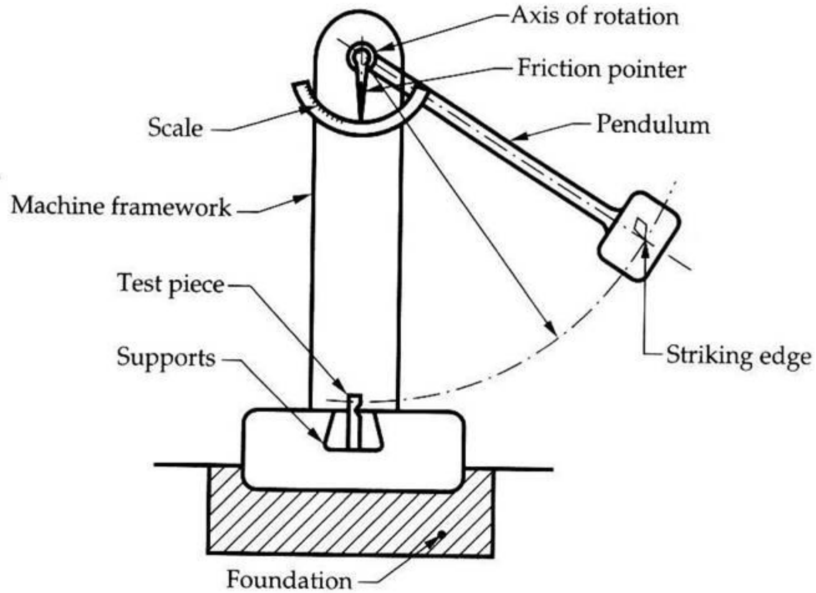
Application : How does it operate under service conditions

Testing : Measuring strength and ductility to add another data point



Iterate the process

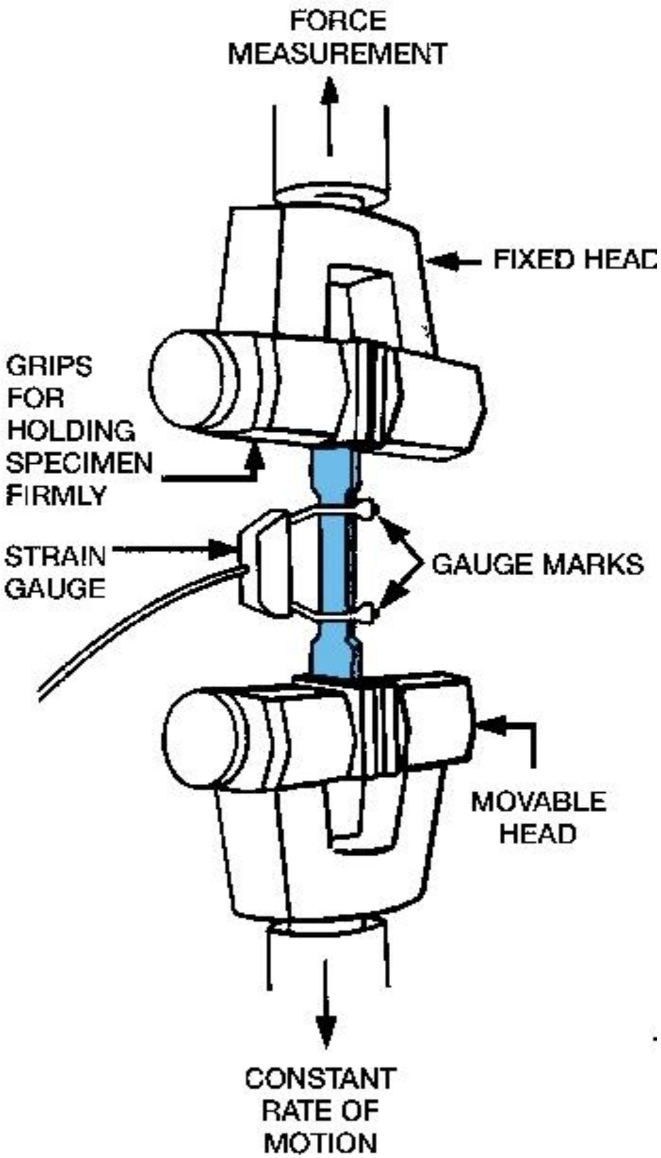
Measuring Strength

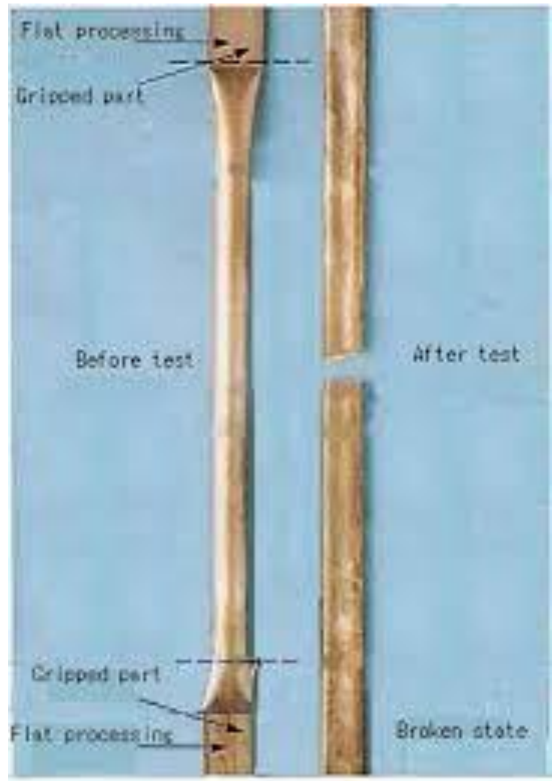


Multiple ways to measure strength: one example is an 'impact test', where the material is hit with a hammer. The more force of the hammer (or alternatively the greater resistance of the material to a given force) required to break the sample corresponds with higher strength.

Strength typically in units of GPa = Force / area --- thus the force of the hammer for a given area.

Measuring Toughness





A common approach to measure toughness (ductility) is to pull on the material and measure how far it stretches before it deforms.

If a material can stretch a large amount before it breaks, then that indicates that the material is tough ; if it breaks without stretching much, than it is brittle.

Toughness reported in % elongation = length at fracture / original length.

Desired Properties of Materials

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Batteries : want to provide large amounts of current and for long time periods

Nanoparticles : Want them to have good properties for the application, but do not want them to be toxic

Magnets : Want high magnetization values, while also being able to operate them at high temperature (eg. Hard disk drives)

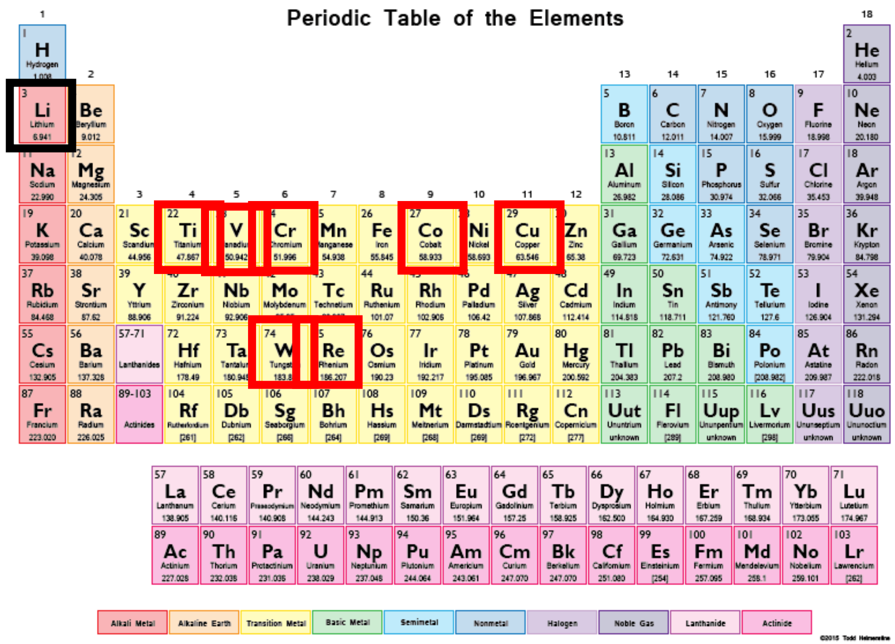
Battery Data

A	B	Average Output Voltage	Capacity
Ca	Co	3.25	242
Ca	Mo	2.44	97
Ca	Ti	1.93	149
Ca	V	2.68	260
Ca	W	1.5	59
Li	Co	3.76	274
Li	Cr	4.01	295
Li	Cu	3.91	262
Li	Mo	2.45	199
Li	Re	1.55	216
Li	Ti	1.78	309
Li	V	2.91	298
Li	W	1.7	120
Mg	Co	3.05	138
Mg	Mo	2.32	191
Mg	Ti	1.21	291
Mg	V	2.54	282
Mg	W	0.78	60
Y	Cu	3.11	436
Y	V	1.84	316
Zn	Mo	1.04	167
Zn	Ti	-0.17	238
Zn	V	1.18	232
Zn	W	-0.86	58

- Average output voltage measures the maximum amount of voltage which can be output
- Capacity describes the amount of current that can be output over a period of time – in units of Milliamp-hours (mAh). A larger capacity means that it will take longer to discharge the battery
- We want to maximize the output voltage possible, while also making it take longer to discharge the battery.

Battery Data

Battery types of AB – for example, first row is a CaCo battery



If we look for example at the elements that could be combined with Li, no clear trend is seen between periodic table and properties

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In the last year, the Samsung cell phones have been in the news due to causing fires --- resulting from Li-ion batteries

The reason behind the fires is due to incorrect selection of battery size --- results in trying to pull more voltage from the battery than the output allows.

Therefore, an increase in output voltage is required to get same performance.

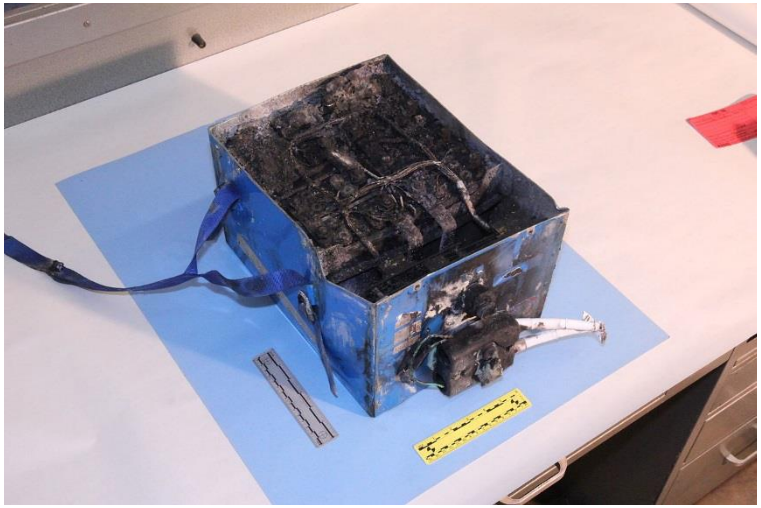
Battery Considerations

Similar issues have resulted recently in the Boeing Dreamliner airplane, as well as for hoverboards.

Lithium-ion batteries, unlike other rechargeable batteries, have a potentially hazardous pressurized flammable liquid electrolyte.

In the case of the Dreamliner, the overheated or overcharged cell resulted in failure after 52,000 hours, as opposed to the 10 million flight hours predicted.

In the case of the hoverboards, the batteries were overcharged due to using charger not certified for the batteries.



Battery Considerations

- Lithium-ion cells are very susceptible to damage outside the allowed voltage range that is typically within (2.5 to 3.65) V
- Exceeding this voltage range results in premature aging of the cells and, furthermore, results in safety risks due to the reactive components in the cells
- So why are we still using Li-ion batteries even with these problems.
- Because, as shown in the graph, they tend to perform better than batteries that use less flammable materials.

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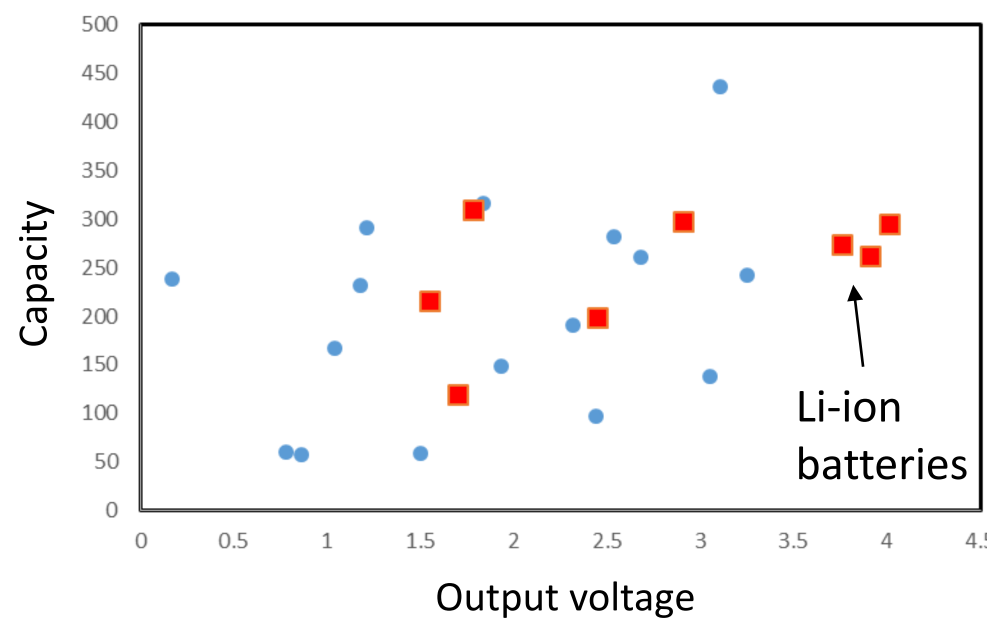
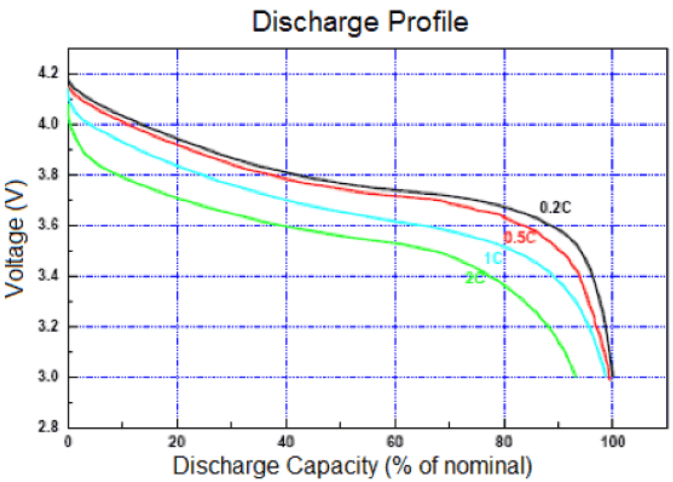


Measuring Battery Properties



Capacity is determined by the equation :

$Q = I * t$, where Q is charge, I is current, and t is time.

Capacity is related to Q, ie. the usable charge

At constant current, can run battery cell until it reaches minimum voltage. From the time (t) and constant current (I), the capacity is estimated.

Taking the area underneath the curve of I versus t gives an exact value of capacitance, as current is unlikely to remain constant.

Desired Properties of Materials

Metals : want strong and tough metals for structural applications : eg. Cars, buildings, etc. Want them to be lighter – use less gas

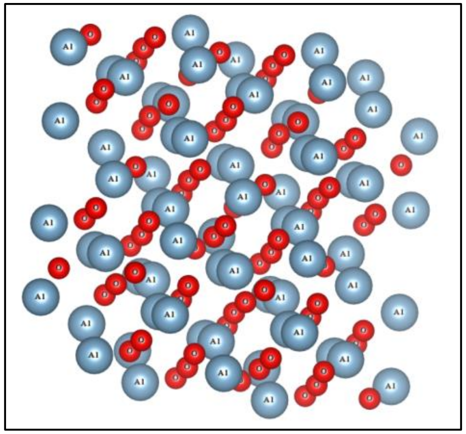
Batteries : want to provide large amounts of current and for long time periods

Nanoparticles : Want them to have good properties for the application, but do not want them to be toxic

Magnets : Want high magnetization values, while also being able to operate them at high temperature (eg. Hard disk drives)

Toxicity Data

Oxide nanoparticle	Toxicity	is.toxic
TiO2	1.74	FALSE
SnO2	2.01	FALSE
ZrO2	2.15	FALSE
SiO2	2.2	FALSE
Fe2O3	2.29	TRUE
Al2O3	2.49	TRUE
Cr2O3	2.51	FALSE
CeO2	2.602	FALSE
Sb2O3	2.64	TRUE
In2O3	2.81	TRUE
Bi2O3	2.82	TRUE
La2O3	2.87	TRUE
Y2O3	2.87	TRUE
V2O3	3.14	TRUE
CuO	3.2	TRUE
NiO	3.45	TRUE
ZnO	3.45	TRUE
CoO	3.51	TRUE



- Toxicity is reported as $\log(1/EC_{50})$

EC_{50} has units of mol/L

Mol : measure of quantity
L : measure of volume

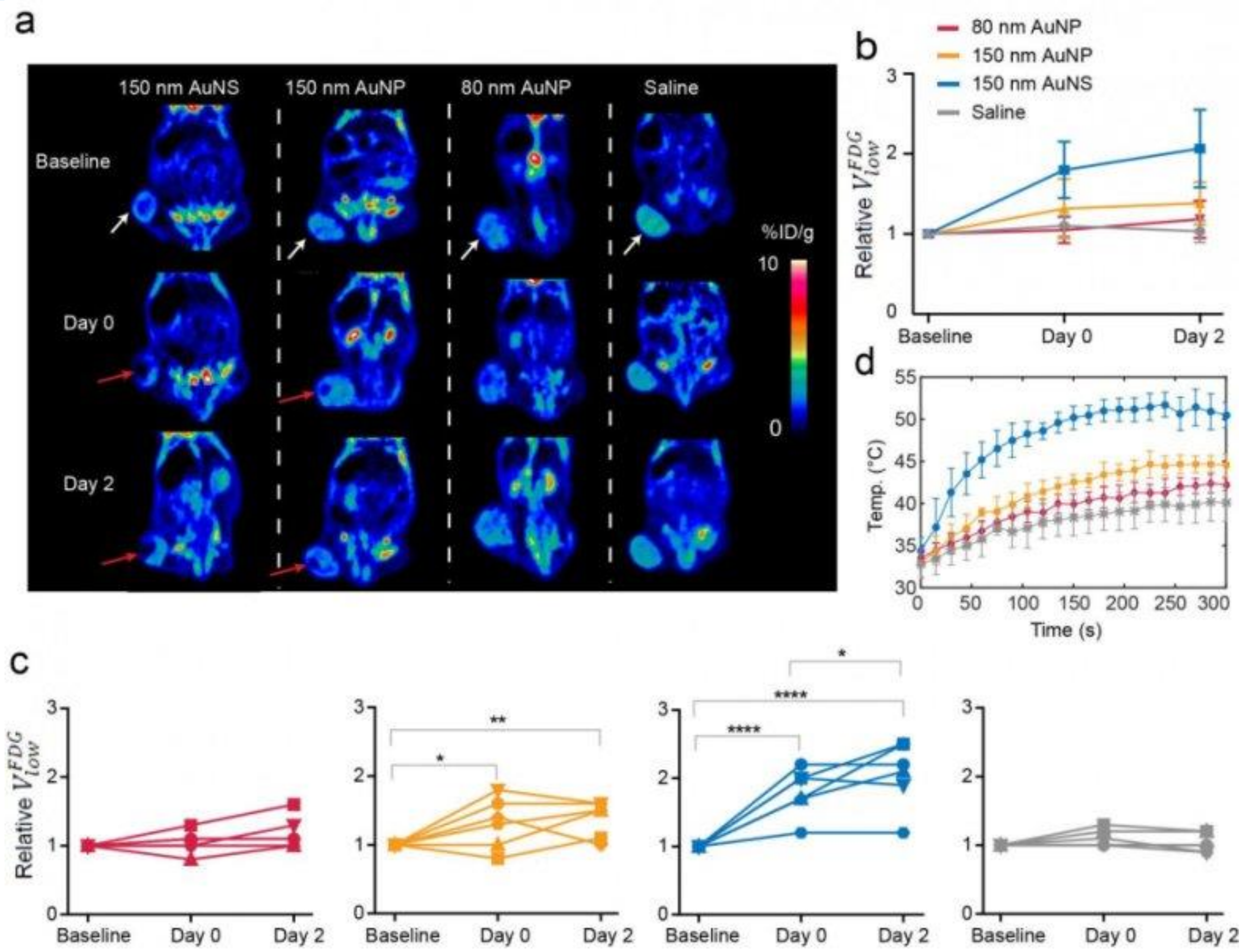
- Mol/L is therefore a density. This measures what density of nanoparticles is required to alter half of the cells. So large EC_{50} means that lots of nanoparticles are needed to affect the cells – thus less toxic.

- Therefore, this would correspond to smaller $1/EC_{50}$ --- ie. larger 1/EC50 corresponds to higher toxicity.

Uses of Nanoparticles

The images show PET scans of a mouse with a large tumor (by the white arrow). The tumor is treated with nanoparticles, which are injected directly into the tumor and are then flashed with near infrared laser light. The laser light heats the nanoparticles, thus damaging or killing the cancer cells (red arrows).

Credit: Kamilla Nørregaard and Jesper Tranekjær Jørgensen, Panum Inst.



Uses of Nanoparticles

Fabrics are being engineered to contain nanosilver – any of a collection of nanoparticles made from silver – are used to kill odor causing bacteria in socks and sports clothing.

Could a seemingly simple clear plastic bag—the kind that you load your fruits and vegetables into at the supermarket—actually be as strong as steel? It could be if it is made from a new composite plastic that blends the strength of nanoparticles with the pliancy of a water-soluble polymer.

Toxicity in Nanoparticles

"Currently, more than 600 consumer products containing nanomaterials are already on the market, used in sporting goods, tires, stain-resistant clothing, sunscreens, cosmetics, and electronics and increasingly utilized in biomedicine for purposes of diagnosis, imaging, and drug delivery.

"[T]he increased presence of nanomaterials in commercial products raises concerns about adverse effects on environment, health, and society (NanoEHS). The key to the long-term growth and sustainability of nanomaterials is to establish end-user confidence that the engineered nanomaterials are safe. Increasing numbers of investigations show that many types of nanomaterials, including carbon nanotubes, fullerenes, quantum dots such as CdS, oxide nanoparticles such as ZnO and TiO_2, have a toxic effect on biological cells."

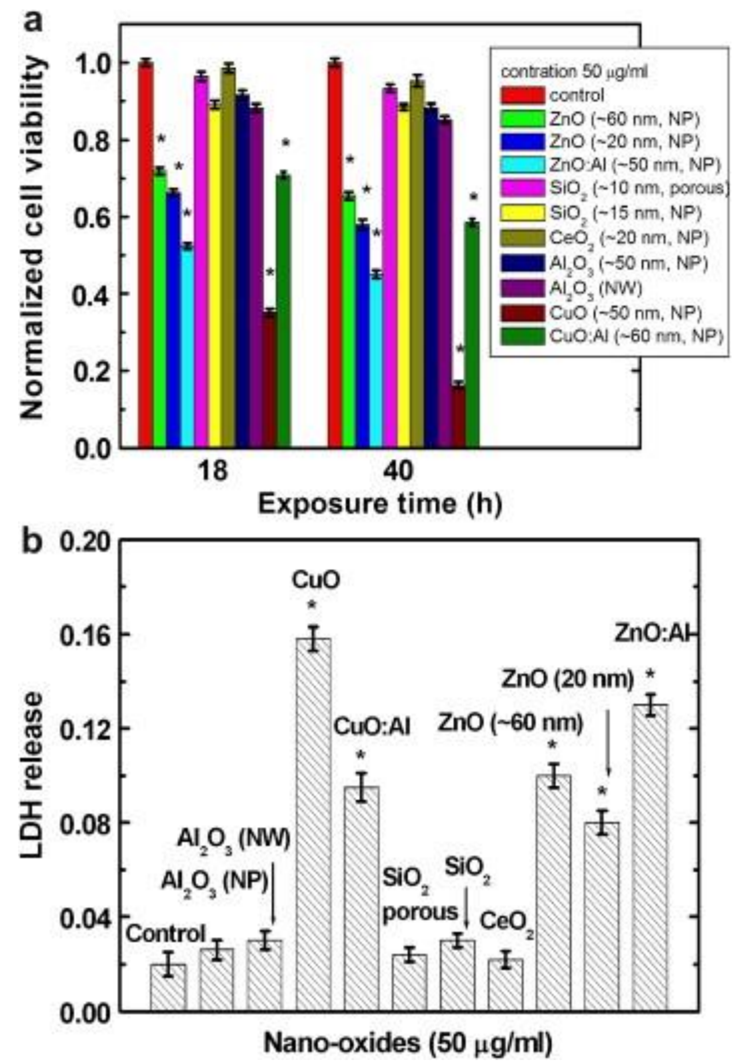
M. Xu, et al, Biomaterials, 31, p. 8022-8031

Measuring EC_{50} Data

In toxicology measurements, dose descriptor is the term used to identify the relationship between a specific effect of a chemical substance and the dose at which it takes place. The dose descriptors are used to derive the no-effect threshold levels for human and environmental health and safety.

Dose descriptors are determined in the toxicological studies on the hazards of the substance and are usually expressed as LC50, LD50, NOAEL, NOAEC, T25, BMD, EC50, NOEC, DT50, etc. They are used for hazard classification and risk assessment.

LC50 is a statistically-derived dose at which 50% of the animals will be expected to die. For inhaled toxicity, air concentrations are used for exposure values. LC50 is measured as **mg/L**.



Desired Properties of Materials

Metals : want strong and tough metals for structural applications : eg. Cars, buildings, etc. Want them to be lighter – use less gas

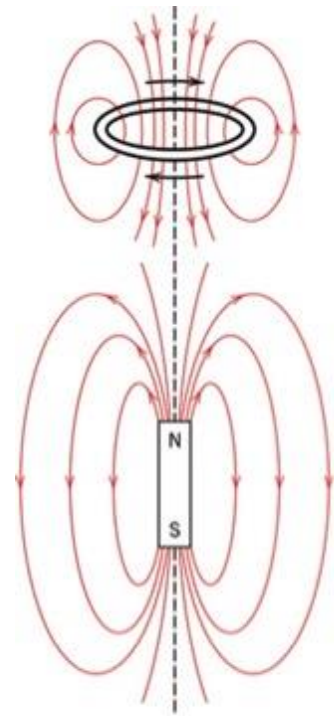
Batteries : want to provide large amounts of current and for long time periods

Nanoparticles : Want them to have good properties for the application, but do not want them to be toxic

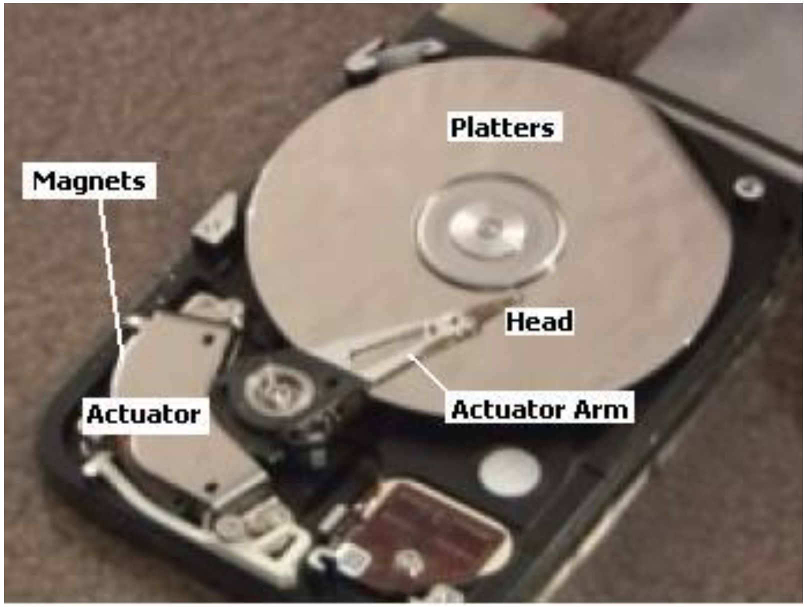
Magnets : Want high magnetization values, while also being able to operate them at high temperature (eg. Hard disk drives)

Magnetic Data

A	B	Maximum Temperature	Saturation Magnetization	Contain RE	Contains Toxic
Ce	Fe	-38	2.5	TRUE	FALSE
Co	Ga	316	0.53	FALSE	TRUE
Co	Pt	567	1.01	FALSE	TRUE
Co	Si	237	0.24	FALSE	TRUE
Co	Sn	366	0.76	FALSE	TRUE
Cr	O	123	0.49	FALSE	FALSE
Dy	Fe	362	5.8	TRUE	FALSE
Er	Fe	314	4.9	TRUE	FALSE
Eu	O	-204	2.36	TRUE	FALSE
Fe	Ni	570	1.04	FALSE	FALSE
Fe	Pd	476	1.38	FALSE	FALSE
Fe	Pt	477	1.43	FALSE	FALSE
Gd	Co	741	0.29	TRUE	TRUE
Gd	Fe	523	3.6	TRUE	FALSE
Ho	Fe	335	5.5	TRUE	FALSE
Mn	Al	377	0.75	FALSE	FALSE
Mn	As	45	0.63	FALSE	TRUE
Mn	Bi	360	0.73	FALSE	FALSE
Ni	Fe	570	1.04	FALSE	FALSE
Ni	Mn	477	1	FALSE	FALSE
Sm	Co	747	0.86	TRUE	TRUE
Sm	Fe	415	2.7	TRUE	FALSE
Tb	Fe	425	0.5	FALSE	FALSE
Tm	Fe	326	2.6	TRUE	FALSE
Y	Co	714	0.85	FALSE	TRUE
Y	Fe	54	0.48	FALSE	FALSE



Magnetic Application --- Computer Hard Disk Drive (HDD)



The magnet controls the spin, and leads to the faster reading of data and leads to larger hard drive capacities and better performance.

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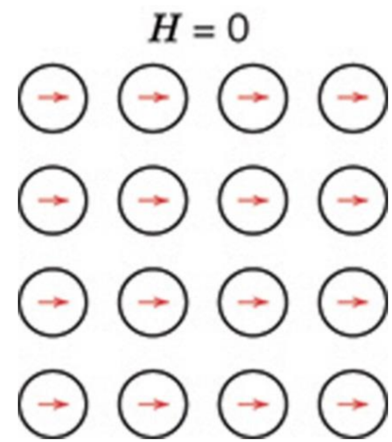
The maximum possible magnetization, or **magnetic saturation, M_s** of a ferromagnetic material represents the magnetization that results when all the magnetic dipoles in a solid piece are aligned to the external field.



Small domains in materials can be magnetically aligned in one of two orientations, corresponding to a 0 or a 1 in digital storage. This technique is used to read and write on magnetic storage media.

Magnetic Data

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Co	Si	237	0.24	FALSE	TRUE
Co	Sn	366	0.76	FALSE	TRUE
Cr	O	123	0.49	FALS	
Dy	Fe	362	5.8	TRU	
Er	Fe	314	4.9	TRU	
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Fe	Ni	570	1.04	FALS	
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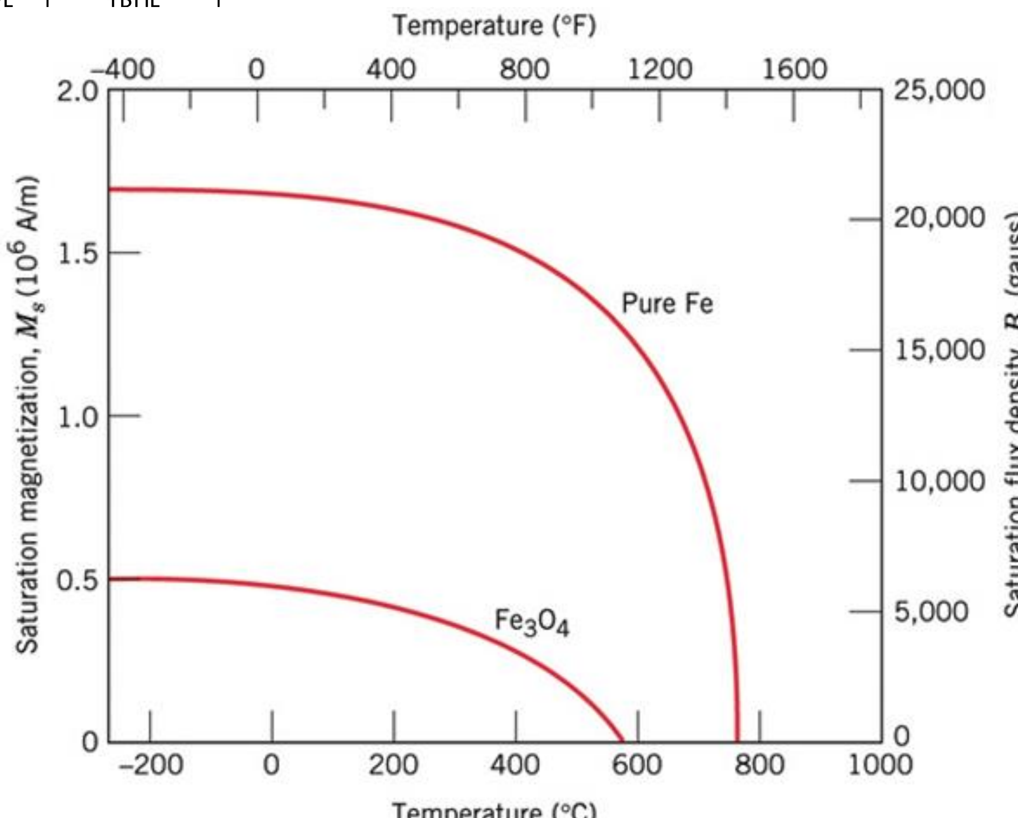
The saturation falls off with temperature, and there is a maximum temperature above which a material cannot be magnetized.



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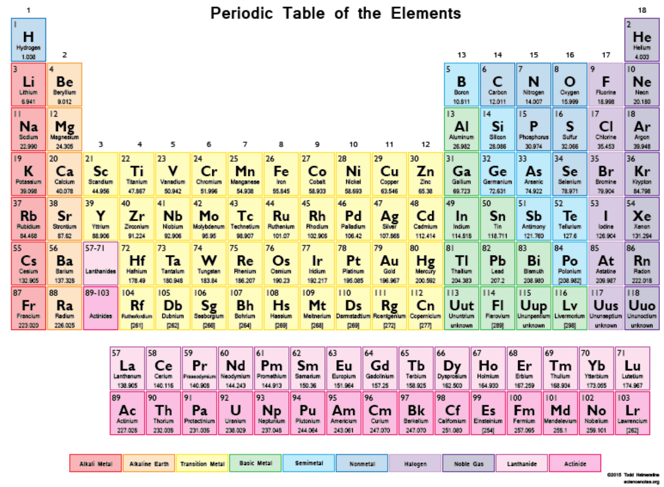
Magnetization is measured as **A/m** – amps per meter.

The ampere is the unit of electrical current, and 1 amp is the current that flows with a charge of 1 Coulomb per second. The Coulomb is dimensionless, and is 6.24×10^{18} – so that's the number of electrons that pass a given point in 1 second.

Summary

What is the link between the elements as described in the periodic table and the application properties when elements are combined.



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