MATERIALS SCIENCE FOR ENGINEERS

~ 4.5 10^9 years, 3^{rd} generation star dust "settles" to form our solar system

~ 10^6 years, humans branch off similar mammals, **Stone tools = Stone Age**

~ 30,000 anatomically modern humans, homo sapiens sapiens, with "same" mindset

~ 10,000 invention of agriculture *in the middle East*, Pottery/Glass *in Mesopotamia*

4000 – 2000 BC **Copper Age**

2000 – 1000 BC **Bronze Age**, i.e. (Cu,Sn) alloys, ***invention of metallurgy***

1000 – 1 BC **Iron Age**

~ 1650 Classical physics - Mechanics

~ **1800 Metallography / Crystallography**

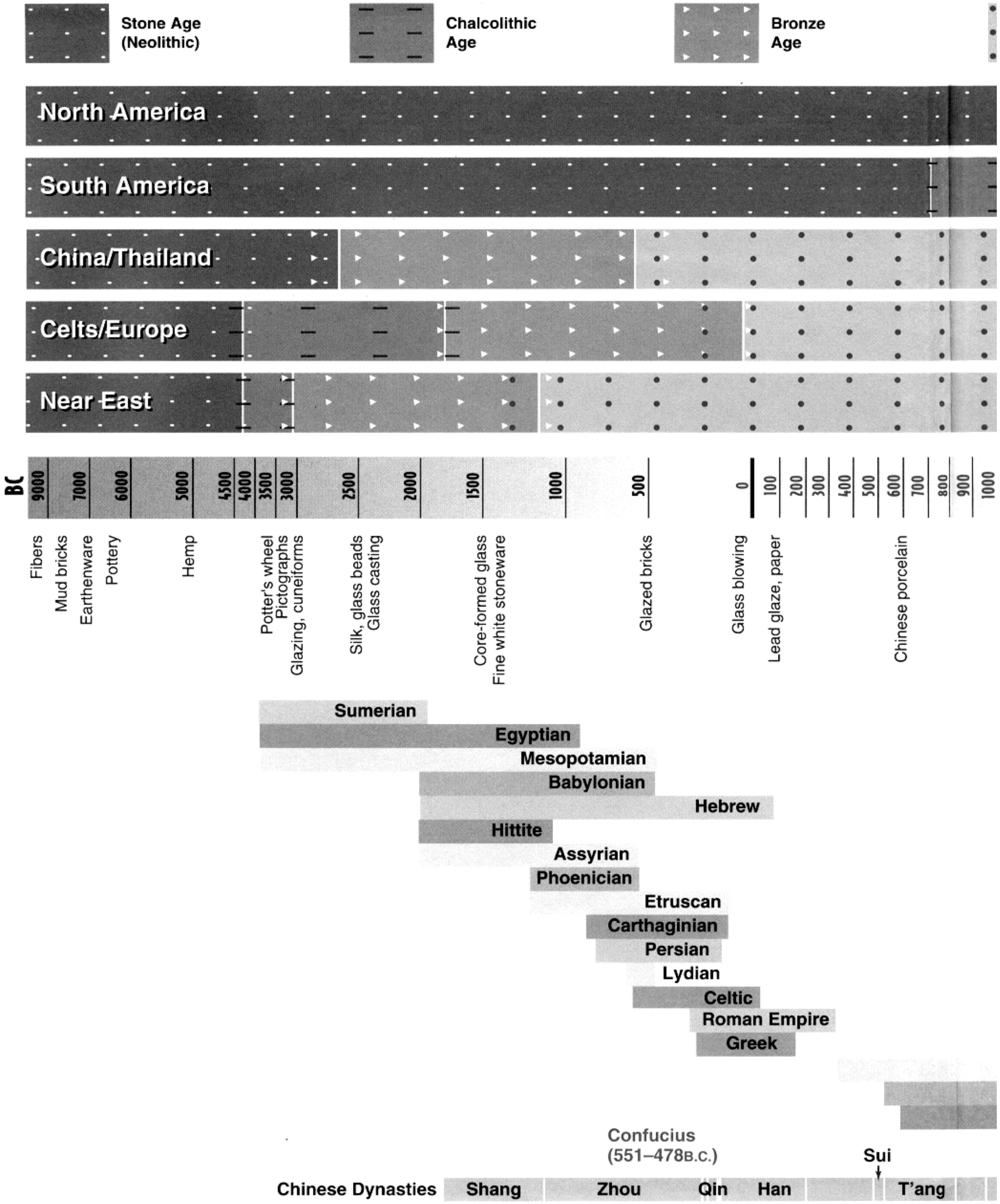
~ **1900 Physical Metallurgy, Crystal Physics, Statistical Physics, Modern Physics, Sold State Physics**

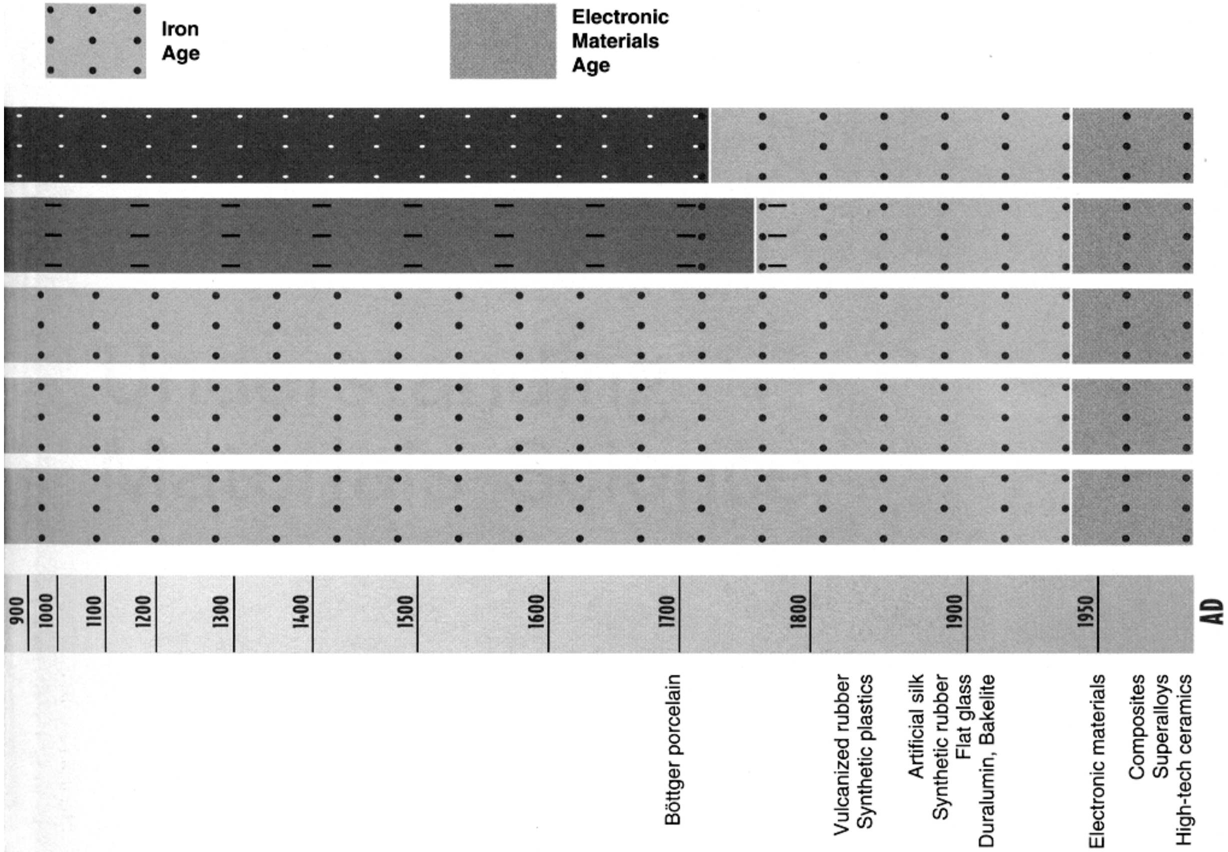
1947 invention of transistor at Bell Labs (Ge), ***Nobel prize*** for Physics 1956 to William Shockley John Bardeen (also 1972) and Walter H. Brattain

~ **1950 Materials Science and Engineering**

~ **1955 Silicon** *(electronic materials, information technology)* **Age**

21st century Nanoscience and Technology


Stone Age (Neolithic)
Chalcolithic Age
Bronze Age
North America
South America
China/Thailand
Celts/Europe
Near East
BC
9000
7000
6000
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
100
200
300
400
500
600
700
800
900
1000
Fibers
Mud bricks
Earthenware
Pottery
Hemp
Potter's wheel
Pictographs
Glazing, cuneiforms
Silk, glass beads
Glass casting
Core-formed glass
Fine white stoneware
Glazed bricks
Glass blowing
Lead glaze, paper
Chinese porcelain
Sumerian
Egyptian
Mesopotamian
Babylonian
Hebrew
Hittite
Assyrian
Phoenician
Etruscan
Carthaginian
Persian
Lydian
Celtic
Roman Empire
Greek
Confucius
(551–478B.C.)
Sui
Chinese Dynasties
Shang
Zhou
Qin
Han
T'ang



Materials ◆ Civilizations ◆ Ages

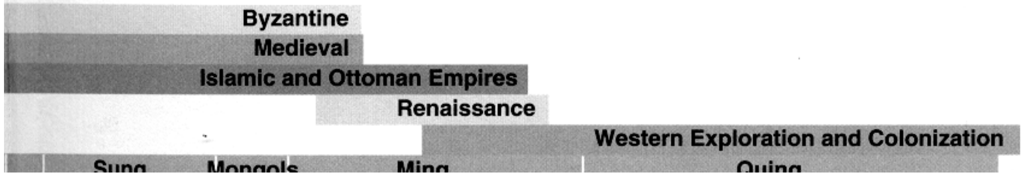
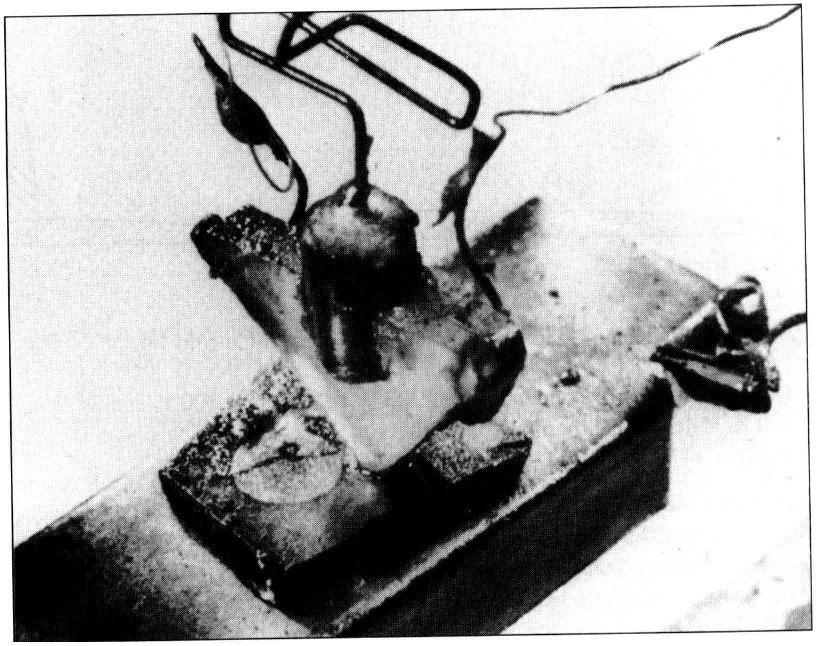


FIGURE 1.1. Copper pendant found in a cave in northeast Iraq; about 9500 B.C. The shape was obtained by hammering native copper or by carving copper ore. (Reprinted by permission from C.S. Smith, *Metallurgy as a Human Experience* (1977), ASM International, Materials Park, OH, Figure 2.)



the world's first semiconductor transistor (Ge)

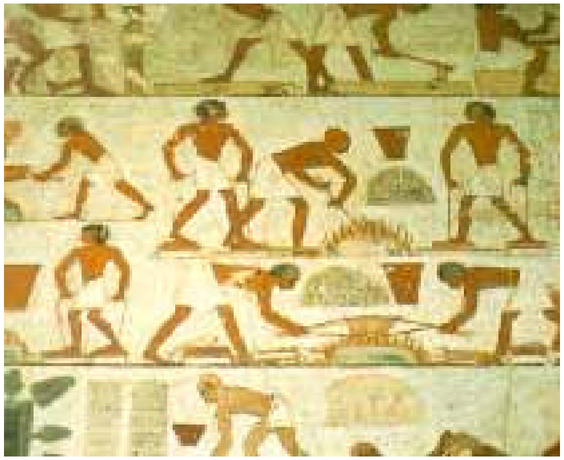
Bell Labs, New Jersey, USA

Nobel prize for Physics 1956 to William Shockley, John Bardeen (also 1972) and Walter H. Brattain

300,000 BC flint, can be easily shaped for tools, beginning of ceramics

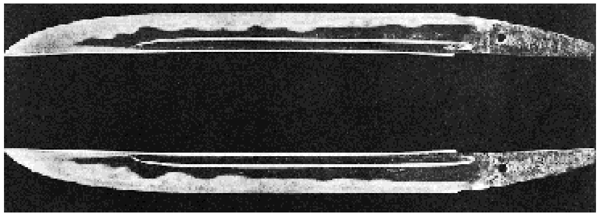
5,500 BC native gold and copper as found on surface of earth used for tools and weapons

4,000 BC, melting and casting of metals, earliest know cast metal object, copper mace head



3,500 Egyptian tomb painting recording metal working

~ 3,000 BC, bronze, the first alloy, metallurgy



Damascus sword,
Fe:C alloys, steal, for blades, guns, canons, tanks, airplanes, depleted U ammunition to destroy tank armor, ….

India **from ˜ 1000 BC to ˜ 650 AD, Wootz steel = (first) Damascus steel**

small pieces of wrought iron together with some wood chips and leaves in small clay crucibles which were sealed with a clay lid and then heated in air-blast enhanced fires, this enabled (less than 2% C) to distribute uniformly, resulting in a steel of superior hardness

book: *Von Stahel and Eysen*, Nürmberg, 1532, by a German alchemist

“Take varnish, dragon’s blood, horn scrapings, half as much salt, juice, made form earthworms, radish juice, tallow, and vervain and quench therein. It is also very advantageous in hardening if a piece that is to be hardened is first thoroughly cleaned and well polished.”

….

“If fault should be found with some of the recipes, pray do not reject the whole book. Perhaps the fault lies in the user himself, because he did not follow the instructions correctly. ***All arts requite practice and long experience, and their mastery is only gradually acquired.”***

Legend: medieval German weapon smith Wieland’s recipe: file a forged piece of iron into coarse powder, fed to your chicken, separate filing from the chickens faces by a magnet, after 7 passes through the chicken bodies, you have the material for swords of superior strength and hardness,
Science in 1930: steel with low C content and some N is indeed produced industrially !

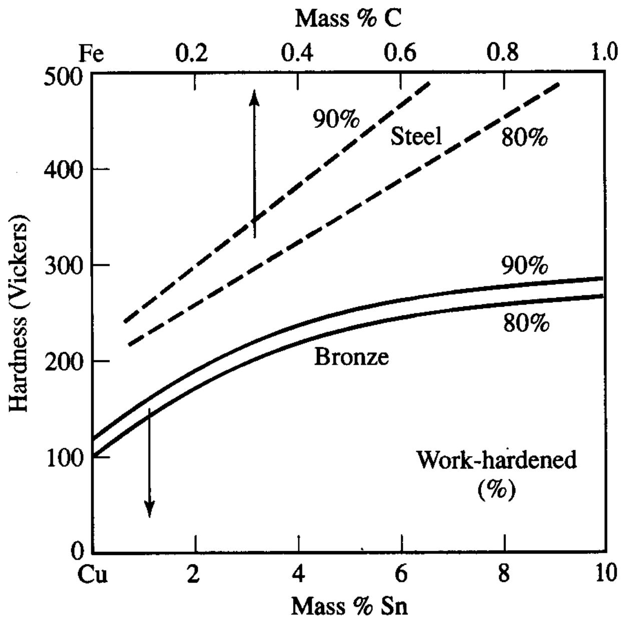


FIGURE 7.1. Hardness of various steels and bronzes as a function of composition and degree of work hardening. The work hardening is given in percent reduction of area (see also Table 2.1).

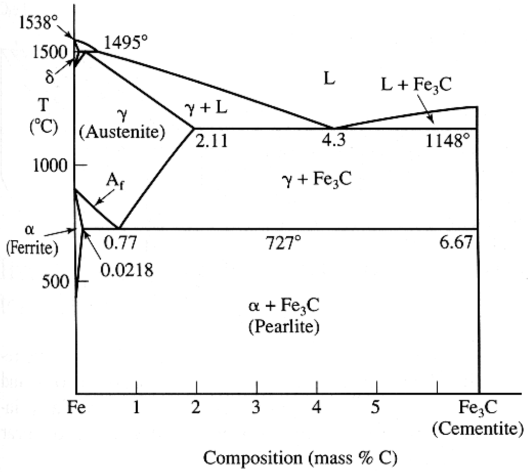


FIGURE 8.1. Portion of the iron–carbon phase diagram. (Actually, this section is known by the name *Fe-Fe$_3$C phase diagram.*) A_f is the highest temperature at which ferrite can form. As before, the mass percent of solute addition is used (formerly called weight percent).

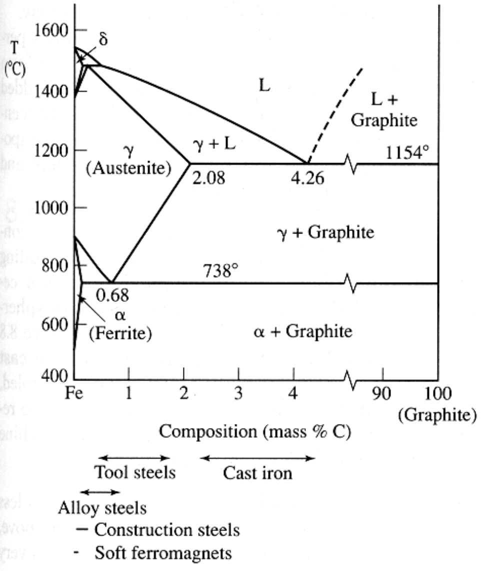


FIGURE 8.7. The equilibrium iron–carbon phase diagram showing graphite as the stable phase. Compare to Figure 8.1, in which the metastable intermetallic phase Fe$_3$C is prominently included. The dashed line marks the solubility of graphite in liquid Fe. Note the carbon contents of common iron-containing materials, which are shown below the phase diagram.

Metallurgy

Vannoccio Biringuccio, "***De la pirotechnia*"**, Venice, **1540**

Georgius Agricola, 1494 – 1555, father of geology and recorder of all known metallurgical practice, "***De re metallica*"**, pubished 1556

˜ 1650, Newton/Descartes/Hooke's time**:**

man-made materials such as bronze, steel, porcelain were generally perceived as not having any "anatomy",
only a very few natural philosophers, early physicists, mineralogists, crystallographers suspected that materials may have internal structure

$\sum \vec{F} \cdot dt = d\vec{p}$, $\vec{F}_{12} = -\vec{F}_{21}$ but how is the material able to put up a resisting force?

Hooke: $\vec{F} = -k\vec{x}$, for small x, but how can the resisting force increase with the deformation? How come that constant of proportionality is different in different directions?

from **Metallography** to **Physical Metallurgy**

René de Réanumar, 1683 – 1757, studies fracture of metals without a microscope

Aloys von Widmanstätten, 1754 – 1849, cuts a metal meteor up, polishes and etches it, ***and observes internal structure,*** extremely slow cooling produced large grains that could be seen with the unaided eye

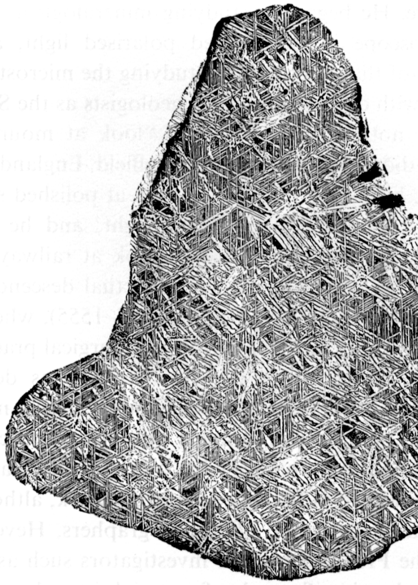


Figure 3.4. (from Smith 1960, p. 151). The Elbogen iron meteorite, sectioned, polished and etched. The picture was made by inking the etched surface and using it as a printing plate. The picture is enlarged about twofold. From a book by Carl von Schreibers published in 1820, based upon the original observation by von Widmanstätten in 1808. (Reproduced from Smith 1960). This kind of microstructure has since then been known as a Widmanstätten structure.

Henry Sorby, 1826 – 1908, amateur scientist in Sheffield, U.K., studies all kinds of materials (rocks, steel, …) with a light microscope, ***steel consist of an array of separate small grains,*** *looking at a railway line through a microscope does make sense*

ridiculed by the geologists: *doesn't make sense to look at a mountain through a microscope?*

Harry Brearley: 1871 – 1948, inventor of stainless steel (1913)

"It would be foolish to deny the fruitfulness of the enormous labor, patient and often unrewarded, which has replaces the old cookery-book method of producing alloyed metals by an understanding intelligence which can be called scientific. But it would be hardly less foolish to imagine, because a subject can be talked about more intelligibly, that the words invariably will be words of wisdom. The operations of an old trade may not lend themselves to complete representations by symbols, and it is a grievous mistake to suppose that what the University Faculty does not know cannot be worth knowing. Even a superficial observer might see that the simplifications, and elimination of interferences, which are possible and may be desirable in a laboratory experiment, may be by no means possible in an industrial process which the laboratory experiment aims to elucidate. … **What a man sees through a microscope is more of less, and his vision has been known to be thereby so limited that he misses what he is looking for, which has been apparent at the first glance to the man whose eye is informed by experience**."

Walter Rosenhain, 1875 - 1934, an engineer by education goes to grad school in Cambridge, U.K., 1897, his supervisor asks him to find out how it is possible that metals can be deformed without loosing their crystalline structure (which was just an unconfirmed hypothesis at the time)

polished steel and other metals, bent them slightly, etched them, looked at them under optical microscope = **metallography**

Figure 3.10. Rosenhain's micrograph showing slip lines in lead grains.

interpretation: plastic deformation entails displacement in shear along particular lattice planes, leaving slip planes which lie in different directions along particular lattice planes in neighboring grains

® **physical metallurgy**

1914 text by Rosenhain: *An Introduction to the Study of Physical Metallurgy,* describes in detail transition of metallurgy from a branch of applied chemistry to an aspect of applied physics

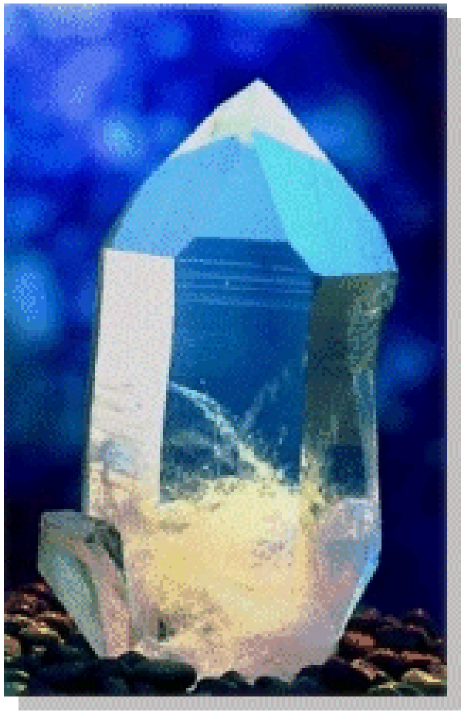
definition: Robert Franklin Mehl, 1967, ardent enemy of defining materials science as a new emerging science that encompasses physical metallurgy

"Physical Metallurgy is a very broad field. ... The US is a pluralistic nation, composed of many ethnic strains, and in this lies the strength of the country. Physical Metallurgy is comparatively pluralistic and has

strength in this. … Theorists and experimentalist interplay." … "What is physical metallurgy? Is it not the primary task of the metallurgist through research to try to define a problem, to do the initial scientific work, nowadays increasingly sophisticated, upon which the solid-state physicist can base his future and relentless probing towards ultimate causes."

all the while there was ***crystallography*** and ***mineralogy***

Johannes Kepler, 1571 – 1630, of Kepler's laws fame: ***"De nive sexangula" = "About the hexagonal show",***
breaking dogma that god just decided to make show hexagonal, conjecture: it is a lowest energy structure, dense packing of smaller units = Demoritus', 460 – 370 BC, atoms, one has to do experiments to find out



Nicholaus Stenson, PhD thesis 1669**,** ***experimental*** the angles between corresponding planes of all quartz crystals are the same, a very brave and fruitful conjecture

R. De L'Isle: text: Crystallographie, 1783, from ***experiment to generalization,*** the angles between corresponding planes of all crystals of any particular mineral are the same

Abbe René Just Haüy, 1743 – 1822**:** J. de Phys. **19**, 1 (1782) one can always device a set of indices for each of these planes, these indices are always rational and vectors in a coordinate system fixed to the crystals of any material, in other words, all crystals consist of many many many repeats of a basic unit cell, there is translational symmetry throughout all crystals, ***also generalization***

this 3D space lattice hypothesis also restricts rotation axes (and other possible symmetry elements), e.g. there are only 1, 2, 3, 4 and 6 fold rotation axes consistent (no 5 fold rotation axis can exist in a crystal)

Hessel, 1830, combinations of translations and rotational symmetry lead to a maximum of 32 point symmetry groups, crystal classes, *from purely mathematical reasoning*

William Hallowes Miller, 1801 – 1880, most convenient labeling system for lattice points, directions, and planes

A. Bravais, 1850, there must be 7 crystal systems and 14 translation lattices *from purely mathematical reasoning*

E.A. Fedorow, 1891, A. Schönflies, 1891, independently, there are 230 space groups, (all translational symmetries and point symmetries combined) *from purely mathematical reasoning*, **any crystal in our**

universe must have one of these space groups, point groups, translation groups, there is simply no other way

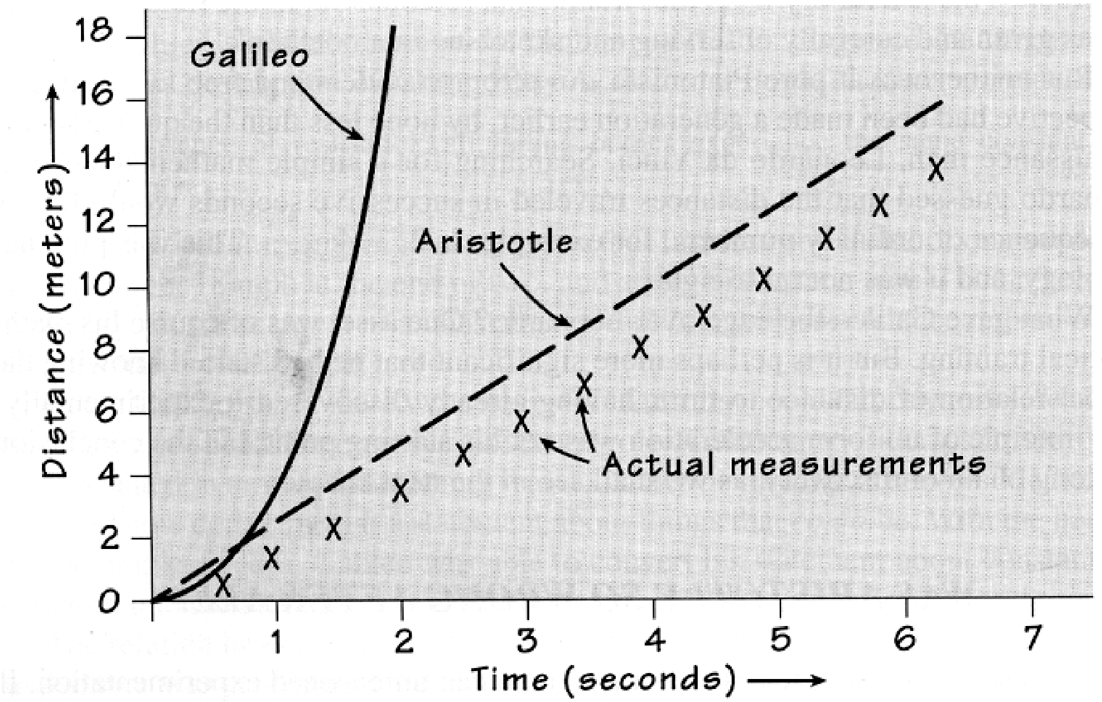
IF CRYSTALS ARE MADE UP OF A PERIODIC ARRANGEMENT OF ATOMS, not proven until 1912 by X-ray diffraction

it is fair to say that this mathematical theory became the structural foundation of modern materials science

Candy sugar grown out of H_20 solution

Siliciumeinkristall für Computerchips

conjecture: **in the absence of air resistance all bodies fall at the same rate**



conjecture: conclusion on basis of insufficient evidence, resulting more from deeper insight how nature is, fist step to theory which then can be falsified by more experiments

the range of velocities and accelerations Galileo could measure was severely limited, there was no accurate stop watch to measure times, in fact Galileo figured out how to use a pendulum to measure times himself

graphs such as to the left were invented only later by Descartes

there was also air resistance resulting in terminal velocities of falling bodies, so the experiment in air actually fits Aristotle's theory better, nevertheless Galileo's conjecture stood the test of time, an mission to the moon took a hammer and a feather and somebody dropped them from the same height and they reached the surface of the moon at the same time

Crystal physics

Franz E. Neumann (1798 - 1895), invents almost single handedly crystal physics, in order to account for physical properties of materials, but does not publish much

"The greatest reward lies in making the discovery; recognition can add little or nothing to that."
(and volunteers fighting Napoleon Bonaparte's armies as a young man)

most of the work is done on single crystals that can be easily prepared, such as NaCl, this is because the science can more easily be developed, physical properties are ordered according to the symmetry classes of the crystals that show them

for the first time in history: scientific approach to Hooke's, 1650, questions: $\vec{F} = -k\vec{x}$
How can the resisting force increase with the deformation? How come that constant of proportionality is different in different directions?

Neumann’s symmetry principle:

the point symmetry group of a physical property is equal or contains the point symmetry group of the crystal that shows this property
in other words, a physical property can not show an anisotropy that is not already contained in the crystal $G_{property} \supseteq G_{crystal}$

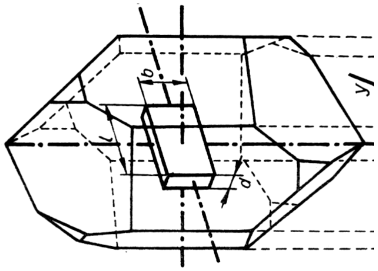
Pierre Curie, 1859 – 1906, (Nobel prize in 1903 for work on radioactivity with this wife Marie and Antoine Henry Becquerel)

Curie’s symmetry principle, *__cause – effect relationship__*

a crystal in an electric or magnetic field (or other cause) possesses a property (effect), it is the crystal that determines the physical effects due to the cause

$$G_{property(effect)} \supseteq G_{crystal\_in\_field} = G_{crystal} \cap G_{field(cause)}$$

if you put the field in certain crystallographic directions, there will be no effect, e.g. quartz crystals have to be employed in certain directions, because there won’t be a piezoelectric effect in other directions regardless of the strength of the applied field



there are about 10 piezo-quartz crystals for every person on earth, there is most likely one in your watch

Neumann’s former student, **Woldemar Voigt**, 1850 – 1919, publishes in 1910 ***Kristallphysik:*** elastic, thermal, electric and magnetic properties of crystals were ordered within a mathematical scheme that comprises scalars, vectors, and tensors (his word for a mathematical entity that mediate causes and effects if both of them are vectors),

so all physical properties and their respective relations are basically understood**,** also derives Lorentz equations, ….

if you can write down and solve an equation that works, you - to some extend - understand the phenomenon

Equilibrium thermodynamics / phase diagrams

Josiah Willard Gibbs, 1839 – 1903, probably the greatest American born Scientist of all times, **initially trained as a mechanical engineer**

“On the equilibrium of heterogeneous substances”, Transactions of the Connecticut Academy of Arts and Sciences, 1876

developed also statistical mechanics nearly independent of Ludwig Boltzmann. and James Clark Maxwell

$$\mathbf{G = H - TS + pV}$$

G, Gibbs free energy, H enthalpy (a from of energy), T absolute temperature (K), S entropy (an measure of disorder in a system, and energy per Kelvin), p pressure, V volume (pV has unit of an energy as well)

if left alone for a long enough time and at sufficiently high temperature, everything goes into a state of minimal G

<u>Gibbs phase rule</u>: *degrees of freedom = components – phases + 2*

component is smallest chemical unit, phase is homogenous and physical distinct entity, e.g. a crystalline precipitate in a crystallographically (or chemically) different matrix

Experimentalist step in, H.W. Bakkhuis Roozeboom, 1856 - 1907

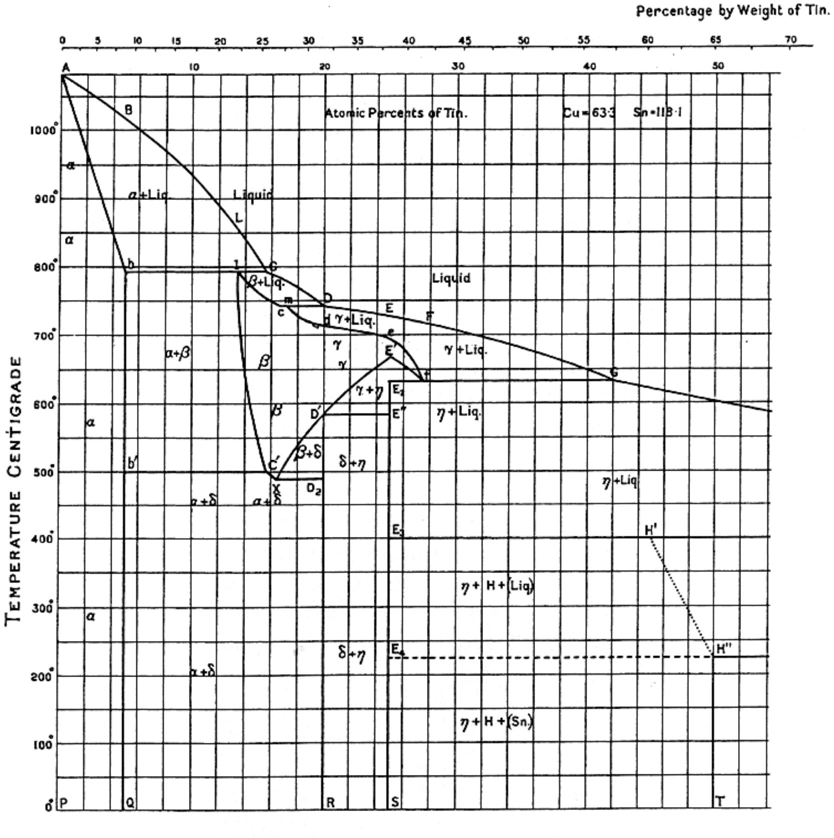


Figure 3.7. Part of Heycock and Neville's Cu–Sn phase diagram.

the world's first high precision phase diagram, about 1890

today there are 10,000 known binary phase diagrams determined experimentally,

more and more phase diagrams get nowadays calculated form fist principles, CALPHAD, so it is back to the theorists

Henri Le Chateleir’s principle: ***If any change of condition is imposed on a system in equilibrium, the system will alter in such a way as to counteract the imposed change.***

Metastability, Wilhelm Ostwald, ***Lehrbuch der Allgemeinen Chemie, 1893*****, also inventor of physical chemistry**

many materials exist in states that are thermodynamically unstable, i.e. not at states of lowest energy, but there is a local minimum in the Gibbs free energy curve, **unless sufficient energy is provided,** e.g. by a heat treatment, **system remains in this metastable state, the process**

either thermodynamics or kinetics determine the states systems are in

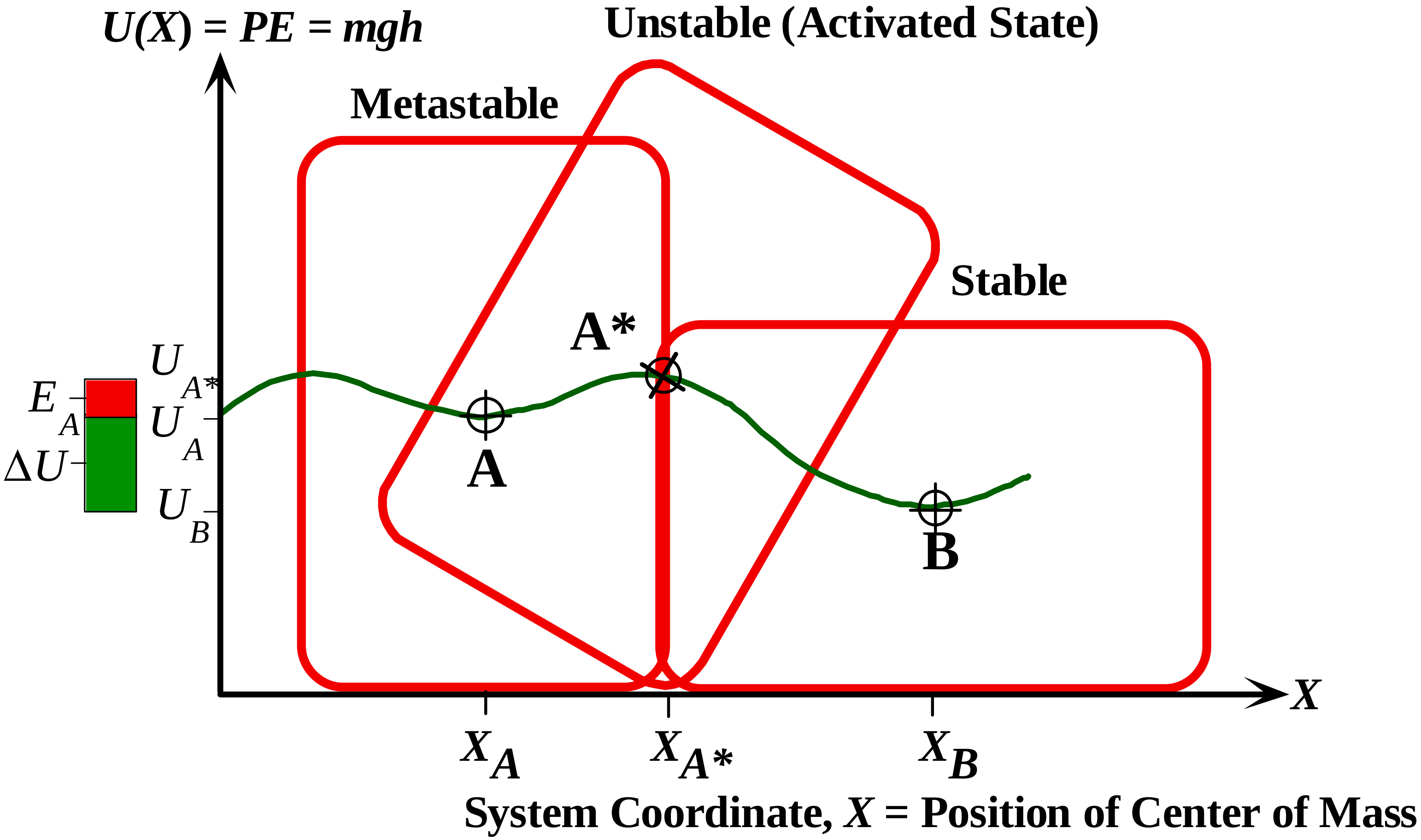
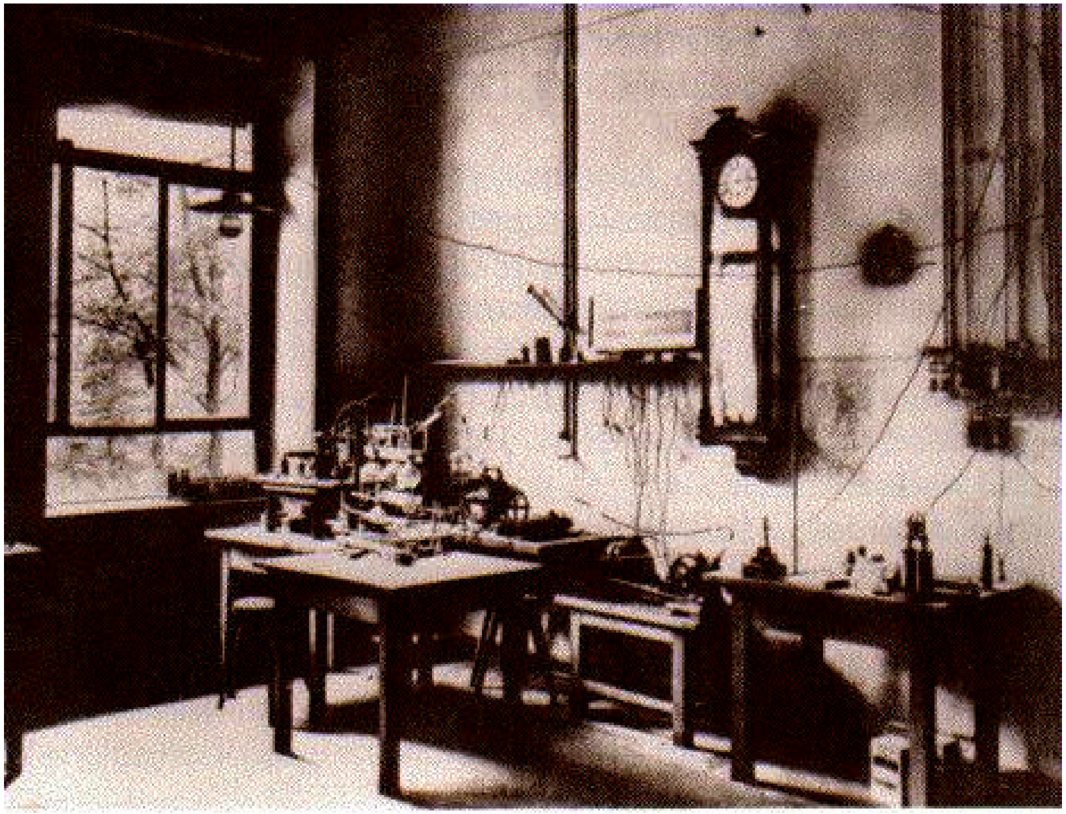


Fig. 1.27: Tilting a filing cabinet from state *A* to its edge in state *A** requires an energy E_A. After reaching *A**, the cabinet spontaneously drops to the stable position *B*. *PE* of state *B* is lower than *A* and therefore state *B* is more stable than *A*.

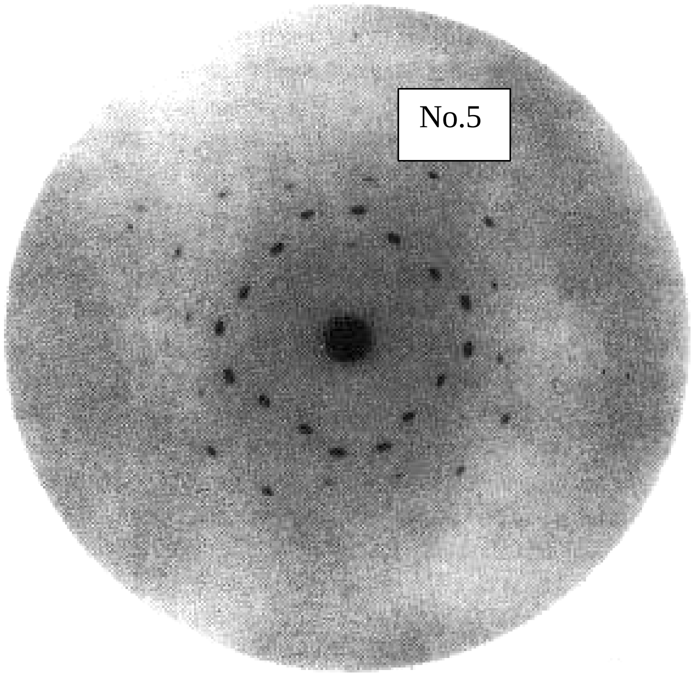
Physicists invent the analytical tools for materials science and using them creates materials science

1895, Wilhelm Konrad Röntgen, 1845 – 1923, X-rays**, Nobel prize in Physics 1901**, initially trained as a **mechanical engineer**



the quintessential case of science and technology emerging from **serendipity**

1912, Max von Laue, 1879 -1960, X-ray diffraction by crystals, Nobel prize in Physics, 1914, **William Lawrence Bragg,** 1890 – 1971, X-ray structure analysis of crystalline materials, together with his father **William Henry Bragg** (working mainly on X-ray spectroscopy) 1862 - 1942, Nobel prize in Physics, 1915



although mentioned in Röntgen's Nobel citation, there has not been a Nobel prize for <u>medical</u> X-rays, as such

so probably that was much less important to the development of mankind as the physical and crystallographic use of X-rays

these spots can all be labeled with Miller's indices, this is definitive proof of both, X-rays possess wave character and crystals are composed of a periodic 3D arrangement of atoms

Nobel prizes Physics:

1914 Max von Laue, 1879 – 1960, X-rays are an electromagnetic wave of about 0.1 nm wavelength, atoms in crystals are arranged in a regular 3D lattice with spacing in the 0.1 nm range, there is X-ray diffraction from crystals, the possibility of analyzing the arrangements of matter in crystals, (Laue equations), 1912

1915 Sir William Henry Bragg and William Lawrence Bragg (son of the former), X-ray crystallography, (W.L.) Bragg equation, X-ray crystal spectrometer, 1913

1924 Karl Manne Georg Siegbahn, X-ray spectroscopy

1937 Clinton Davidson and Sir George P. Thompson (J.J. Thompson's son who first showed electrons are particles), electron diffraction by crystals, in other words electrons are waves, 1927

1986 Ernst Ruska, inventing the electron microscope where one operation mode is electron diffraction (1932) *together with* Gerd Binning and Heinrich Rohrer, scanning tunneling microscope, (completely unrelated)

1994 Clifford G. Schull and Bertram N. Brockhouse, pioneering neutron diffraction and spectroscopy

Nobel Prizes Chemistry

1936 Peter J. Debye, *X-ray and electron diffraction analyses of molecules*

1962 Max F. Perutz, John C. Kendrew, *X-ray diffraction analysis of haemoglobin und myoglobin*

1964 Dame Dorothy Crowfoot Hodgkin, *X-ray diffraction analysis of biochemical macromolecules*

1976 William N. Lipscomb, *X-ray diffraction analysis of borhydrids*

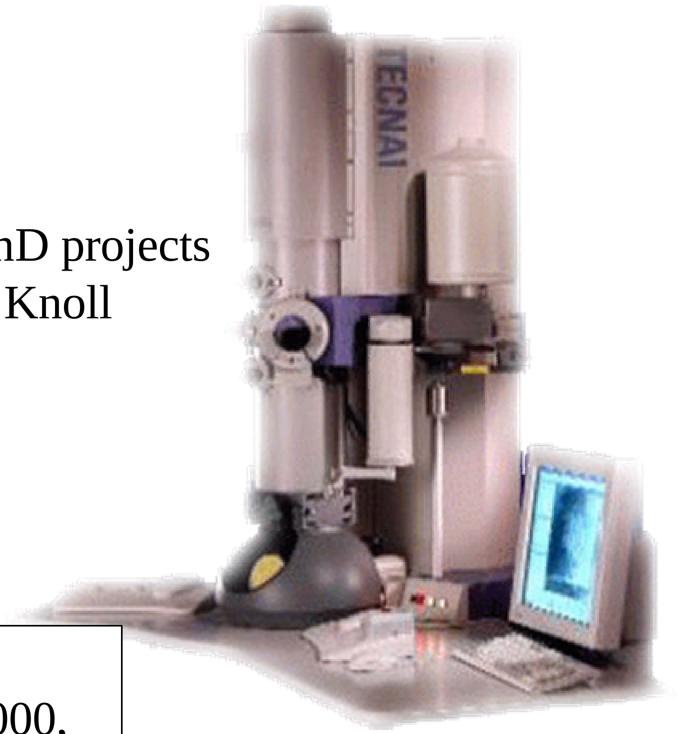
1982 Aaron Klug, *X-ray diffraction analysis of nucleic acids and protein complexes*

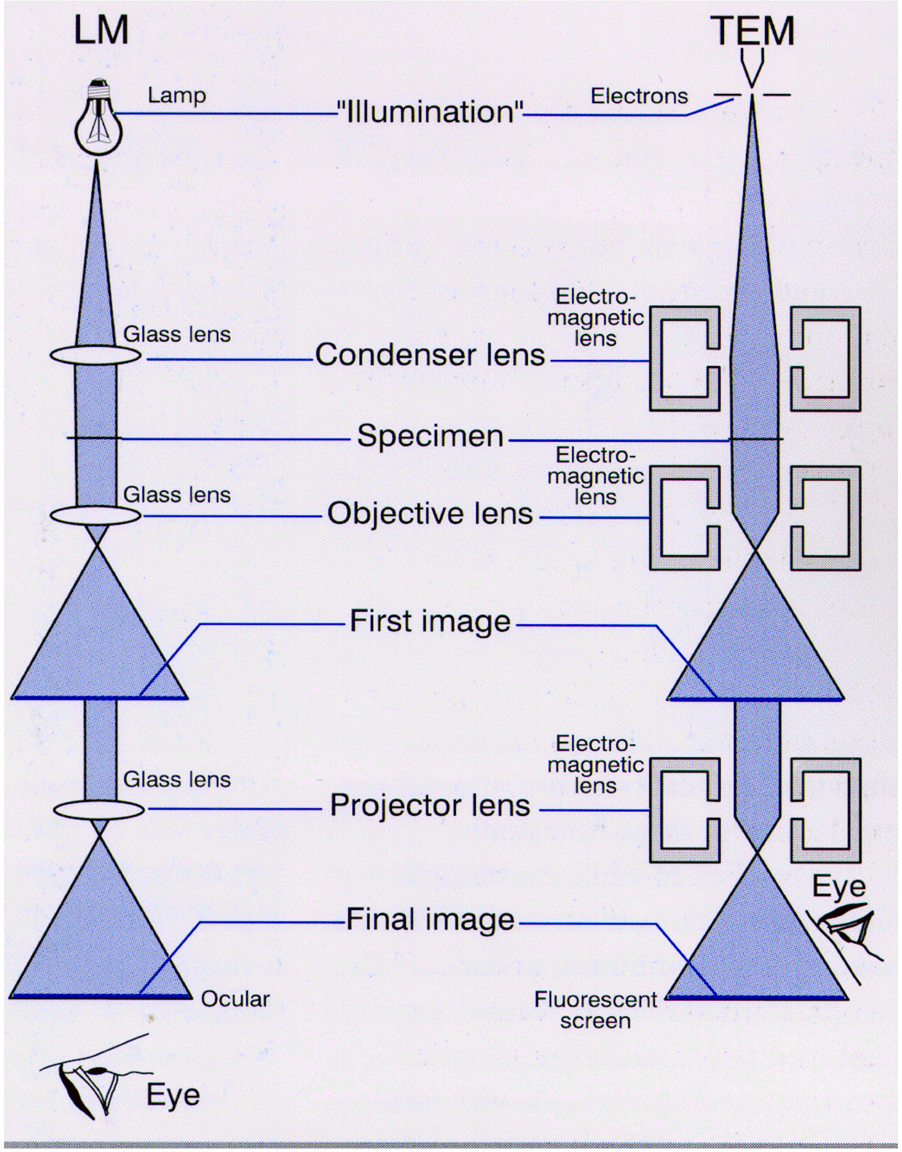
1985 Herbert A. Hauptmann, Jerome Karle, *direct methods of X-ray crystallography*

1988 Johann Deisenhofer, Robert Huber, Hartmut Michel, *structure and function of protein-chromophor-complex*

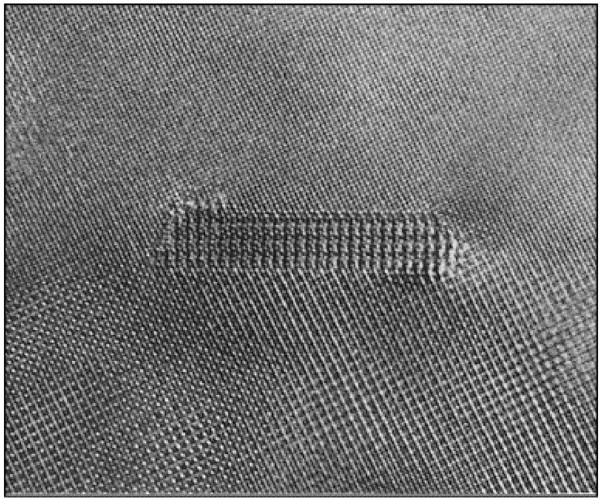
Nobel Prize Medicine, 1962 James D. Watson, Francis H.C. Crick, Maurice H.F. Wilkins, *X-ray diffraction analysis of DNA (**actually Rosalind Franklin's work !**) and its importance for genetic code*

1932 Ernst Ruska, invents and builds the first
Transmission Electron Microscope, engineering MSc, PhD projects
under Max Knoll





magnifications
~ 500 – 1 000 000,
atomic resolution !



(c)

Figure 8.2.8c
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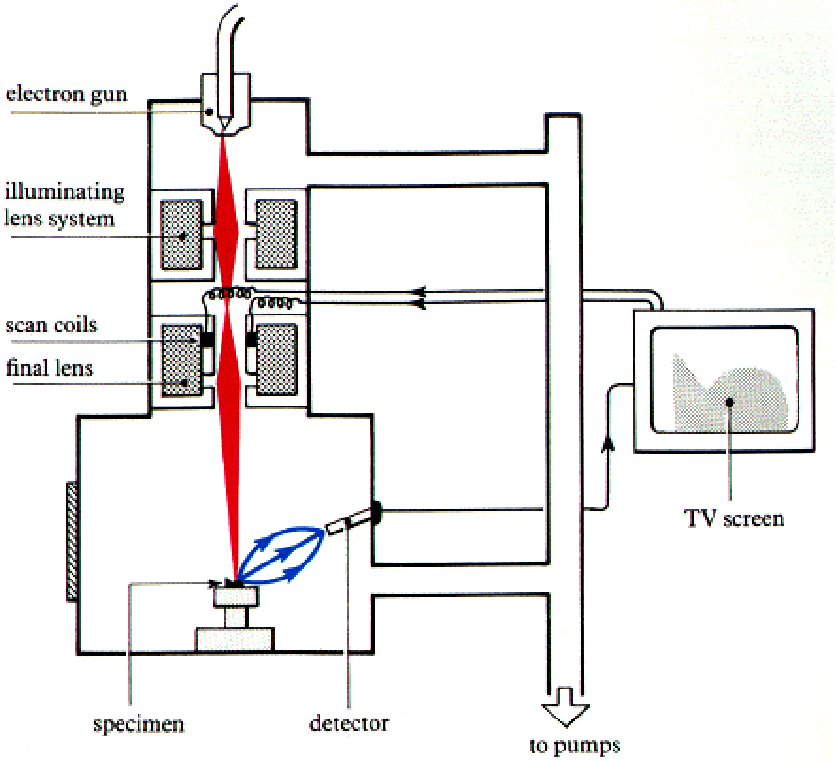
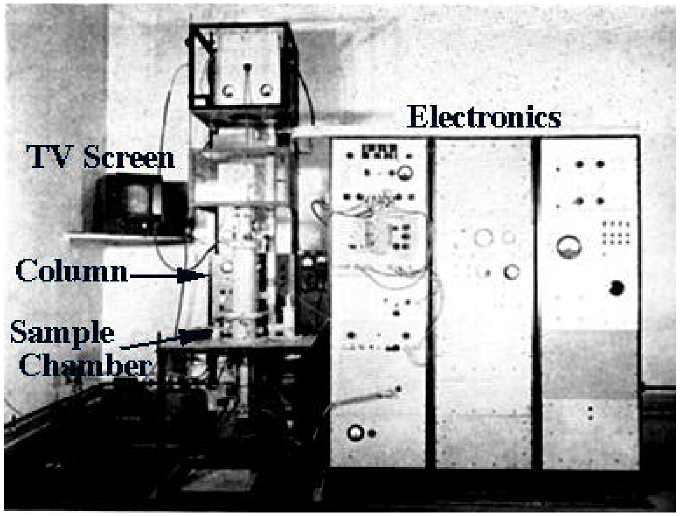
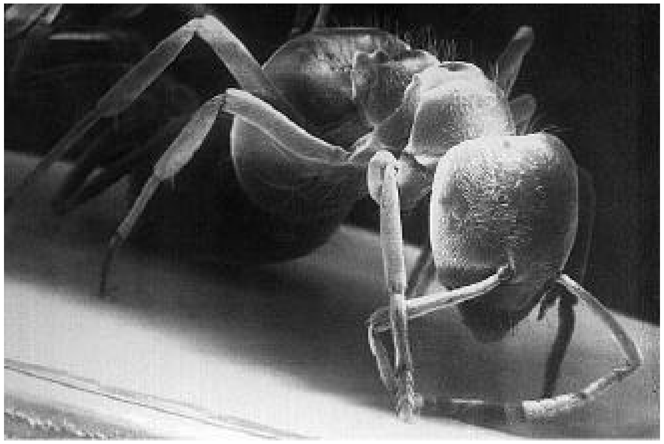
t/a Schaffer: The Science and Design of Engineering Materials, 2/e

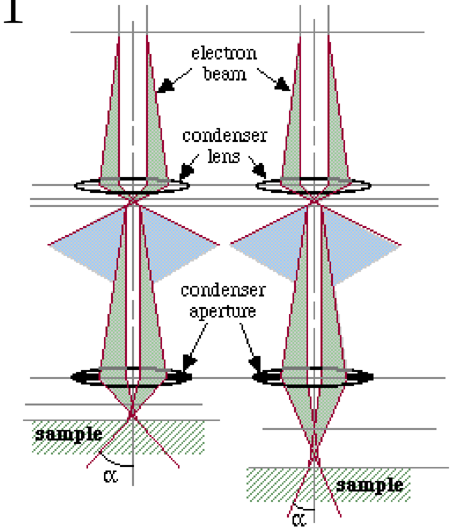
1935 **Max Knoll** invents the Scanning Electron Microscope (to analyze surfaces), Z. Techn. Phys. **11,** 467 (1935)





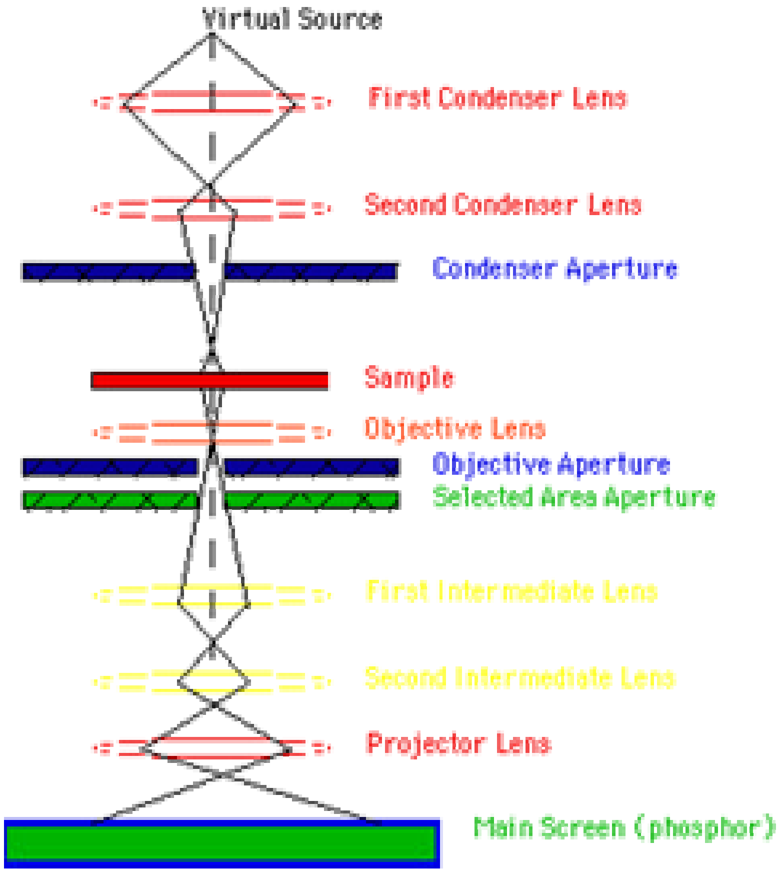
D. McMullan at Cambridge University, builds first reliable SEM, 1951

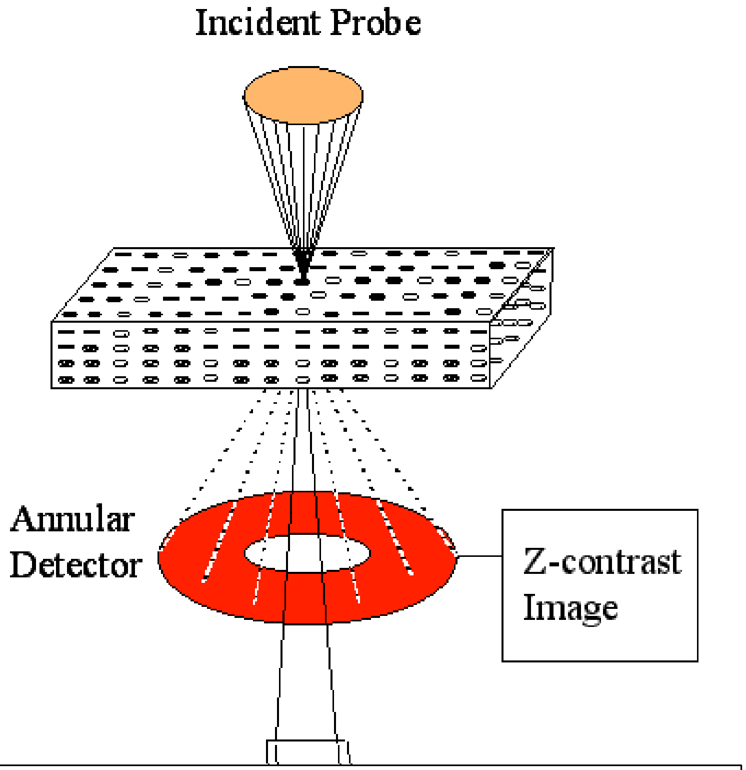




there is a wide range of parameters, it takes experience to operate a SEM; to get a large depth of focus, one has to have a small α, but this also reduces the resolution and signal/noise ratio

hybrid: Scanning Transmission Electron Microscope, two microscopes in one, **TEM/STEM**





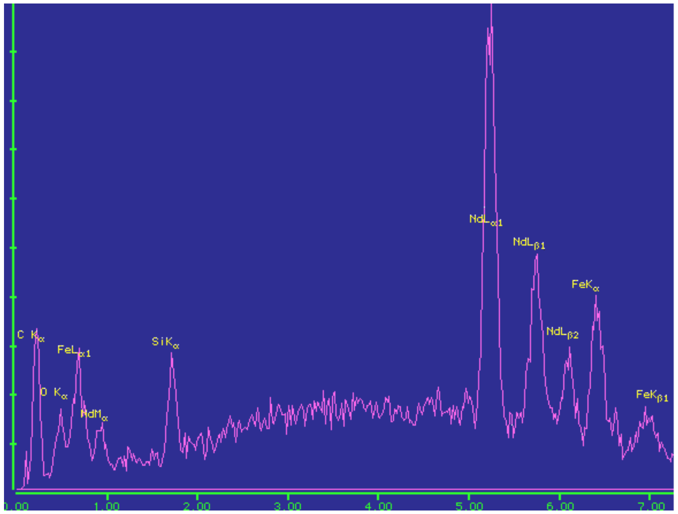
Bright field image, electron energy loss spectroscopy in almost atomic column resolution

TEM and STEM are related by principle of reciprocity, by reversing the path of the electrons, one can in principle get the same contrast in images

STEM “invented” by Manfred von Ardenne in mid/late 30s, a German count without advanced degrees and an engineering background who spend lots of his money on equipment

analytical STEM/TEM

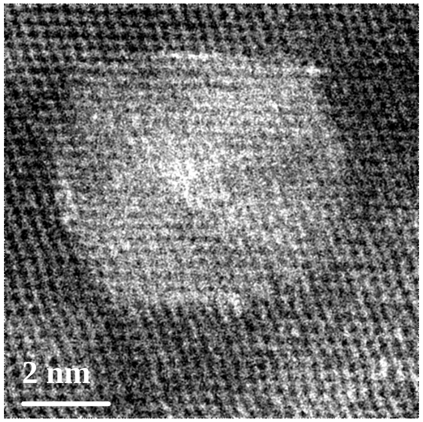
count of X-ray photons ?

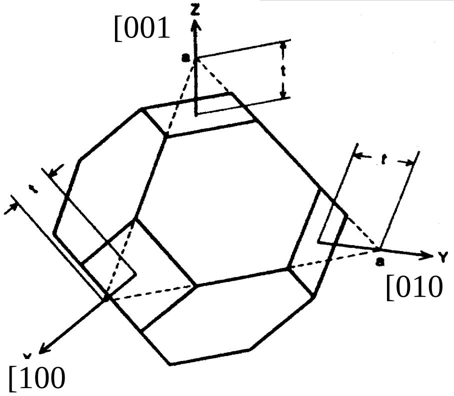


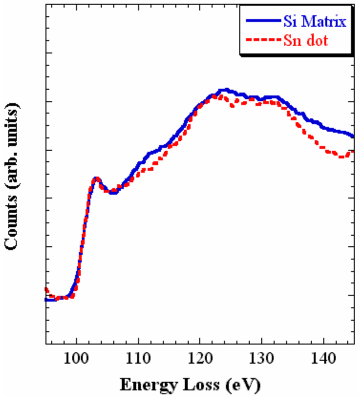
energy of X-ray photons in keV →

the tool for structure analysis at all microscopic levels, atomic, mesoscopic 1-100 nm, macroscopic up to ˜ 100 µm
then one has to take an optical microscope that only magnifies 10 – 1 000 times

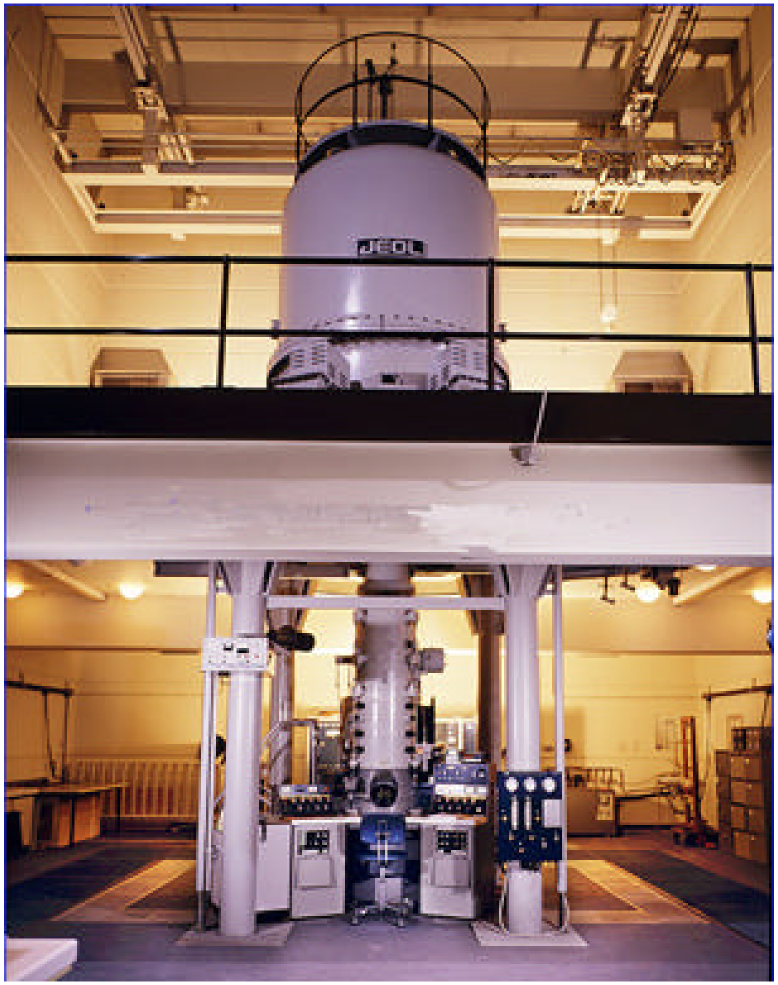
X-ray spectroscopy for quantification of chemical composition in µm areas, excited by impinging electron beam







formation of an α-Sn quantum dot in Si by endotaxy, ***left***, Z-contrast STEM, ***middle***: tetrakaidecahedron, ***right,*** electron energy loss spectroscopy (EELS) from same area for quantification of chemical composition in nm areas, nearly for single atomic columns !!

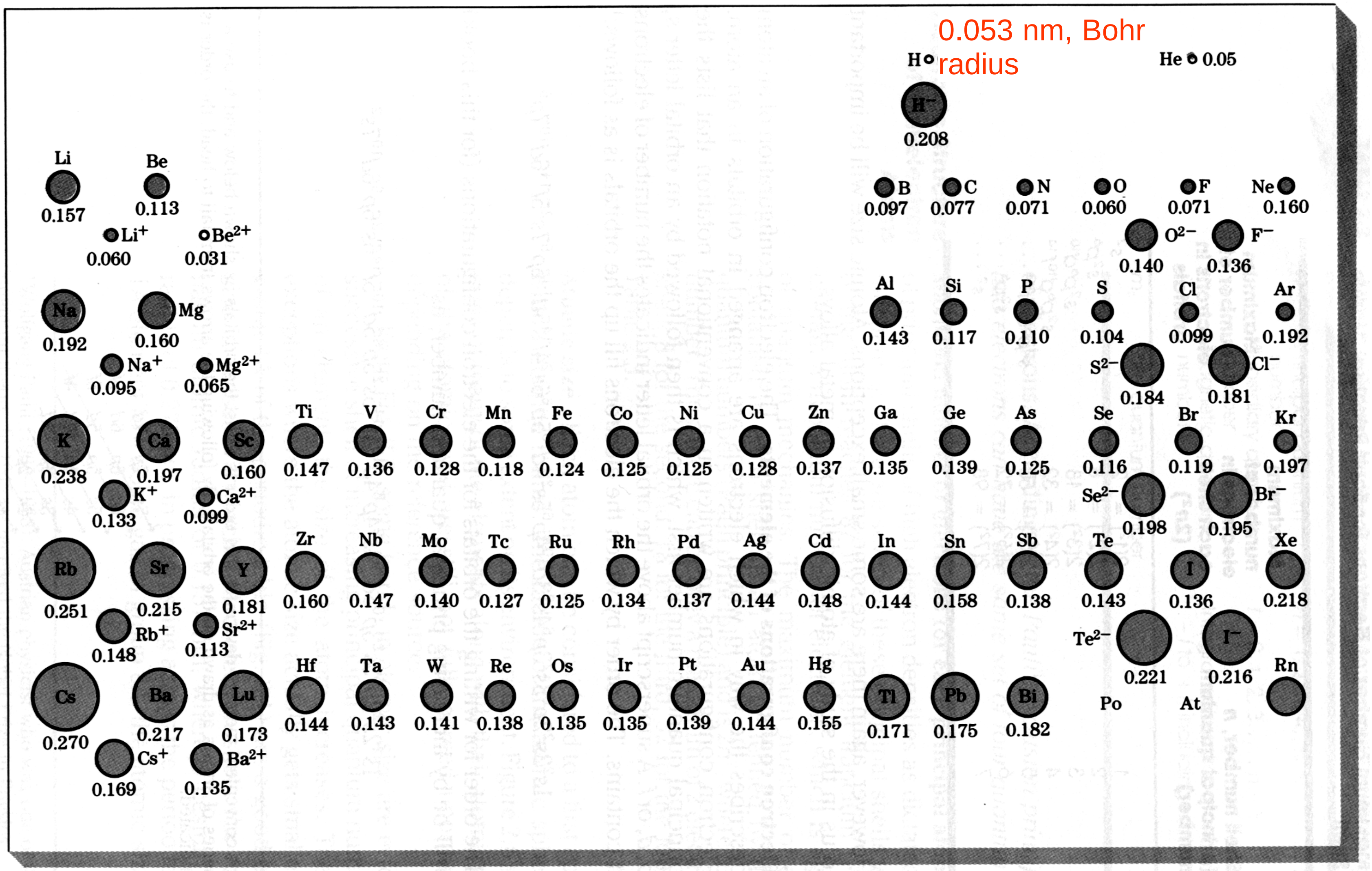


1250 keV U of Antwerp (Belgium)

400 – 800 keV, National Center for Electron Microscopy Berkeley

atomic resolution microscope, at Berkeley: 0.15 nm directly interpretable, point-to-point resolution

$$res_{Scherzer\_Phase-HRTEM} \approx 0.66 \cdot C_s^{1/4} \cdot l^{3/4}$$



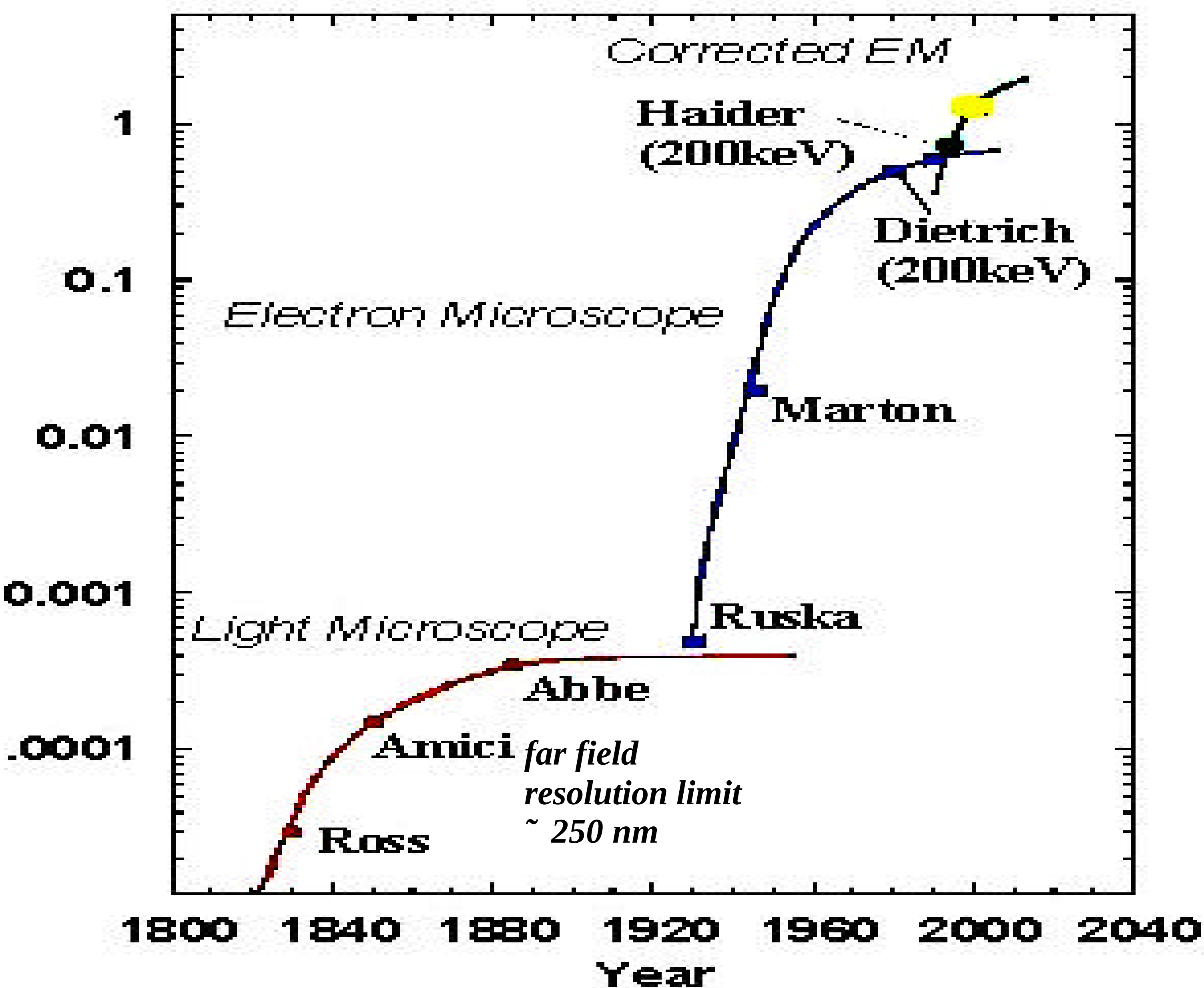
0.053 nm, Bohr radius

FIGURE 2.6 Relative sizes of some atoms and ions. Values are given in nanometers for the radii of the atoms and ions. Metallic radii are given for atoms where applicable. (*Adapted from F. M. Miller, "Chemistry: Structure and Dynamics," McGraw-Hill, 1984, p. 176.)*

Feynman anticipates physical basis for chemical behavior and role of electron microscope

"It would be very easy to make an analysis of any complicated chemical substance; all one would have to do would be to look at it and see where the atoms are. The only trouble is that the electron microscope is one hundred times too poor… I put this out as a challenge: Is there no way to make the electron microscope more powerful?"

– Richard P. Feynman, 1959,
"There's Plenty of Room at the Bottom"



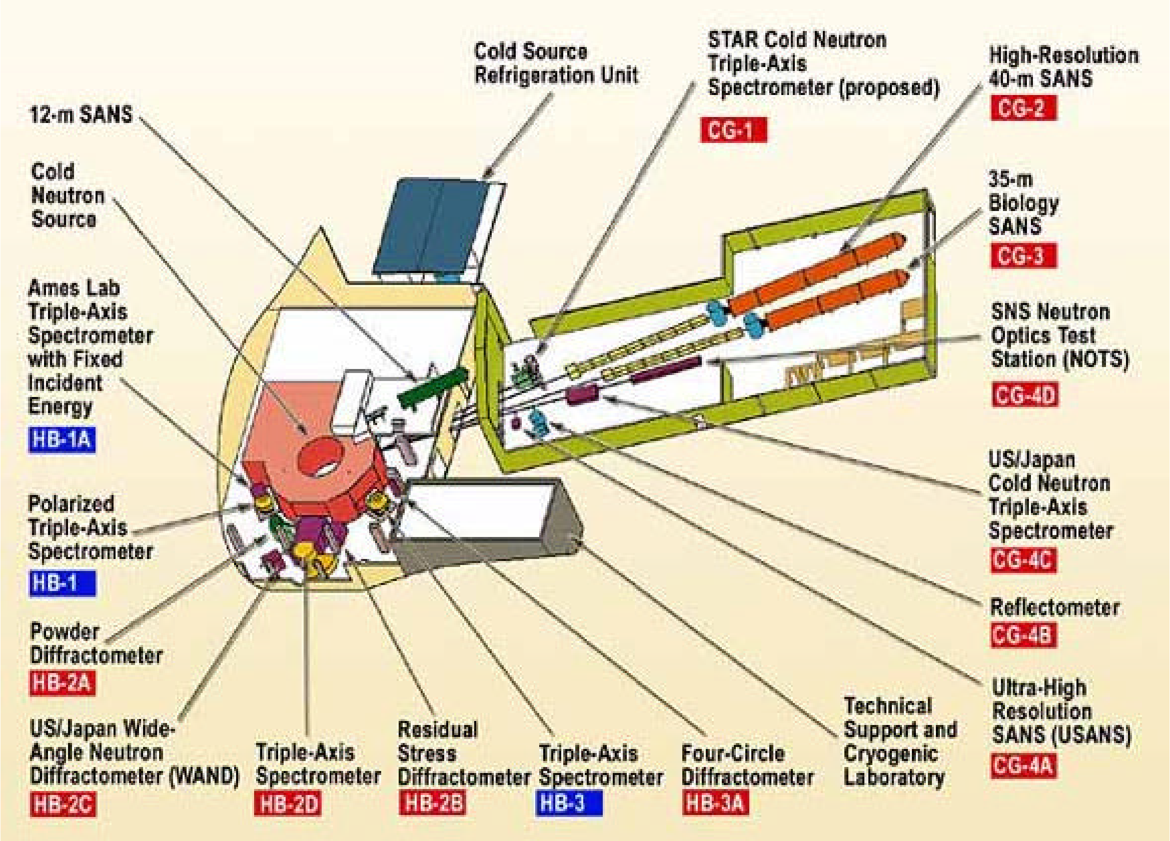
far field resolution limit ~ 250 nm

$$res_{Scherzer\_Phase-HRTEM} \approx 0.66 \cdot C_s^{1/4} \cdot l^{3/4} \quad res_{Scherzer\_Z-STEM} \approx 0.4 \cdot C_s^{1/4} \cdot l^{3/4}$$

out of Nuclear Physics, **Otto Hahn**, 1879 – 1968, Novel prize in Chemistry for fission of ^{235}U in 1944 comes

Neutron diffraction and Spectroscopy

Clifford G. Schull, (1915 – 2001), Nobel prize physics 1994 (for neutron diffraction) together with **Bertram N. Brockhouse**, 1918 – (for neutron spectroscopy)



typically multi-user facilities, here at Oak Ridge National Laboratory, one needs a nuclear reactor as source of the neutrons,
each station is a laboratory on it's own, some 20-100 m^2

from Physical Metallurgy to Materials Science, 1950s

		Years	
Department Titles	**1964**	**1970**	**1985**
Metallurgy	31	21	17
Minerals and Mining	9	7	5
Materials	11	29	51

Northwestern University, Evanston (Illinois) had undergraduate courses on ***Principles of the Properties of Materials*** in the early 50s, first undergraduate textbook Jack Frankel, 1957, with this title
Graduate Department of Metallurgy (up to 1958) → Graduate Department of Materials Science

at MIT: Department of Metallurgy (up to 1967) → Department of Metallurgy and Materials Science (up to 1974) → Department of Materials Science and Engineering now more than 80 colleges and universities in US with degree programs in materials/metallurgical/ ceramics

Materials	**Metals**	**Ceramics**	**Materials and Metals**	**Materials and Ceramics**	**Materials, Metals and Ceramics**
42	12	7	5	4	3

web sites of US schools/departments that offer the above courses at http://www.crc4mse.oeg/resources/colleges.html

well before these changes in US *there was in U.K.:* Daniel Hanson, Sir Alan Cottrell, Frank Nabarro, John Eshelby, … from 1946 onwards at University of Birmingham, changed “more qualitative” approach to metallurgy (physical metallurgy in German “Metallkunde”, i.e. metal knowledge) to what was to become quantitative Materials Science at OXFORD, UK, Department of Metallurgy (until late 60s) → Department of Metallurgy and the Science of Materials (until mid 90s) → Department of Materials

out of these departments above come the best books and undergraduate text on the subject, e.g. ***MIT Series in Materials Science and Engineering***

without being able to quantify effects, one does not really understand them, can't make quantitative predictions/calculations

is not much better off than Agricola in the first half of the 16th century !

There is something fascinating about science. One gets such wholesale returns of conjecture out of such trifling investment of facts.

Mark Twain, Life on the Mississippi

“In fact: one of the key issues in materials engineering is to be able to understand and model the interaction between external variables and atomic scale structures.”

Schaffer et al., The Science and Design of Engineering Materials

Definitions Materials Science

David Turnbull: “the characterization, understanding, and control of the **structure** of matter at the ultra-molecular level and the relating of this structure to properties (mechanical, magnetic, electrical, ect.)”

“COSMAT report”, 1974 commissioned by National Academy of Sciences: “concerned with the generation and application of knowledge relating the composition, **structure**, and processing of materials to their properties and uses”

Robert W. Chan, FRS, at Sussex, later Cambridge, U.K. 1965, “... the materials scientist has to work at several levels of organization, each of which is under-pinned by the next level. Here, again, he is brother under the skin of the biologist, who does just the same: starting with the cell wall, say, he goes on to study the morphology and economy of the cell as a whole, then isolated organs (made up of cells), then the organism as a whole.”

“… the most worrying trend is precisely the reactionary pressure to separate the students of metals and alloys from all the rest.”

Merton Flemmings at MIT: **“to view the broad engineering study of structure/property/processing/performance relations of materials, with engineering emphasis … as a discipline.”**
also devises the materials science tetrahedron, 1989

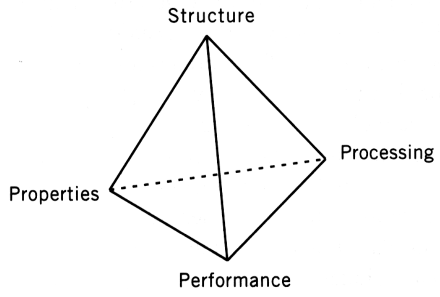


Figure 1.1 The MSE tetrahedron emphasizes the connections between structure, processing, properties, and performance. We place *structure* in the primary position.

S. M. Allan and E. L. Edwin at MIT: **”…** ***there is a common set of principles governing the structure and properties of many different types of materials***

… an understanding of these principles forms the foundation of a modern education in the field of materials science and engineering
… Facility with crystallography is the primary skill for communication in materials science and engineering”

Bernhardt Wuensch at MIT**:** **materials science** is primarily about ***“relation between the structure of matter and its properties”***
materials engineering is primarily about ***“modification of properties and performance during and after processing, and with manufacture”,***

one may define the materials science and engineering super-discipline loosely as being about communications between materials scientist and materials engineers surely a “language” is needed for this communication to happen, as far as the crystalline state is concerned, this “language” is in our opinion crystallography and its “words” are the crystallographic core concepts

Herbert Hollomon, 1958: ***“Out of metallurgy, by physics, comes materials science”***

Materials Science relationship to Materials Engineering

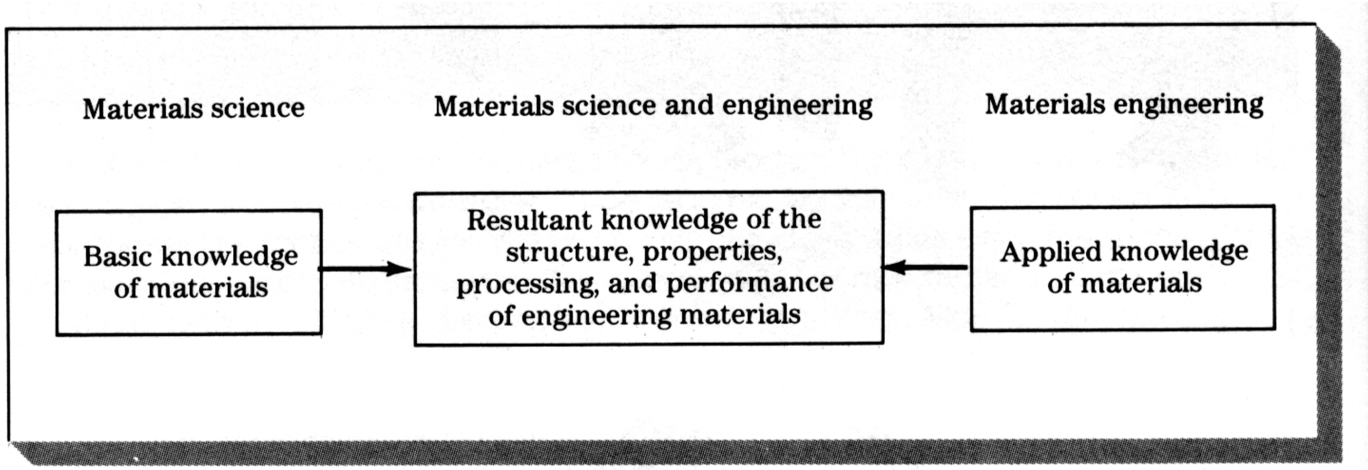
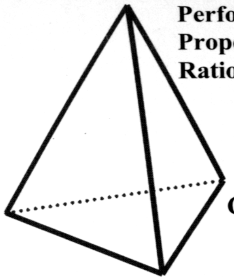


FIGURE 1.3 Materials knowledge spectrum. Using the combined knowledge of materials from materials science and materials engineering enables engineers to convert materials into the products needed by society.

What is Materials Science and Engineering?

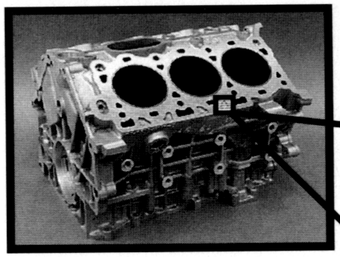


Performance or Properties to Cost Ratio

Synthesis and Processing

Composition

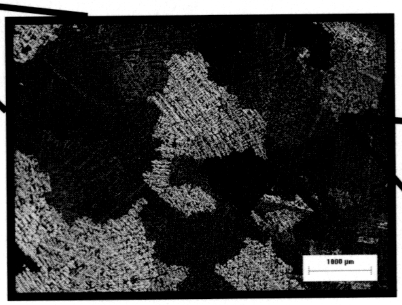
Structure



Macro-Scale Structure
Engine Block
≅ upto 1 meter

Performance Criteria

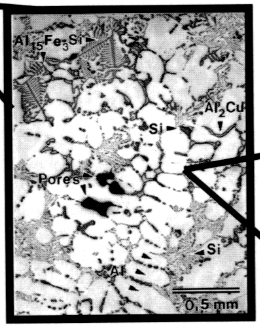
- **Power generated**
- **Efficiency**
- **Durability**
- **Cost**



Microstructure
- Grains
≅ 1 – 10 millimeters

Properties affected

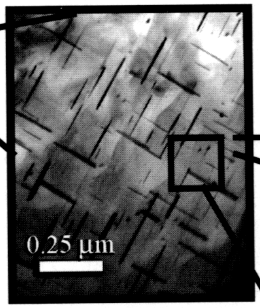
- High cycle fatigue
- Ductility



Microstructure
- Dendrites & Phases
≅ 50 – 500 micrometers

Properties affected

- Yield strength
- Ultimate tensile strength
- High cycle fatigue
- Low cycle fatigue
- Thermal Growth
- Ductility

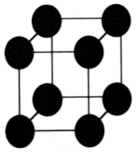


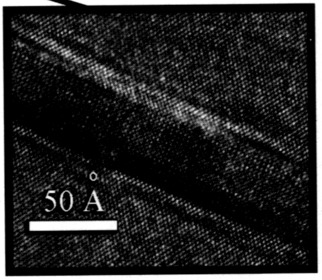
Nano-structure
- Precipitates
≅ 3-100 nanometers

Properties affected

- Yield strength
- Ultimate tensile strength
- Low cycle fatigue
- Ductility

Unit Cell





Atomic-scale structure
≅ 1-100 Angstroms

Property affected

- Young's modulus
- Thermal Growth

note the different usages of a very common word

structure: complex construction or entity, arrangement and interrelationship of parts in a construction, such as a building, manner of construction of organization,….
Chem. arrangement of atoms in a molecule
Geology way in which a mineral, rock, rock mass or stratum is made up of its constituent parts

A real-world example of important microstructural features at different length-scales, resulting from the sophisticated synthesis and processing used, and the properties they influence. The atomic, nano, micro,and macro-scale structures of cast aluminum alloys (for engine blocks) in relation to the properties affected and performance are shown. The materials science and engineering (MSE) tetrahedron that represents this approach is shown in the upper right corner.

(Illustrations Courtesy of John Allison and William Donlon, Ford Motor Company).

every corner is linked to every other corner, so they seem to indicate equal importance, ***but***

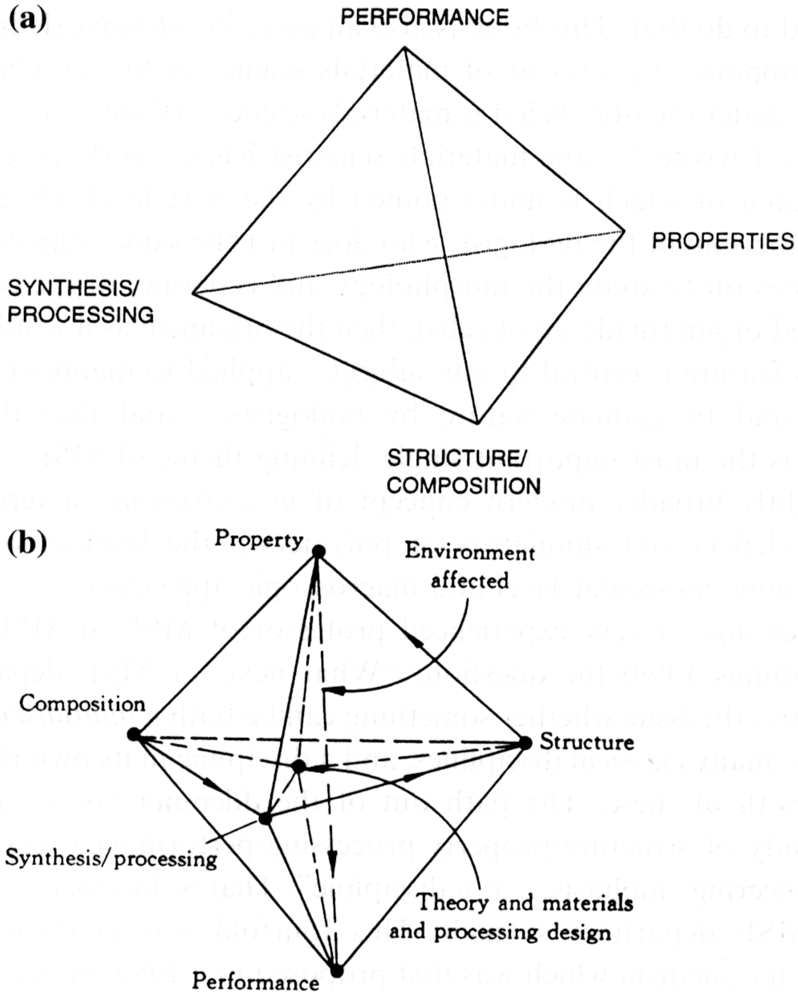


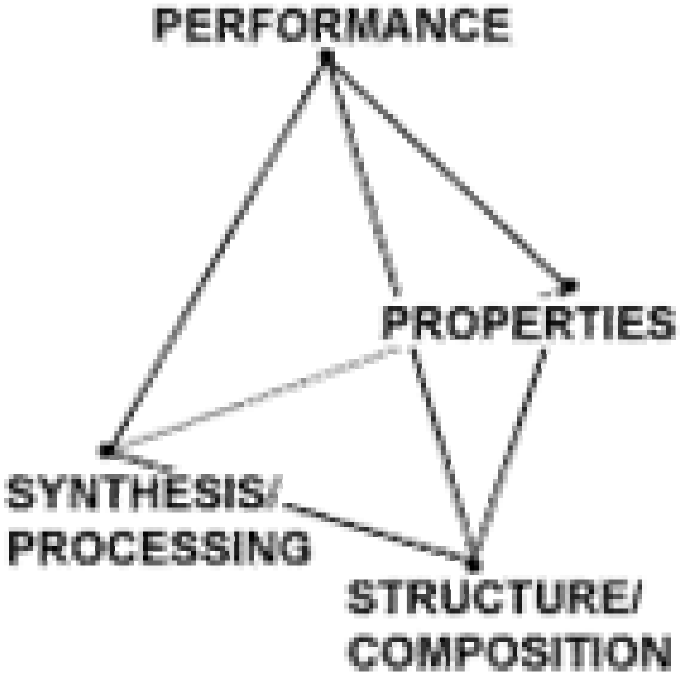
Figure 15.1. (a) The four elements of materials science and engineering, (after Flemings). (b) The six elements of materials science and engineering (after Shi).

R.W. Chan:
“**microstructure** is the central component that best distinguishes Materials Science and Engineering from other disciplines”

makes it a science or engineering discipline in its own right

cover of **Acta (and Scripta) Materialia** *Incorporating Nano structured Materials*
previously Acta (and Scripta) Metallurgica et Materialia, renamed in 1996, previously Acta (and Scripta) Materialia since 1953.

“Emphasis is placed on those aspects of the science of materials that are concerned with the **relationship between the structure of solids and their properties (mechanical, chemical, electric, magnetic and optical)**; with the thermodynamics, kinetics and mechanisms of processes occurring within solids; with experiments and models which help in **understanding the macroscopic properties of materials in terms of microscopic mechanisms**; …



version of the Materials Science & Engineering Career Resource Center http://www.crc4mse.org/Index.html endorsed by The Minerals, Metals & Materials Society

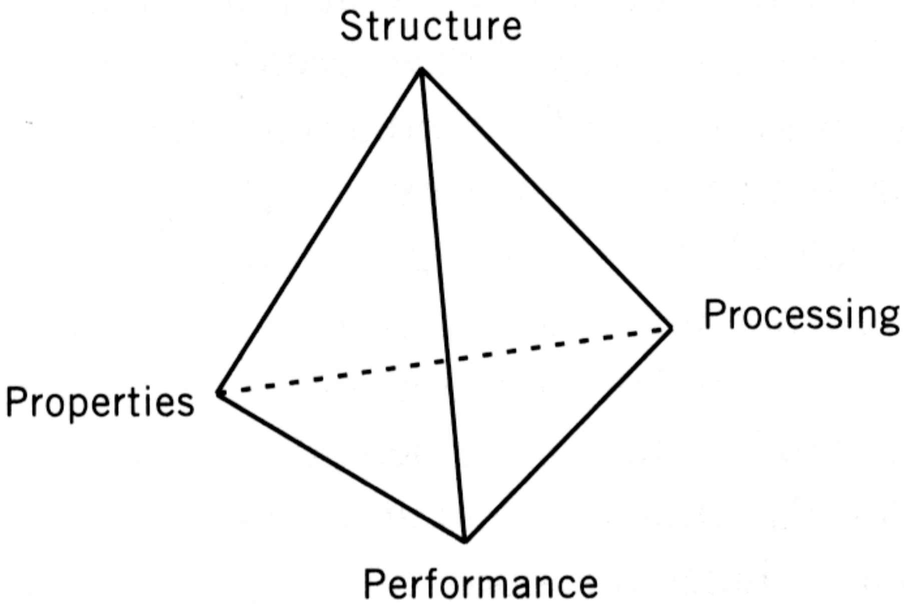
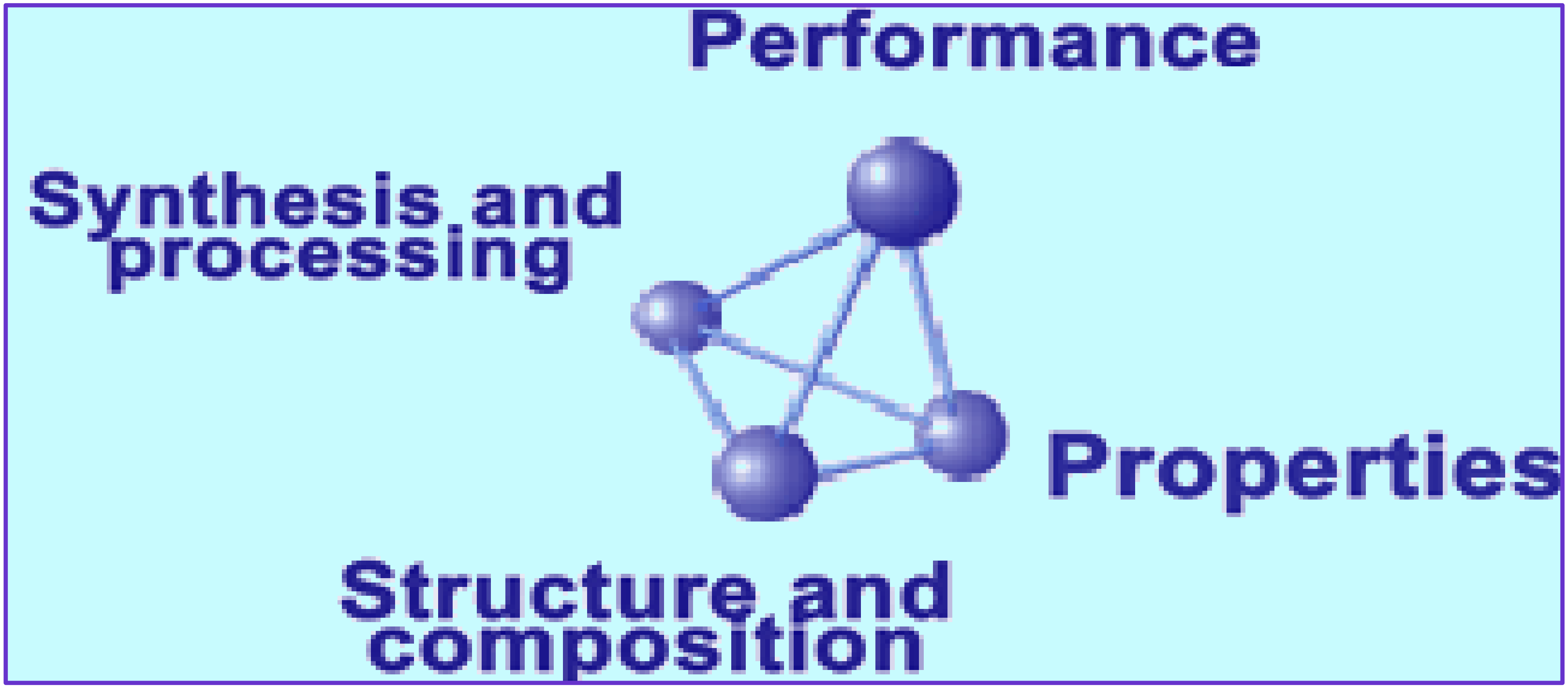
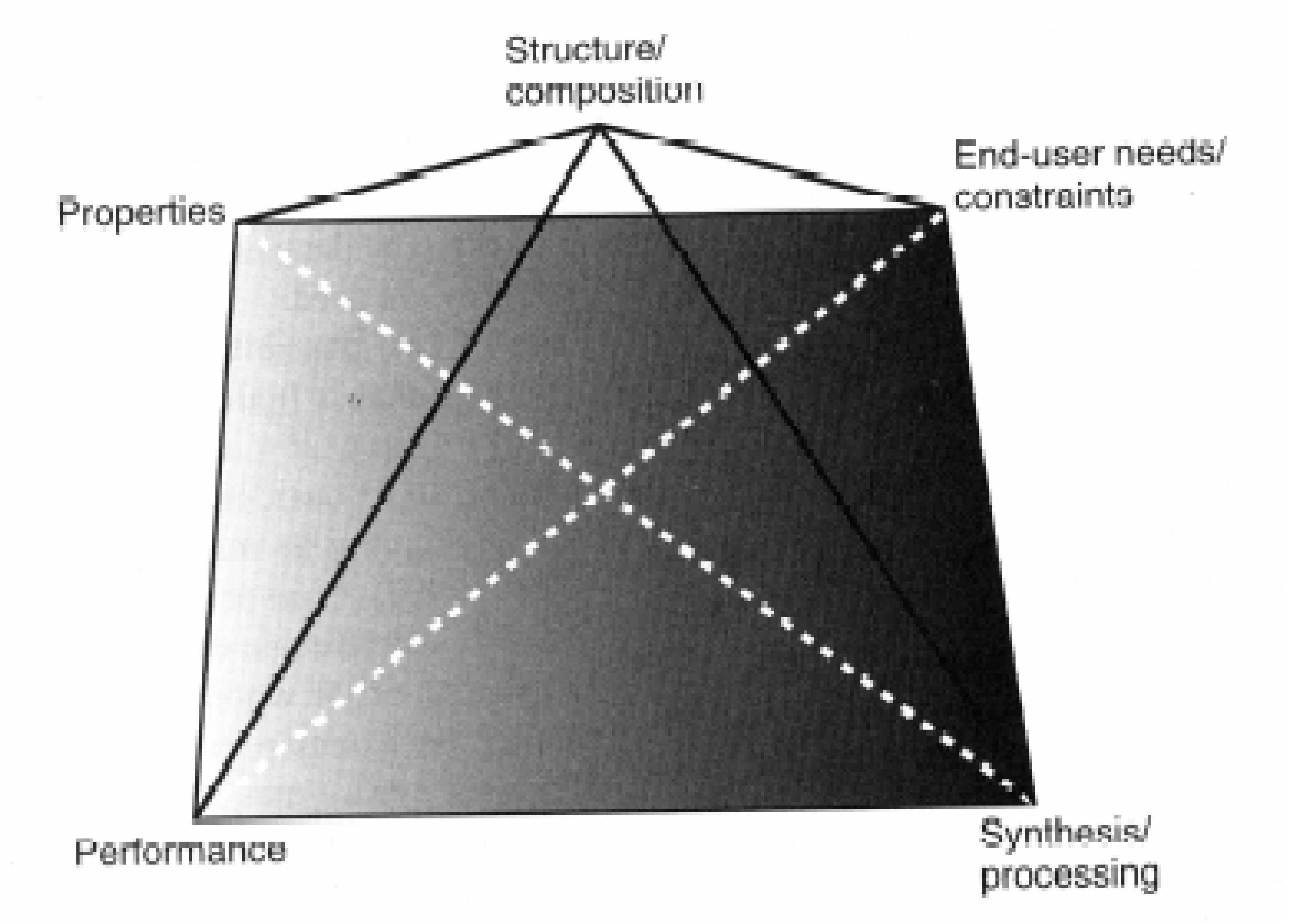


Figure 1.1 The MSE tetrahedron emphasizes the connections between structure, processing, properties, and performance. We place *structure* in the primary position.

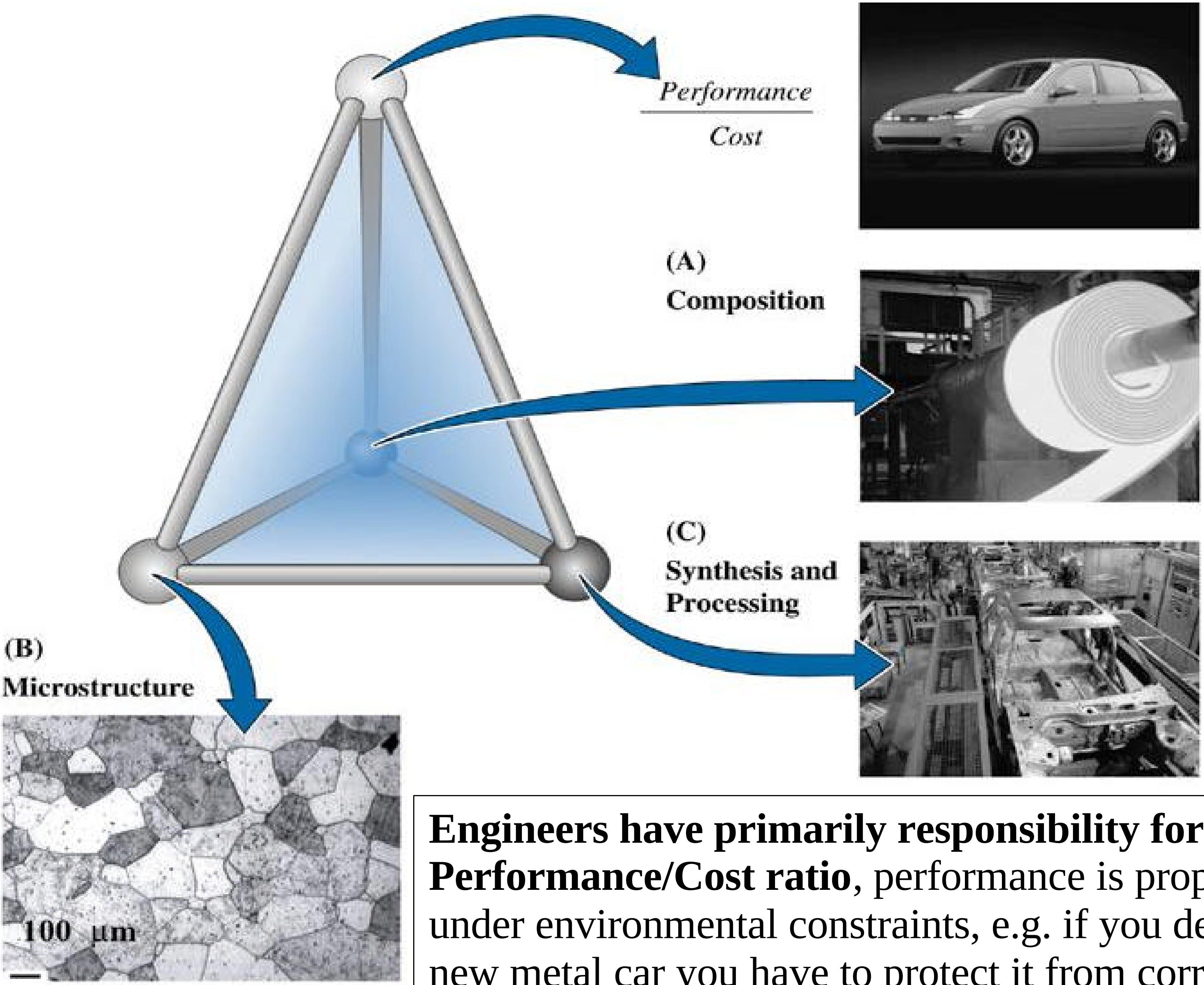
S.M. Allen, E.L. Thomas, The Structure of Materials, Wiley, 1999



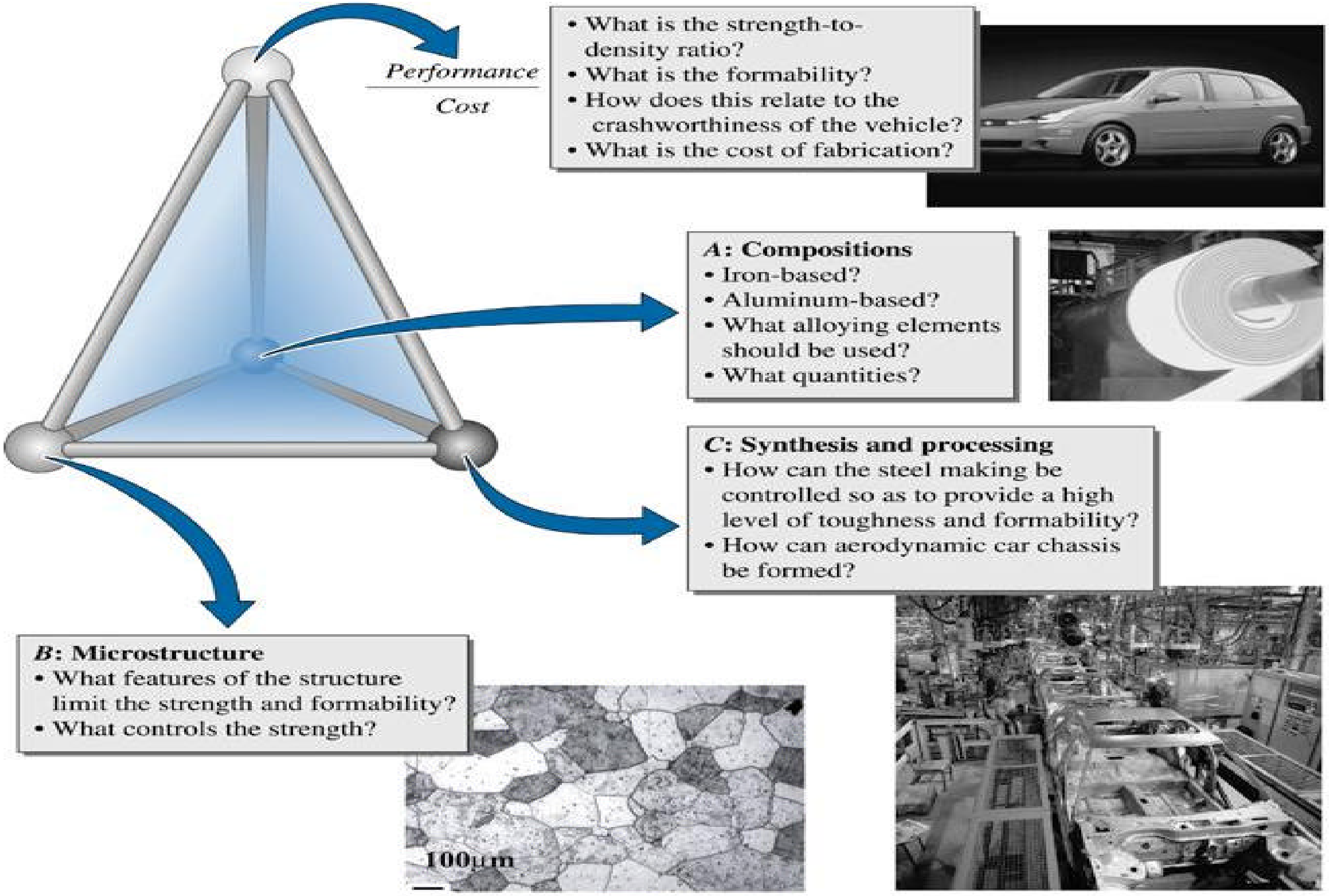
Logo of the Department of Materials Science and Engineering, University of California, Berkeley



That is how a marketing specialists / economists / social scientists may see materials science and engineering, 1999



Engineers have primarily responsibility for Performance/Cost ratio, performance is properties under environmental constraints, e.g. if you design a new metal car you have to protect it from corrosion so that it can keep up its properties



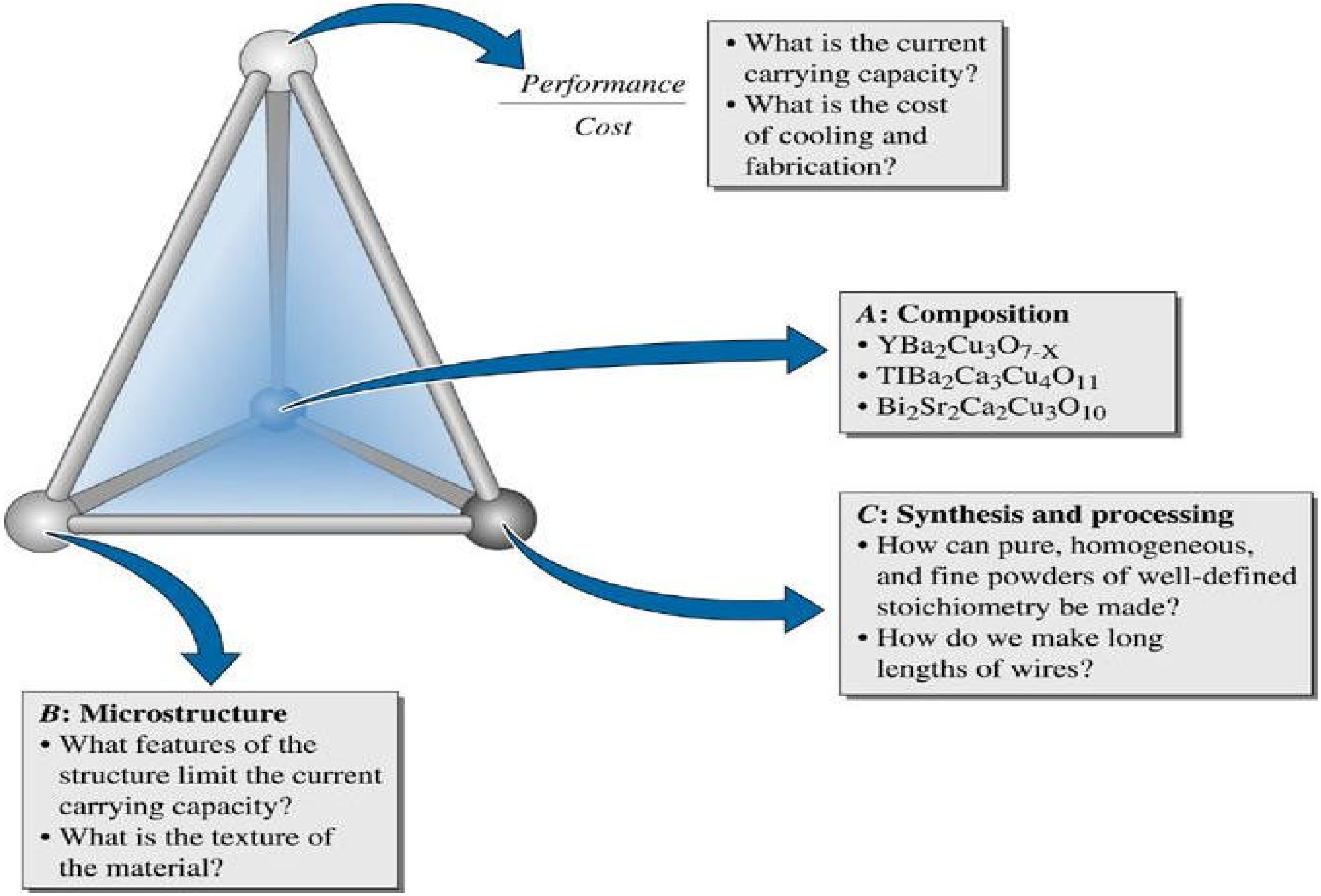
- What is the strength-to-density ratio?
- What is the formability?
- How does this relate to the crashworthiness of the vehicle?
- What is the cost of fabrication?

***A*: Compositions**
- Iron-based?
- Aluminum-based?
- What alloying elements should be used?
- What quantities?

***C*: Synthesis and processing**
- How can the steel making be controlled so as to provide a high level of toughness and formability?
- How can aerodynamic car chassis be formed?

***B*: Microstructure**
- What features of the structure limit the strength and formability?
- What controls the strength?

Application of the tetrahedron of materials science and engineering to **sheet steels for automotive chassis**. Note that the microstructure-synthesis and processing-composition are all interconnected and affect the performance-to-cost ratio.



Performance
Cost

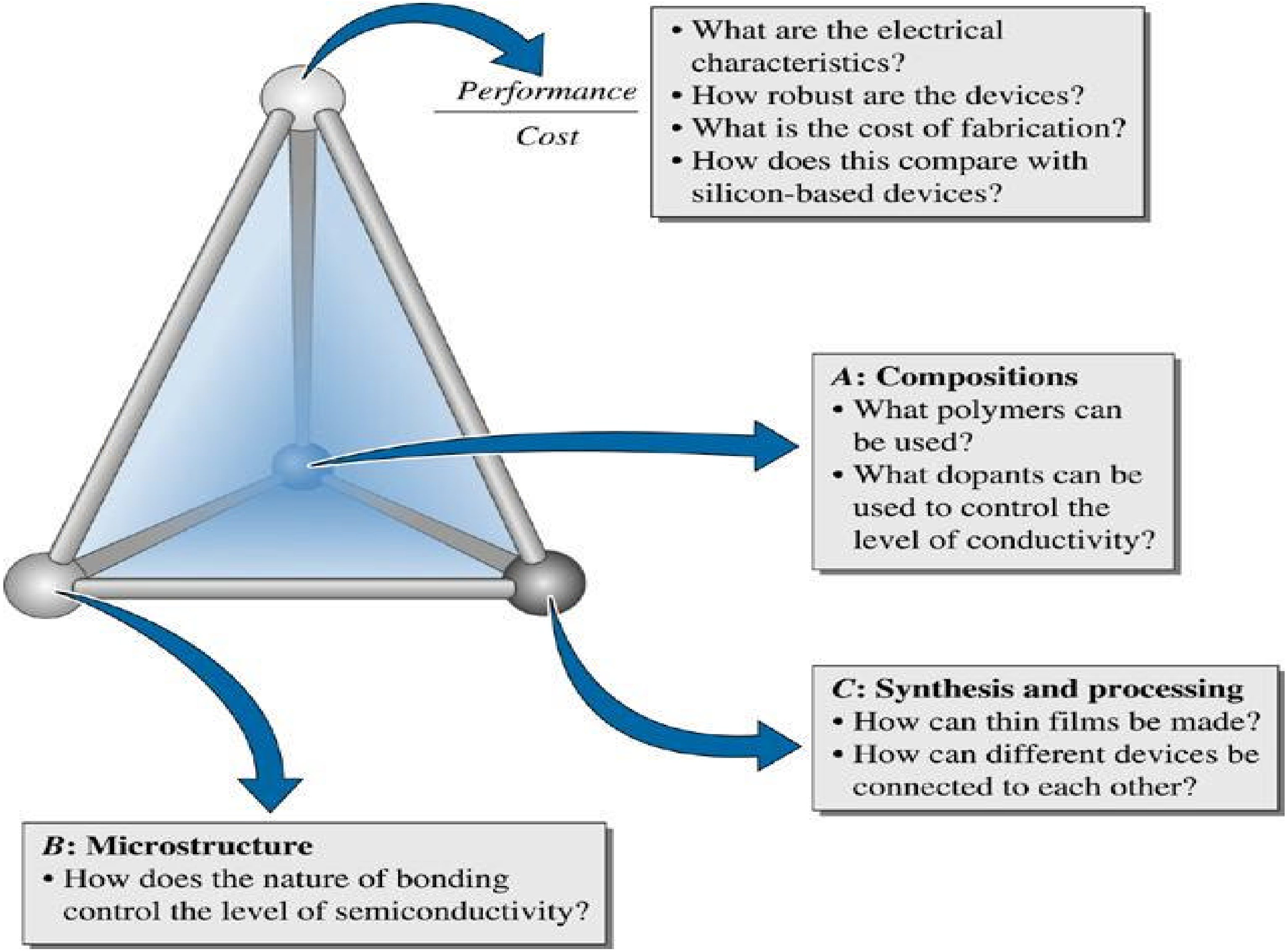
- What is the current carrying capacity?
- What is the cost of cooling and fabrication?

***A*: Composition**
- $YBa_2Cu_3O_{7-X}$
- $TIBa_2Ca_3Cu_4O_{11}$
- $Bi_2Sr_2Ca_2Cu_3O_{10}$

***C*: Synthesis and processing**
- How can pure, homogeneous, and fine powders of well-defined stoichiometry be made?
- How do we make long lengths of wires?

***B*: Microstructure**
- What features of the structure limit the current carrying capacity?
- What is the texture of the material?

Application of the tetrahedron of materials science and engineering to **ceramic superconductors**. Note that the microstructure-synthesis and processing-composition are all interconnected and affect the performance-to-cost ratio.



- What are the electrical characteristics?
- How robust are the devices?
- What is the cost of fabrication?
- How does this compare with silicon-based devices?

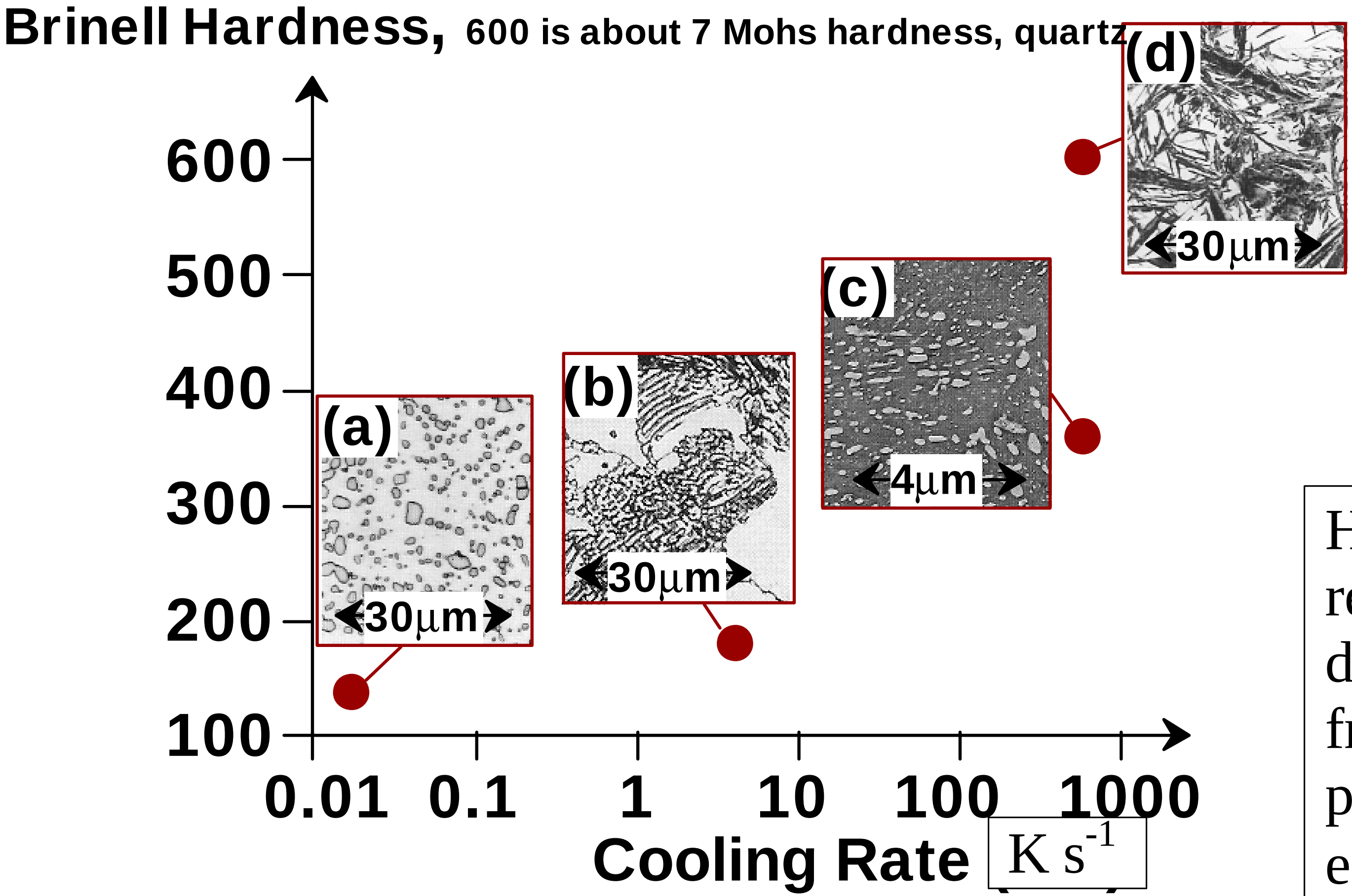
***A*: Compositions**
- What polymers can be used?
- What dopants can be used to control the level of conductivity?

***C*: Synthesis and processing**
- How can thin films be made?
- How can different devices be connected to each other?

***B*: Microstructure**
- How does the nature of bonding control the level of semiconductivity?

Application of the tetrahedron of materials science and engineering to **semiconducting polymers** for microelectronics

So properties do crucially depend on structure at different levels, structures themselves do depend on processing, …



4 wt % C cast iron, just differently processed, results in different mechanical properties

Hardness is the resistivity against plastic deformation, it's derived from many other properties, no simple equation to describe it

some (engineering) definitions of mechanical properties:

Ductility: ability of metals and alloys to retain strength (and freedom form cracks) when shape is altered, absolute elongation to fracture

Brittleness: a tendency to fracture without appreciable deformation and under low stresses, e.g. glass

Stress (s): a force per unite area, measured in Pa = N m^{-2}

Strain (e): a measure of the deformation a materials exhibits under an applies stress, dimensionless or in %; under an applied tensile stress, strain is the change in length per unit original length

Toughness: a combined measure of strength and ductility, $\int s \cdot de$, area under a stress versus strain curve, energy needed to fracture a material

Elasticity: tendency of a body to return to its original size or shape after having been stretched, compressed or deformed / **elastic deformation**, non-permanent, linear function of stress versus strain / **elastic modulus (E)**, also Young's modulus: ease (or difficulty) by which a solid can be deformed, constant of proportionality between strain and stress, i.e. s = E e

Yield strength, intersection of stress versus strain curve with a straight line parallel to the elastic portion and offset by 0.2% on strain axis, i.e. stress necessary to generate this small amount of plastic deformation; *in a more qualitative way:* stress at which stress versus strain curve is no longer (essentially) linear, point where plastic deformation sets in. (There may be an upper and a lower yield strength.)

Plasticity: property of certain materials by which the deformation due to a stress is largely retained after removal of the stress / plastic deformation, permanent deformation associated with the distortion or reformation of atomic bonds

Ultimate strength: highest point in a stress versus strain curve

Rapture/Fracture strength, the stress at which the material fails

there is no simple definition for **strength of a material**. yield strength, fracture strength, ultimate strength, tensile strength, or specific strength, i.e. strength per unit volume, have to be used specifically

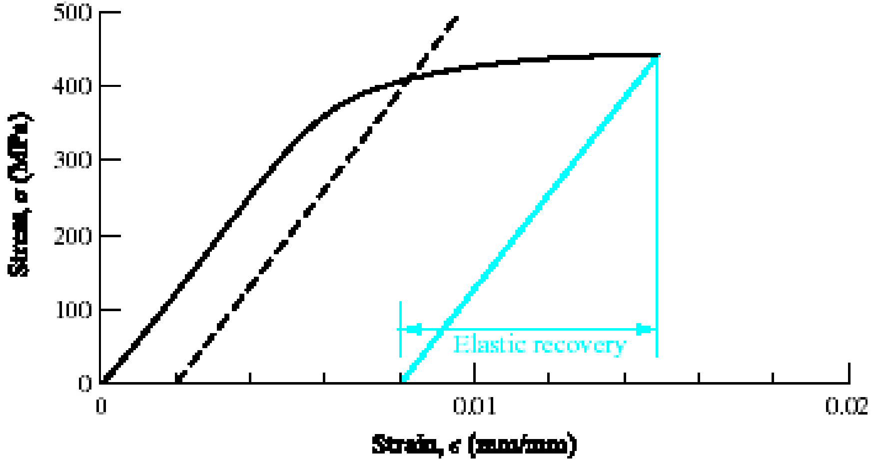


Figure 6-5 *Elastic recovery occurs when stress is removed from a specimen that has already undergone plastic deformation.*

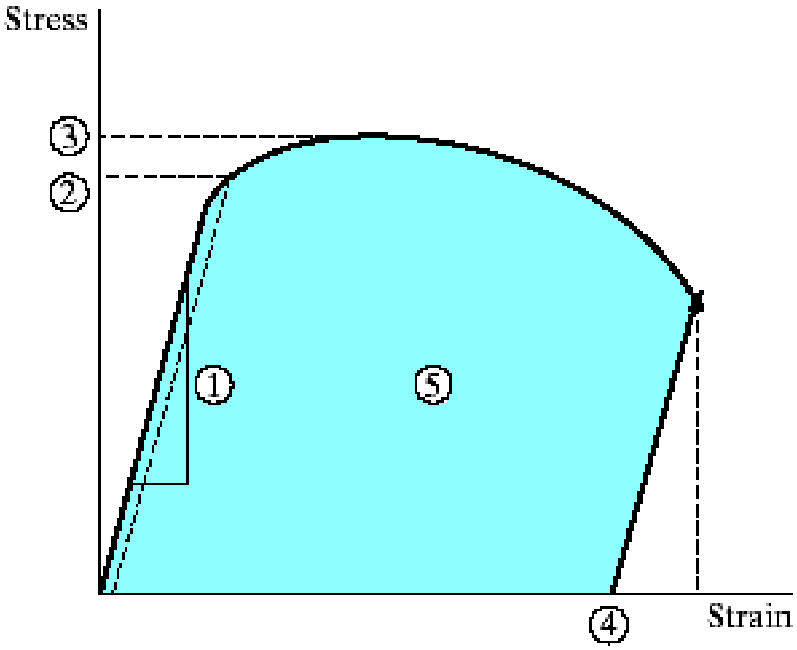


Figure 6-6 *The key mechanical properties obtained from a tensile test: 1, modulus of elasticity, E; 2, yield strength, Y.S.; 3, tensile strength, T.S.; 4, ductility,* 100 × $\epsilon_{\text{failure}}$ *(note that elastic recovery occurs after fracture); and 5, toughness =* $\int \sigma \, d\epsilon$ *(measured under load; hence, the dashed line is vertical).*

more generally, when this curve does not result from a tensile test, the highest point of the curve is the ultimate strength of the material

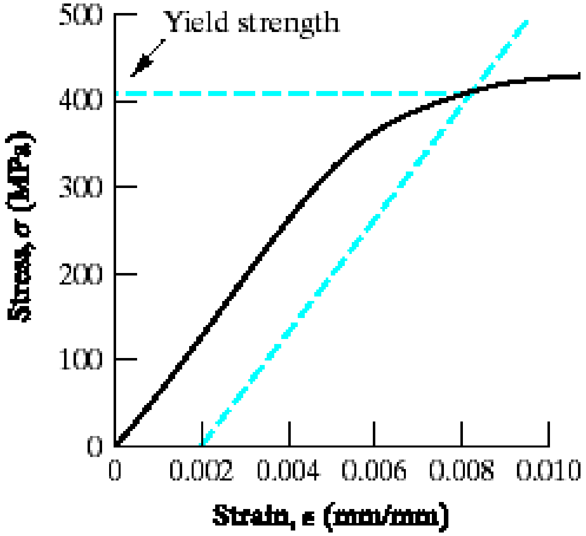


Figure 6-4 *The yield strength is defined relative to the intersection of the stress–strain curve with a "0.2% offset." This is a convenient indication of the onset of plastic deformation.*

Stress versus strain curves do depend on: microstructure of the specimen, geometrical factors, the way a test is administered, e.g. tensile or compression. Furthermore these curves do depend critically on temperature!

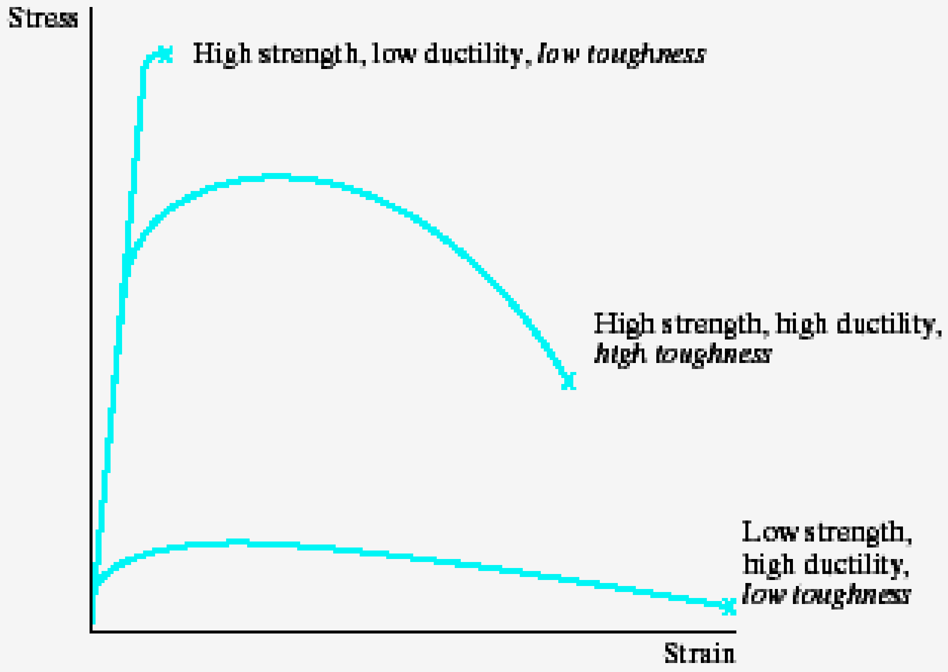


Figure 6-9 *The toughness of an alloy depends on a combination of strength and ductility.*

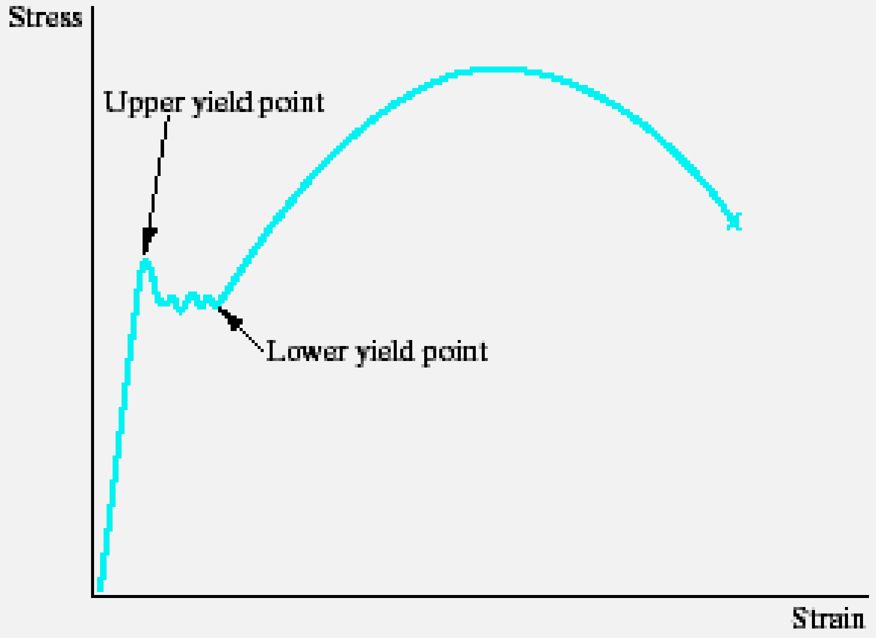


Figure 6-10 *For a low-carbon steel, the stress-versus-strain curve includes both an upper and lower yield point.*

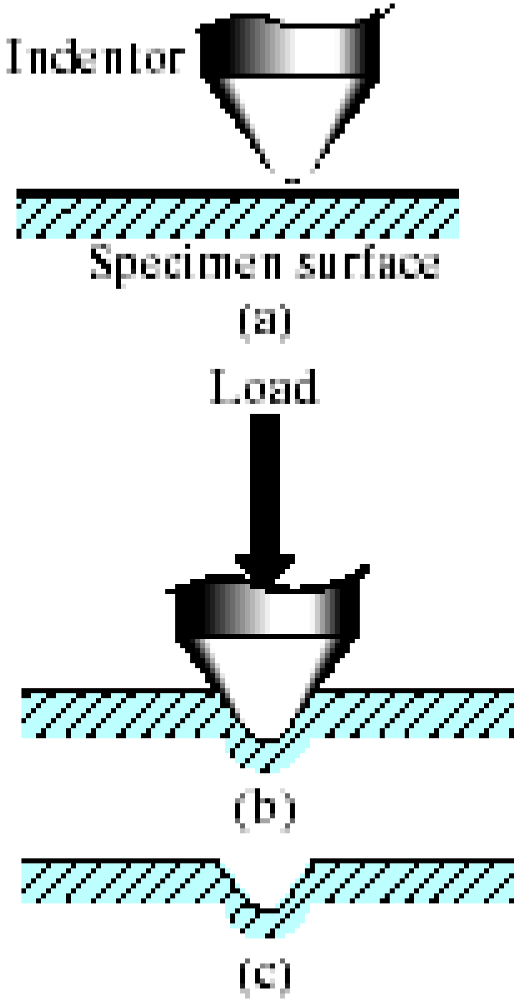
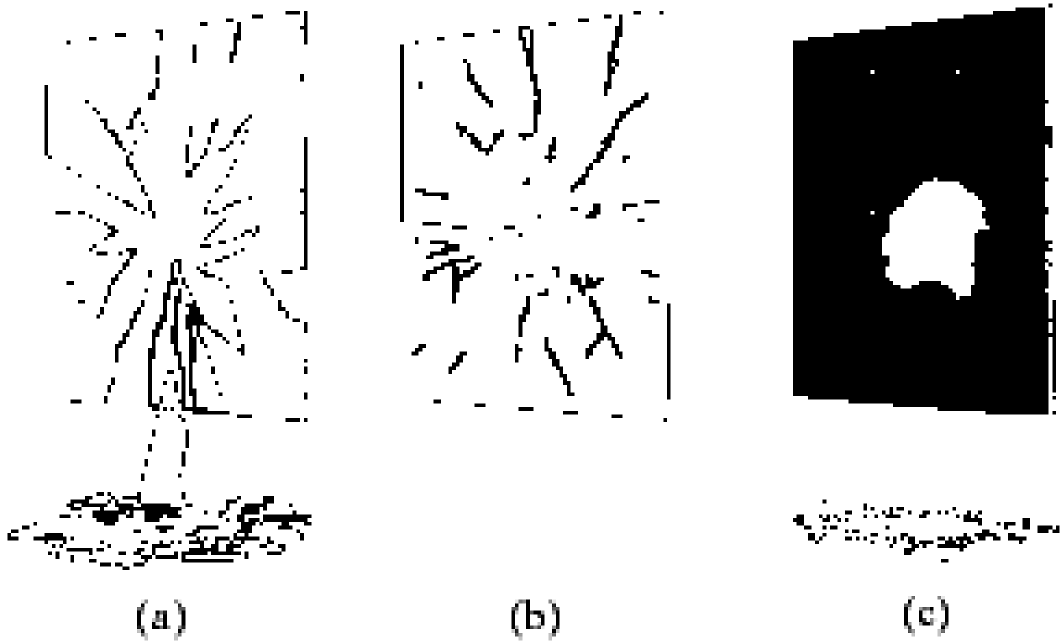


Figure 6-27 *Hardness test. The analysis of indentation geometry is summarized in Table 6.10.*



Break pattern of three states of glass used in commercial and consumer applications. (a) Annealed. (b) Laminated. (c) Tempered. (From R. A. McMaster, D. M. Shetterly, and A. G. Bueno, "Annealed and Tempered Glass," in *Engineered Materials Handbook*, Vol 4, *Ceramics and Glasses*, ASM International, Materials Park, Ohio, 1991.)

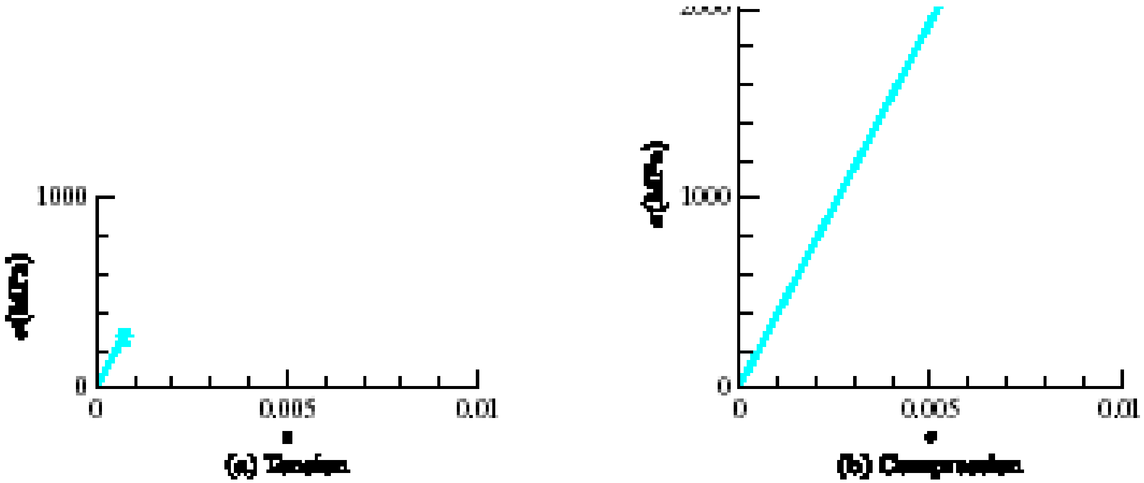
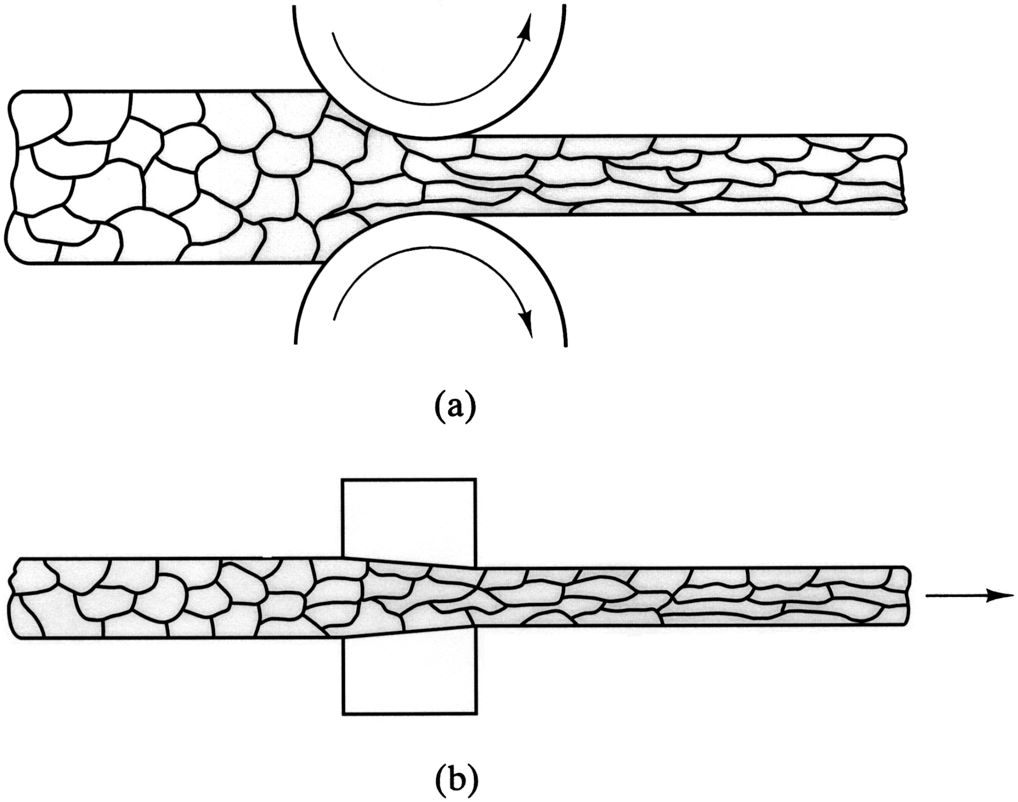


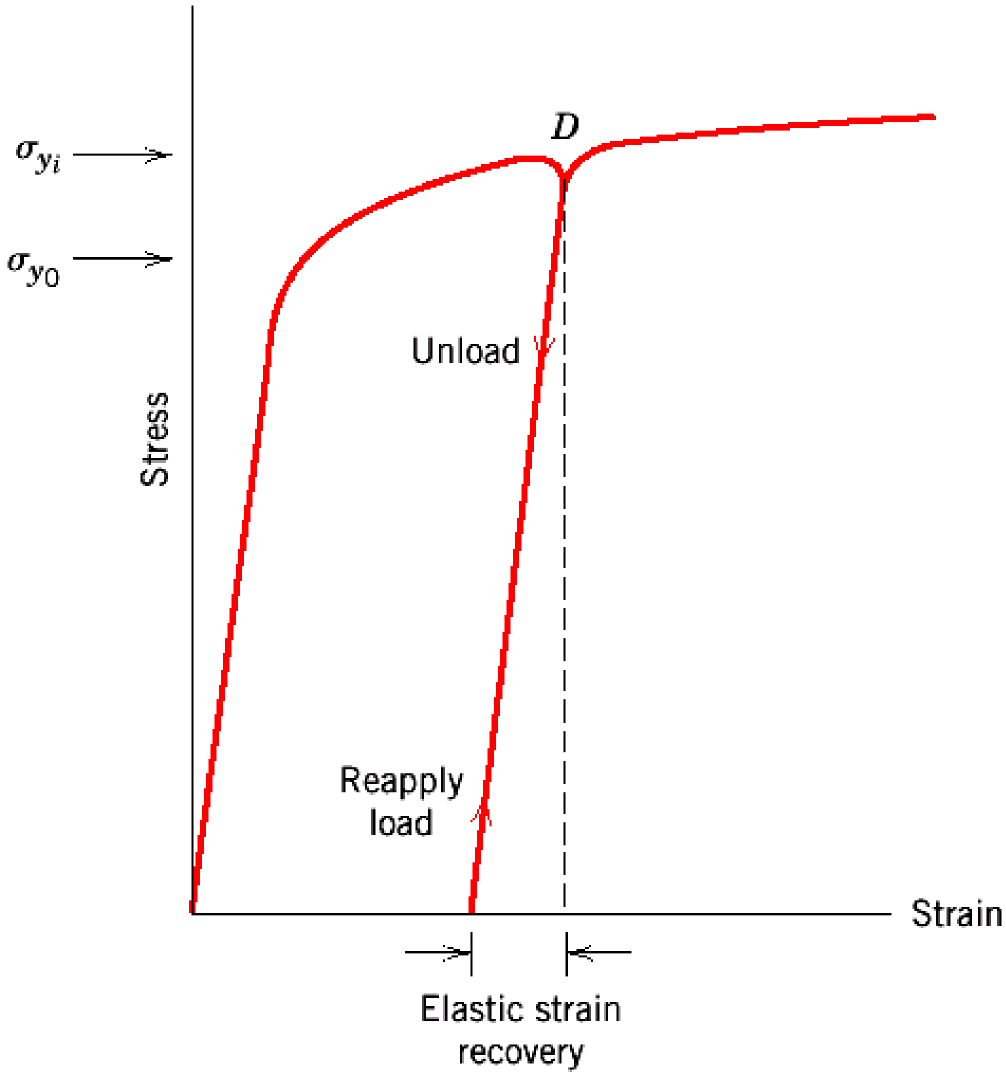
Figure 6-13 *The brittle nature of fracture in ceramics is illustrated by these stress–strain curves, which show only linear, elastic behavior. In (a), fracture occurs at a* tensile *stress of 280 MPa. In (b) a* compressive *strength of 2100 MPa is observed. The sample in both tests is a dense, polycrystalline Al_2O_3.*

One technically important type of **processing of metals is cold rolling**, it is also know as work hardening or strain hardening, cold working, …


(a)

(b)

Figure 10-29 *Examples of cold-working operations: (a) cold-rolling of a bar or sheet and (b) cold-drawing a wire. Note in these schematic illustrations that the reduction in area caused by the cold-working operation is associated with a preferred orientation of the grain structure.*

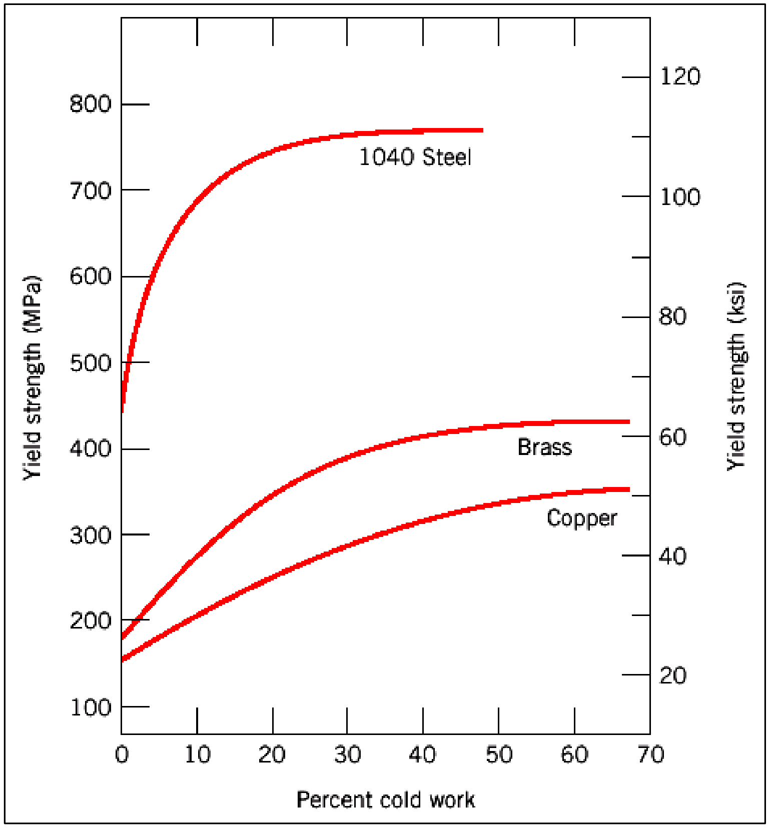


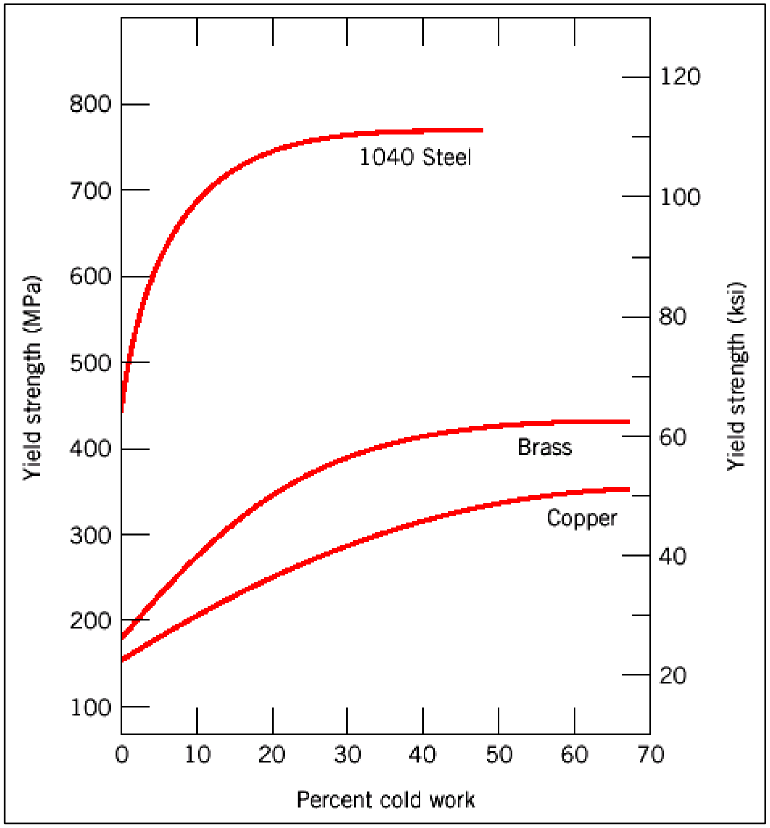
the new yield strength s_{yi} is higher than the initial yield strength s_{y0}

strain energy is stored in the system in form of dislocation strain fields and elastic distortions within grains

this stored energy allows for a larger elastic region in the strain stress diagram, i.e. the cold rolled material got mechanically stronger due to the plastic deformation that was inflicted by processing, the cold rolling

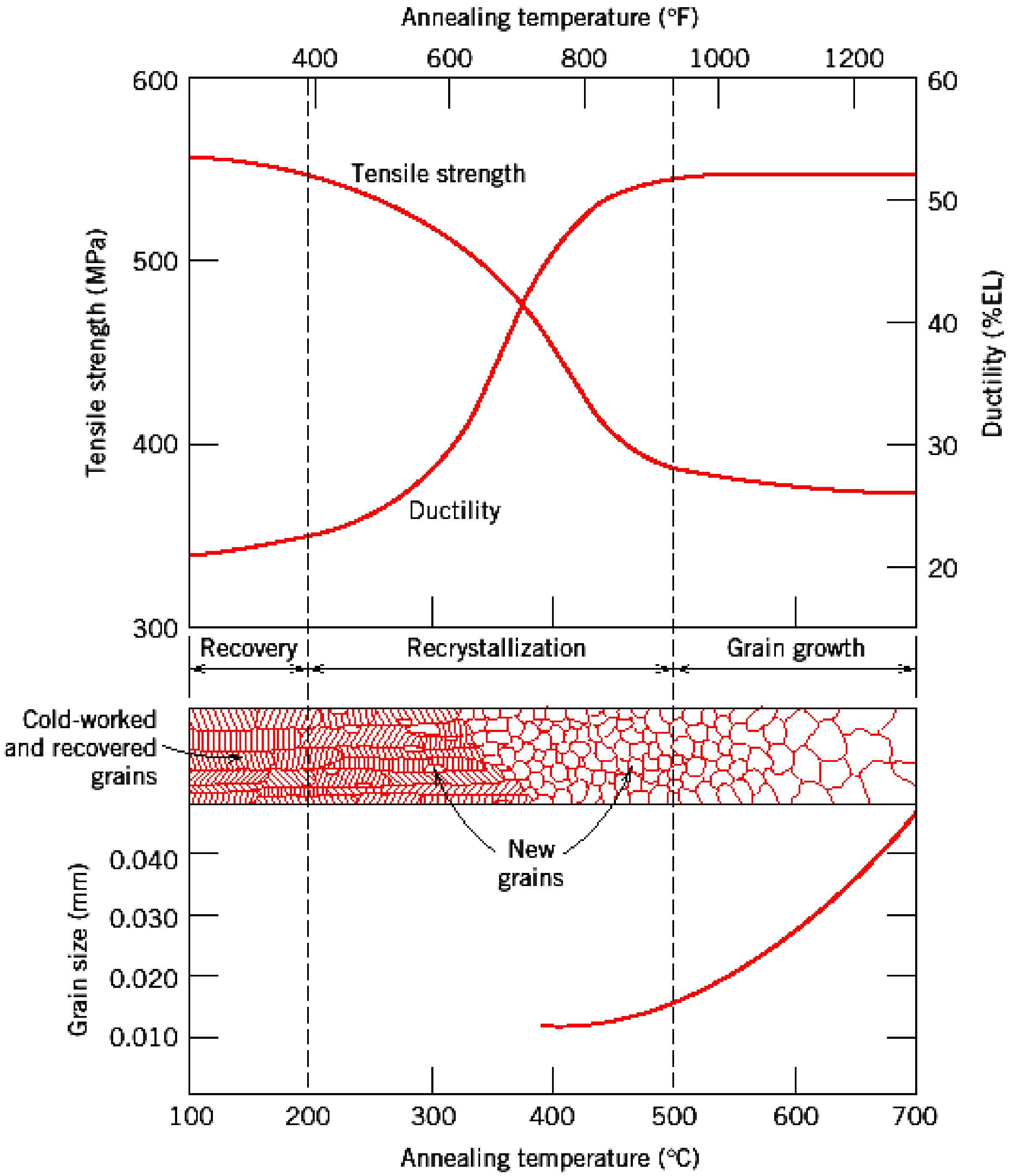
that cold rolling changed the microstructure, ….



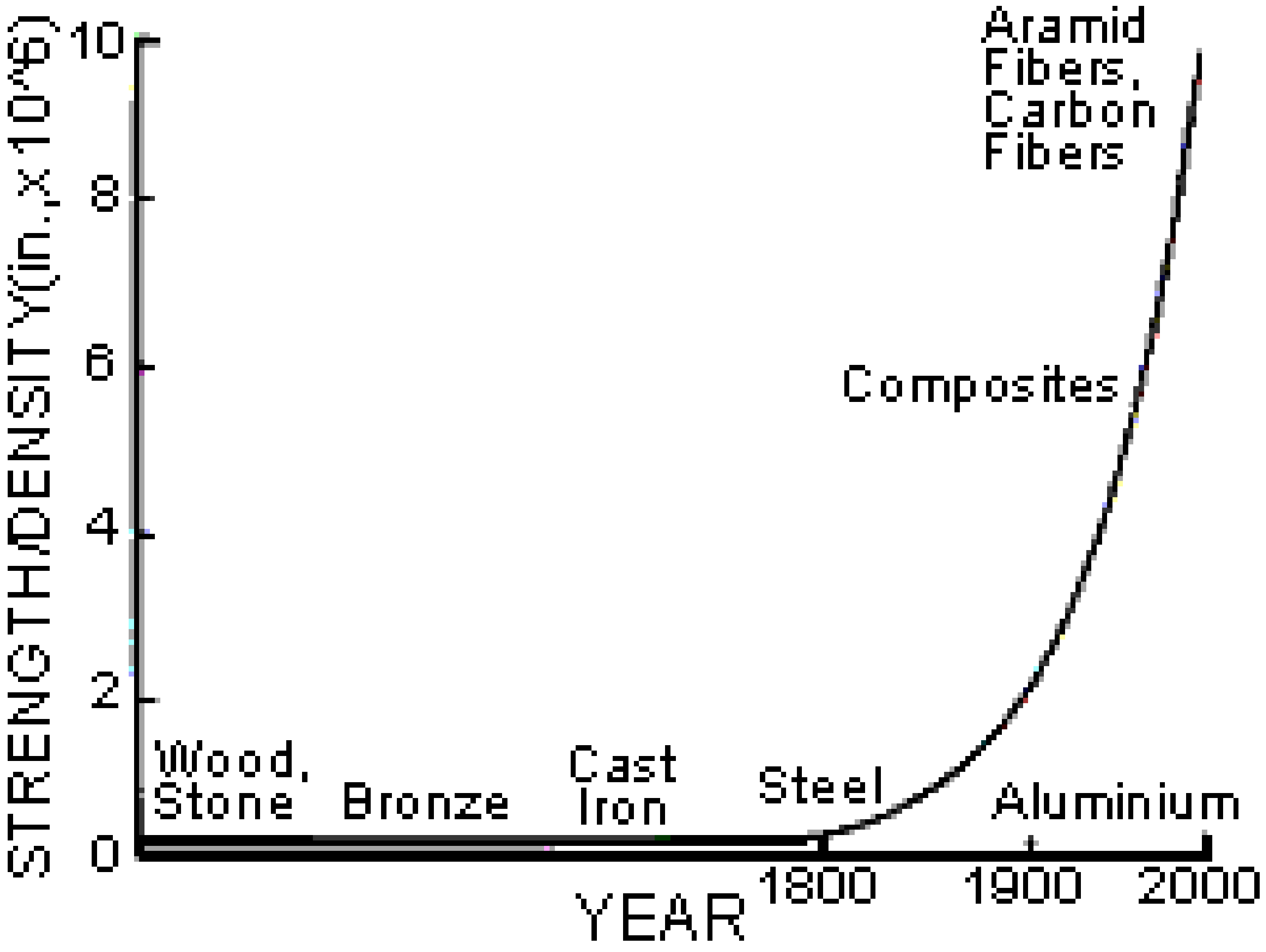


There is no such thing as a free lunch, increasing the yield strength and hardness of a material by cold rolling has to be "paid for" by a decreasing ductility and brittleness,

annealing of a cold rolled metal at about $^{1}/_{3}$ to ½ of its melting temperature releases much of that stored energy by changing the microstructure, i.e. brings the metal closer to thermodynamic equilibrium which is a minimal free energy state, with that change of microstructure we have again a change in mechanical properties, now it's an increased ductility and reduced brittleness



Annealing temperature (°F)
400
600
800
1000
1200
600
500
400
300
Tensile strength (MPa)
60
50
40
30
20
Ductility (%EL)
Tensile strength
Ductility
Recovery
Recrystallization
Grain growth
Cold-worked and recovered grains
New grains
Grain size (mm)
0.040
0.030
0.020
0.010
100
200
300
400
500
600
700
Annealing temperature (°C)



note how the increase in strength per unit density of materials correlates with the emergence of firstly physical metallurgy and secondly materials science

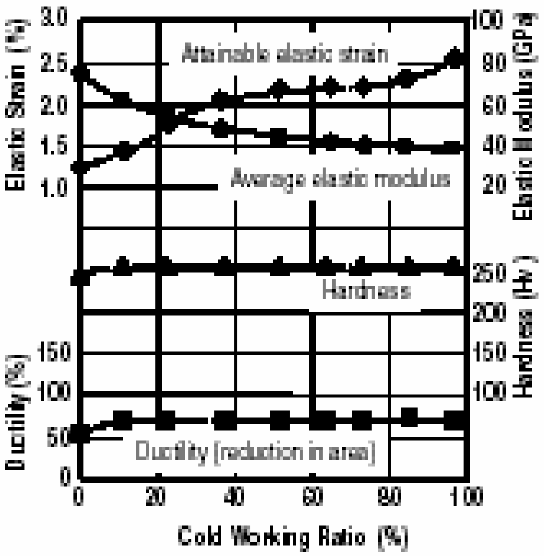
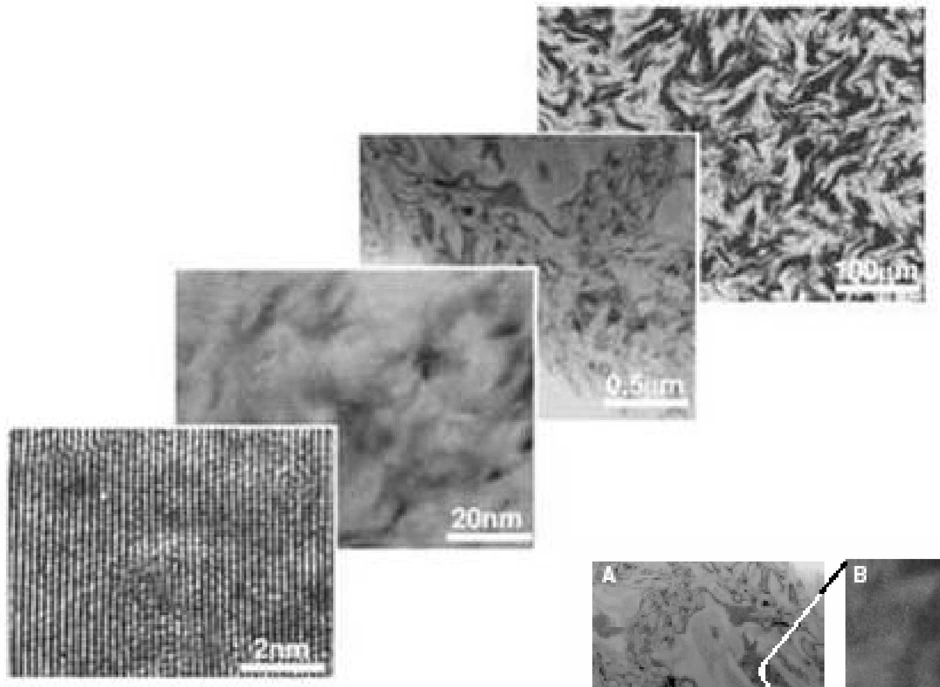


Fig. S1. Changes in mechanical properties of Ti-12Ta-9Nb-3V-6Zr-1.5O alloy with cold working ratio. The elastic modulus (average value of non-linear elasticity) decreases with increasing the cold working ratio, falling below 40 GPa at 90%-working; accordingly the elastic strain increases to 2.5% after 60% cold working. Meanwhile, Vickers hardness and tensile ductility (reduction in area) are both independent of the cold working ratio, which suggests that the alloy has super cold workability at room temperature. Note that the fracture strain that represents the amount of uniform tensile elongation shown in Fig.1 is fairly small; however, the material shows a curious work-softening behavior and very large local elongation (reduction in area) even after cold working to more than 99.9%. This work softening interferes with the uniform elongation in tensile specimen seen in Fig. 1.



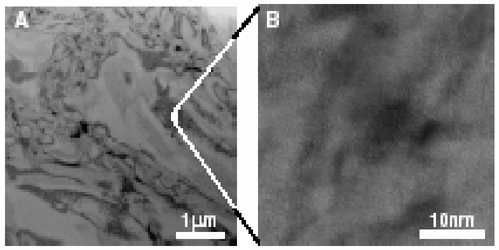
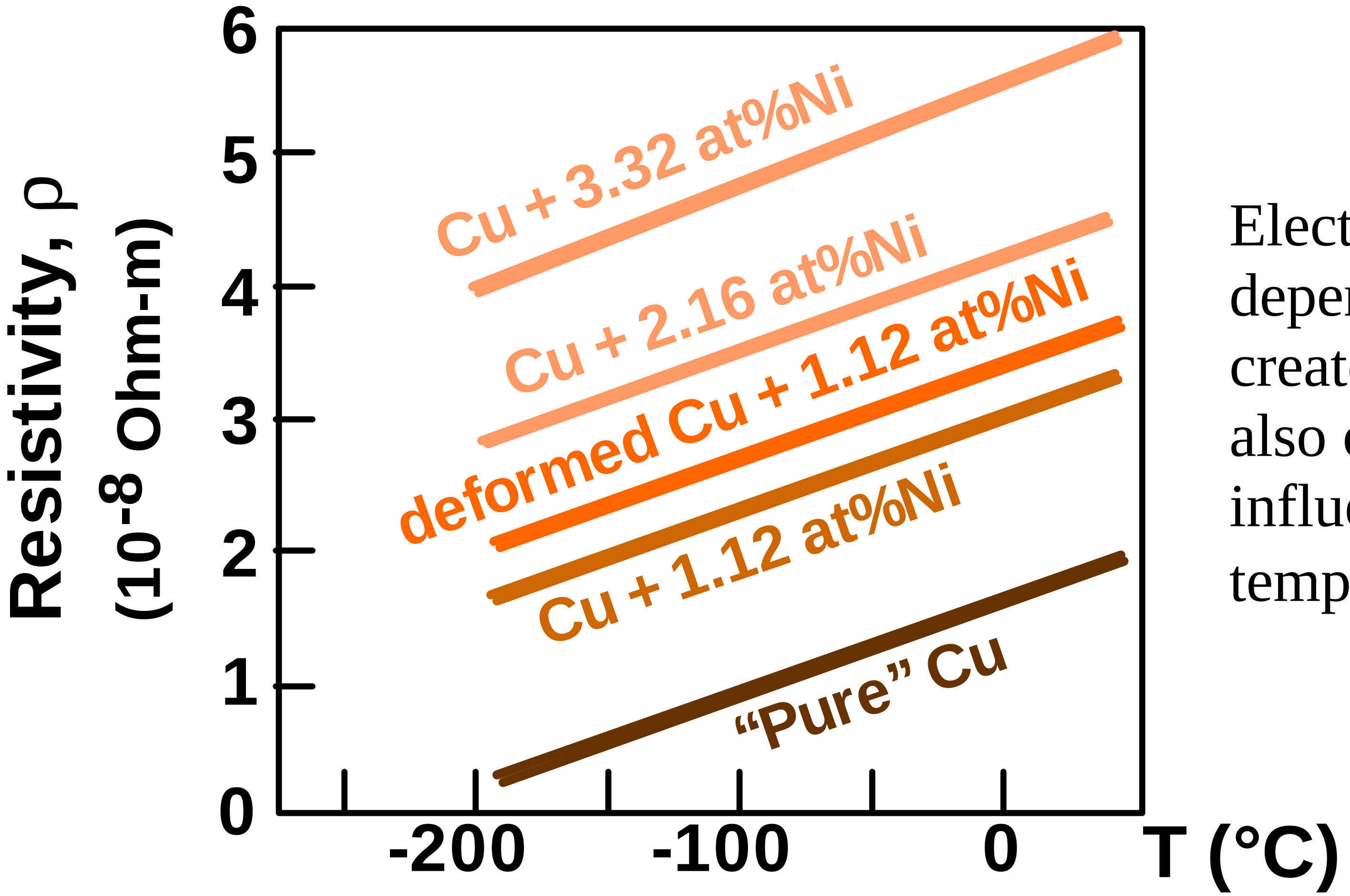


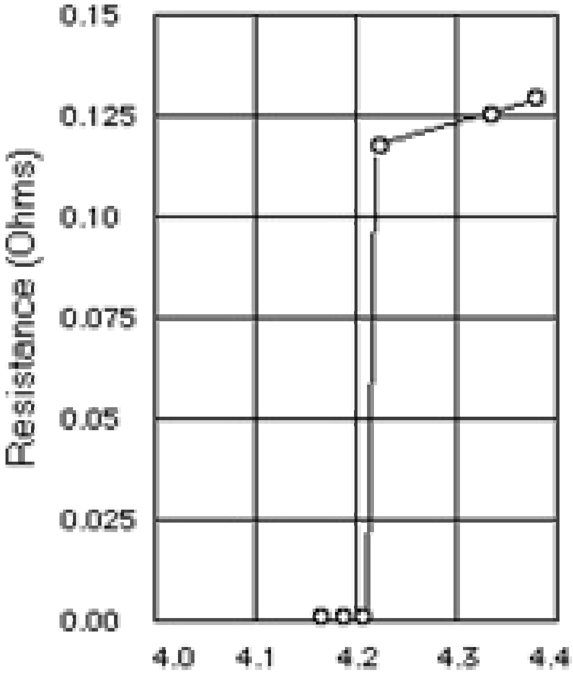
Fig. S2. TEM images of 90 % cold-worked Ti-23Nb-0.7Ta-2Zr-1.2O alloy. In spite of a large amount of plastic deformed condition, no dislocation is visible in the micrographs; rather, strange nanometer size strain contours are observed throughout the specimen.

super-elastic metal alloys have very complex microstructure at different levels, they deform without dislocation formation and slip, the dependence of mechanical properties on cold work is different, so there is still more to discover in metals, Science, April 2003

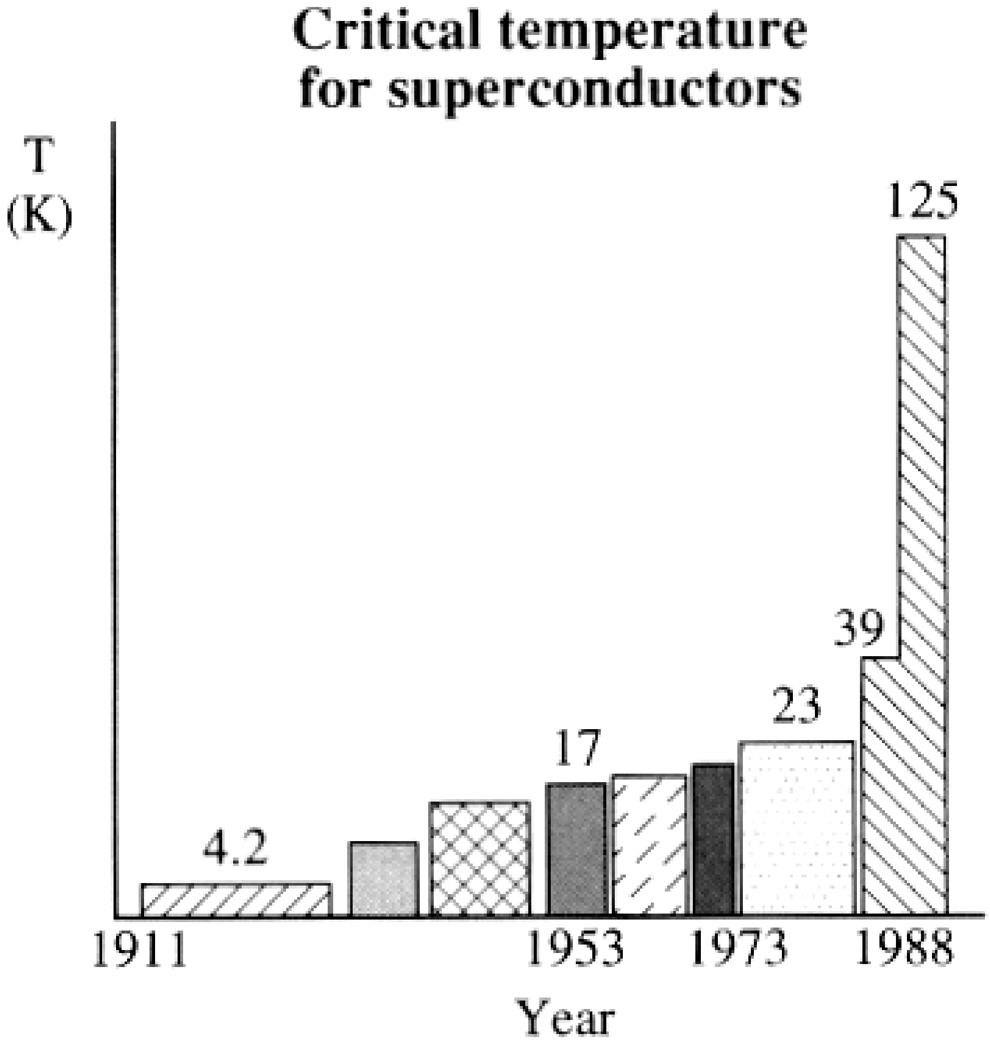


Electric resistivity of Cu depend on microstructure created by alloying and also on environmental influences such as temperature

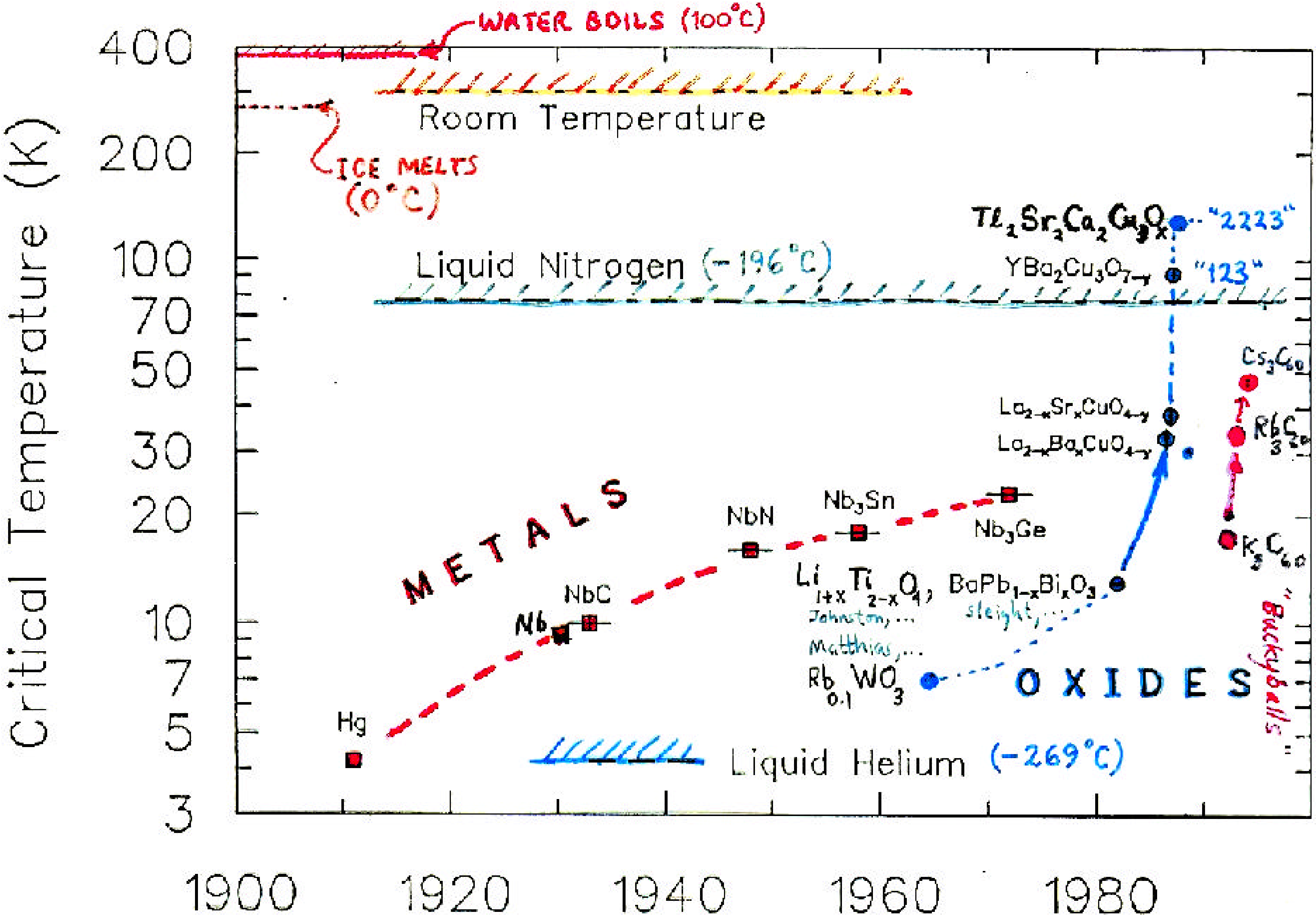
Fig. 1

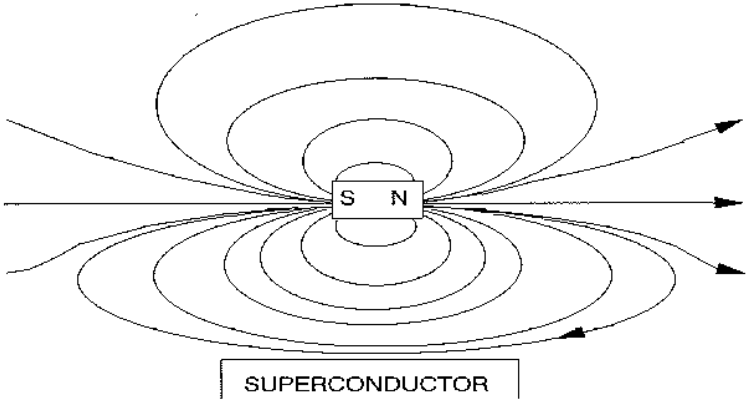


Heike Kamerlingh Onnes’ original data for Hg, 1911



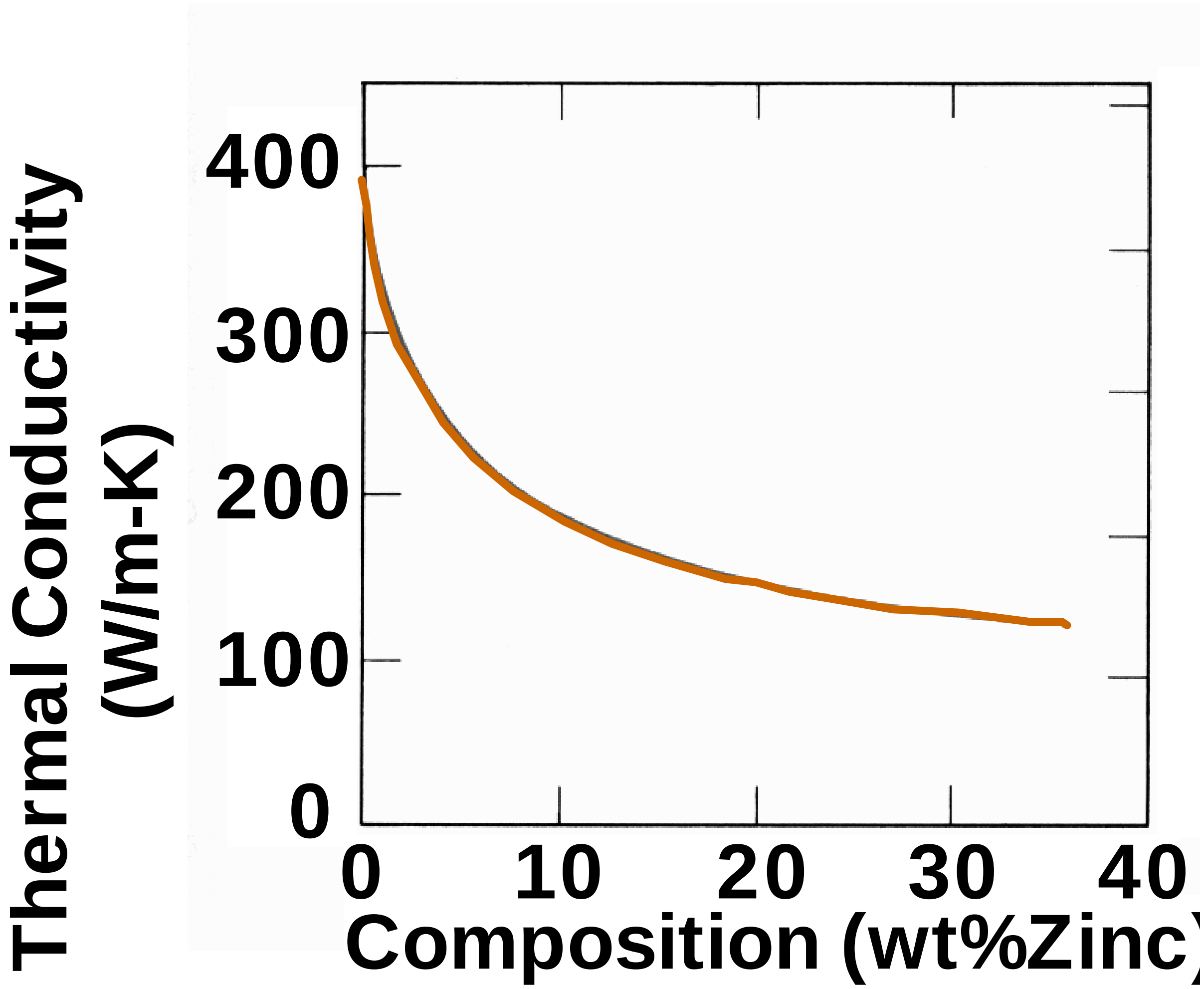
A Short History of Superconductors



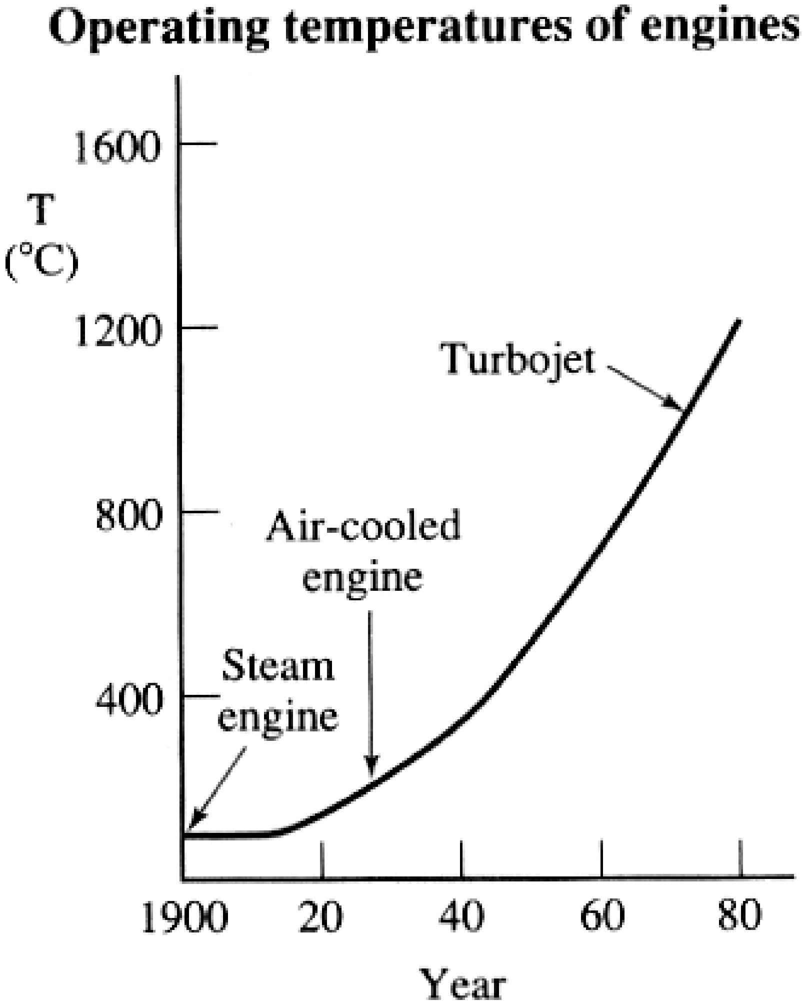


Superconductors are more than perfect conductors of electricity, they also have an interesting magnetic property of excluding a magnetic field. A superconductor will not allow a magnetic field to penetrate its interior. It causes currents to flow that generate a magnetic field inside the superconductor that just balances the field that would have otherwise penetrated the material. **Understanding and Designing high temperature superconductors are important materials science and engineering problems.**

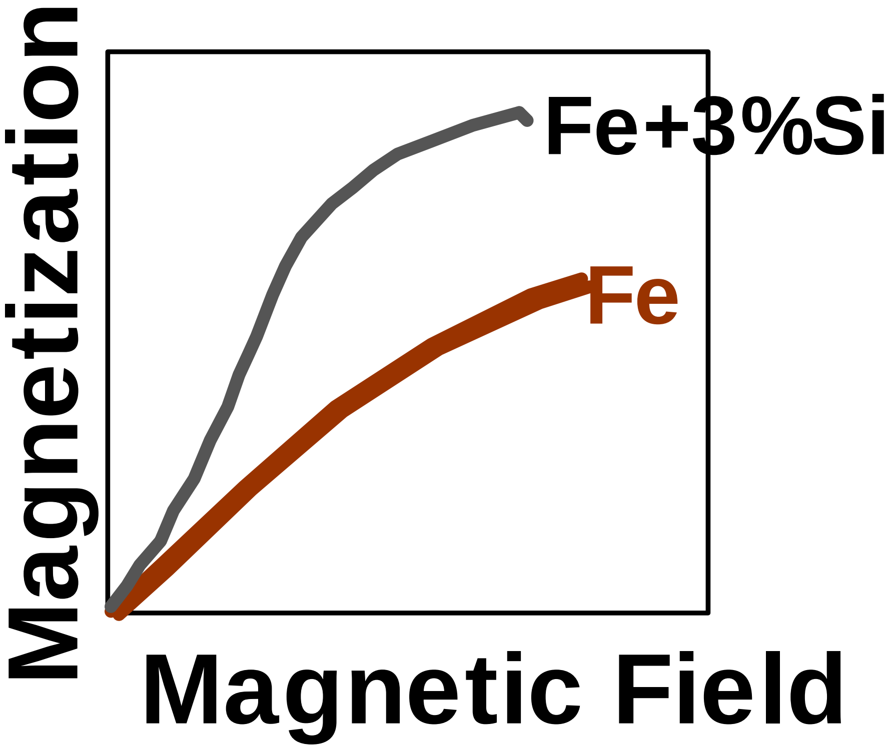
Meissner Effect: magnet levitating above a superconductor occurs only for small magnetic fields. If magnetic field too large, it penetrates the interior of the superconductor and its superconductivity.

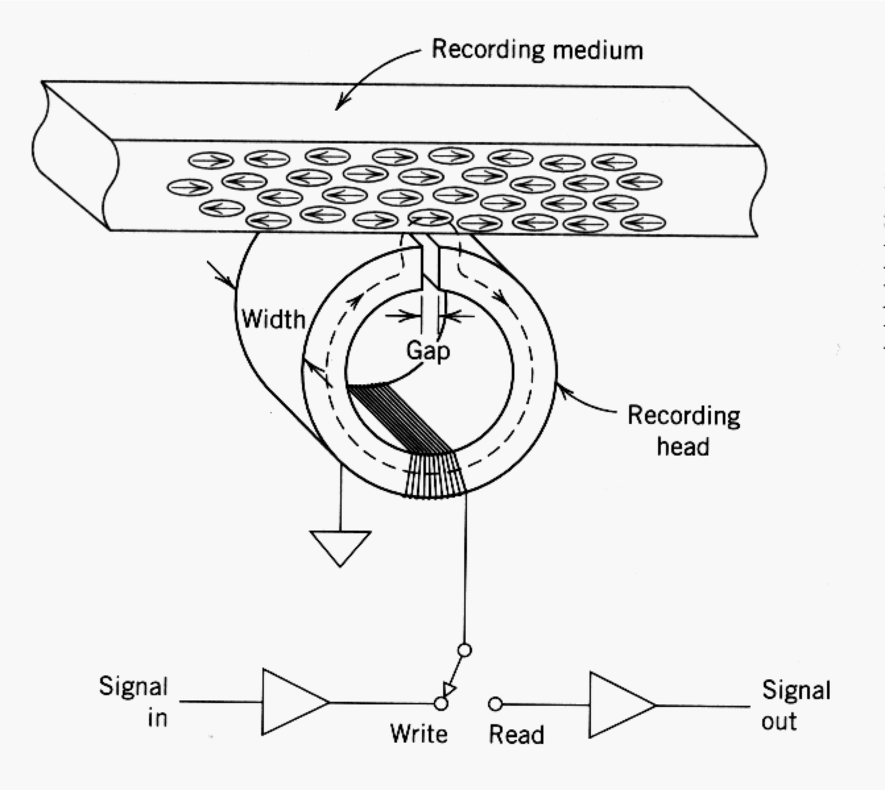


Thermal conductivity of Cu depends on microstructure created by alloying (brass), microstructure itself depends on processing

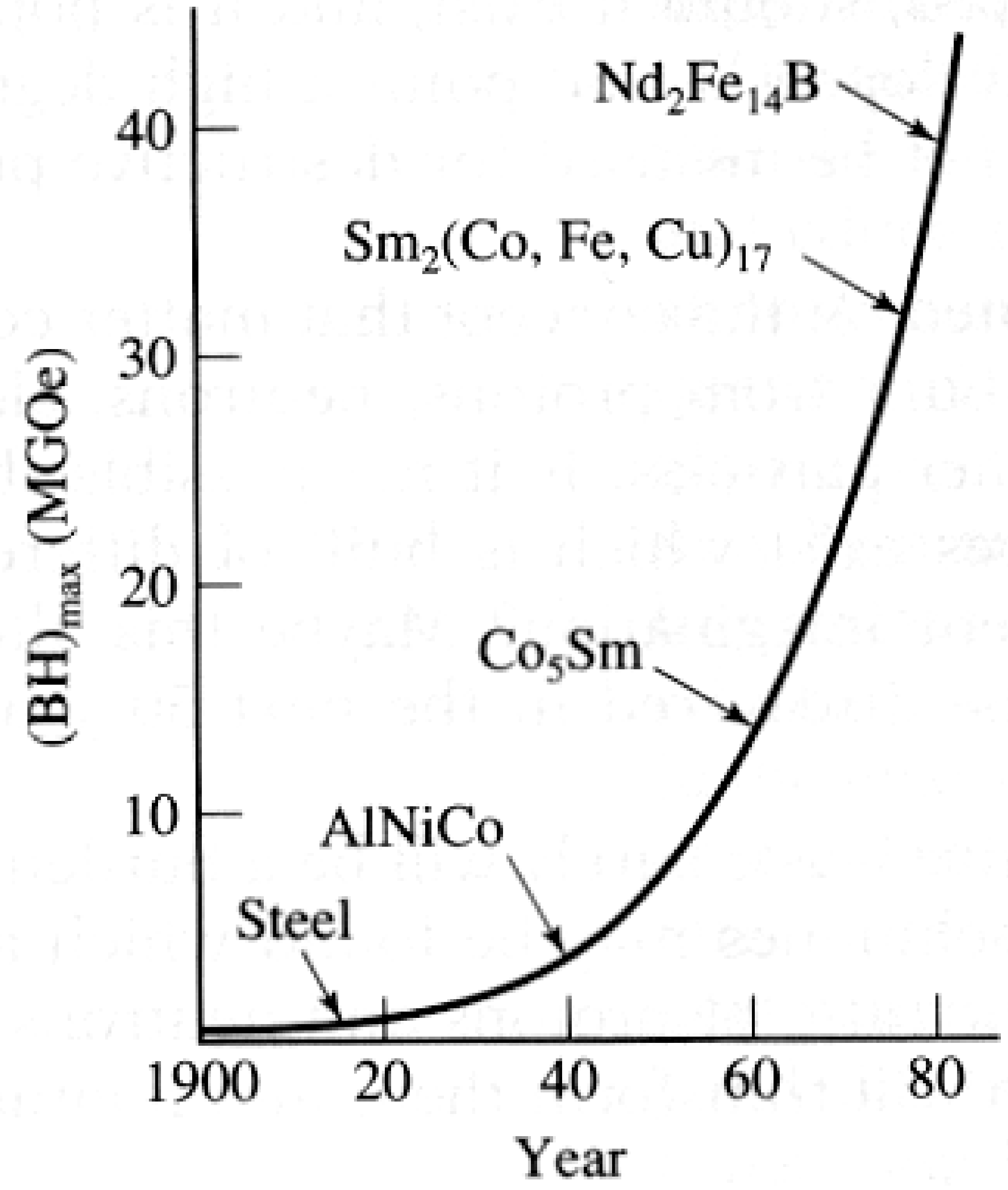


<u>Basic thermodynamics</u>: **Ideal** Carnot heat engine is the more effective the larger the difference between the hot (Th) and cold (Tc) reservoirs that are in thermal contact is, $e = 100\ \% - {}^{Th}/_{Tc}$ also **<u>real engines</u>** that are very hot are more effective for the same thermal environment, of course this is also a materials science and



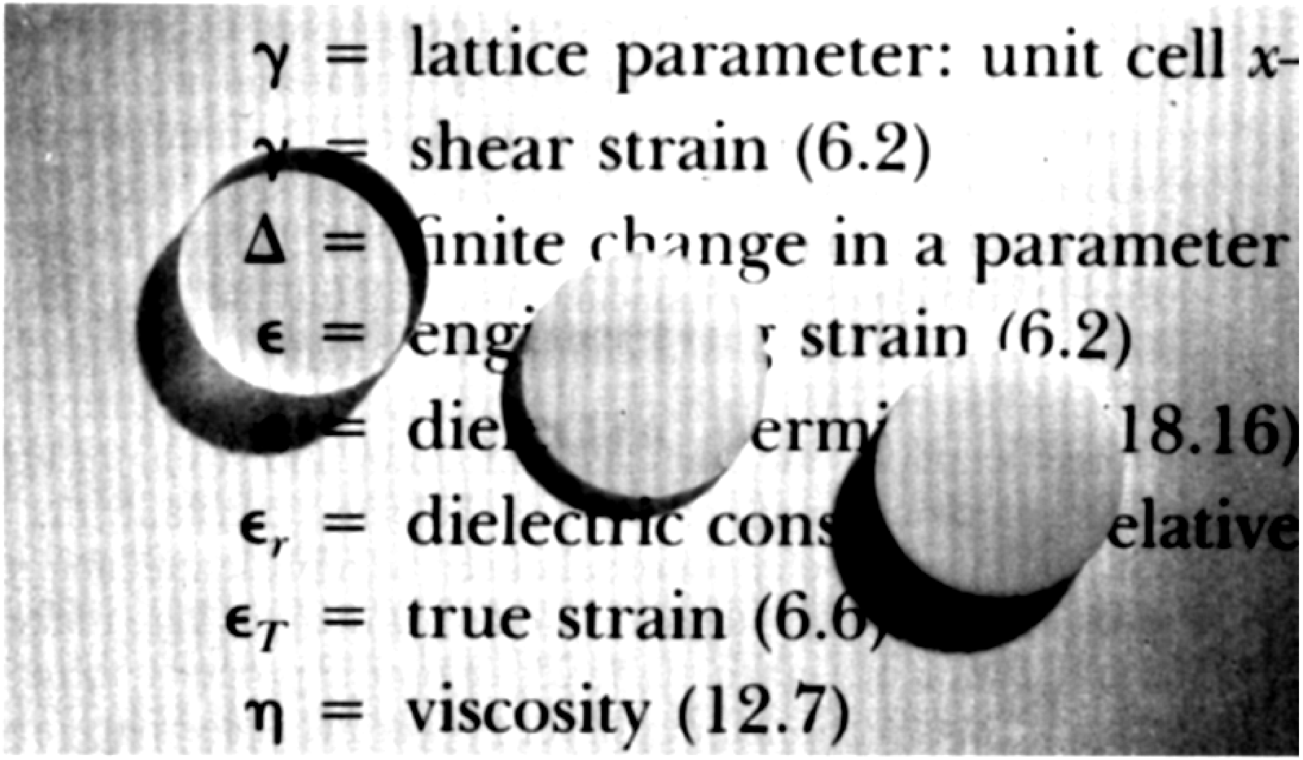


Magnetic Polarization (Magnetization) depends on environmental influences, here magnetic field strength and microstructure of the particles that carry information on a magnetic tape


Strength of permanent magnets

Frederik H. Norton at MIT about his department: **“The Metallurgy Department had interests in process metallurgy, physical metallurgy, chemical metallurgy and corrosion, but, in truth, *the properties and uses of metals are not very exciting …”***

metal: ***they are considered to be mature materials with relative little potential for major breakthroughs”*** Schaffer at al.



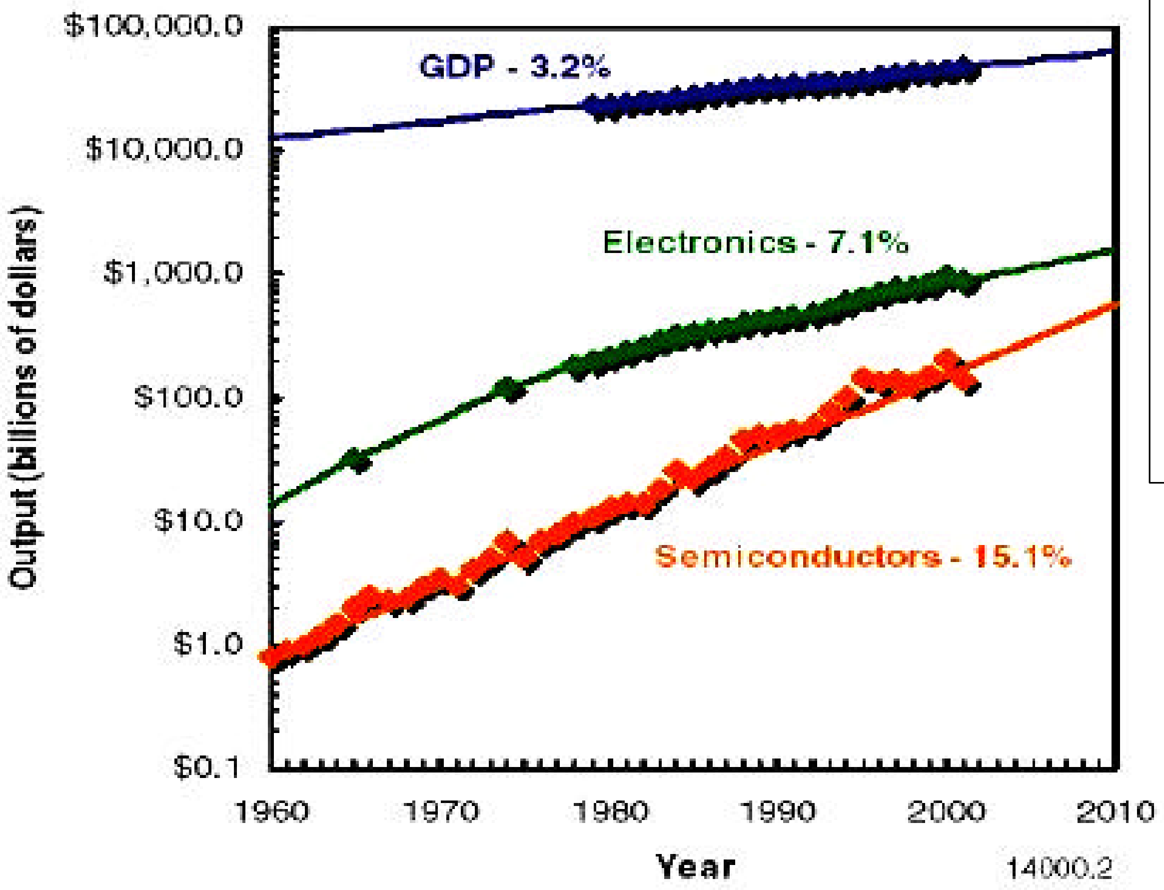
Optical properties depend on microstructure, microstructure depends on processing, all Al_2O_3

single crystal sapphire is transparent

poly-crystal without micro-pores is translucent

poly-crystal with 5 % porosity is opaque

Semiconductors: Sutton's Law of R&D



March, 29, 2004

Si: 130,000,000
Silicon: 7,100,000
Semiconductor: 4,060,000
GaN 2,000,000
GaAs 587,000

Steel: 24,000,000
Fe: 13,800,000

Google hits:
Silicon 3,530,000
GaAs 305,000

October 2003

Steel: 10,200,005

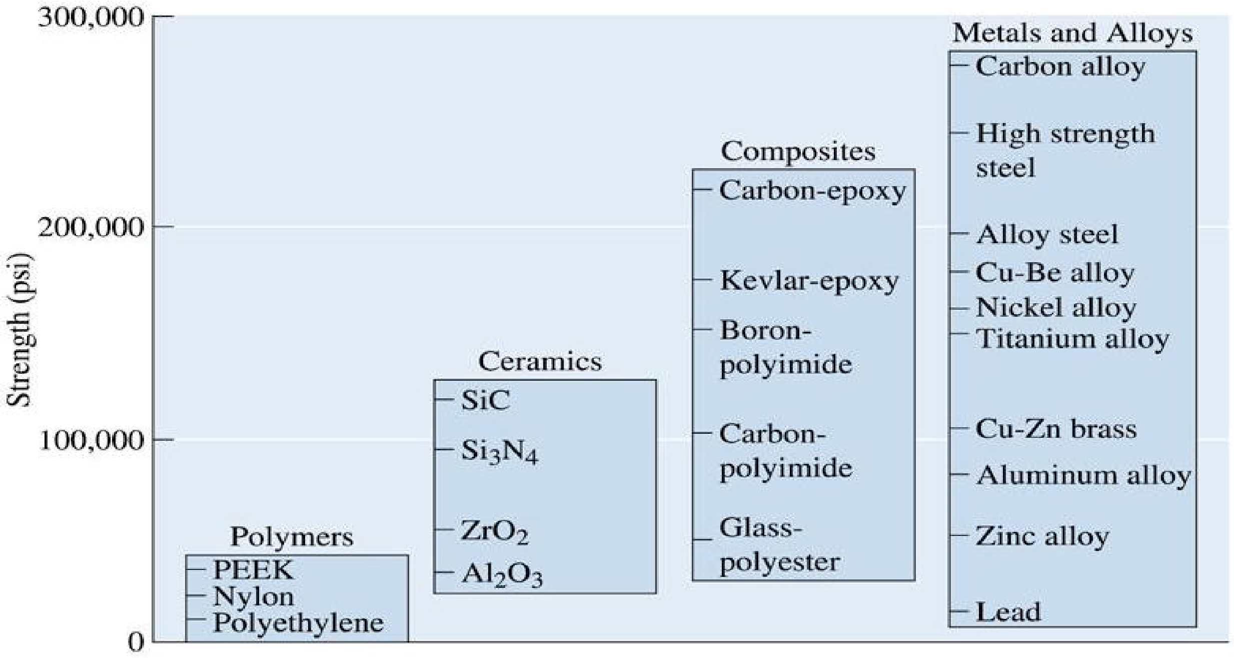
"It's where the money is" W.Sutton

"Breakthrough for Everlasting Prosperity of Semiconductor Industry" T.Ohmi

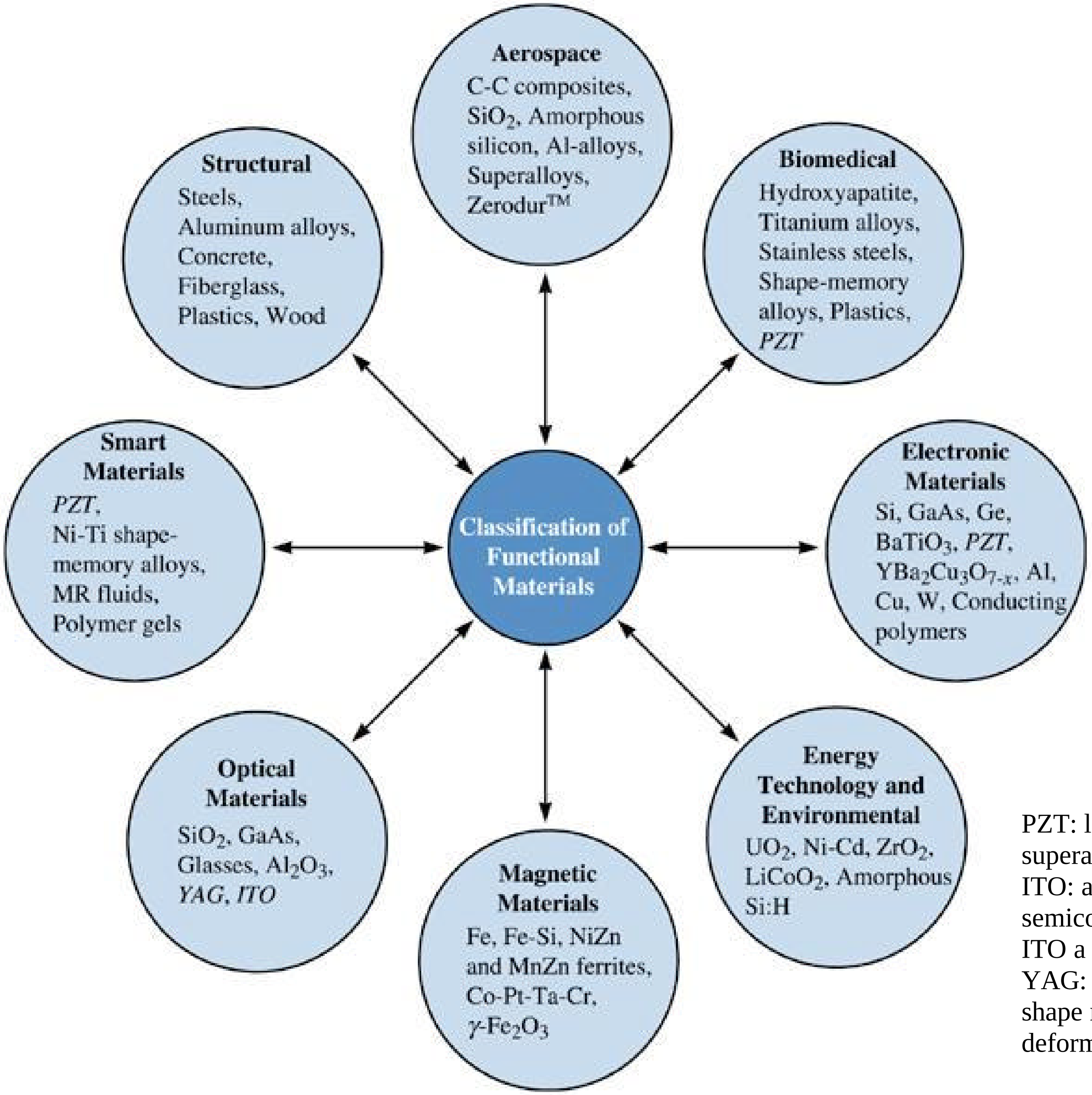
Major Classes of Materials

metals, ceramics (semiconductors), composites, polymers,

better: semiconductors, metals, composites (semiconductor devices),ceramics, polymers ?



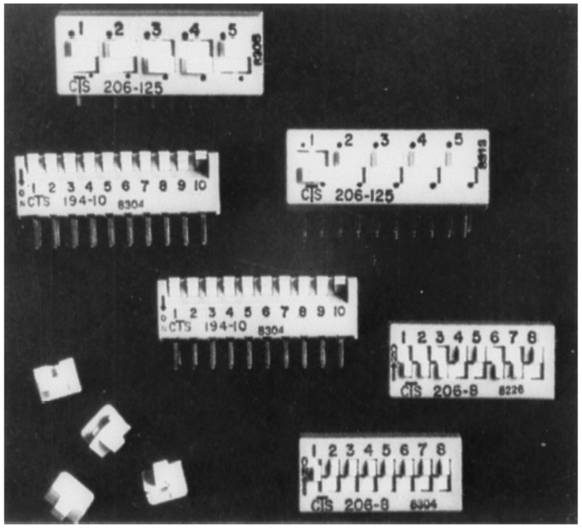
Representative strengths of various categories of materials, metals, some composites and some ceramics (e.g. concrete) are considered “structural materials” the other materials are **functional materials**, 1 psi ˜ 6.897 10^{-3} MPa (a force N per area m^2)



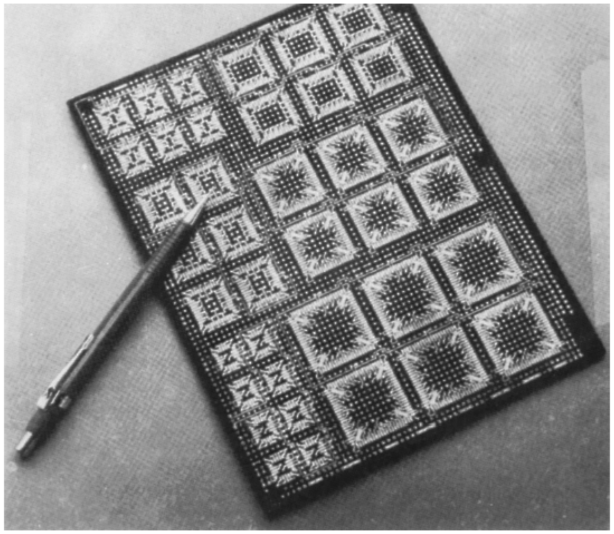
Functional classification of materials.
Note that metals, plastics, and ceramics occur in different categories.
A limited number of examples in each category is provided

Structural Materials sometimes also considered functional materials

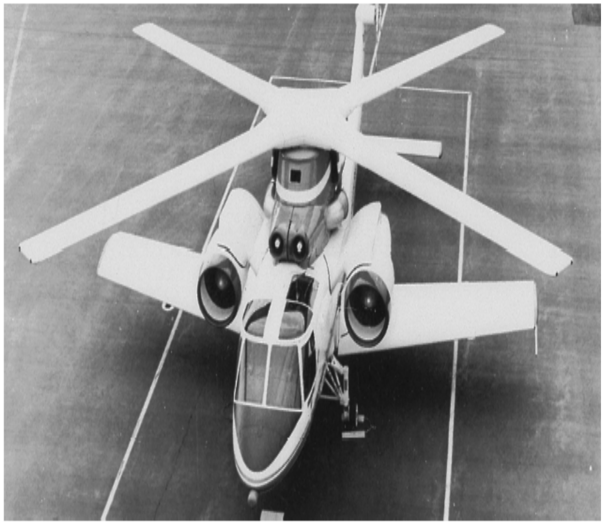
PZT: lead zirconate titanate ($PbZr0_3$, $PbTi_{0.48}$ $Zr_{0.52}0_3$
superalloy: heat resisting alloy
ITO: a layer structure under development in semiconductor industry,
ITO a transparent conductor
YAG: Y-Al-Garnet: a crystal used for lasers
shape memory alloy, remembers its original form after deformation followed up by heat treatment



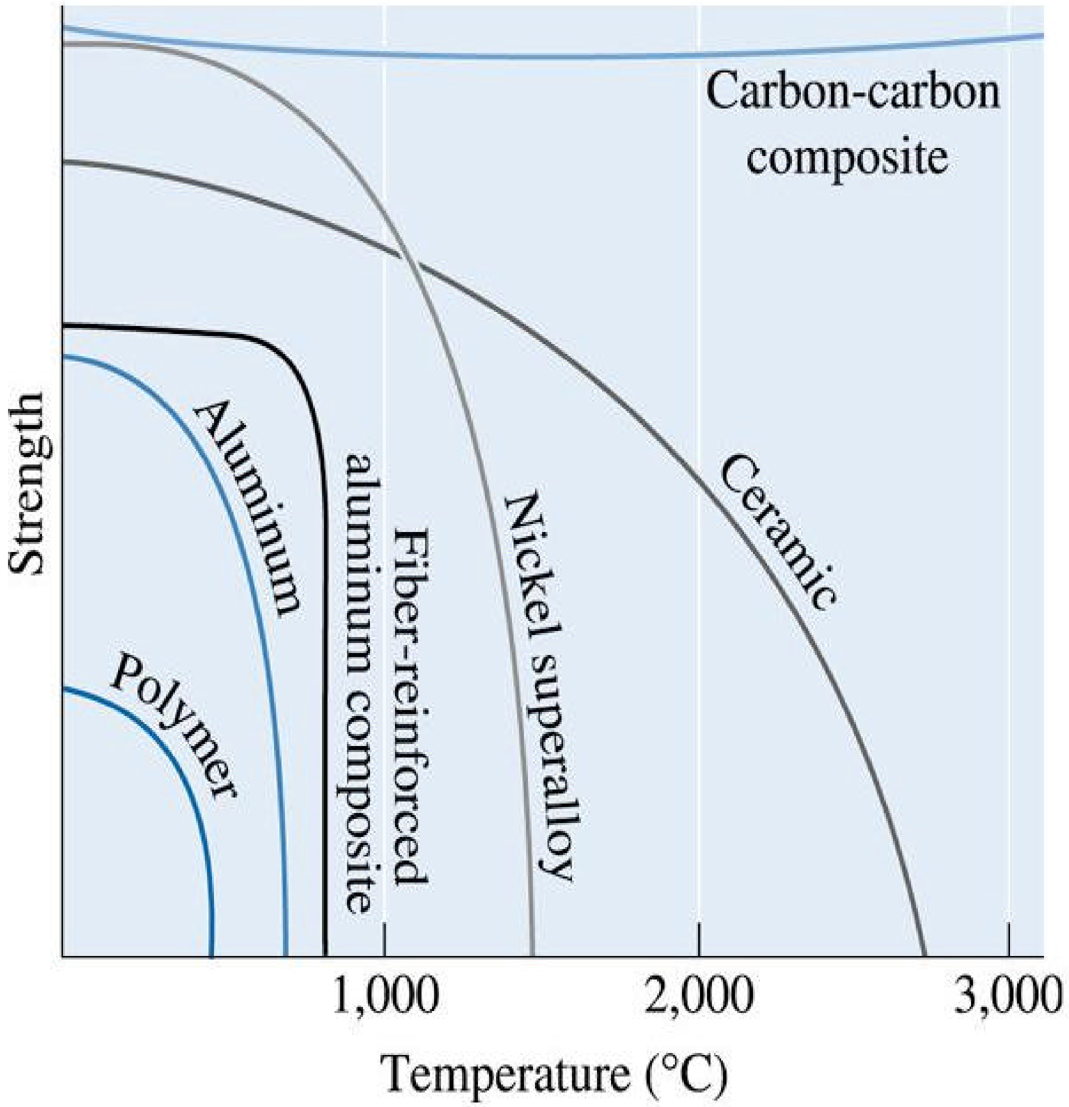
Polymers are used in a variety of electronic devices, including these computer dip switches, where moisture resistance and low conductivity are required.



Integrated circuits for computers and other electronic devices rely on the unique electrical behavior of semiconducting materials.



The X-wing for advanced helicopters relies on a material composed of a carbon-fiber-reinforced polymer.



Usage of Materials depend on environmental constraints, e.g.

increasing temperature normally reduces the strength of a material. Polymers are suitable only at low temperatures. Some composites, special alloys, and ceramics, have excellent properties at high temperatures

As Hooke ~ 1650 already noticed, physical properties are typically anisotrope, i.e. have different values in different lattice or macroscopic directions

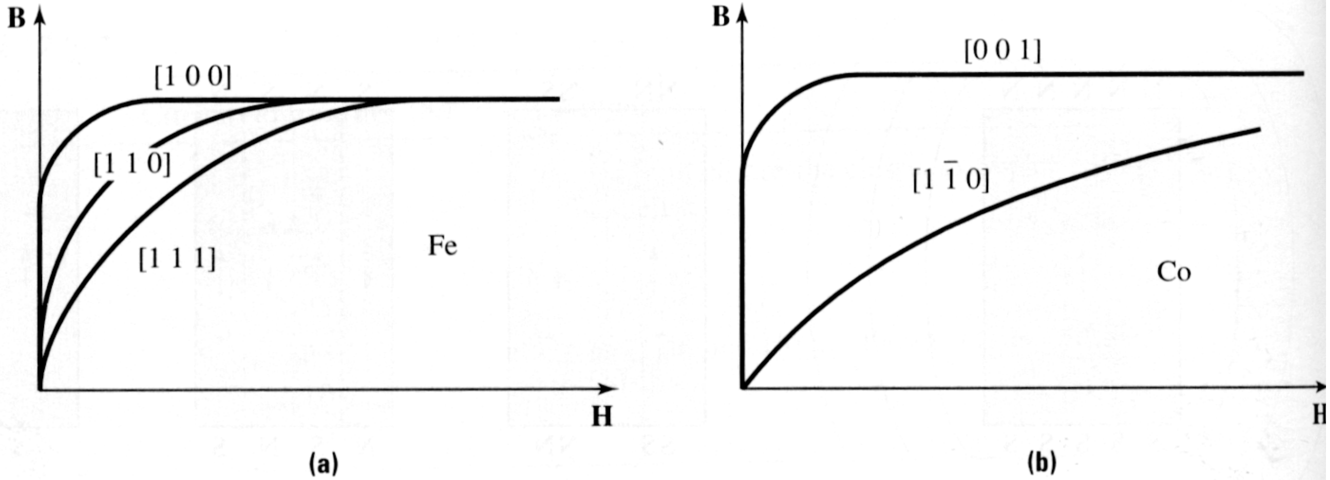
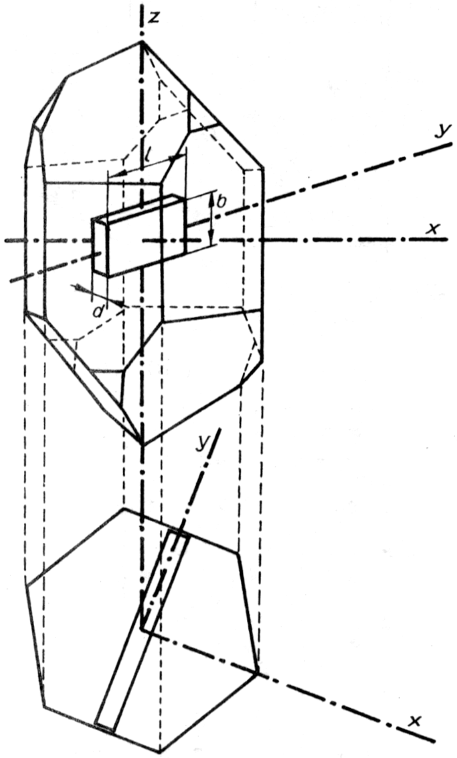


FIGURE 12.6–3 The soft magnetization directions for two of the common ferromagnetic elements: **(a)** Fe and **(b)** Co. (*Source: L. L. Hench and J. K. West,* Principles of Electronic Ceramics, *Copyright © 1990 by John Wiley & Sons. Reprinted by permission of John Wiley & Sons, Inc.*)



this anisotropy is especially strong if the structure is highly anisotrope, e.g. in polymers, or single crystals of low symmetry, going back to Crystal Physics: certain effects can only exist in crystals of low symmetry

Nanostructured materials – the next really big thing

1953 **Lifshitz and Kosevich,** predict quantum size effects in dimension reduced semiconductor entities, quantum wells, wires, and dots

1959, ***Richard P. Feynman's*** *vision "There is plenty of room at the bottom":*

"Up to now, we have been content to dig in the ground to find minerals. We heat them and we do things on a large scale with them. And we hope to get a pure substance with just so much impurity, and so on.

But we must always accept some atomic arrangement that nature gives us. We haven't got anything, say with a "checkerboard arrangements, with the impurity atoms exactly arranged 1,000 angstroms apart, on in some other particular pattern.

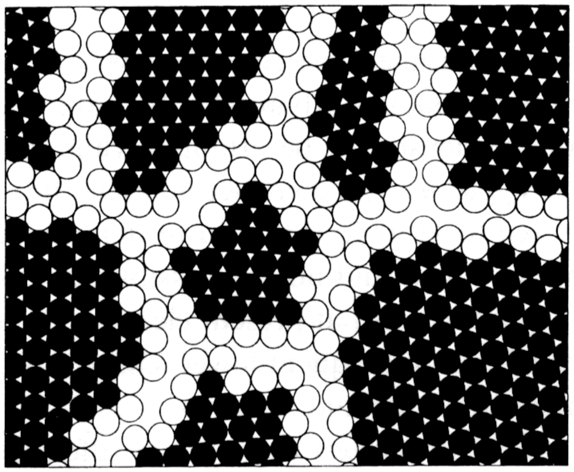
I can hardly doubt that when we have some control of the arrangements of things on a small scale, we will get an enormously greater range of possible properties that substances can have.”

so that is what it is all about novel physical properties for applications,

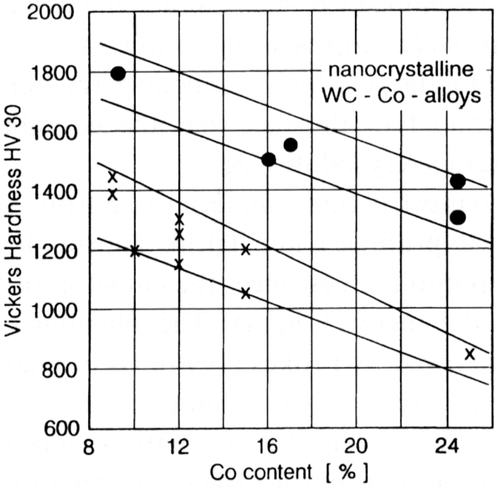
in short: if mesoscopic structures are in the nm range, materials have very different properties,

e.g. small specs of matter (< 100 nm) have a different melting point than large bulks

Herbert Gleiter, 1981, polycrystalline solids of extremely small grain size, are much harder than exactly the same material when it is “microstructured” !!!



Schematic of the microstructure of a nanostructured single-phase material (after Gleiter 1996).



Hardness of WC–Co cermets with nanostructured and conventional grain sizes (after Gleiter 1996, reproduced from a report by Schlump and Willbrandt).

this is because there isn’t much opportunity for dislocation to glide anymore as a large part of the material is basically “grain boundary”

many nanostructures are not in equilibrium, but stabilized by large grain boundary/surface area to volume ratio, lots and lots of novel phases with interesting properties that only exist due to the nanometer size of the crystals

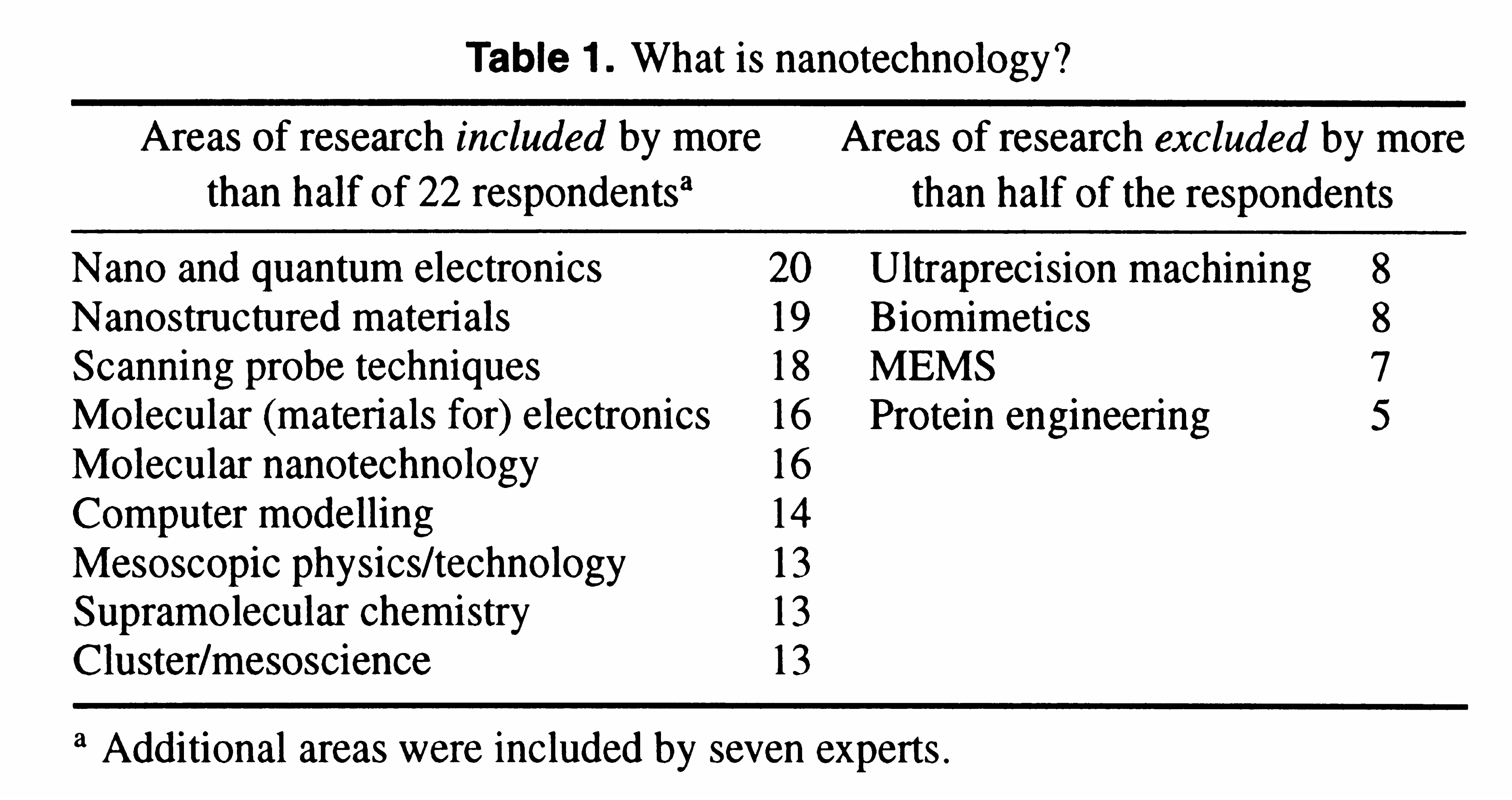


Table 1. What is nanotechnology?

Areas of research *included* by more than half of 22 respondents[a]		Areas of research *excluded* by more than half of the respondents	
Nano and quantum electronics	20	Ultraprecision machining	8
Nanostructured materials	19	Biomimetics	8
Scanning probe techniques	18	MEMS	7
Molecular (materials for) electronics	16	Protein engineering	5
Molecular nanotechnology	16		
Computer modelling	14		
Mesoscopic physics/technology	13		
Supramolecular chemistry	13		
Cluster/mesoscience	13		

[a] Additional areas were included by seven experts.

I. Malsch, *Nanotechnology* **10** (1999) 1 *"There are a variety of nanotechnologies, not just on."* ***But quantum electronics and growth and characterization of self-assembled compound semiconductor quantum dots are right at the core of it!***

Neal Lane, 1999**:** ***"If I were asked for an area of science and engineering that will most likely produce the breakthroughs of tomorrow, I would point to nanoscale science and engineering."*** Former President William J. Clinton's chief science adviser

NSF projects: **$ 1 trillion of products worldwide affected by nanotechnology, 2 million nanotechnology workers in 10 to 15 years**

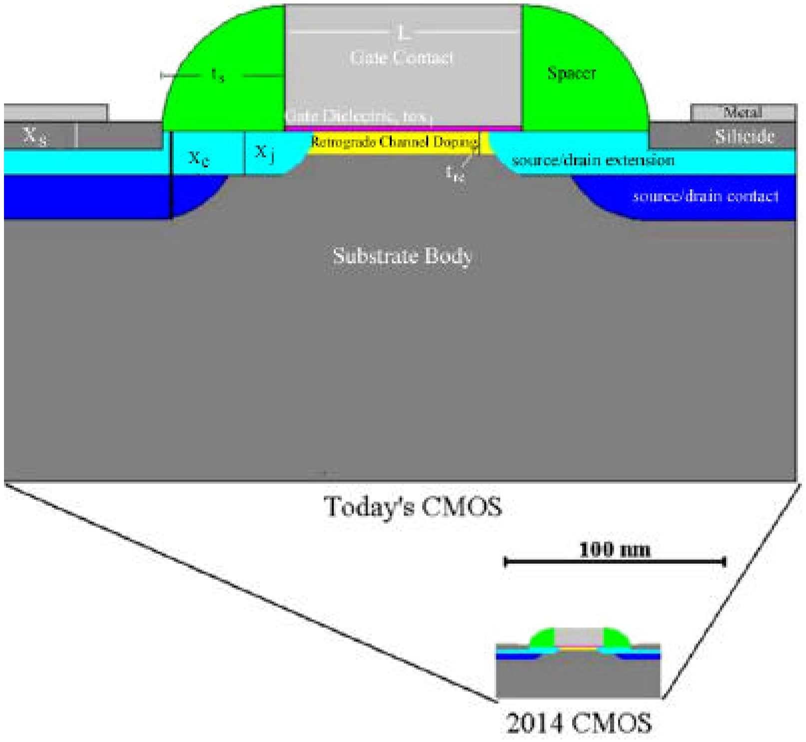
amongst many other applications, replacement for Si microelectronics, so the "Si age" might soon be over, the information age may continue

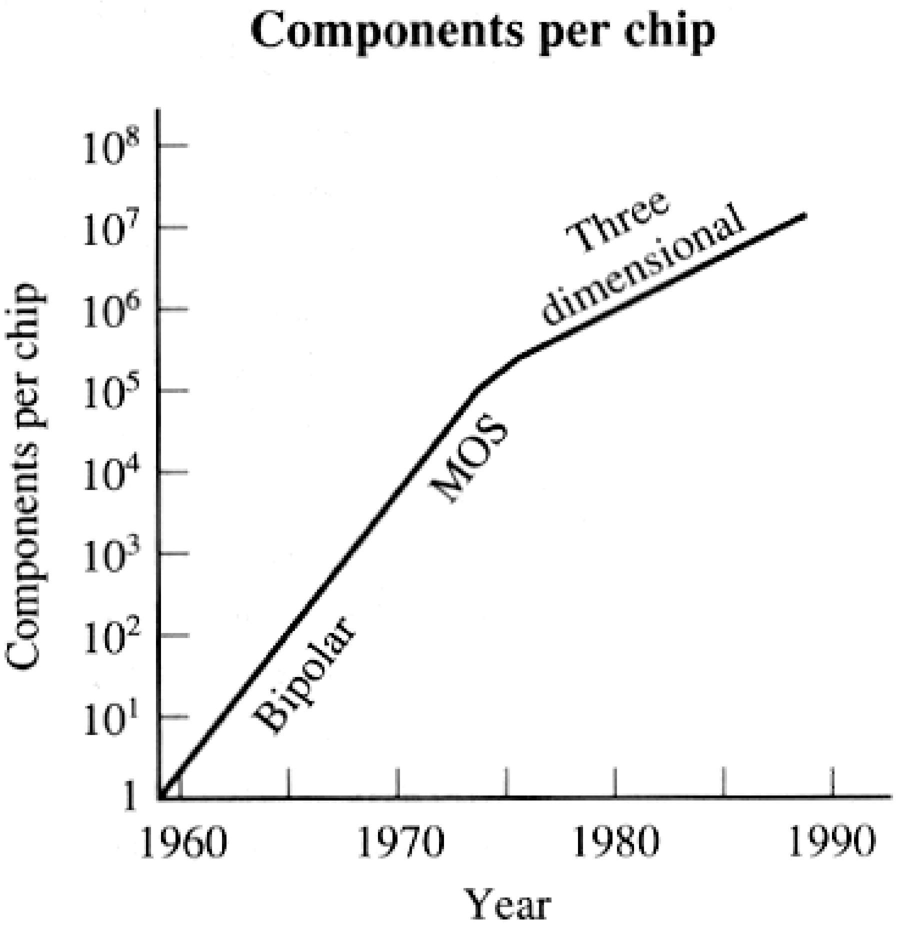
Moore's law: the number of components fabricated on a chip will double every 18 month

Gordon Moore, 1965, co-founder of Intel, philanthropist,
major ($ million +) benefactor of PSU's school of engineering

so that is an exponential "law",

extremely fast growth





prizes for new fabrics rise also exponentially

currently it is projected that at below about 35 nm structure size the CMOS technology will no longer work, due to quantum mechanical effects

in 2007, we should be at a structure size of 65 nm, this shall still be applicable, 2014 the design below will be completely obsolete

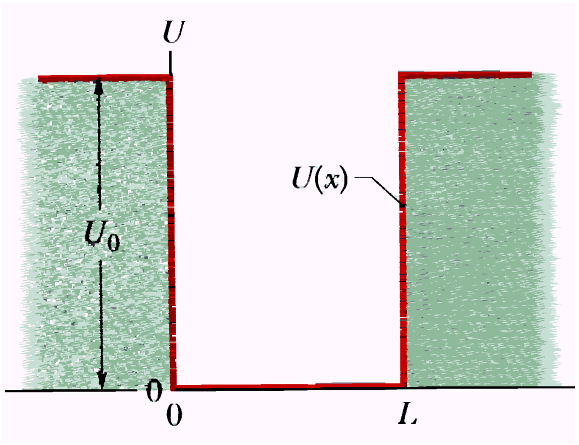
Dimension	**2002 (nm)**	**2014 (nm)**
Gate length (L)	120 (<20%)	22(<20%)
Equivalent gate dielectric thickness (t_{ox})	1.9-1.5 (<4%)	0.5-0.6 (<4%) (equivalent oxide-actual thickness greater)
Sidewall spacer length (t_s)	72-144 (<10%)	3.7-7.5 (<10%)
Silicide thickness (X_s)	55	12
Contact depth (X_c)	75-145	15-35
Drain extension depth (X_j)	42-70	8-13
Retrograde channel depth (t_{rc})	21-35	4-8

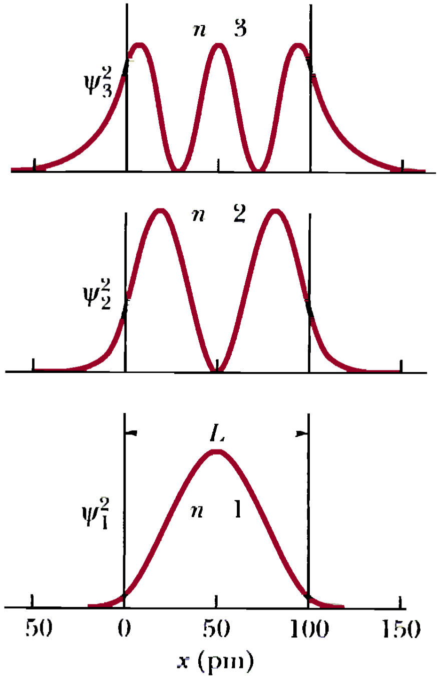
Self-assembled semiconductor quantum dots: *what are they*?

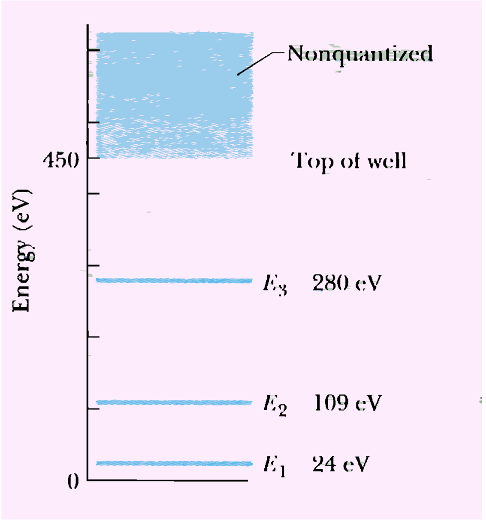
Traps for matter waves, artificial pseudo-atoms, entities with discrete energy levels

one-dimensional, time independent Schrödinger’s equation

$$\frac{d^2y}{dx^2} = -\frac{8 \cdot m \cdot p^2}{h^2}[E - U(x)] \cdot y$$





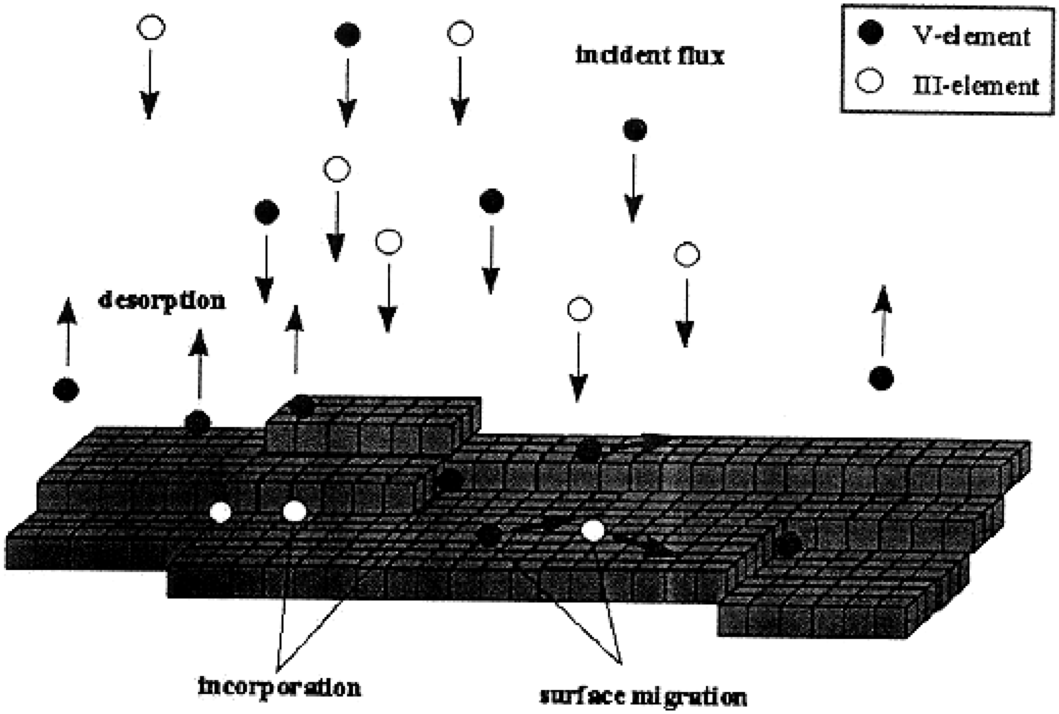


Electron in real atom: U_0 ˜ 10 eV, L = 0.1 nm

Exciton in semiconductor quantum dot: ? E ~ 0.1 eV, L ~ 10 nm

D. Halliday et al., *Fundamentals of Physics*, John Wiley & Sons Inc., 2001, p. 988-999

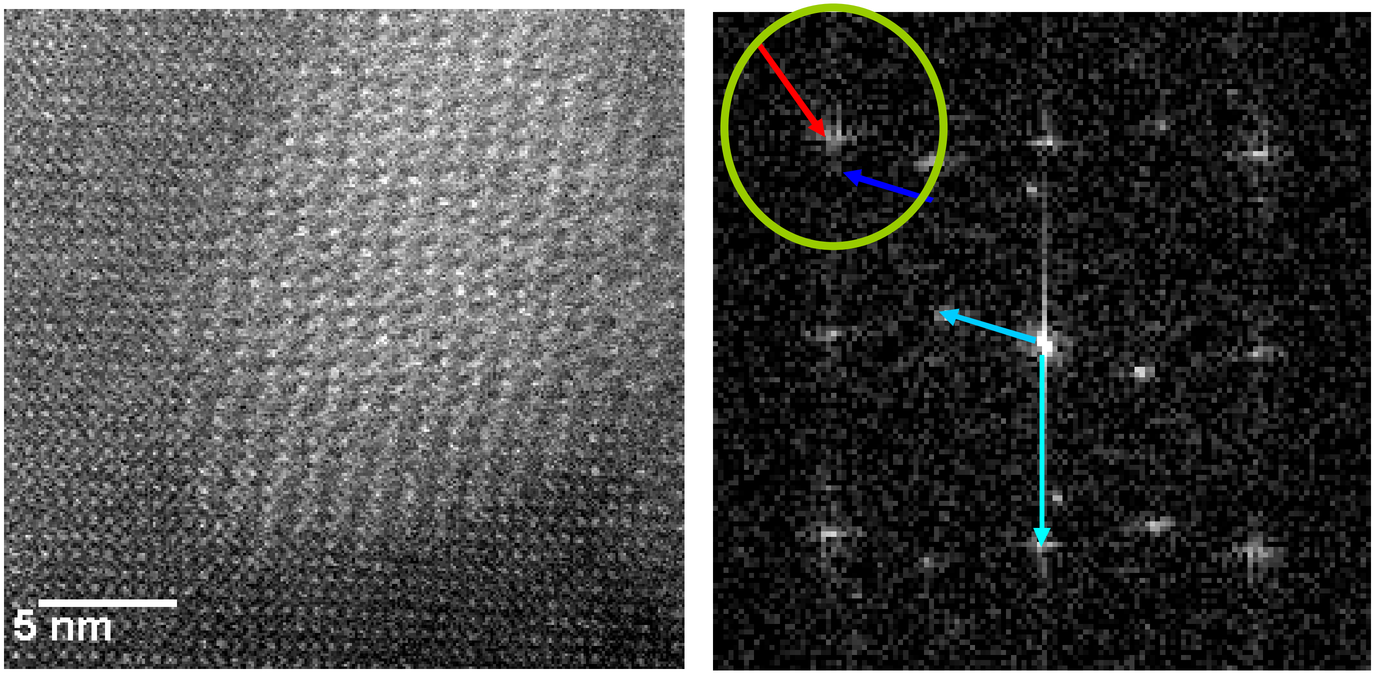
How are quantum dots made? Molecular beam epitaxy



deposition, surface diffusion, interdiffusion are random events, smaller bandgap semiconductor (alloy) usually larger lattice constant, *(one way of self-assembly, resulting in "cake with raisins")*

***KEY ISSUE*: uniformities of size, shape, chemical composition, strain distribution, crystallographic phase, mutual alignment, …**

Dogma until (2001): epitaxially grown quantum dots always compressively strained and possess random distribution of atoms in sphalerite, diamond, halite alloys



***Atomically ordered* In(Sb,As) quantum dot in InAs**

left: atomic resolution Z-contrast image, [001] plan view; ***right***: Power Spectrum (Fourier transform) showing superlattice spots of projected superlattice cell 3 times larger, than matrix cell, ~ 1.3 nm anion order, **(110)$_{\mathbf{matrix}}$** ¦ **(210)$_{\mathbf{quantum\ dot}}$**

2001 we began creating "checkerboard" arrangements (and other particular patterns) with periodicities of ˜ 10 angstroms, <u>beating Feynman's vision by a factor of ˜ 100!</u>

so all that is materials science:

How are we going to proceed from here? ***As foundation is structure on all levels***

atomic scale structure, **ideal crystal** structures, **real crystal** structures, i.e. point, line, area and volume defects and how they move, diffusion and dislocation slip and how this influences the mechanical and other properties

diffraction and other **methods to analyze structures** at all levels

and how structures cause/determine/modify mechanical, electrical, optical & dielectric, magnetic, and thermal properties of materials

laboratory visits: SEM, TEM, FIB *(hands-on, just to get a feel for how it is done), course assignment: answer puzzlers 1 – 7 and a few more questions from* http://www.umsl.edu/~fraundor/nanowrld/dtemspec.html