Conceitos e Principios dos Materiais

ma·te·ri·al [muh-teer-ee-uhl]
noun

1. The substance or substances of which a thing is made or composed: *Stone is a durable material.*

2. Anything that serves as crude or raw matter to be used or developed: *Wood pulp is the raw material from which paper is made.*

3. Any constituent element.

4. A textile fabric: *Material for a dress*

5. A group of ideas, facts, data, etc., that may provide the basis for or be incorporated into some integrated work:*To write material for a comedy show*.

A Material Girl

- Focus on Materials as in “Making Stuff”
-
- UK Center for Materials Education: “It has recently proved extremely difficult for the members of the Materials Benchmarking panel to agree on a definition of Materials for the Benchmarking statement …”
- What is a material according to one Materials Scientist?

  (Prof. Adrian Sutton, Oxford U.)

- “… All matter is potentially 'a material'. Whether we decide to call something a material depends on whether its structural, mechanical, electrical, magnetic or optical properties enable us to understand an existing role, or to suggest a new role, in some phenomenon or process. These are often called 'engineering' properties of materials, but the function they enable may be in biology or geology as well as traditional engineering...”

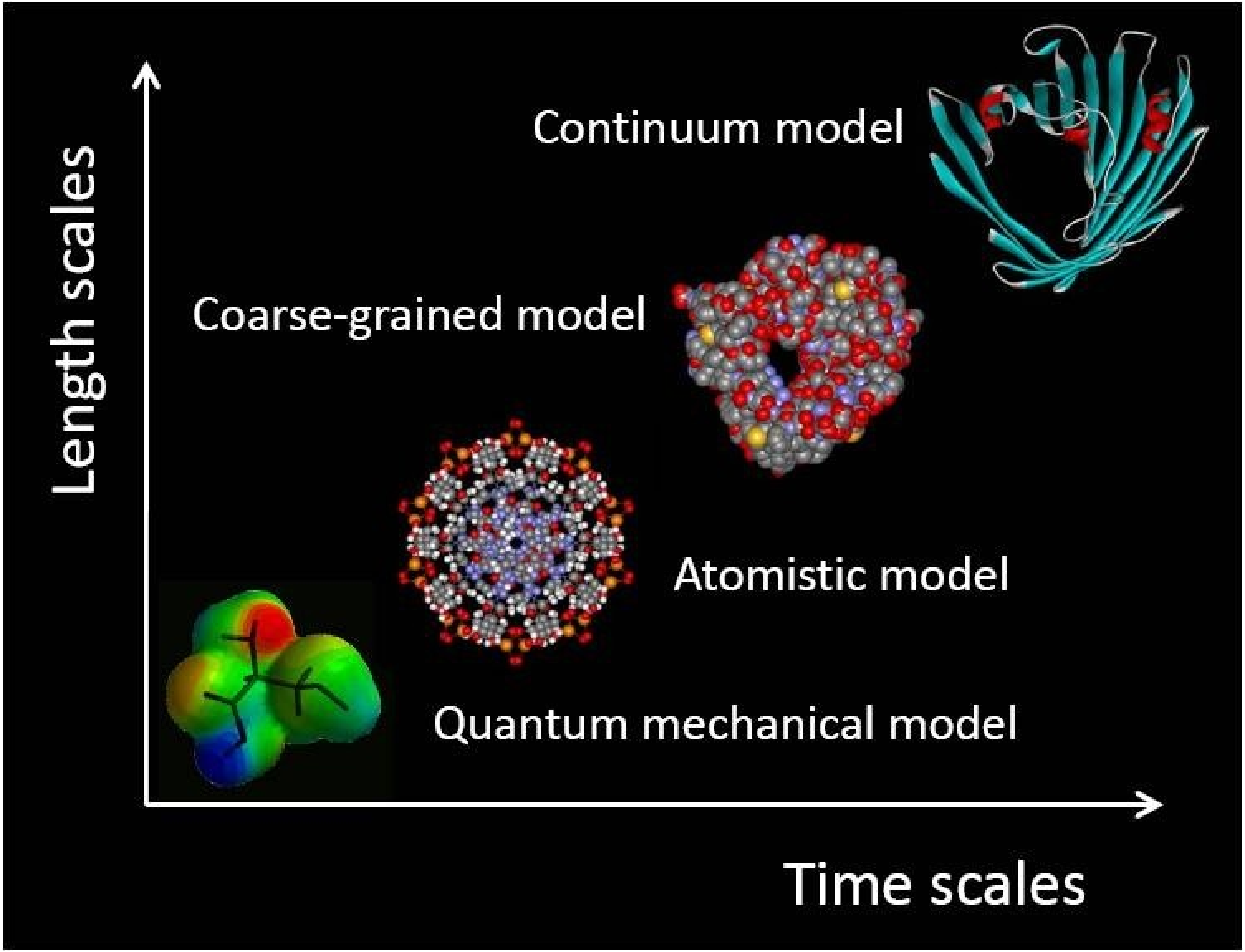
- So what is materials science?
- Perhaps the simplest way to answer this question is to look at what materials scientists do.
- First, they determine the structure of materials.
- Second, they measure properties of materials.
- Third, they devise ways of processing materials, i.e. creating materials, transforming existing materials, and making useful things out of them.
- Fourth, they think about how a material is suited to the purpose it serves already, and how it may be enhanced to give better performance for particular applications.

One way of classifying materials is:

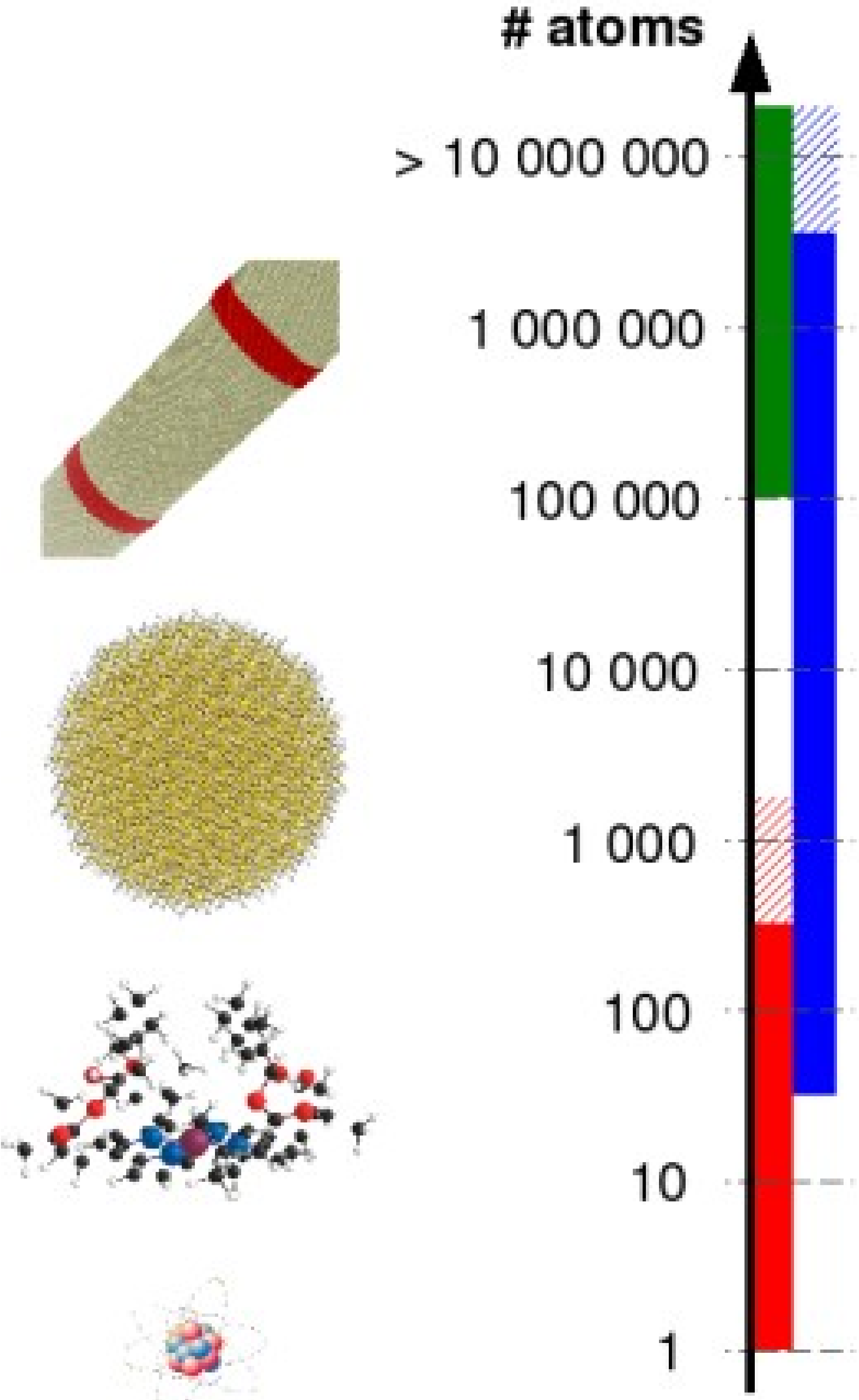
- Biomaterials
- Carbon
- Ceramics
- Composites
- Glass
- Metals
-

- Nanomaterials
- Polymers
- Refractory
- Semiconductors
- Thin Films
- Functionally Graded Materials

It is generally understood that multiscale modeling and simulation is required for understanding a complex system. That surely applies to all materials.



Multi-scale modeling



Continuous medium approximations

Examples : Classical elasticity, effective mass

Atomistic « semi-empirical » methods

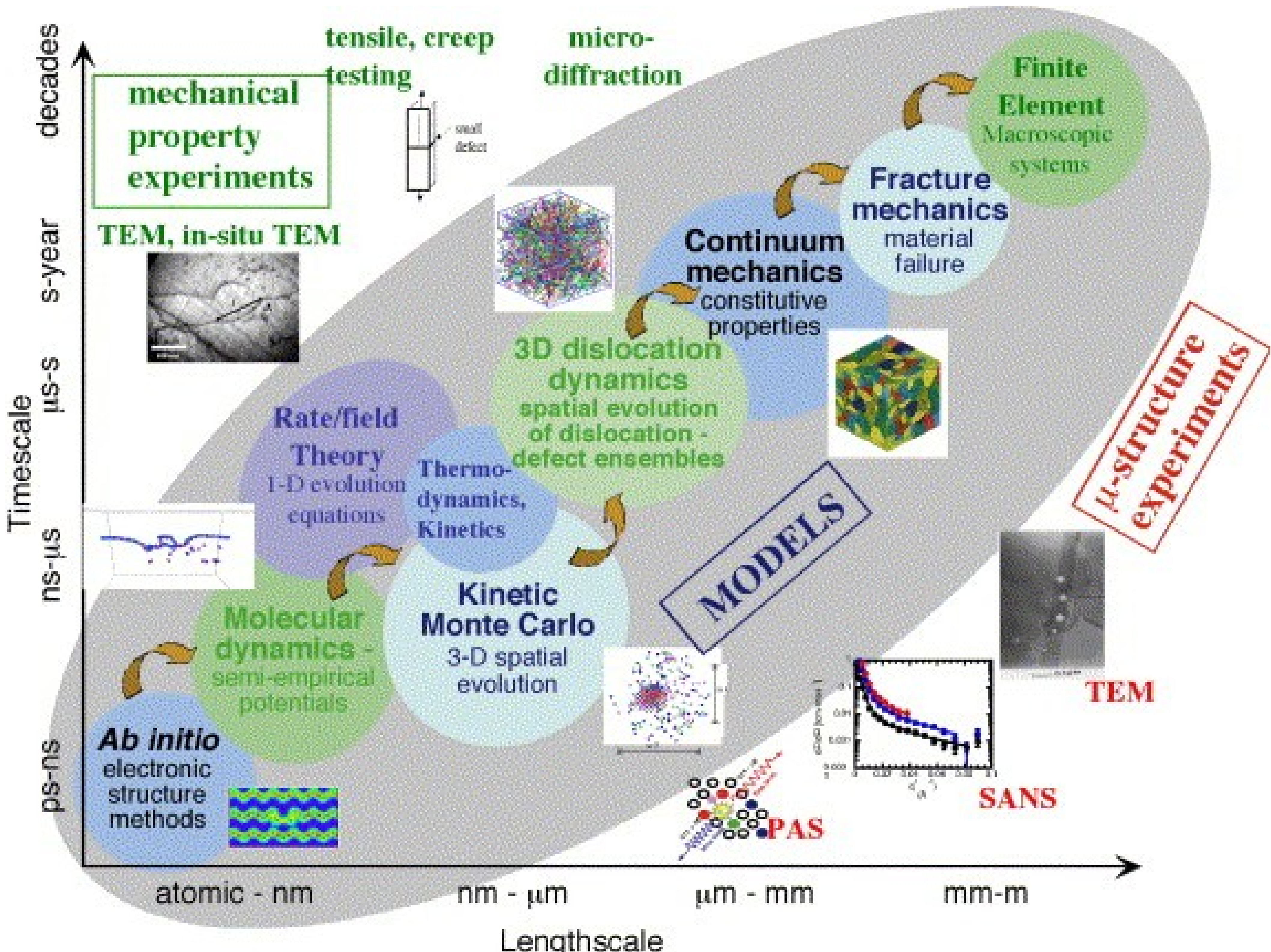
Simplified and parametrized hamiltonians
Classical or quantum mechanics

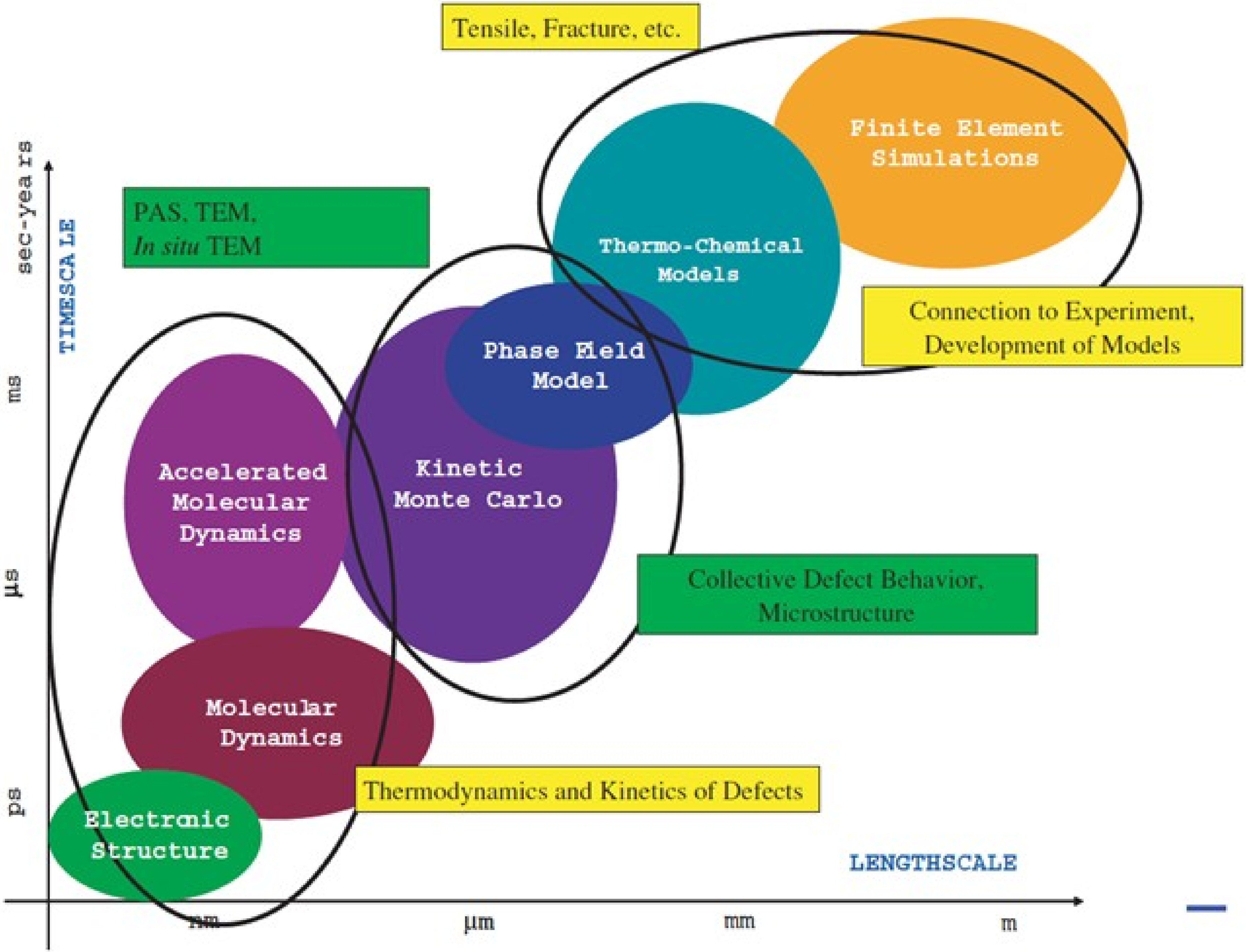
Examples : Inter-atomic potentials (structure)
Tight-binding (electronic properties)

« *Ab initio* » methods (« first principles »)

No « adjustable parameter »
(≠ « no approximations »)
Quantum mechanics

Example : Density Functional Theory (DFT).


decades
s-year
µs-s
ns-µs
ps-ns
Timescale
mechanical property experiments
tensile, creep testing
small defect
micro-diffraction
TEM, in-situ TEM
Finite Element
Macroscopic systems
Fracture mechanics
material failure
Continuum mechanics
constitutive properties
3D dislocation dynamics
spatial evolution of dislocation - defect ensembles
Rate/field Theory
1-D evolution equations
Thermo-dynamics, Kinetics
Kinetic Monte Carlo
3-D spatial evolution
Molecular dynamics -
semi-empirical potentials
Ab initio
electronic structure methods
MODELS
µ-structure experiments
TEM
SANS
PAS
atomic - nm
nm - µm
µm - mm
mm-m
Lengthscale


Tensile, Fracture, etc.
Finite Element Simulations
Thermo-Chemical Models
Connection to Experiment, Development of Models
PAS, TEM, *In situ* TEM
Phase Field Model
Kinetic Monte Carlo
Accelerated Molecular Dynamics
Collective Defect Behavior, Microstructure
Molecular Dynamics
Thermodynamics and Kinetics of Defects
Electronic Structure
TIMESCALE
sec-years
ms
µs
ps
LENGTHSCALE
nm
µm
mm
m

We can proceed formally, by studying the different experimental and theoretical methods used at various epochs, and scales,

Or

We can proceed by looking at examples: Examples are more efficient and more fun.

F = m a = m dv/dt = dp/dt

$$\begin{aligned} \nabla \bullet \varepsilon \mathbf{E} &= \rho \\ \nabla \bullet \mu \mathbf{H} &= 0 \\ \nabla \times \mathbf{E} &= -\mu \frac{\partial \mathbf{H}}{\partial t} \\ \nabla \times \mathbf{H} &= \mathbf{J} + \varepsilon \frac{\partial \mathbf{E}}{\partial t} \end{aligned}$$

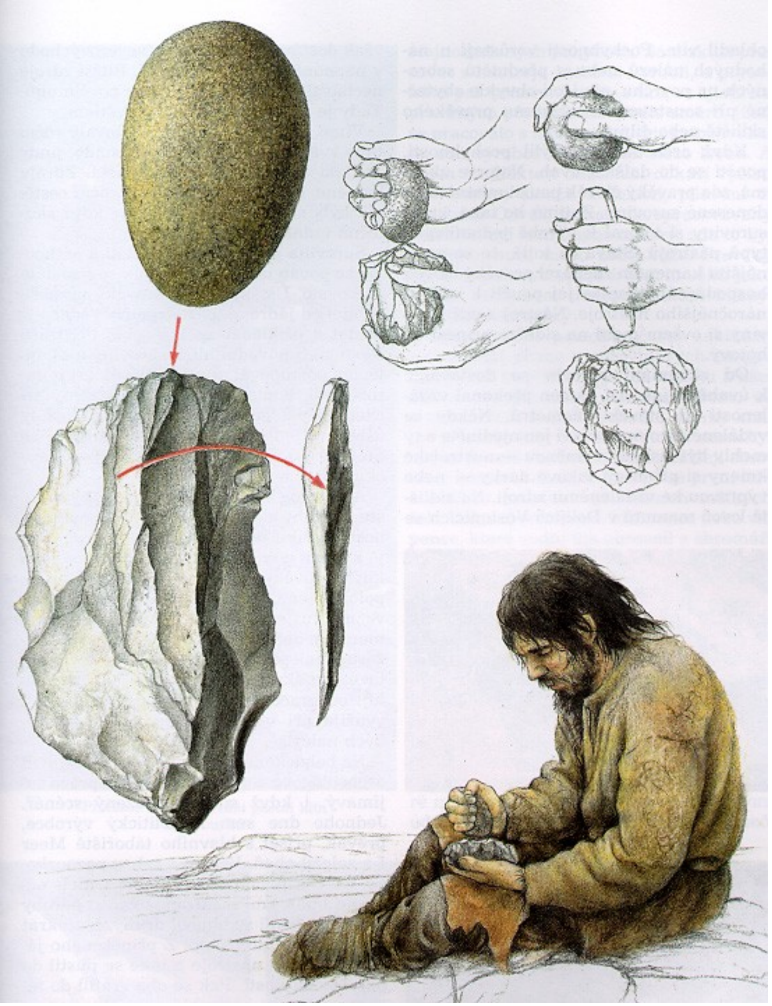
$$H(t) \mid \psi(t)\rangle = i\hbar \frac{d}{dt} \mid \psi(t)\rangle$$

Newton, Maxwell and Schrödinger, that's enough!

The Stone Age: Aww, it's just a rock...

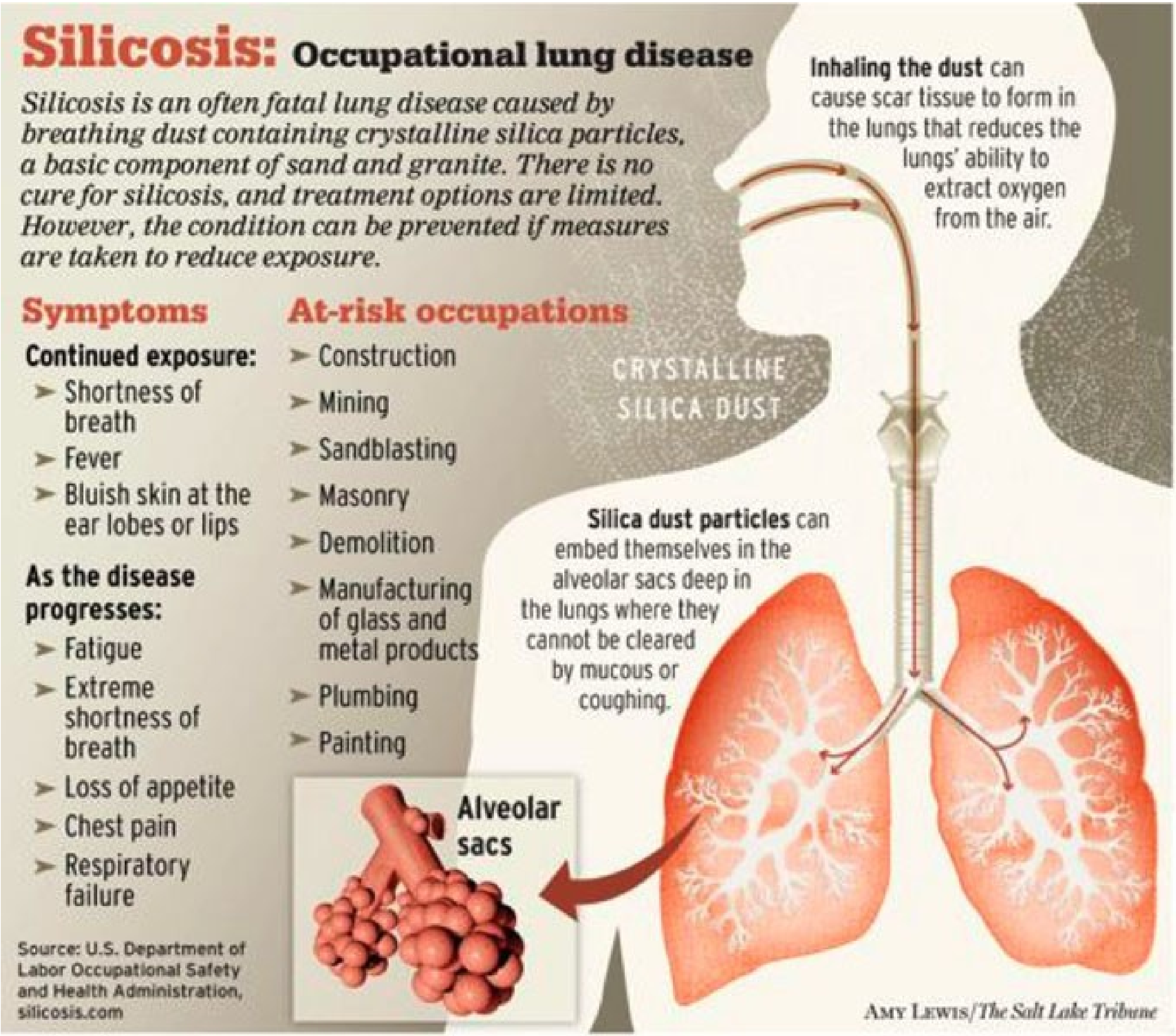
Owww, that's sharp!!

The earliest flintknapped stone tools were simple flakes from Olduvai Gorge in Tanzania, Africa. The sharp edges could have been used for cutting into the hides of animals. A flake tool measuring 33mm long dates to somewhere between 1.5 and 2 million years ago.



Manual mechanical processing of flint and other stones changed little from prehistoric times to the 19th century- producing skin scrapers, knives, projectile points, gunflints,...

slomo_flintknapper



Silicosis: Occupational lung disease

Silicosis is an often fatal lung disease caused by breathing dust containing crystalline silica particles, a basic component of sand and granite. There is no cure for silicosis, and treatment options are limited. However, the condition can be prevented if measures are taken to reduce exposure.

Symptoms

Continued exposure:

- Shortness of breath
- Fever
- Bluish skin at the ear lobes or lips

As the disease progresses:

- Fatigue
- Extreme shortness of breath
- Loss of appetite
- Chest pain
- Respiratory failure

At-risk occupations

- Construction
- Mining
- Sandblasting
- Masonry
- Demolition
- Manufacturing of glass and metal products
- Plumbing
- Painting

Inhaling the dust can cause scar tissue to form in the lungs that reduces the lungs' ability to extract oxygen from the air.

Silica dust particles can embed themselves in the alveolar sacs deep in the lungs where they cannot be cleared by mucous or coughing.

Source: U.S. Department of Labor Occupational Safety and Health Administration, silicosis.com

Amy Lewis/*The Salt Lake Tribune*

Flintknappers tended to die young, as a result of silicosis. One of the earliest occupational diseases.

Left: Fragment of 20k-yr old cooking/fermentation pot from Hunan, China

Right:Reconstruction of 16-18k-yr old pot from same site.

So fired pottery was invented in the hunter-gathering epoch, prior to the agricultural revolution.. a big surprise!

Kaolinite is a clay mineral, part of the group of industrial minerals, with the chemical composition $Al_2Si_2O_5(OH)_4$. It is a layered silicate mineral, with one tetrahedral sheet linked through oxygen atoms to one octahedral sheet of alumina octahedra. Rocks that are rich in kaolinite are known as kaolin or china clay.

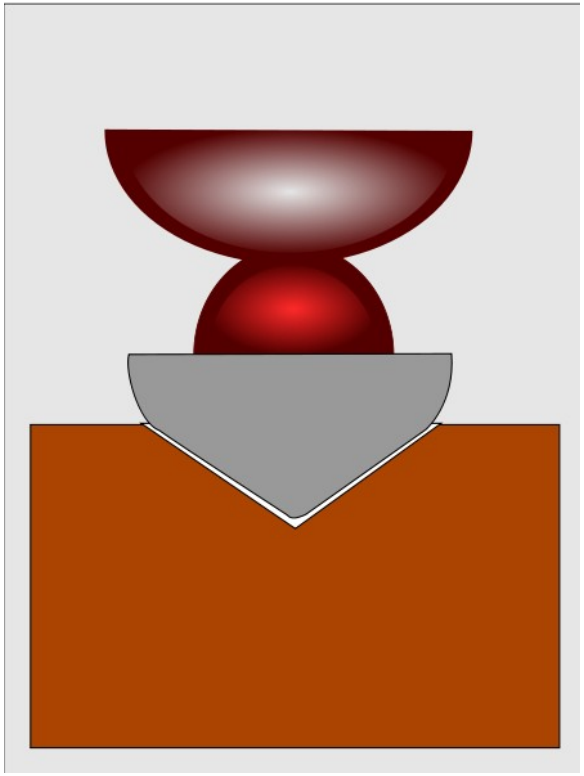
The name is derived from Kao-ling (Chinese: 高岭 / 高嶺 ; pinyin: Gaoling), a village near Jingdezhen, Jiangxi province, China. The name entered English in 1727 from the French version of the word: "kaolin", following Francois Xavier d'Entrecolles's reports from Jingdezhen.

To make a pot, you must first find a suitable material:

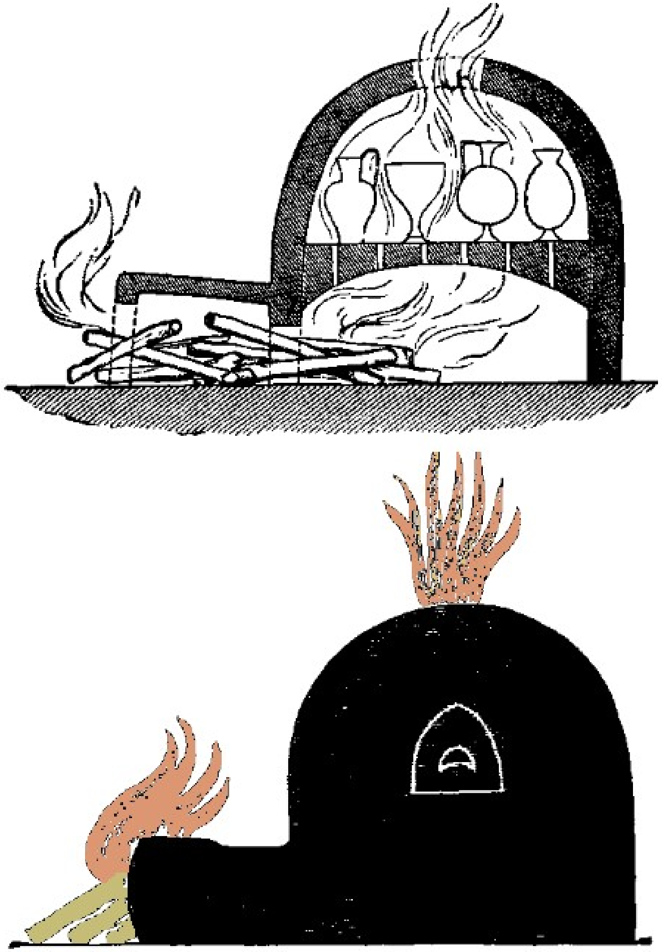
With a good moist clay you can make pot by paddling, by roping, and pretty soon by turning on a wheel. Mechanical processing techniques and control of plasticity are developed!

Paddling

Roping



Turntable set into ground



Now **thermal processing** is discovered, and progresses from open fires to the updraft kiln. Fired pottery is not only more fracture resistant, it can be really beautiful. A new decorative art is born!

Olla with linked serrated scrolls on a field of fine-line hatching, A.D. 1100-1250. West-central New Mexico, Anasazi; Tularosa Black-on-white. 38.1 x 39.4 cm (15 x 15 1/2 inches).

The swirling, dynamic appearance of the rim of this deep bowl is one of the most recognizable characteristics of wares made during Japan's oldest known civilization, the Jomon. And forming a dramatic contrast to the flamboyant ornamentation along the top is the relatively simple cord-marked lower portion of the vessel.(ca. 1500 BCE)

Some basic properties of materials:
Acoustical, Atomic, Chemical, Electrical, Environmental, Magnetic, Manufacturing, Mechanical, Optical, Radiological, Thermal properties

- e.g. Mechanical: Brittle vs Ductile- The behavior of materials can be broadly classified into two categories; brittle and ductile. Steel and aluminum usually fall in the class of ductile materials. Glass and cast iron fall in the class of brittle materials. The two categories can be distinguished by comparing the stress-strain curves- or, if it breaks when you drop it, it's brittle; if it stretches when you pull it, it's ductile. More on stress-strain later.
- e.g. Melting Point: To do metallurgy, you must be able to process material at and above its melting point. On the other hand, refractory materials must be chemically and physically stable at high temperatures. More on thermal processing later.

HDPE tensile test

Stone age, copper age, bronze age, iron age, silicon age, information age??

- The Copper Age, also called the Eneolithic or the Chalcolithic Age, has been traditionally understood as a transitional period between the Neolithic and the Bronze Age, in which a gradual introduction of the metal (native copper) took place, while stone was still the main resource utilized. 3400-2300 BC- Central Europe, Europe, later in Andes.
- Metallurgy begins

Copper axes

- Stage A: Although native copper nowadays is frequently displayed in museum showcases of mineral collections, it once occurred copiously during prehistoric times. In Cyprus or Crete, collecting the mineral was once as easy as simply picking it up from the ground. In fact, native copper is no longer as easy to find in that state these days. The treatment of this native mineral was also uncomplicated through cold-hammering. This permitted the production of only a limited range of artifacts like awls, pins, or beads. In larger objects, the metal cracks when it is cold-hammered.
- Stage B: Annealing the metal on an open fire (200–300 °C is hot enough) reduces its hardness considerably and earns in malleability. This permits the confection of slightly more sophisticated objects, like bracelets, but is still a rather limited technique.
- Stage C: In the first two steps, the mineral used was native copper that does not actually need specialized technology. Probably due to the situation that native copper was increasingly difficult to find, copper ore is used in this third step. This is a very significant development. In fact, this is truly the beginning of the metallurgy, as the mineral has to be smelted to separate the copper from the gangue, requiring technology.

Native Cu, and its ore

- Copper smelting.

  Illustration of the copper production process in ancient Japan. One of the workers (at centre left) is working at the furnace while the other (lower right) is cooling the freshly smelted metallic copper in water. The process used the same principle as modern copper production. Copper ore contains a small amount of metal among a great amount of impurities. When the ore is heated above copper's melting point (1083 degrees Celsius) the copper will melt and sink below the solid impurities. It is at this point that the copper metal can be removed from the furnace.

Metallurgy and trade evolved, then the Bronze age dawned

Bronze is an alloy of copper and tin, sometimes zinc, with additional elements (e.g. P, Sb) added to increase hardness.

- The Aegean Bronze Age begins around 3200 BC when civilizations first established a far-ranging trade network. This network imported tin and charcoal to Cyprus, where copper was mined and alloyed with the tin to produce bronze. Bronze objects were then exported far and wide, and supported the trade. Isotopic analysis of the tin in some Mediterranean bronze objects indicates it came from as far away as Great Britain.
-

Apa type swords (Romania), 17th century BC

Ceremonial jewelry, Denmark 400-600BC

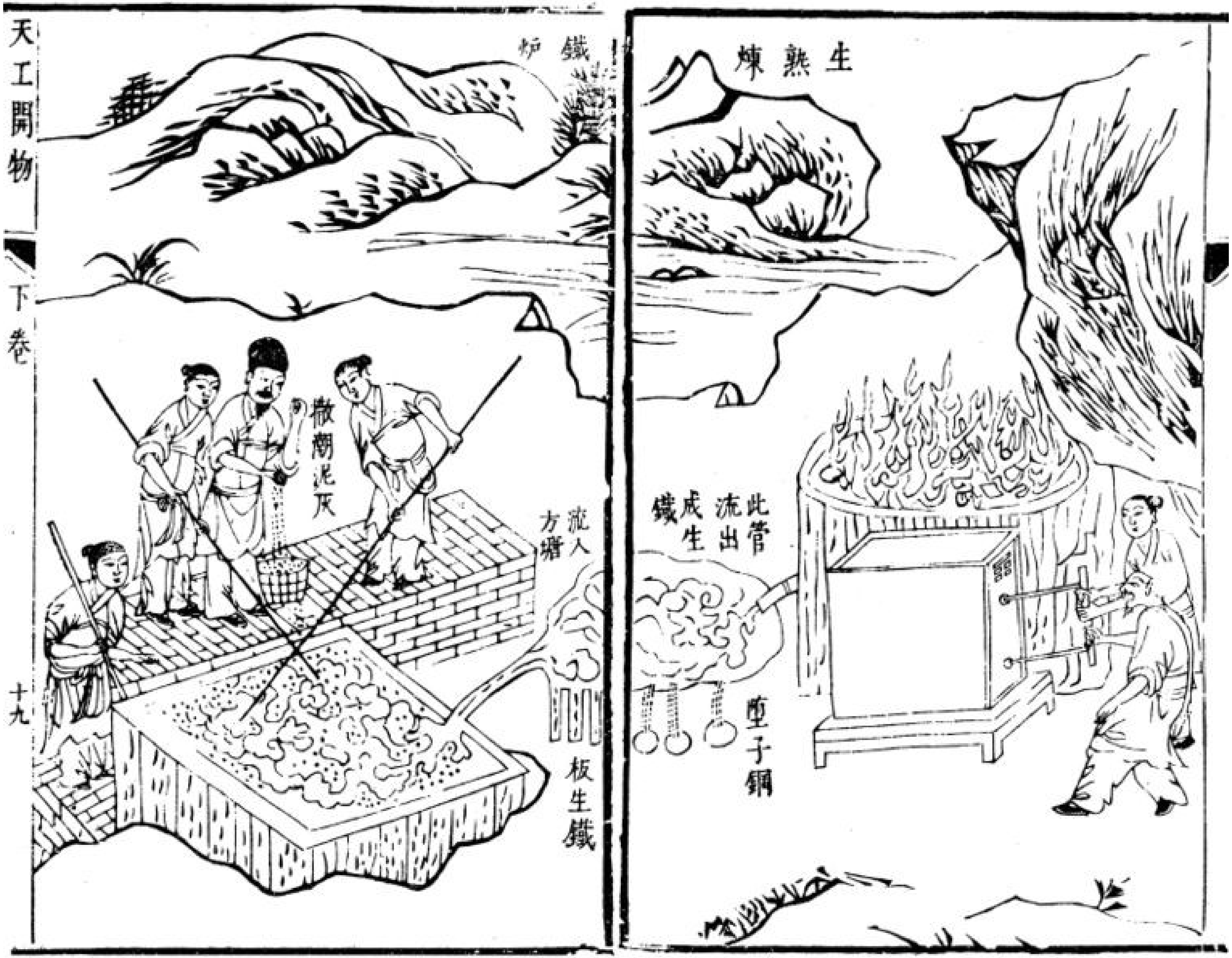
~1500BC: Iron starts to be interesting, but only gets going ~1100BC with discovery that carbon additions make a metal superior to bronze:STEEL

The next great development in metallurgy involves a metal which is the most abundant in the earth's surface but which is much more difficult to work than copper or tin. It is iron, with a melting point too high (1536C) for primitive furnaces to extract it in pure form from its ore. The best that can be achieved is a cluster of globules of iron mixed with sludgy impurities. This unpromising substance can be turned into a useful metal by repeated heating and hammering, until the impurities are literally forced out.

The development of the *bloomery*, a forced-air oven using a mixture of charcoal as fuel and reducing agent, opened the door to *wrought iron* as a useful material.

It is critical to control the carbon content to 2-4% in the product, to be malleable. Excess carbon leads to *pig iron* which is brittle and requires further processing.

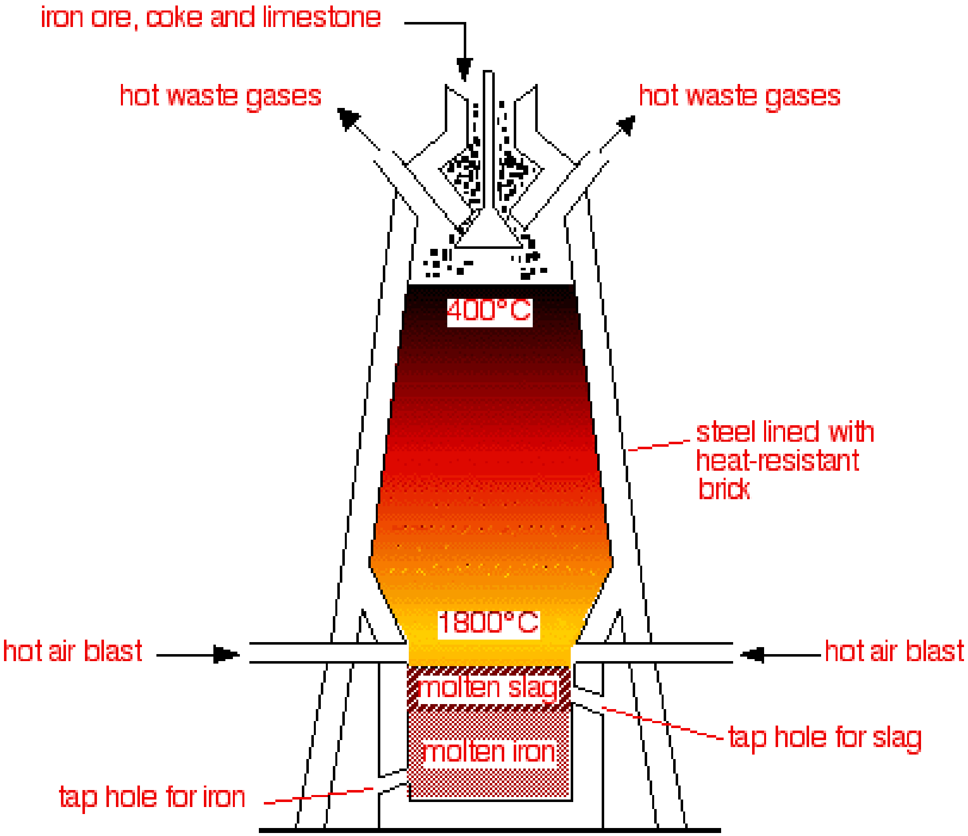
And then the blast furnace was invented....



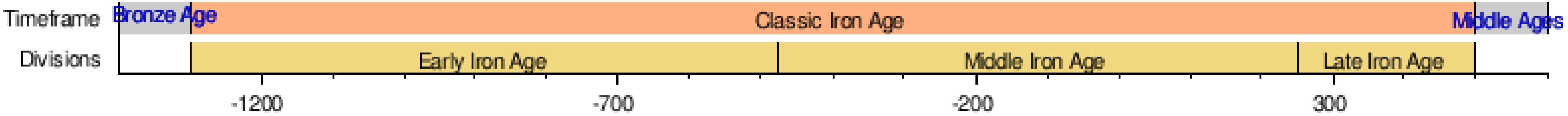
Chinese iron workers smelting iron ore to make pig iron and wrought iron. The left half of the illustration shows the puddling process, while the right half displays men operating a blast furnace. From the Tiangong Kaiwu encyclopedia printed in 1637.

Blast furnaces existed in China from about the 5th century BC and in the West from the High Middle Ages. They spread from the region around Namur in Wallonia (Belgium) in the late 15th century, being introduced to England in 1491. The fuel used in these was invariably charcoal. The successful substitution of coke for charcoal is widely attributed to Abraham Darby in 1709. The efficiency of the process was further enhanced by the practice of preheating the blast, patented by James Beaumont Neilson in 1828.

Model of first German blast furnace..
hundreds of employees, Beginning of Industrial Revolution and Age of Steel.



Schematic of modern blast furnace.



Historians consider that the Age of Iron ended ~500AD, with the beginning of the Middle Ages... What happened to materials during the following period, up to the beginning of the Industrial Revolution ~1750? The Ironbridge at Coalbrookdale in Shropshire, England, completed in 1779, was the first major structure to be constructed entirely of iron.

At 60m length, it was heavily over-designed, but still developed structural cracks very early.

....From 1850 to 1865 great advances in iron and steel processing took place. The Steel Age began about 1860. Up to this time only two types of iron were made, brittle cast iron and soft wrought iron. Steel, which is both hard and strong, was made in only small quantities and was expensive. The first major structure built entirely of steel was the cantilevered Forth Bridge in Scotland, completed in 1890.The 2.5 km Forth Railway Bridge, the world's first major steel bridge, has gigantic girder spans of 521 m. The balanced cantilever principle was adopted. The main crossing comprises tubular struts and lattice-girder ties in three double-cantilevers each connected by 105 m 'suspended' girder spans resting on the cantilever ends and secured by man-sized pins. The outside double-cantilever shoreward ends carry weights of about 1000 tonnes to counter-balance half the weight of the suspended span and live load. It is still in use today.

Firth of Forth
Rail Bridge

It didn't take long for architects to realize the potential of steel as a building framework. William Le Baron Jenney became known as the Father of the American skyscraper. Iron frame buildings have greater usable interior space, are more fire-resistant, and can be made much taller than with other materials.

Home Insurance Building, Chicago 1884

Burj Khalifa, Dubai 2009, height 830m