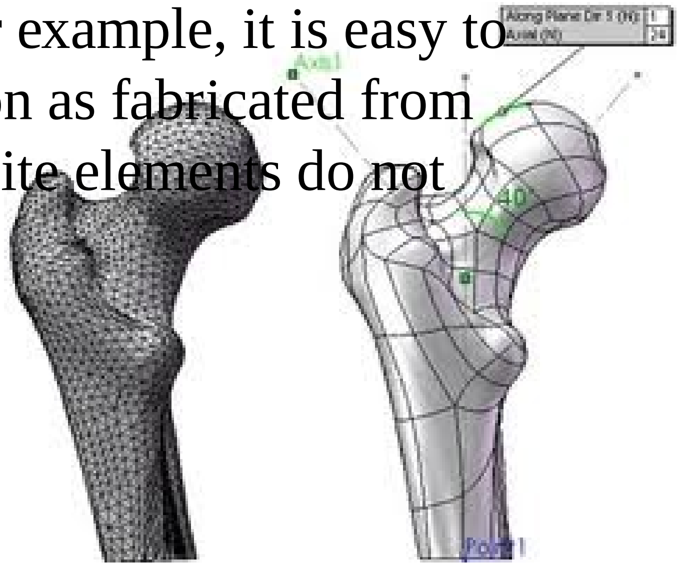
What is the Finite Element Method?

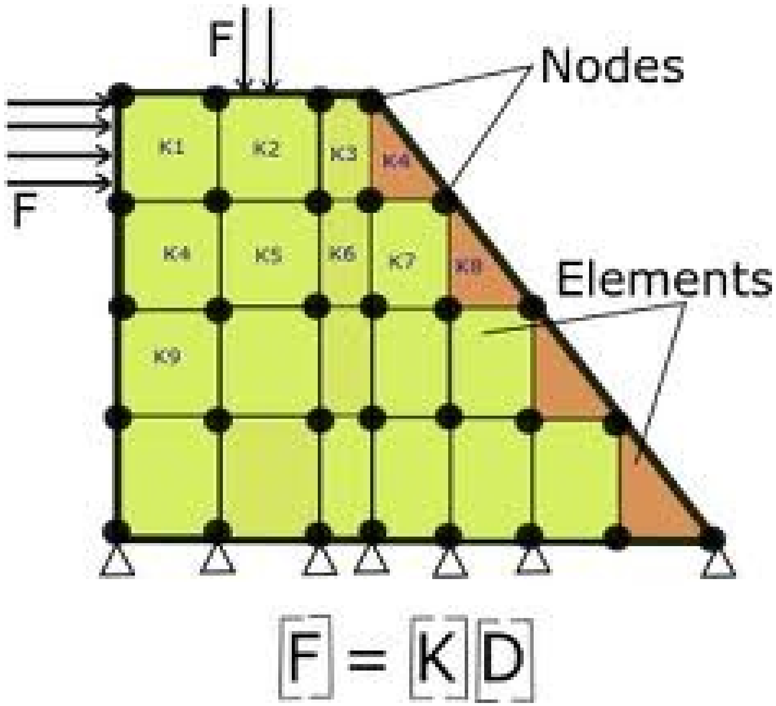
The finite element method (FEM) is the dominant discretization technique in structural mechanics. The basic concept in the physical interpretation of the FEM is the subdivision of the mathematical model into disjoint (non-overlapping) components of simple geometry called finite elements or elements for short. The response of each element is expressed in terms of a finite number of degrees of freedom characterized as the value of an unknown function, or functions, at a set of nodal points.

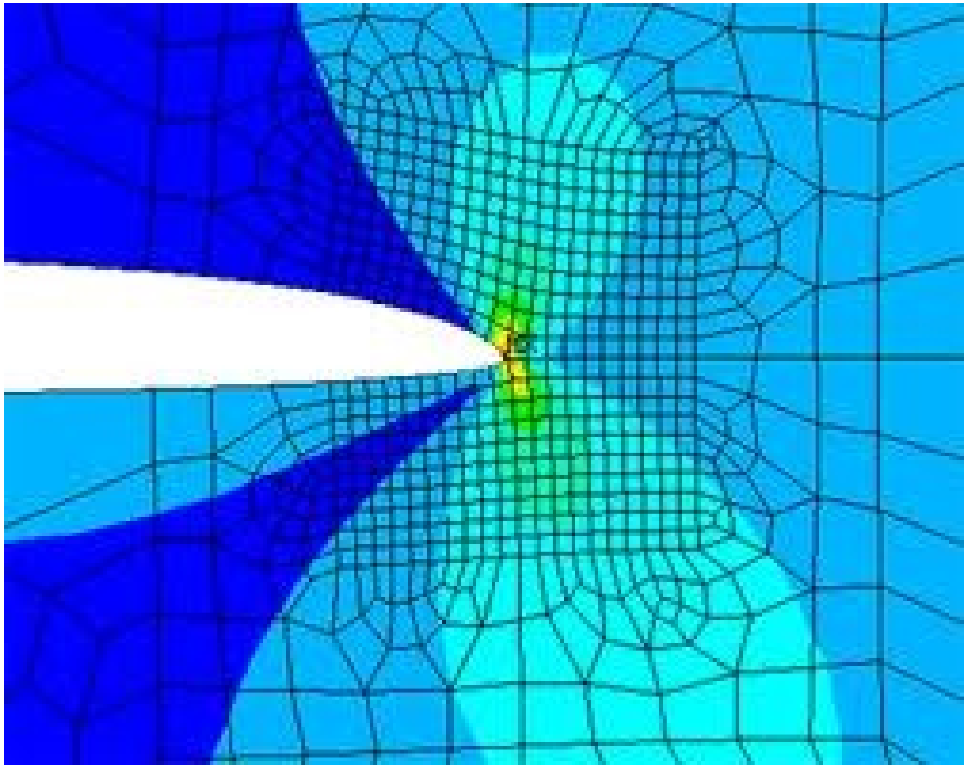
The response of the mathematical model is then considered to be approximated by that of the discrete model obtained by connecting or assembling the collection of all elements. The disconnection-assembly concept occurs naturally when examining many artificial and natural systems. For example, it is easy to visualize an engine, bridge, building, airplane, or skeleton as fabricated from simpler components. Unlike finite difference models, finite elements do not overlap in space.



FEM model of femur; coarse grid for whole body mechanics, fine grid for prosthesis design/simulation

Density and shape of elements is determined by local 'areas of interest'- e.g. high stress/rapidly varying regions

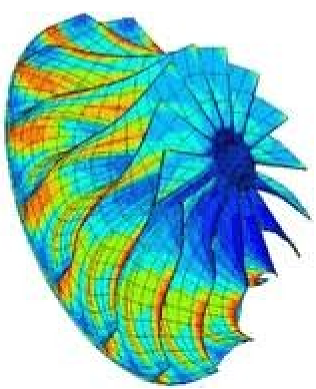




Rectangular and triangular elements in a 2D cross-section. The driving force and response are approximated in a set of linear equations, K(x,y) describing the material properties.

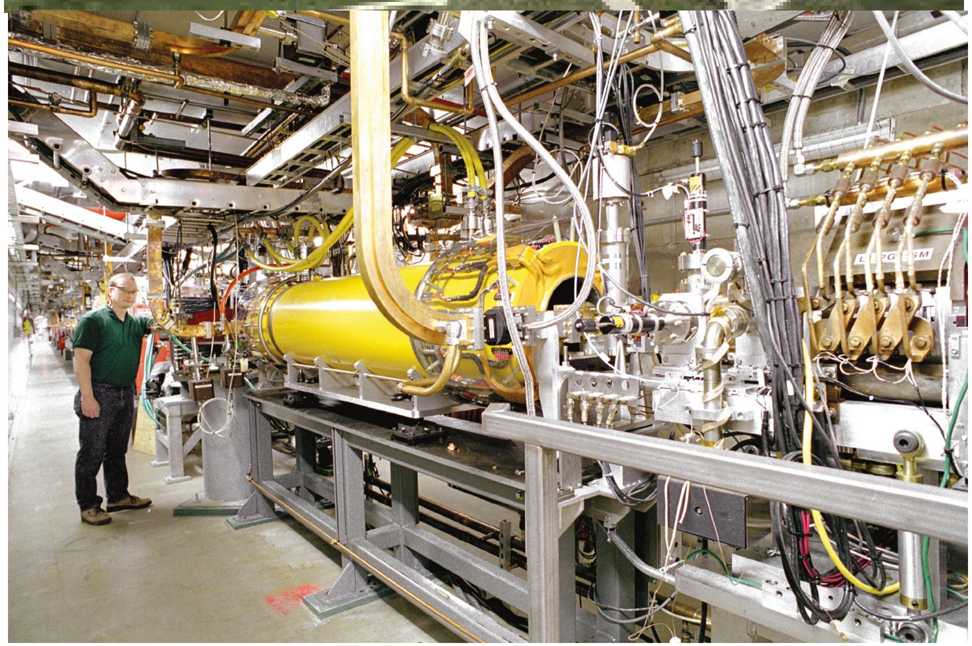
Crack-tip propagation in a solid. In a more complete model there is a MD region around the tip, and a QM region at the center of the propagating crack.

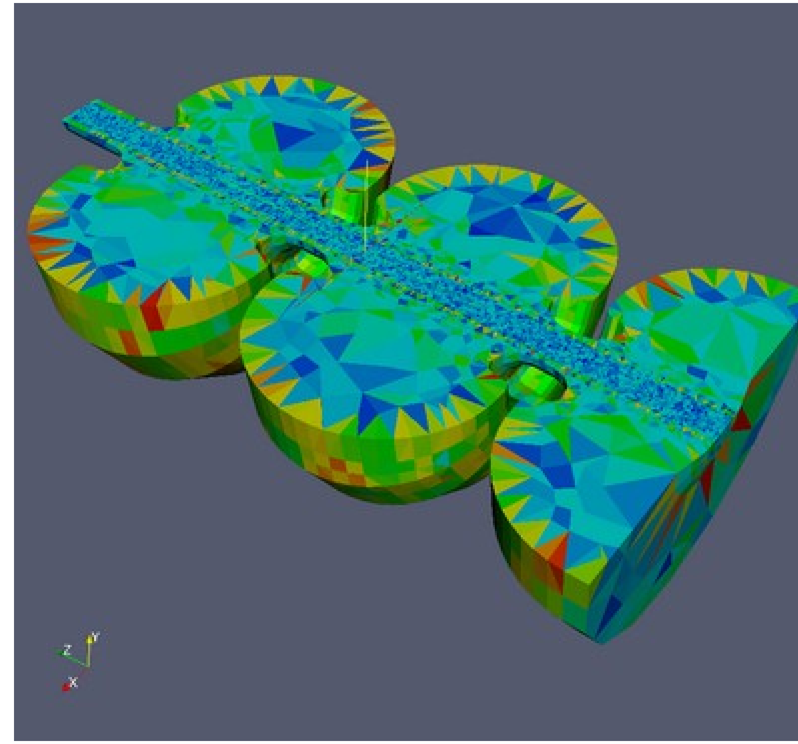
Video games rely on 'realistic' physics engines for natural-looking action



High performance compressor impeller blades have to survive 100g centrifugal stresses.

Auto- and aircraft seating and compartment designs are developed by simulation, before the expensive crash tests with dummies. Accident analysis is also carried out via FEM modeling.





Portion of FEM design for electron gun component of linear accelerator segment at Advanced Photon Source, Argonne IL

Basic Theory

The way finite element analysis obtains the temperatures, stresses, flows, or other desired unknown parameters in the finite element model is by minimizing an energy functional. An energy functional consists of all the energies associated with the particular finite element model. Based on the law of conservation of energy, the finite element energy functional must equal zero.

FEM obtains the correct solution for any finite element model by minimizing the energy functional. The minimum of the functional is found by setting the derivative of the functional with respect to the unknown grid point potential for zero.

Thus, the basic equation for finite element analysis is $\partial F / \partial p = 0$

where F is the energy functional and p is the unknown grid point potential

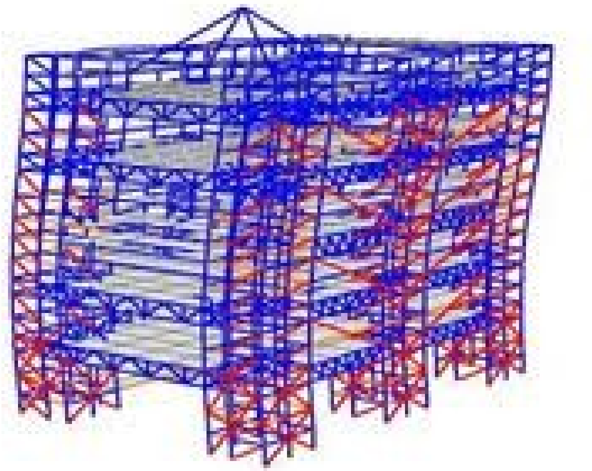
(In mechanics, the potential is displacement.) to be calculated. This is based on the principle of virtual work, which states that if a particle is under equilibrium, under a set of a system of forces, then for any displacement, the virtual work is zero. Each finite element will have its own unique energy functional.

FEM is used to design functional components, to predict their modes of failure. Optimized design can reduce material and fabrication costs **a lot.**

nastran_promo_fem

Auto manufacturers and govt. regulators use FEM to predict and analyze crash data.

two_car_crash_fem



fem_earthquake_bldj

Building construction and building retrofits are guided by FEM simulations of earthquake response.

To solve a given problem, formulate a potential energy function as an integral, then approximate the integral by a sum over elements.

As an example, in stress analysis, the governing equations for a continuous rigid body can be obtained by minimizing the total potential energy of the system. The total potential energy Π can be expressed as:

$$\Pi = 1/2 \int_{\Omega} \sigma^T \varepsilon \, dV - \int_{\Omega} d^T b \, dV - \int_{\Gamma} d^T q \, dS$$

where σ and ε are the vectors of the stress and strain components at any point, respectively, **d** is the vector of displacement at any point, **b** is the vector of body force components per unit volume, and **q** is the vector of applied surface traction components at any surface point. The volume and surface integrals are defined over the entire region of the structure Ω and that part of its boundary subject to load Γ. The first term on the right hand side of this equation represents the internal strain energy and the second and third terms are, respectively, the potential energy contributions of the body force loads and distributed surface loads. The integrands are generalized dot products of tensors and vectors.

FEM Solution Process Procedures

1. Divide structure into pieces (elements with nodes) (discretization/meshing)

2. Connect (assemble) the elements at the nodes to form an approximate system of equations for the whole structure (forming element matrices)

3. Solve the system of equations involving unknown quantities at the nodes (e.g., displacements)

4. Calculate desired quantities (e.g., strains and stresses) at selected elements

$$u(X,t) = \sum_i N_i(X)\ u_i^e(t) = \mathbf{N}\ \mathbf{u}^e$$

$$\varepsilon(X,t) = \sum_i N_{i,X}\ u_i^e(t) = \mathbf{B}_0\ \mathbf{u}^e$$

$$F(X,t) = \sum_i N_{i,X}\ x_i^e(t) = \mathbf{B}_0\ \mathbf{x}^e$$

$$\mathbf{f}_{\text{int}}^e = \int_{\Omega_0^e} \mathbf{B}_0^T P\ d\Omega_0$$

$$\mathbf{f}_{\text{ext}}^e = \int_{\Omega_0^e} \rho_0 \mathbf{N}^T b\ d\Omega_0 + \left[\mathbf{N}^T A_0 t_X^0\right]_{\Gamma_t^e}$$

$$\mathbf{M}^e = \int_{\Omega_0^e} \rho_0 \mathbf{N}^T \mathbf{N}\ d\Omega_0$$

$$\mathbf{M}\ \ddot{\mathbf{u}} = \mathbf{f}_{\text{ext}} - \mathbf{f}_{\text{int}}\ .$$

Some Areas in which FEM is successfully applied:

Application Problem	State Vector *d*	Forcing Vector *f*
Structures, Solid Mechanics	Displacement	Mechanical force
Heat Conduction	Temperature	Heat flux
Acoustic fluid	Displacement potential	Particle velocity
Potential flows	Pressure	Particle velocity
General flows	Velocity	Flux
Electrostatics	Electric potential	Charge density
Magnetostatics	Magnetic potential	Magnetic intensity

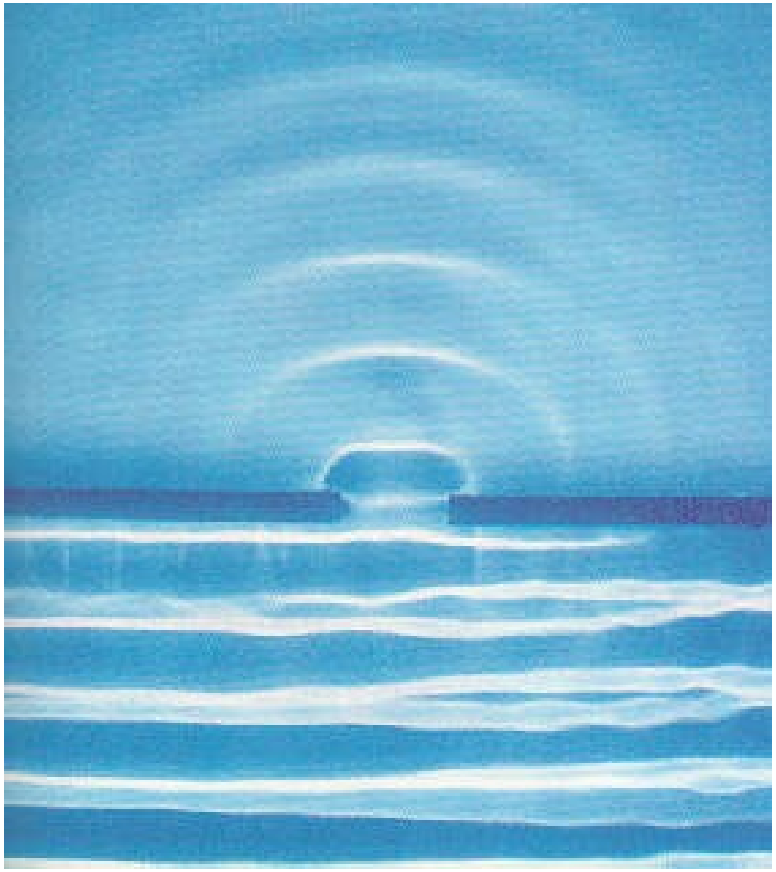
Entertainment Industry: fastest growing budgets on the planet. 3D FEM modeling is at the center of imaginary beings/imaginary worlds. Move over Pentagon!

Principios de analise 3: Experimentos na escala Nanometrica ou de Angstroms:

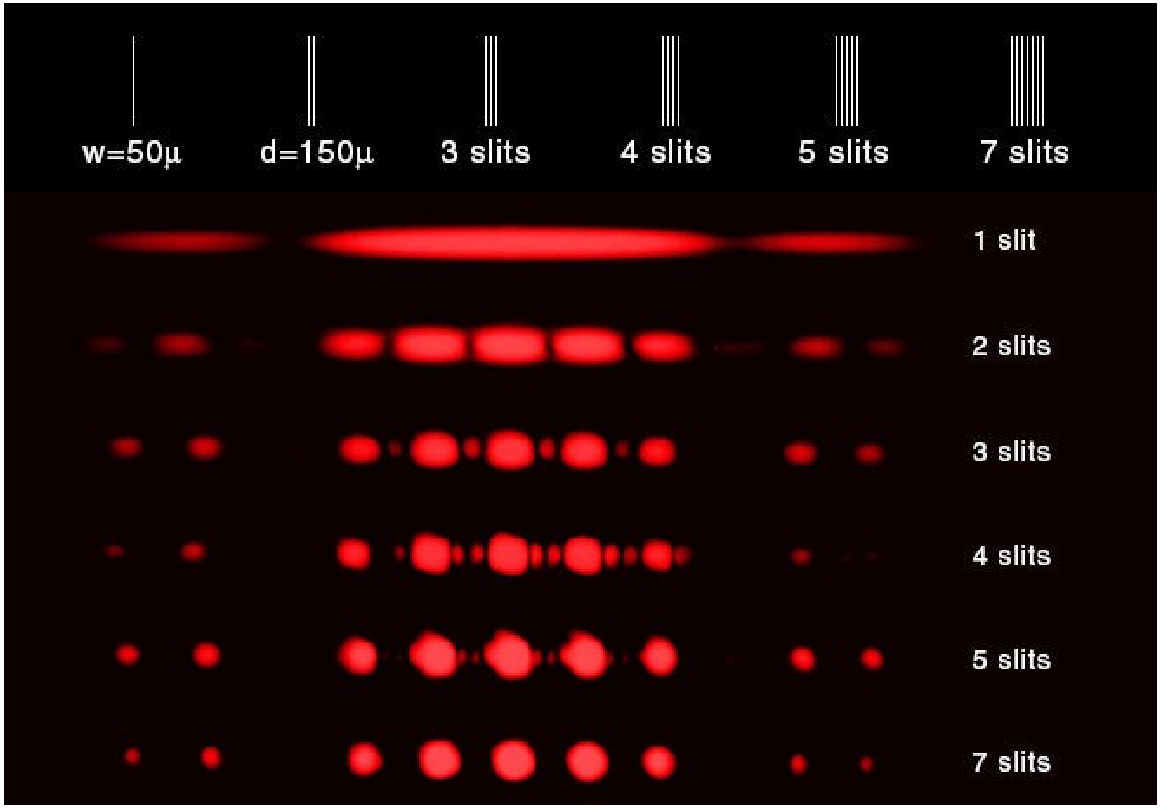
Difracao de raios-X, eletrons, neutrons, ions

Microscopia UV, XPS, IR, NMR, Raman
(e muitos outros letras, ex: SMOKE)

Diffraction: X-rays, electrons, neutrons,...

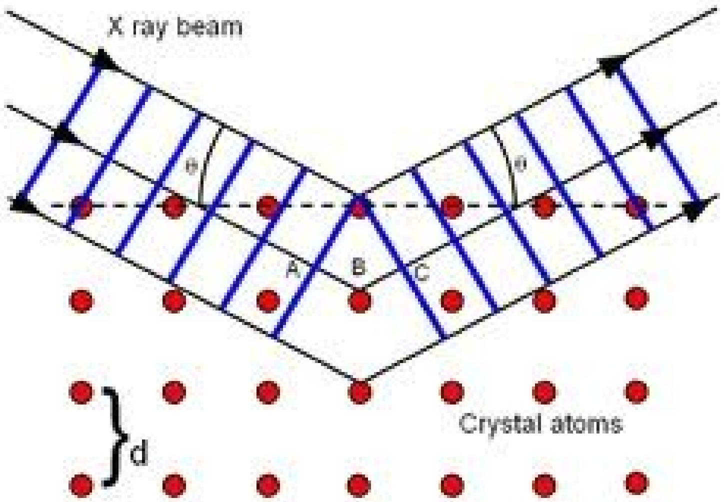


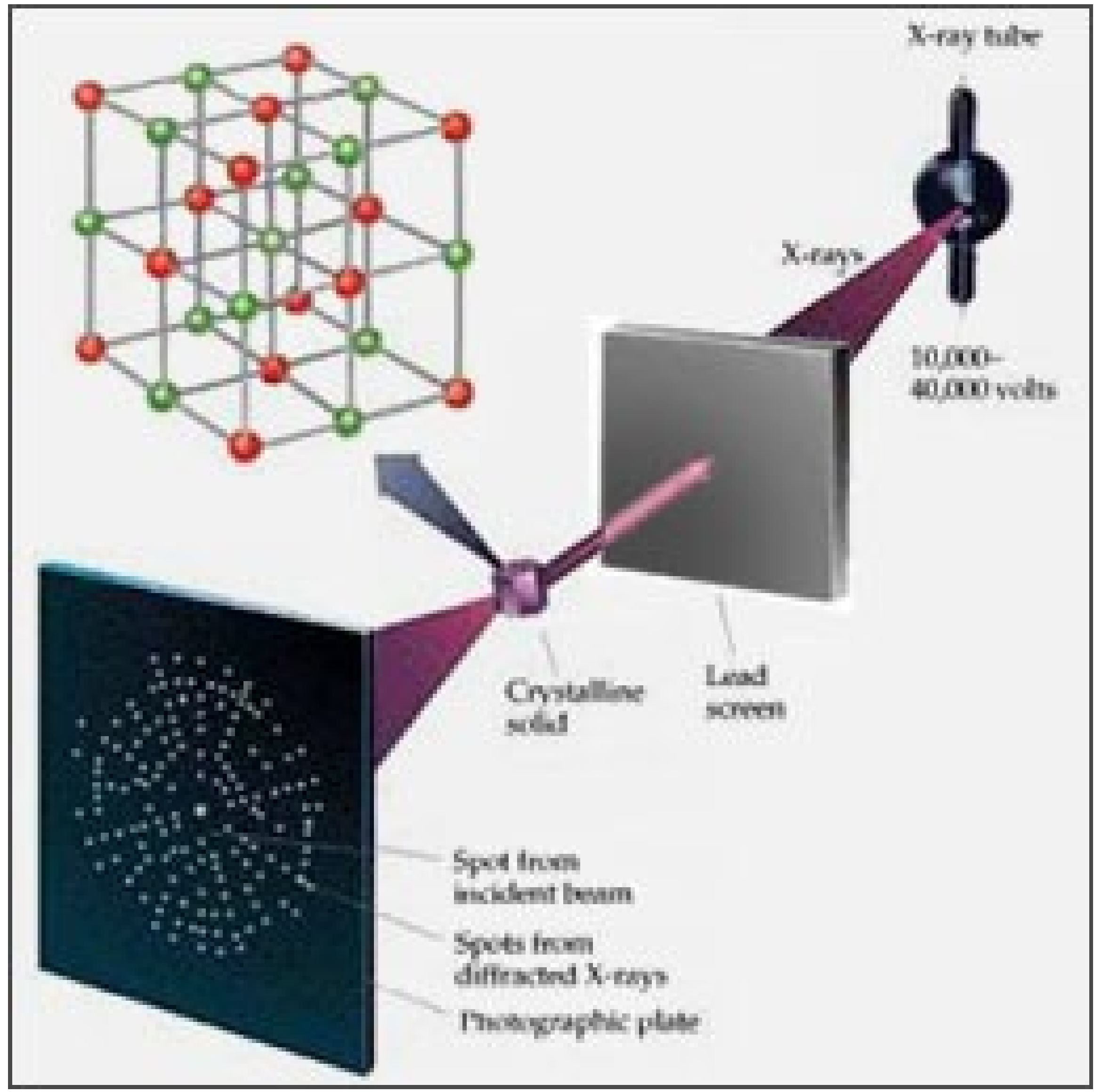
Water waves in a tank with a single slit aperture.



Visible laser light seen through 1,2,...7 slits
Energy, wavelength, frequency relations:
$E = pc = hc/\lambda$

X-ray diffraction



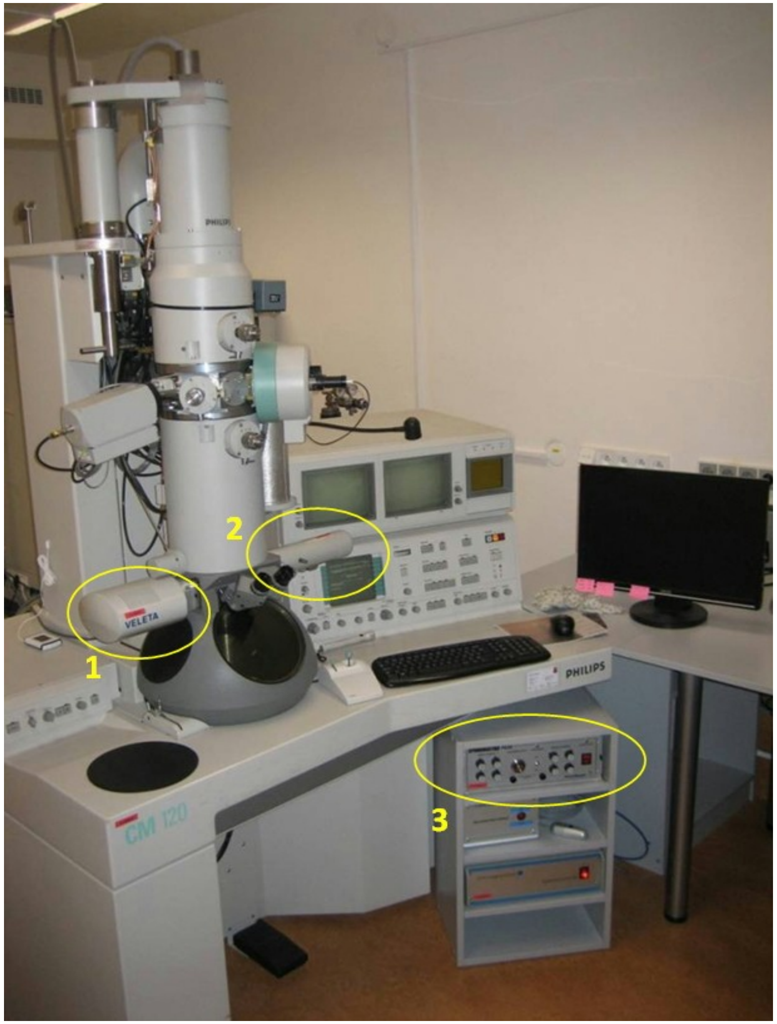


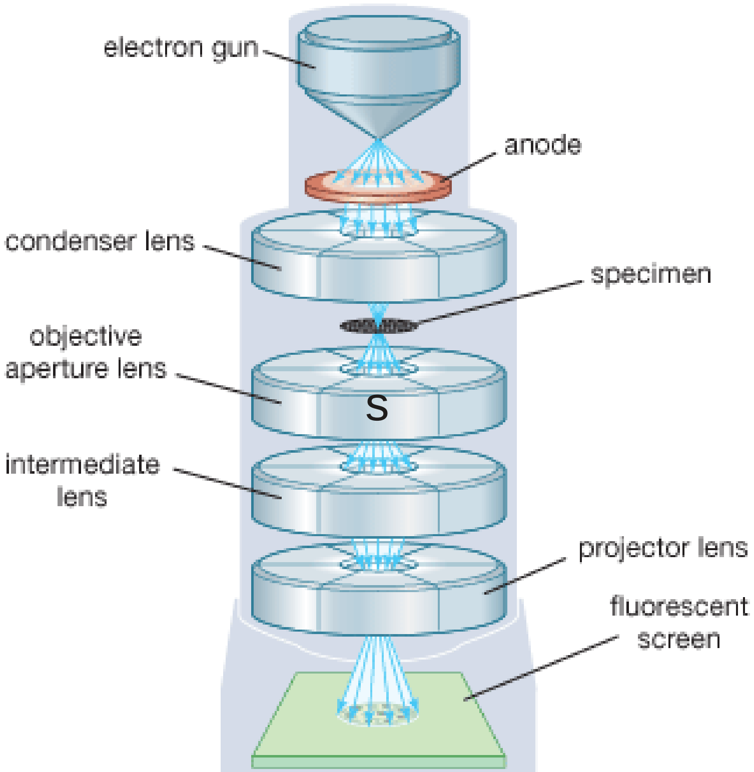
The path difference between two waves undergoing constructive interference is given by 2*d*sin*θ*, where *θ* is the scattering angle. This leads to **Bragg's law**, which describes the condition for constructive interference from successive crystallographic planes (*h*, *k*, and *l*, as given in Miller Notation) of the crystalline lattice:

$$2d \sin \theta = n \lambda$$

where *n* is an integer determined by the order given, and *λ* is the wavelength. A diffraction pattern is obtained by measuring the intensity of scattered waves as a function of scattering angle.

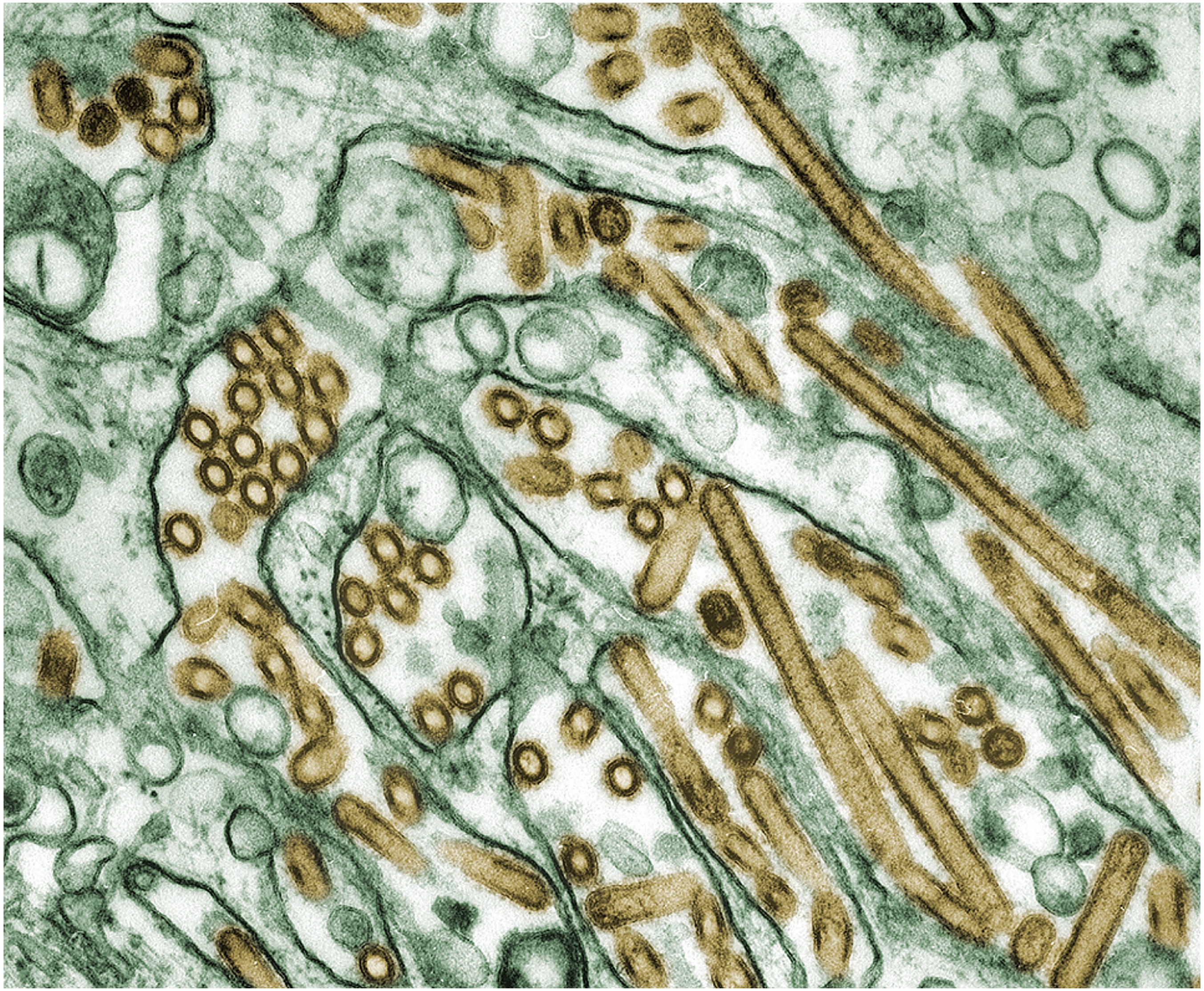
Electron diffraction





Electrons have a wavelength: $E^2 = (pc)^2 + (mc^2)^2$ $\lambda = h/p$

For E = 150 eV λ = 1.0 Å Thanks, DeBroglie!

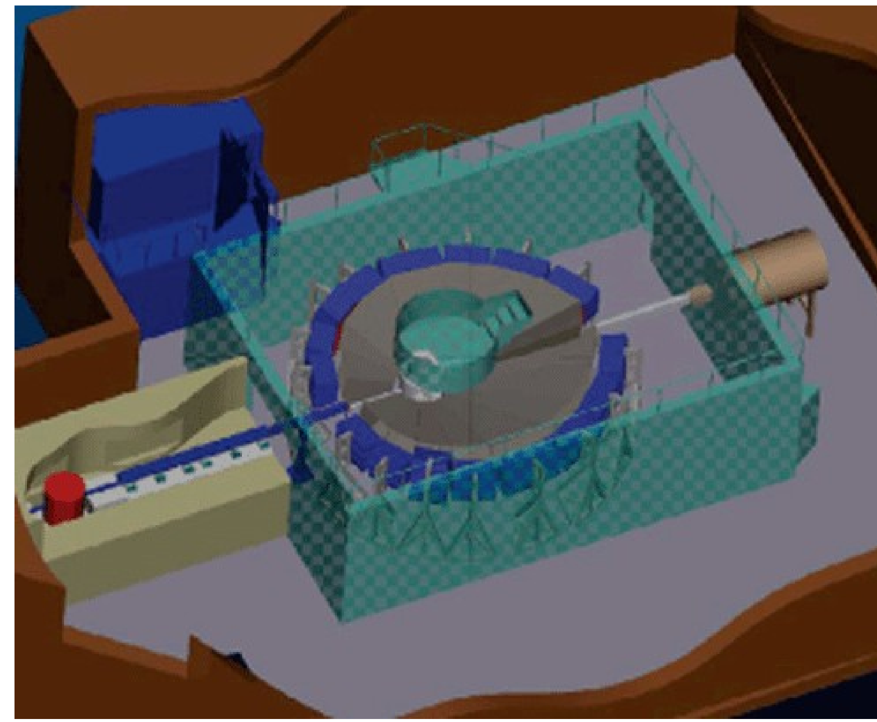


Transmission Electron Microscope (TEM) image of Avian influenza virus A H5N1 (gold) cultivated in MDCK cells (green).
MDCK=Madin-Darby canine kidney (Cocker spaniel 1958)

Neutron Diffraction

Neutron sources are generally large; beam handlers and detectors are large; typically operated at national centers.

Detector at Los Alamos Neutron Science Center

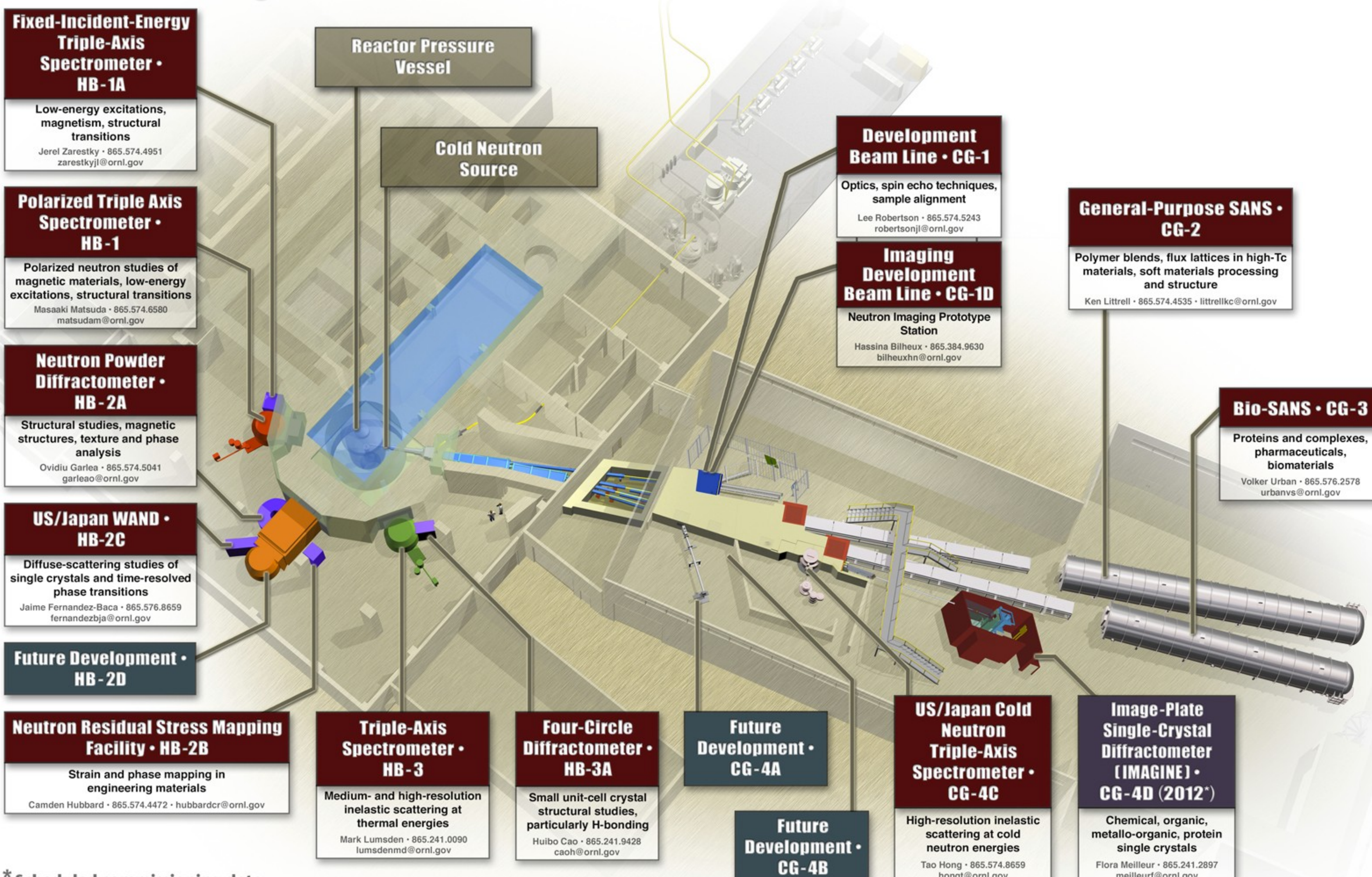


Schematic of beam handling and detector At Oak Ridge Spallation Neutron Source

High Flux Isotope Reactor at Oak Ridge National Laboratory

The United States' highest flux reactor-based neutron source

HFIR



* Scheduled commissioning date.

LEGEND

- Installed, commissioning, or operating
- In design or construction
- Under consideration

07-G00244K/gim

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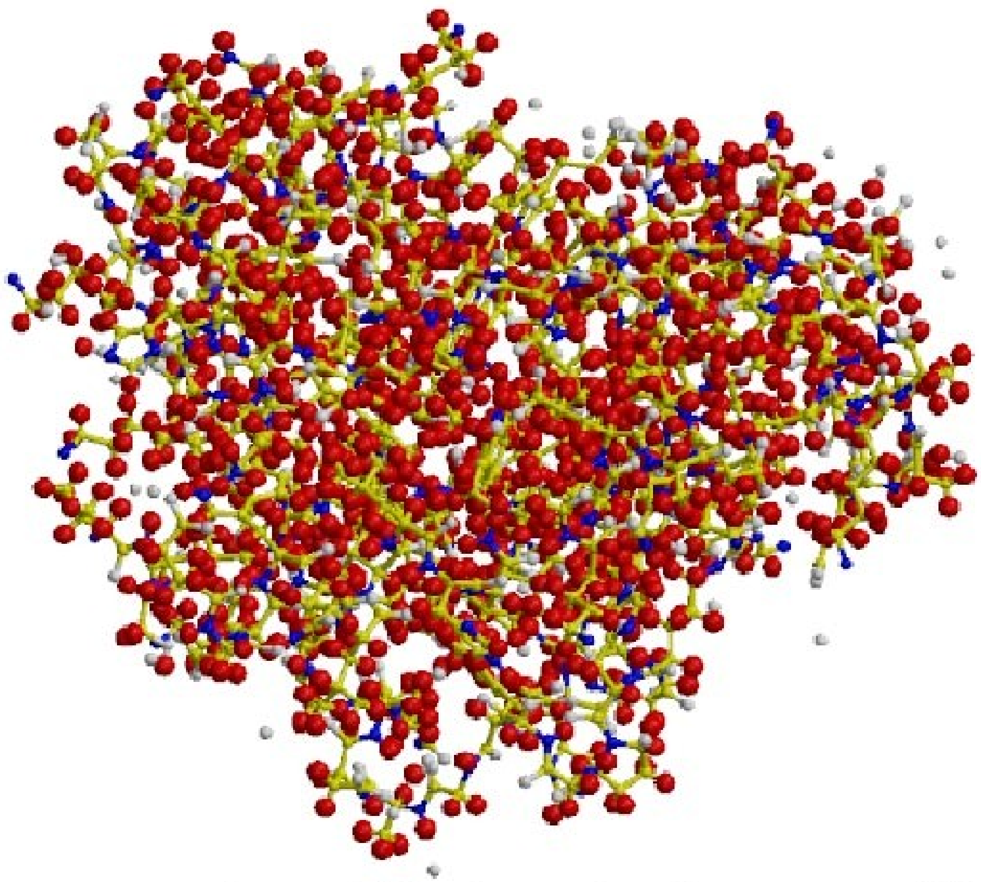
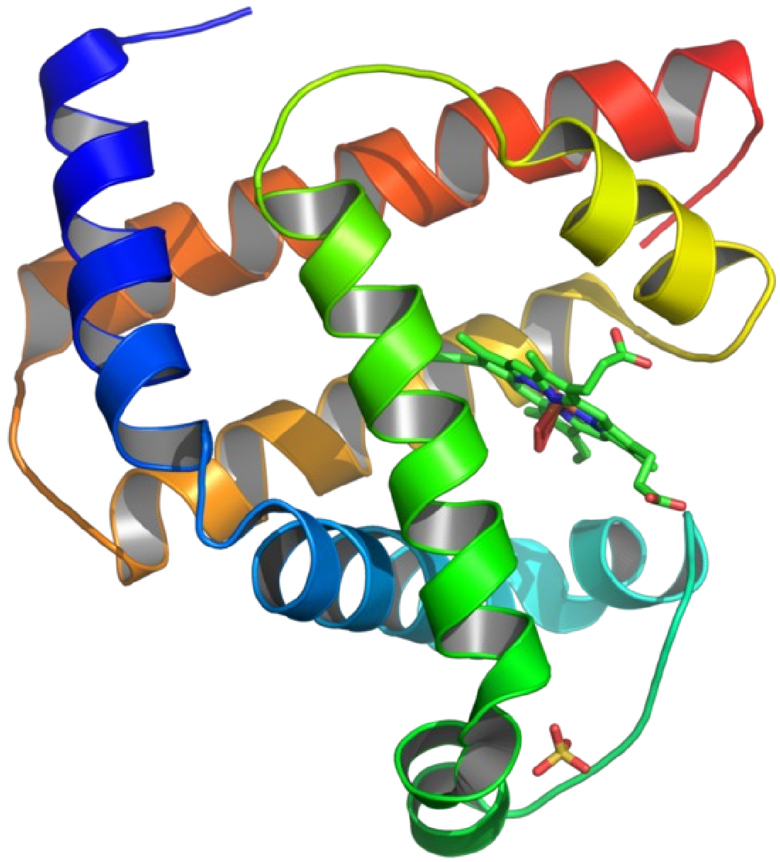
Myoglobin (abbreviated Mb) is a single-chain globular protein of 153 or 154 amino acids, containing a heme (iron-containing porphyrin) prosthetic group in the center around which the remaining apoprotein folds. It has eight alpha helices and a hydrophobic core. It has a molecular weight of 17,699 daltons (with heme), and is the primary oxygen-carrying pigment of muscle tissues.



Tertiary structure of myoglobin determined by neutron diffraction

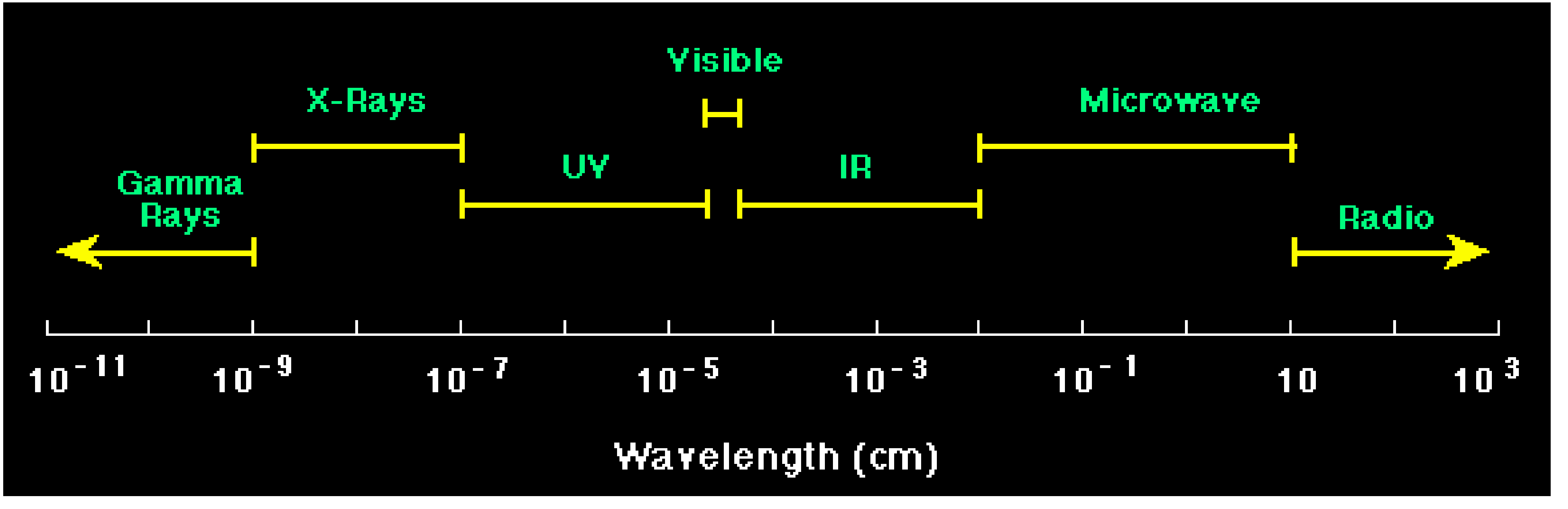
nitrogen, carbon, oxygen, hydrogen



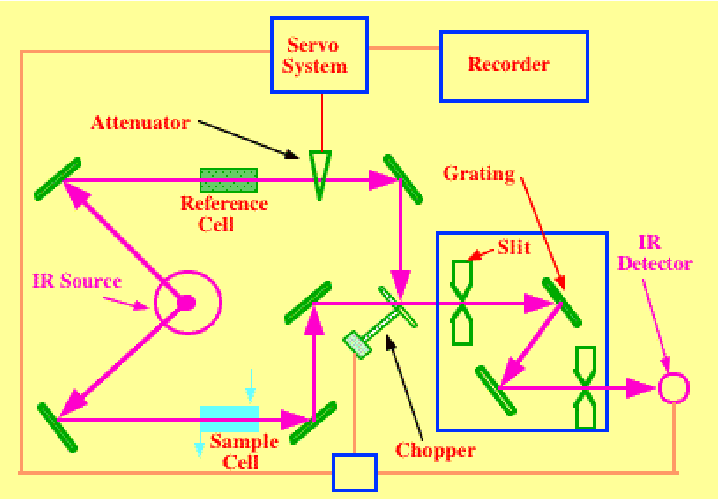
Simplified ribbon model of myoglobin

IR,VIS,UV,XP Spectroscopy

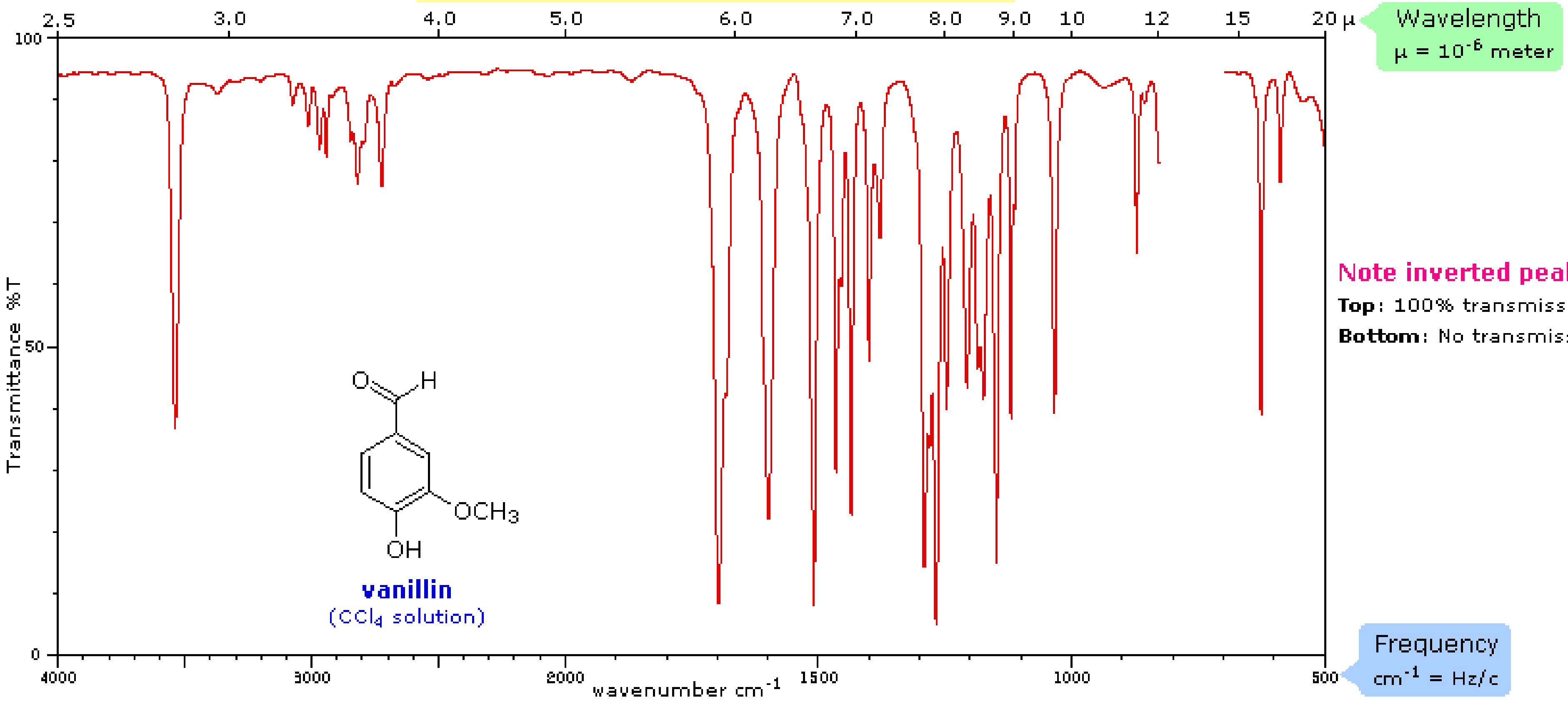
IR= InfraRed 2.5 < λ < 20μ $1.2\text{x}10^{14} < \nu < 1.9\text{x}10^{13}$ Hz
VIS=Visible 400 < λ <700nm $7.5\text{x}10^{14} < \nu < 4.3\text{x}10^{14}$ Hz



Old-fashioned grating IR Spectroscopy



Try this:
formaldehyde vibrations

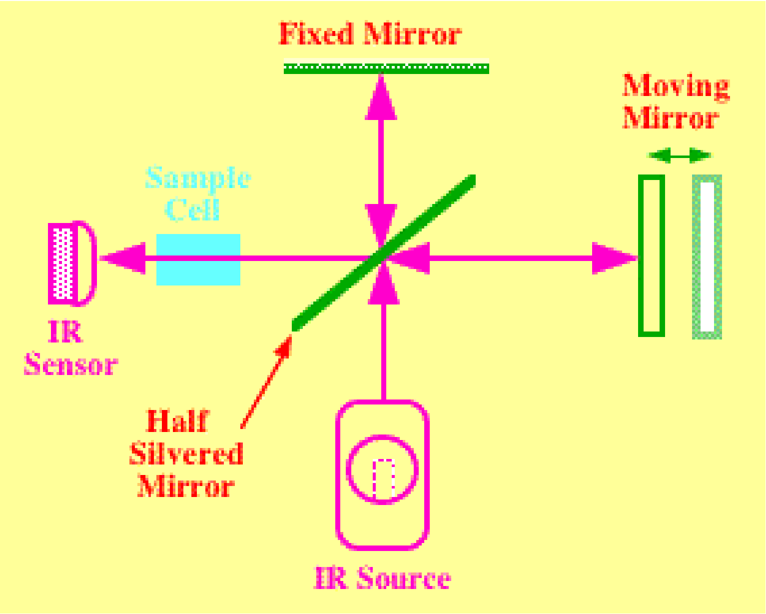


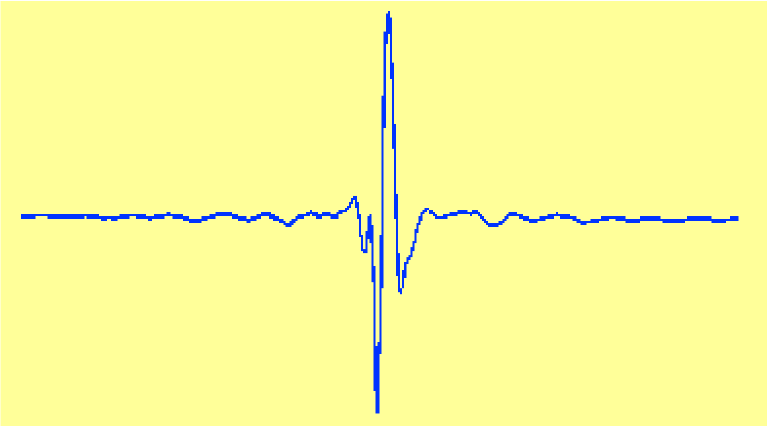
Note inverted peaks

Top: 100% transmission

Bottom: No transmission

State-of-the-art Fourier Transform FTIR Spectroscopy

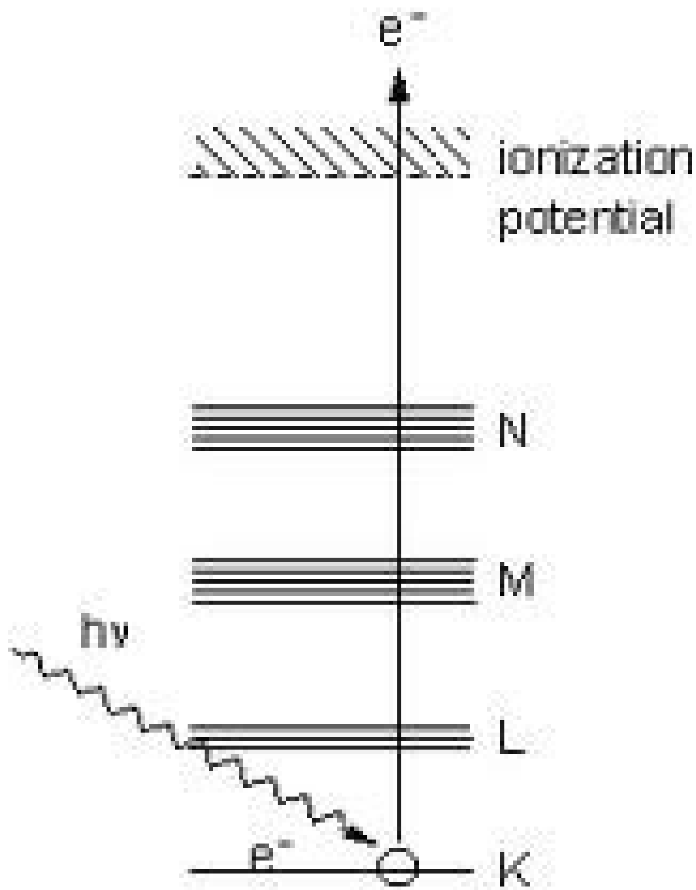


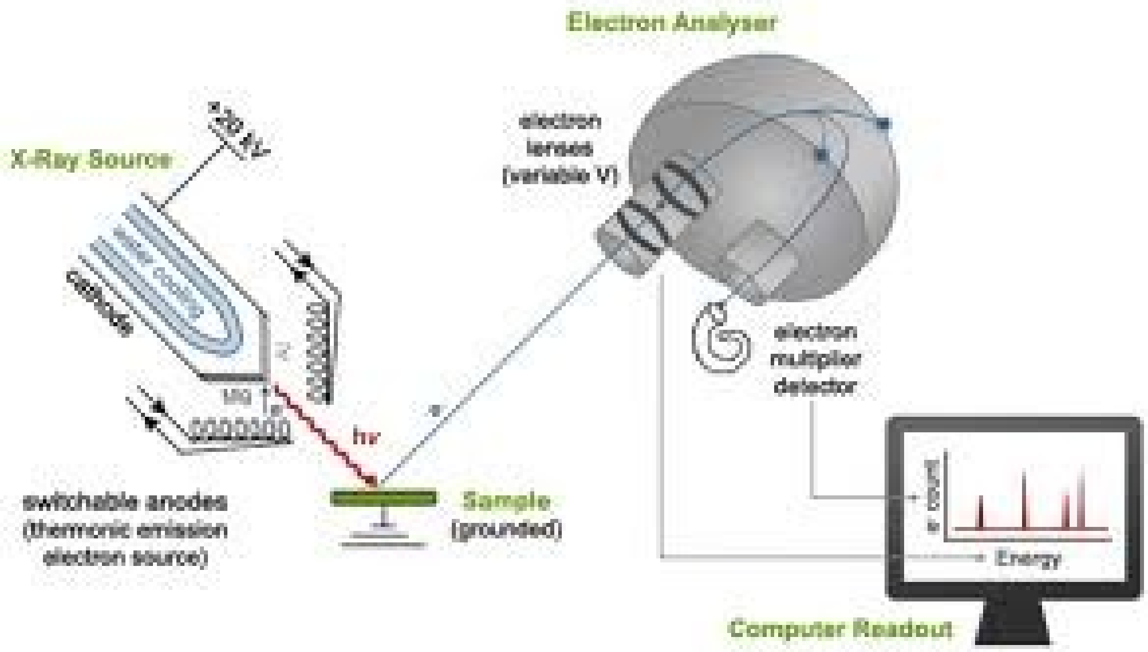


FTIR output signal

Sweet, hi-tech, but requires significant data processing to interpret. Has essentially replaced the direct grating-style instrumentation.

XPS- X-ray Photoelectron Spectroscopy

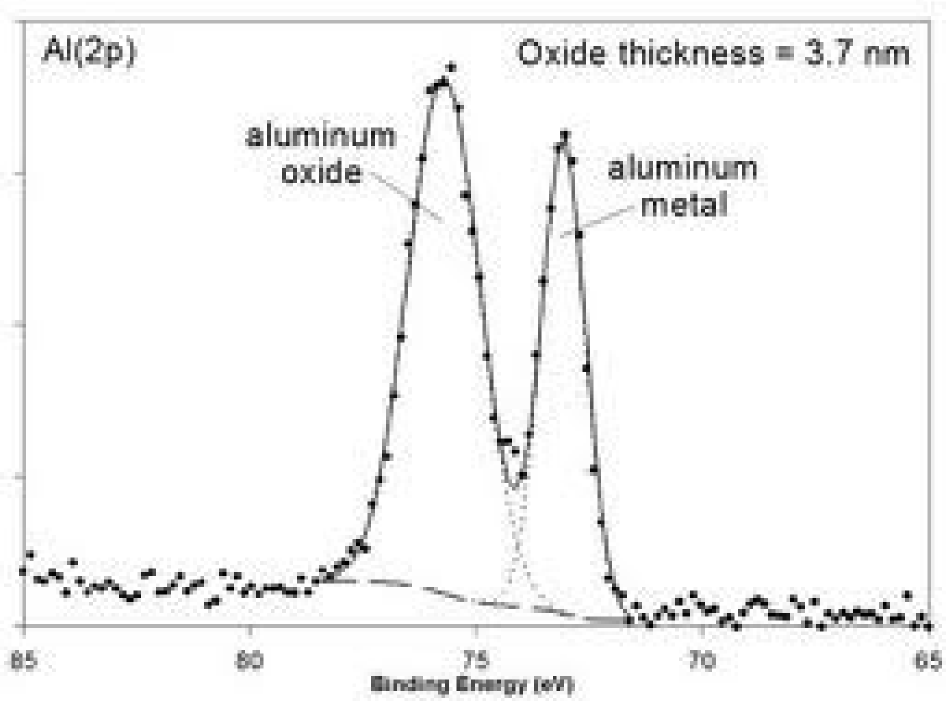


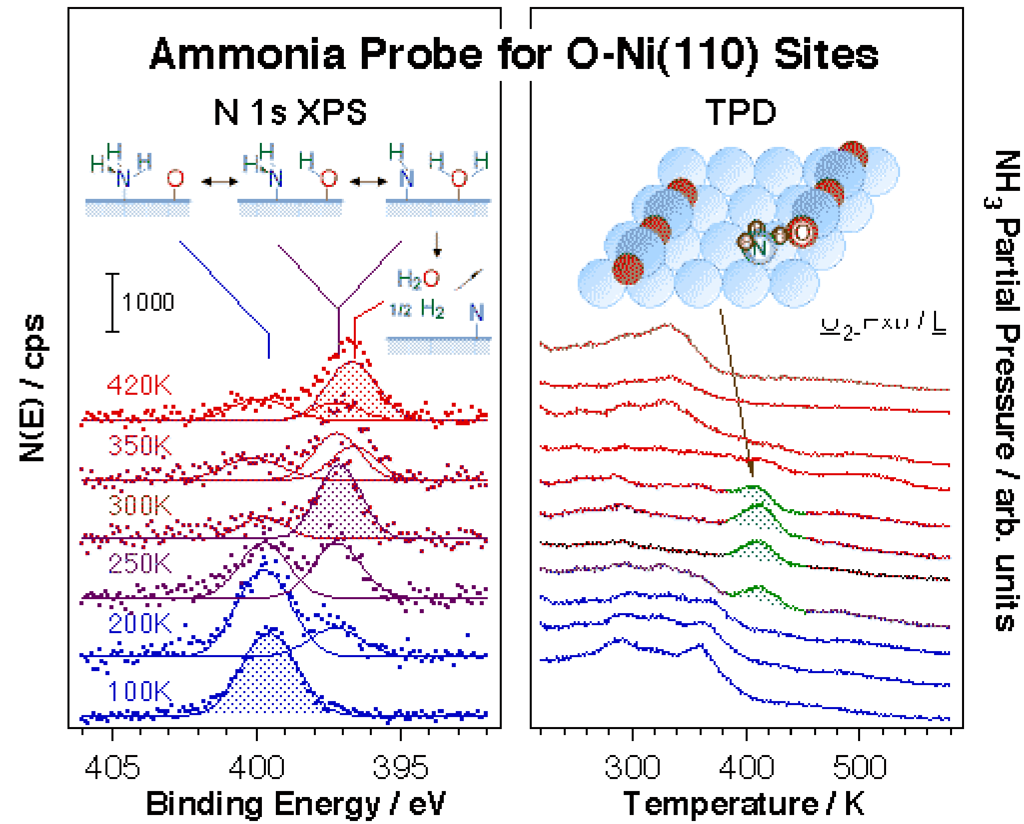


High energy photon in, electron out; measure its kinetic energy

XPS equipment schematic-clever detectors can measure count rates at a large number of energies simultaneously.

XPS is a surface probe





A simple story: Aluminum oxide over Al metal, seen via excitation of Al (2p)

A complex story: Ammonia and its dissociation products on Oxygen-doped Ni(110). Here TPD (temperature programmed desorption) is used to drive different species off the surface at different T. XPS from N(1s) states.