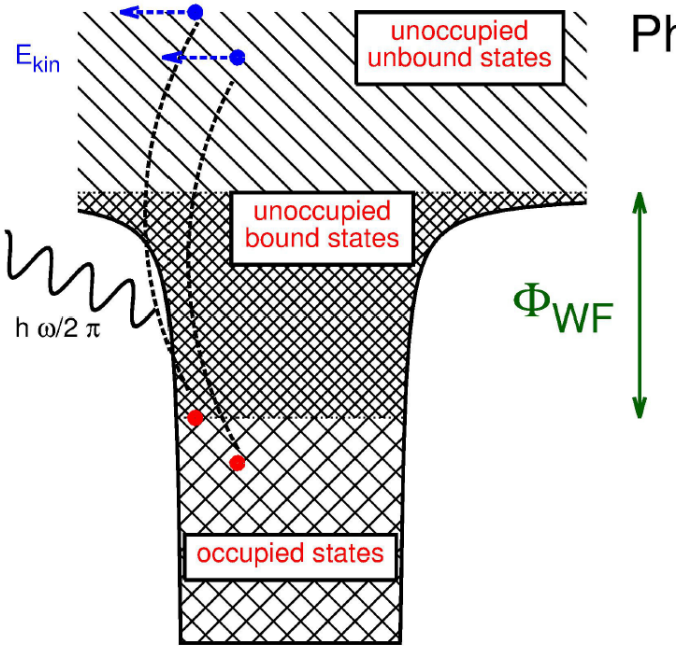
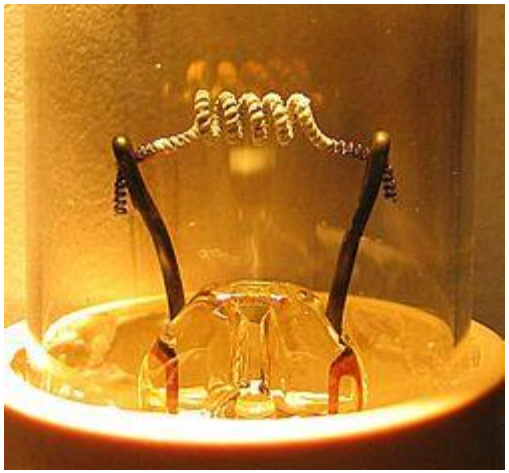
Scattering (Experiments)

Photoelectric Effect

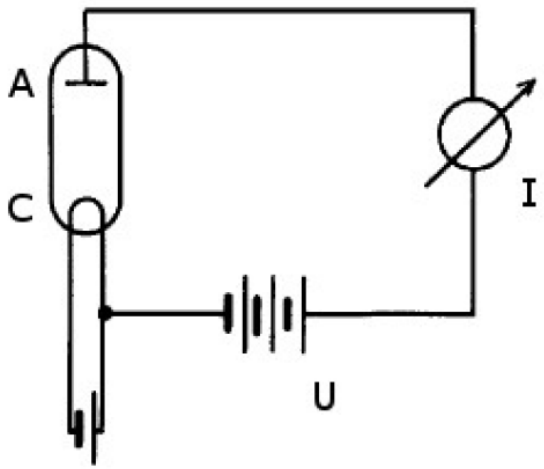
$$\hbar\omega = E_{kin}^{max} + \Phi_{WF}$$

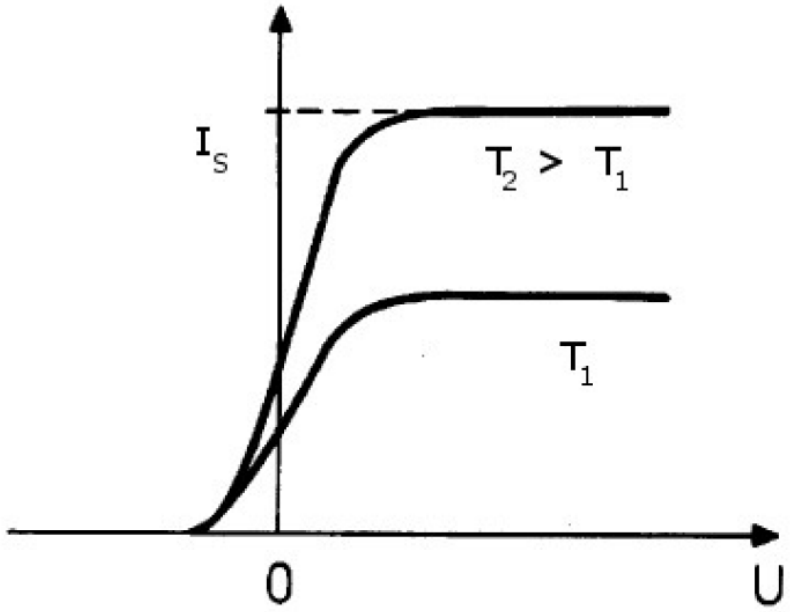


Thermionic Emission

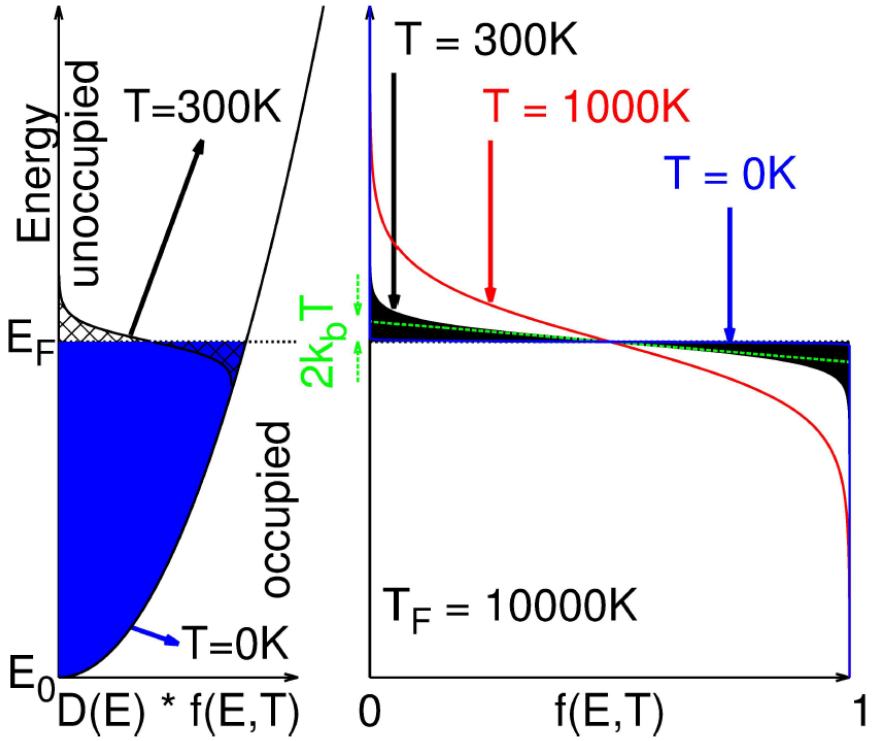


Thermionic Emission





Boltzmann Distribution: $N_2/N_1 = \exp\{(E(N_1)-E(N_2)/ k_B T\}$

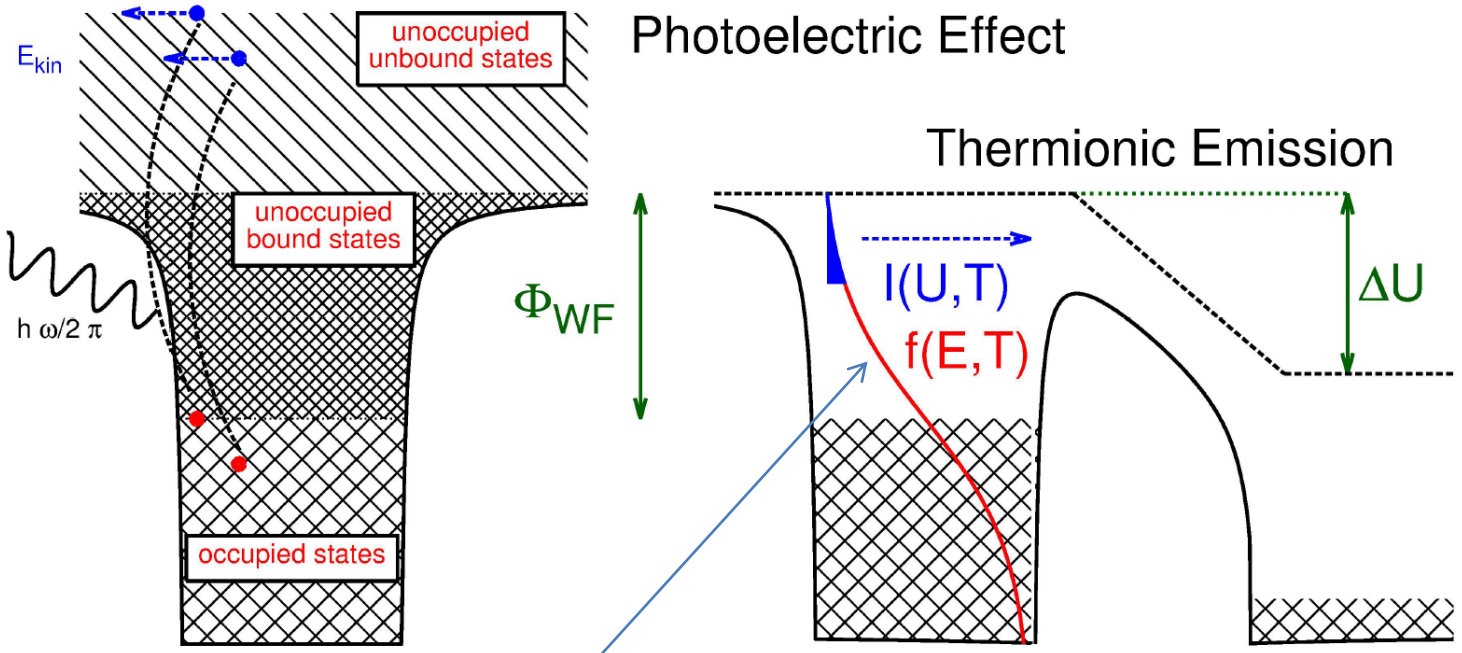


$$f(E_i, T) = \frac{1}{e^{E-\mu_i/k_B T} + 1}$$

Fermi Function

Photoelectric Effect as explained by A. Einstein (1905)

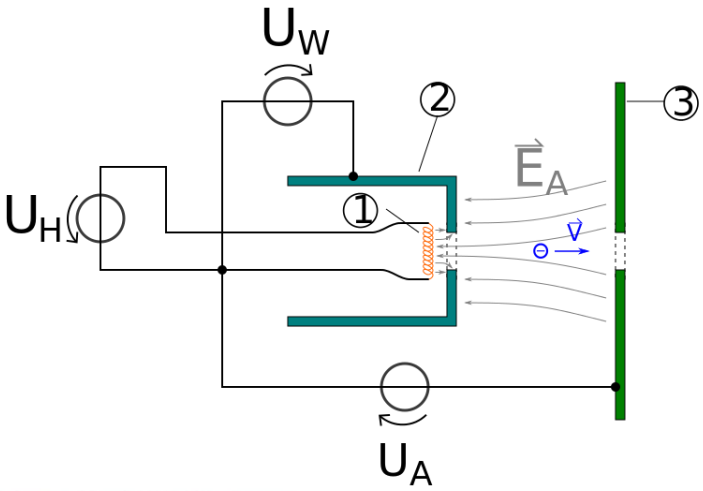
$$\hbar\omega = E_{kin}^{max} + \Phi_{WF}$$

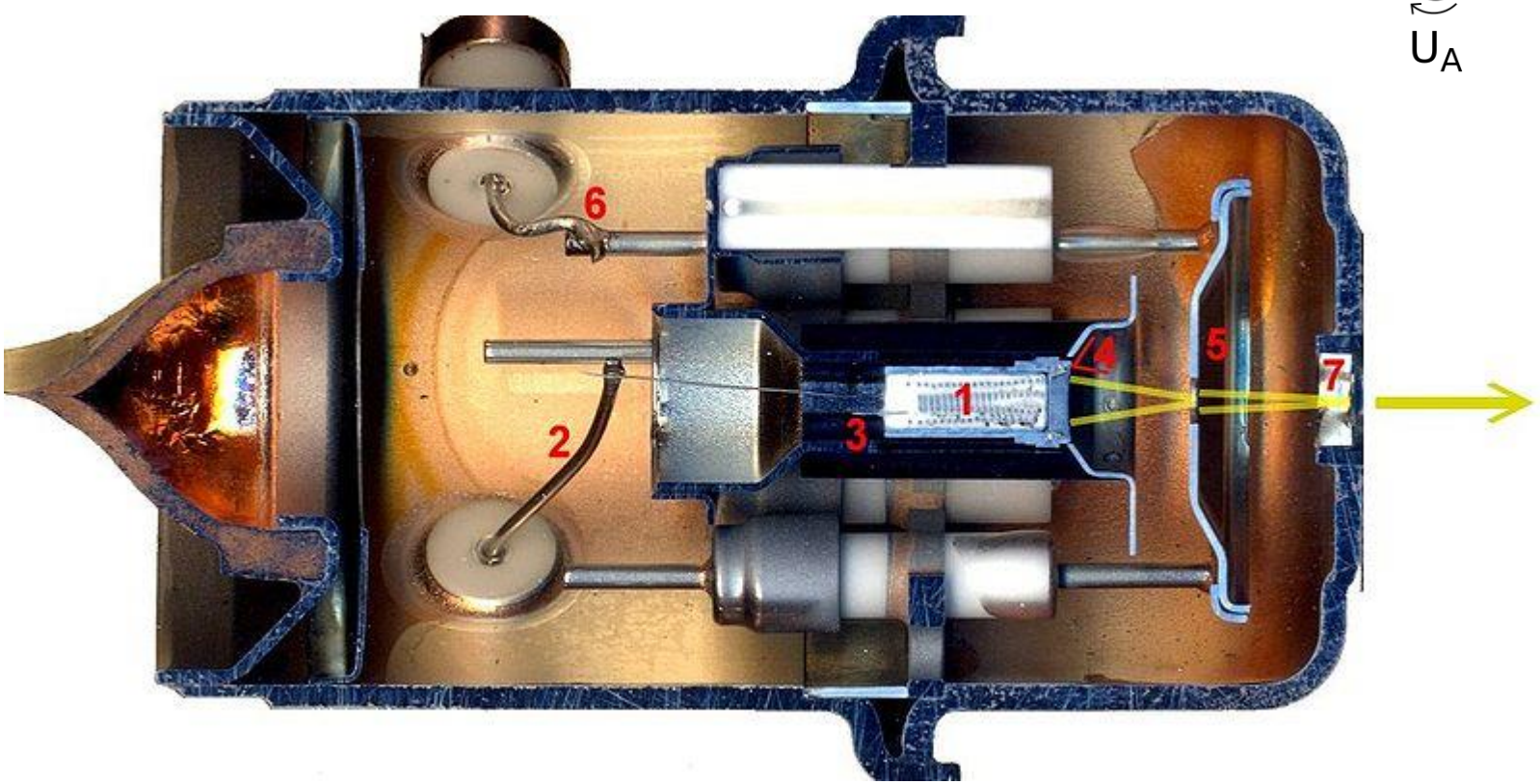


$$f(E_i, T) = \frac{1}{e^{E-\mu_i/k_B T} + 1}$$

Fermi Function

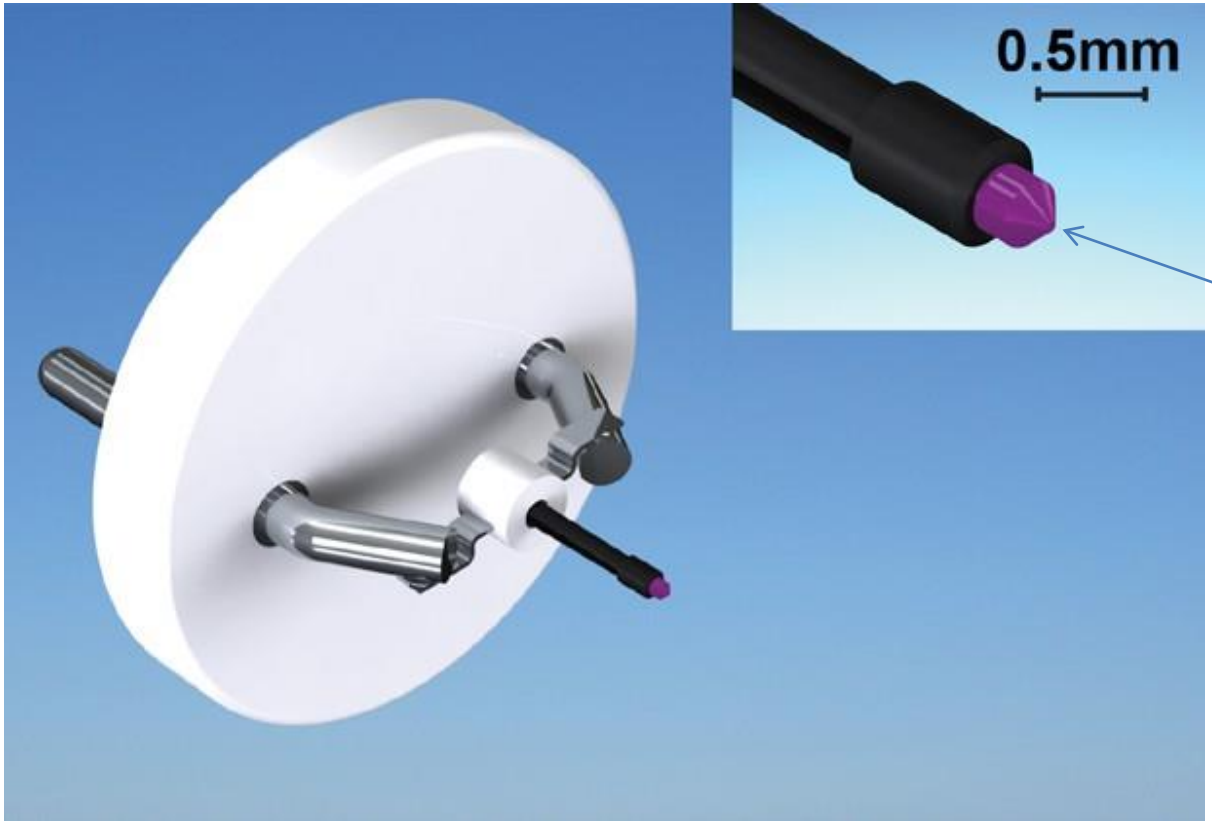
Electron Gun





Li	Be											B	C		
2,9	4,98											4,45	5,0		
Na	Mg											Al	Si	P	S
2,75	3,66											4,28	4,85	–	–
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se
2,30	2,87	3,5	4,33	4,3	4,5	4,1	4,5	5,0	5,15	4,65	4,33	4,2	5,0	3,75	5,9
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te
2,16	2,59	3,1	4,05	4,3	4,6	–	4,71	4,98	5,12	4,26	4,22	4,12	4,42	4,55	4,95
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po
2,14	2,7	3,5	3,9	4,25	4,55	4,96	4,83	5,27	5,65	5,1	4,49	3,84	4,25	4,22	–

Figure 7.12: Work function of various polycrystalline materials.



www.kimballphysics.com

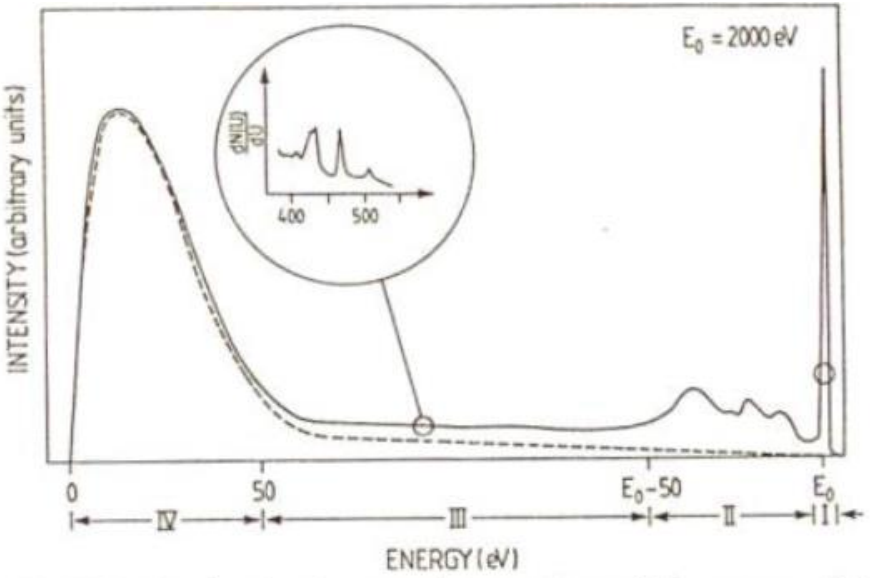
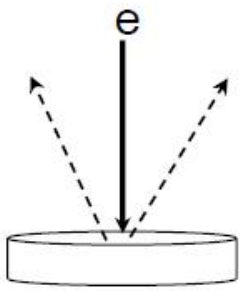


Fig. V.2. Qualitative large-scale overview of the energy distribution of electrons emitted from a surface which is irradiated by an electron beam of primary energy E_0.

Electron diffraction and microscopy:

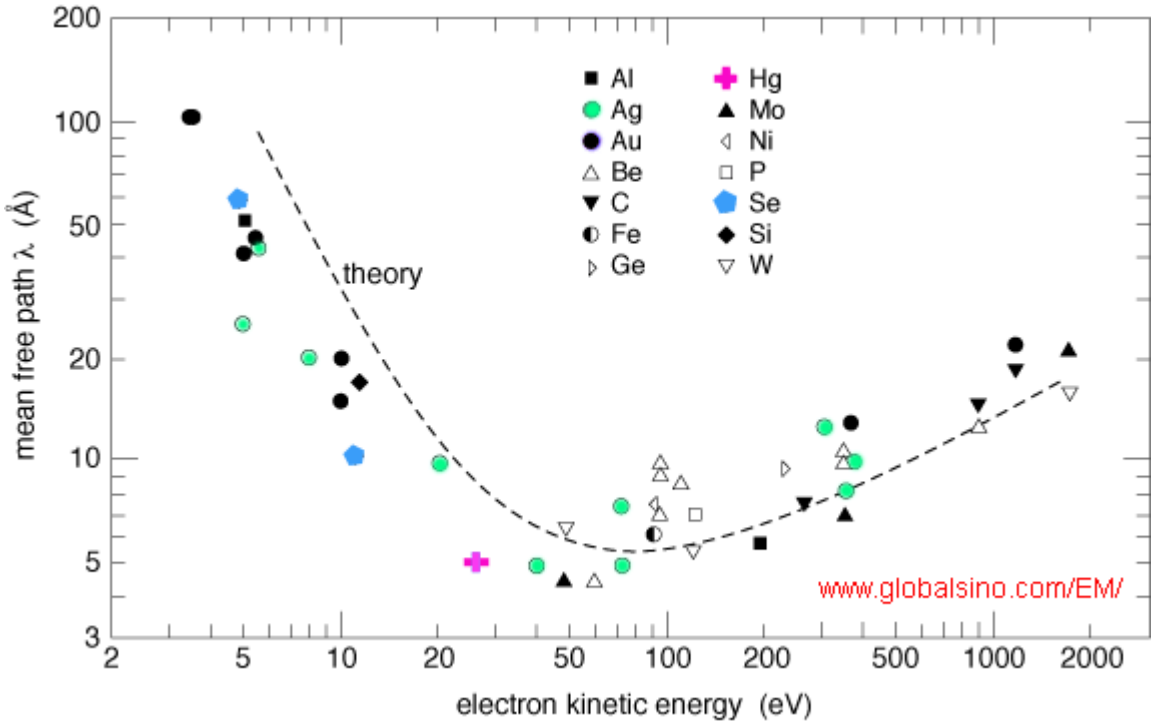
Elastic backscattered e^-, ~ few % at 100eV



Let us take a 20 eV electron:

$p = mv = \sqrt{2mE}$ ..... $= 2.4 \times 10^{-24}$ kg m / s

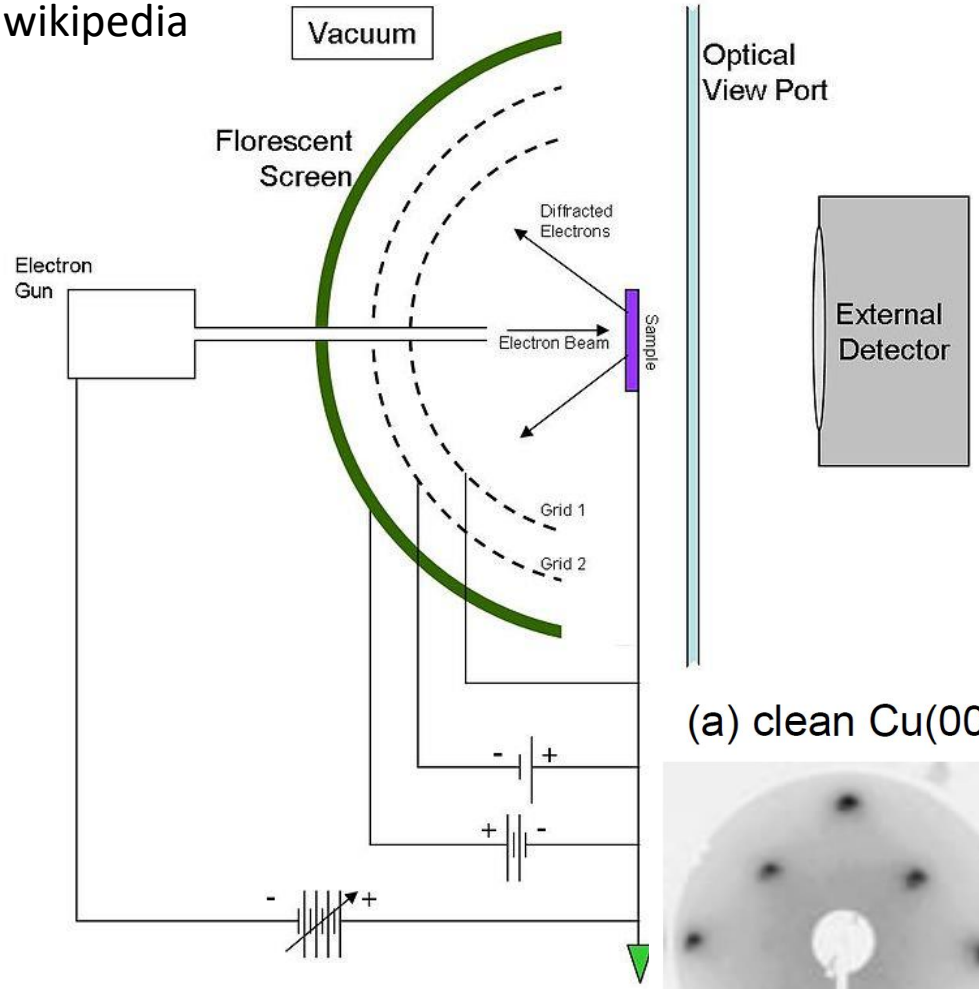
$\lambda = hc / E = 2.7$ Å



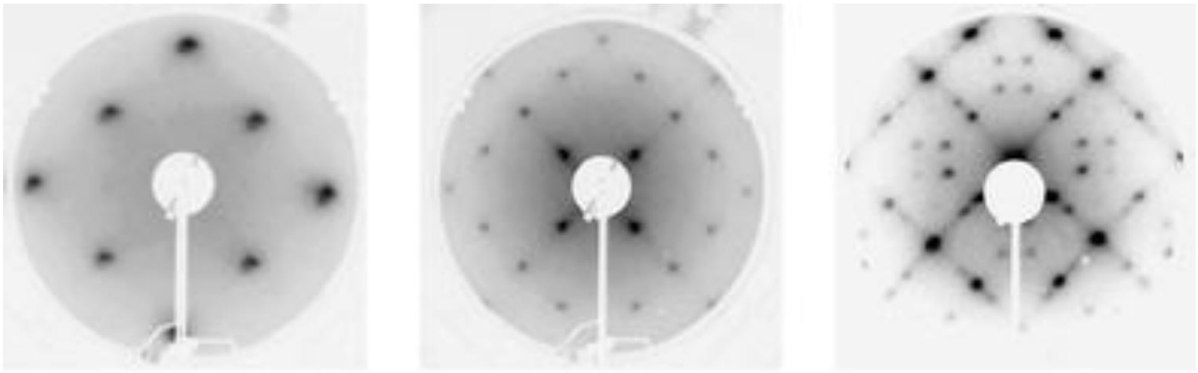
LEED – Low Energy Electron Diffraction

www.scientaomicron.com

wikipedia



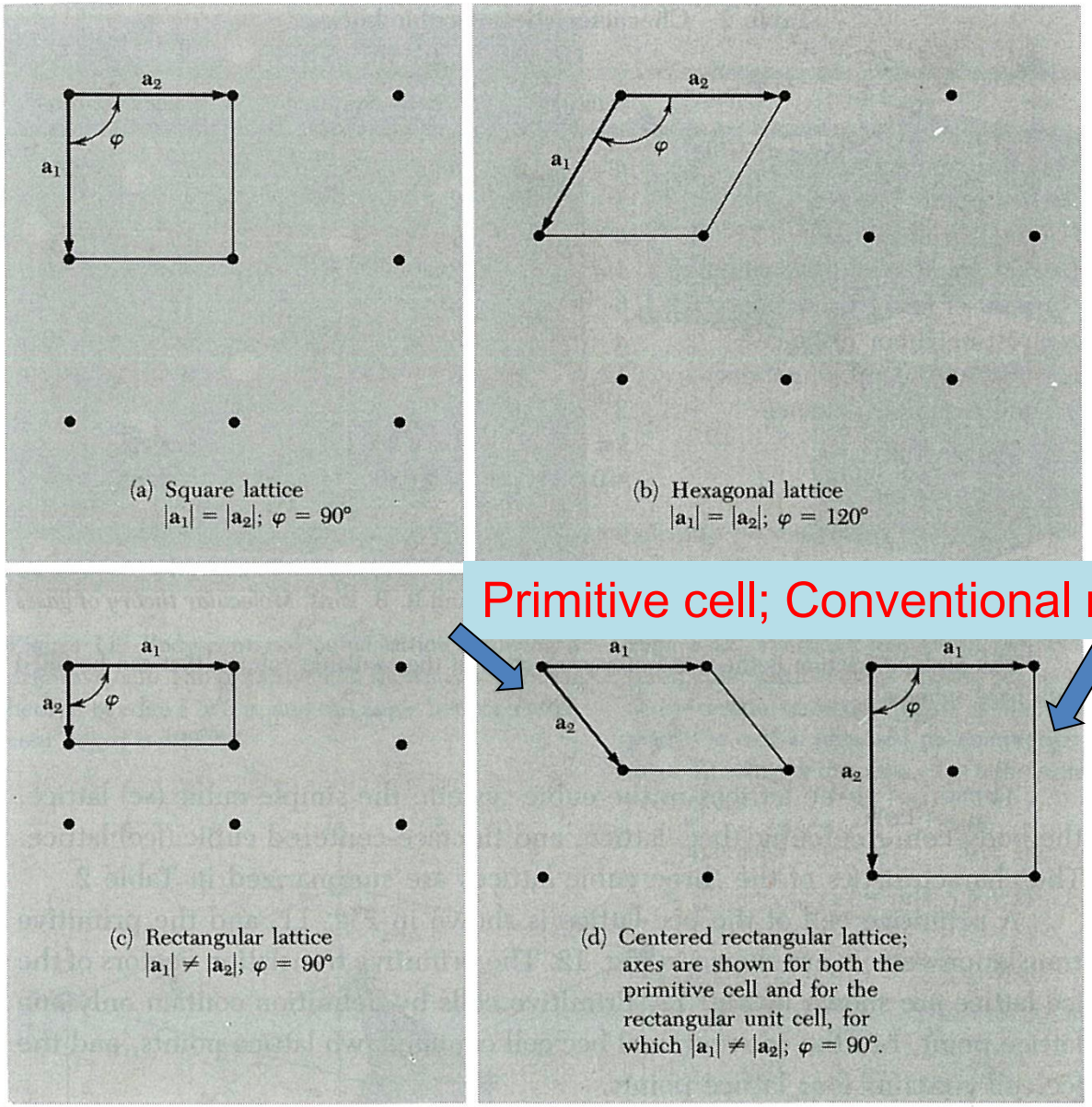
(a) clean Cu(001); (b) $p(2 \times 1)$ O; (c) $c(2 \times 3)$O /Cu(001)



(a) (b) (c)

Two - Dimensional lattices (1 oblique + 4 special)

Chapter 1



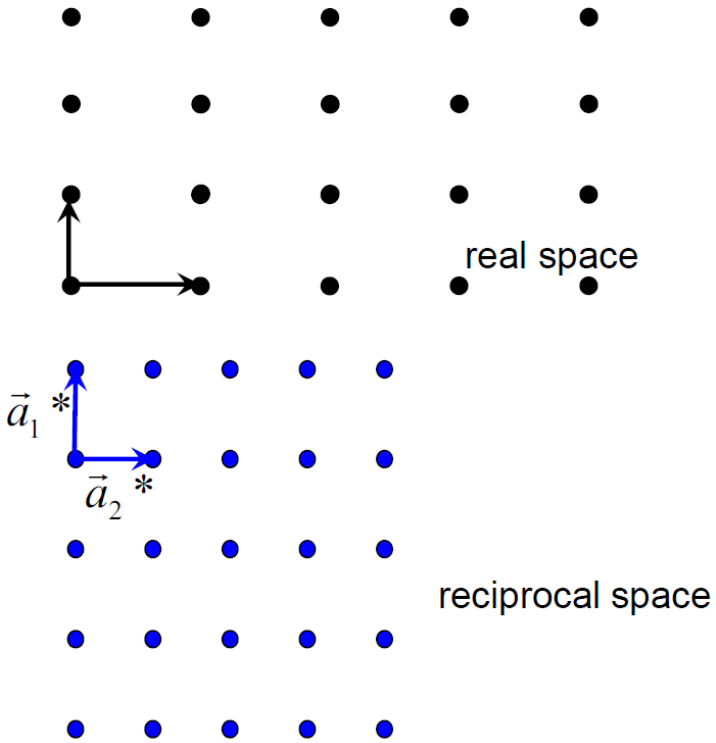
Primitive cell; Conventional rectangular cell

Figure 9 Four special lattices in two dimensions

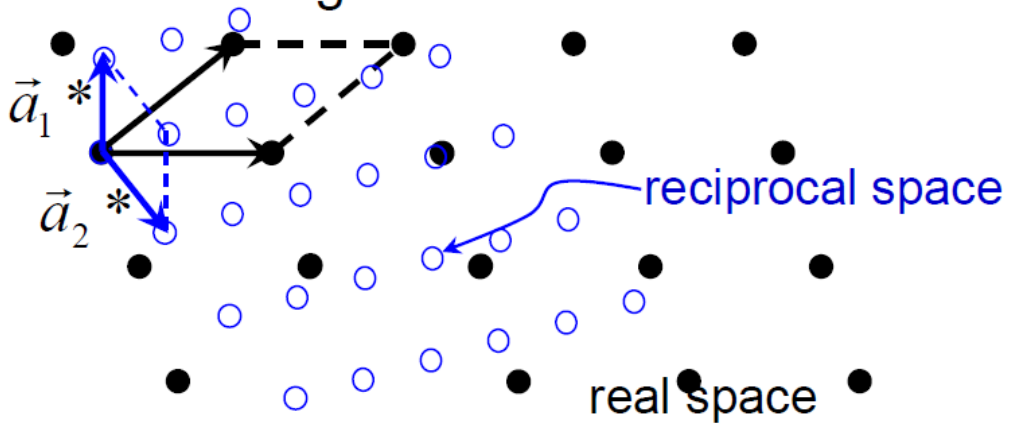
- Given a unit cell with basis vectors $(\vec{a}_1, \vec{a}_2)$
- There is a complementary reciprocal lattice $(\vec{a}_1{}^*, \vec{a}_2{}^*)$

$\vec{a}_i \cdot \vec{a}_j{}^* = \delta_{ij} \quad (i, j = 1, 2) \Rightarrow \vec{a}_1{}^* \perp \vec{a}_2 \quad \text{and} \quad \vec{a}_2{}^* \perp \vec{a}_1$

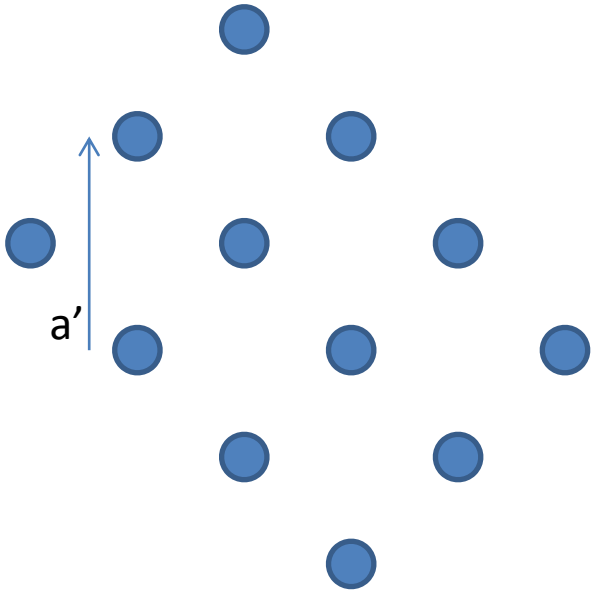
Rectangular Lattice

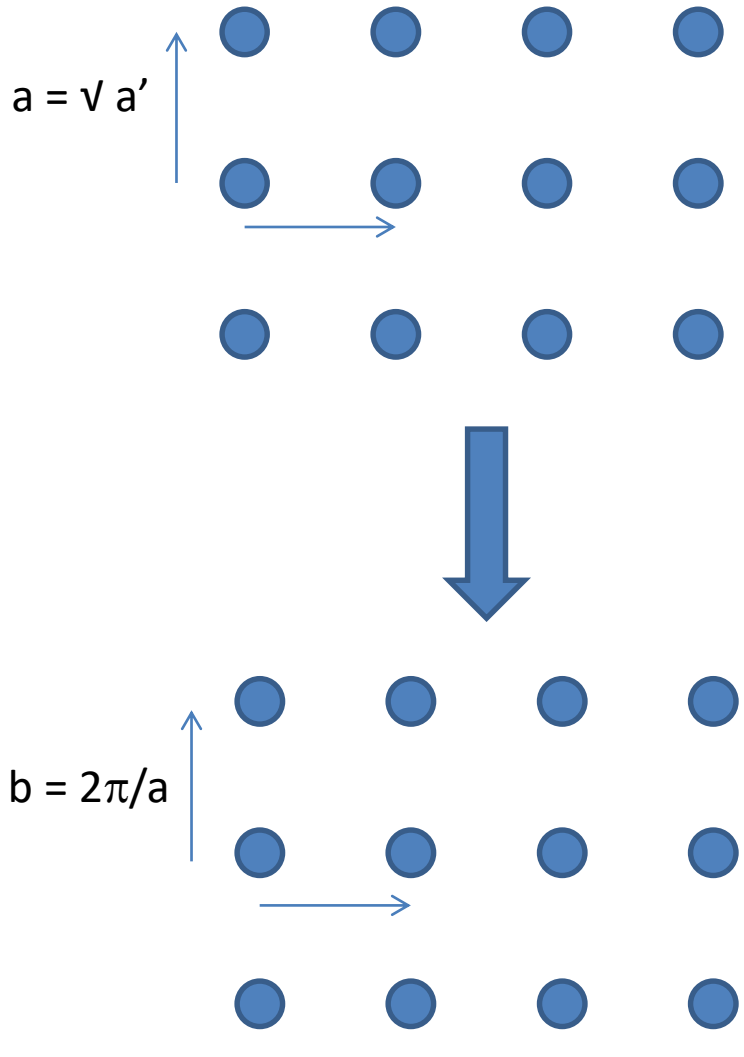


Non-rectangular lattice

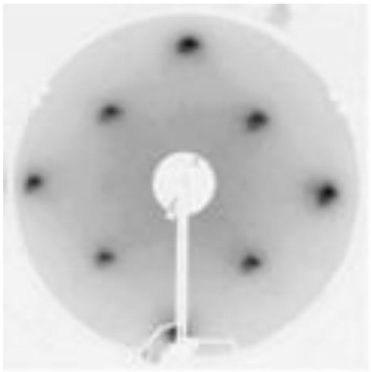


Cu(100) (fcc)





(a) clean Cu(001); (

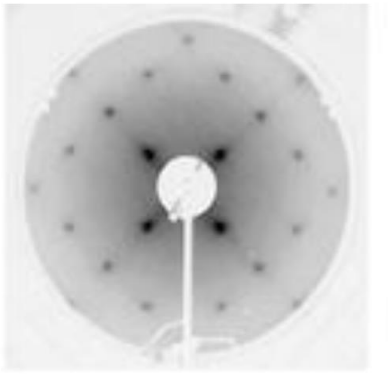


(a)

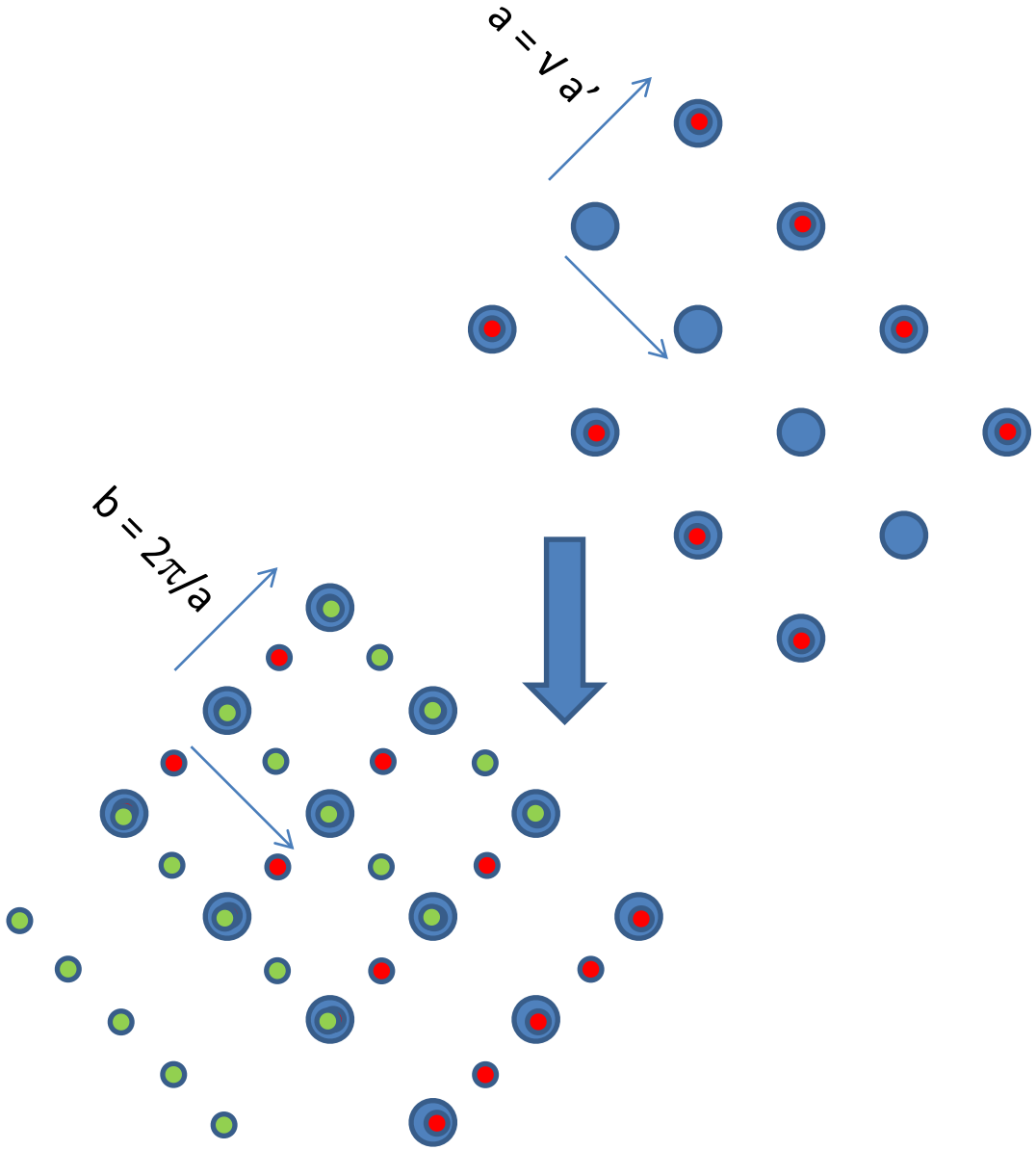
Cu(100): p(2x1)O

2 domain structure

(b) $p(2 \times 1)$ O; (c) $c(2$



(b)

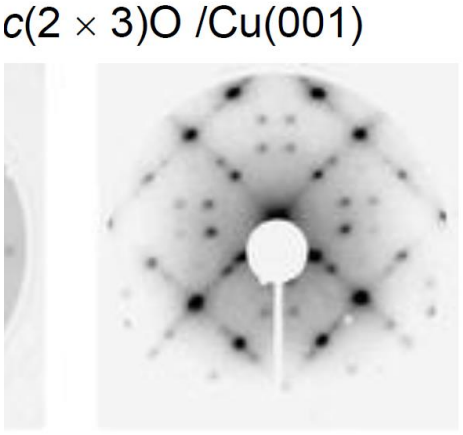


Cu(100): c(2x3)O

a1 = (a x) b1* = (2π/a x)
a2 = (a y) b2* = (2 π/a y)

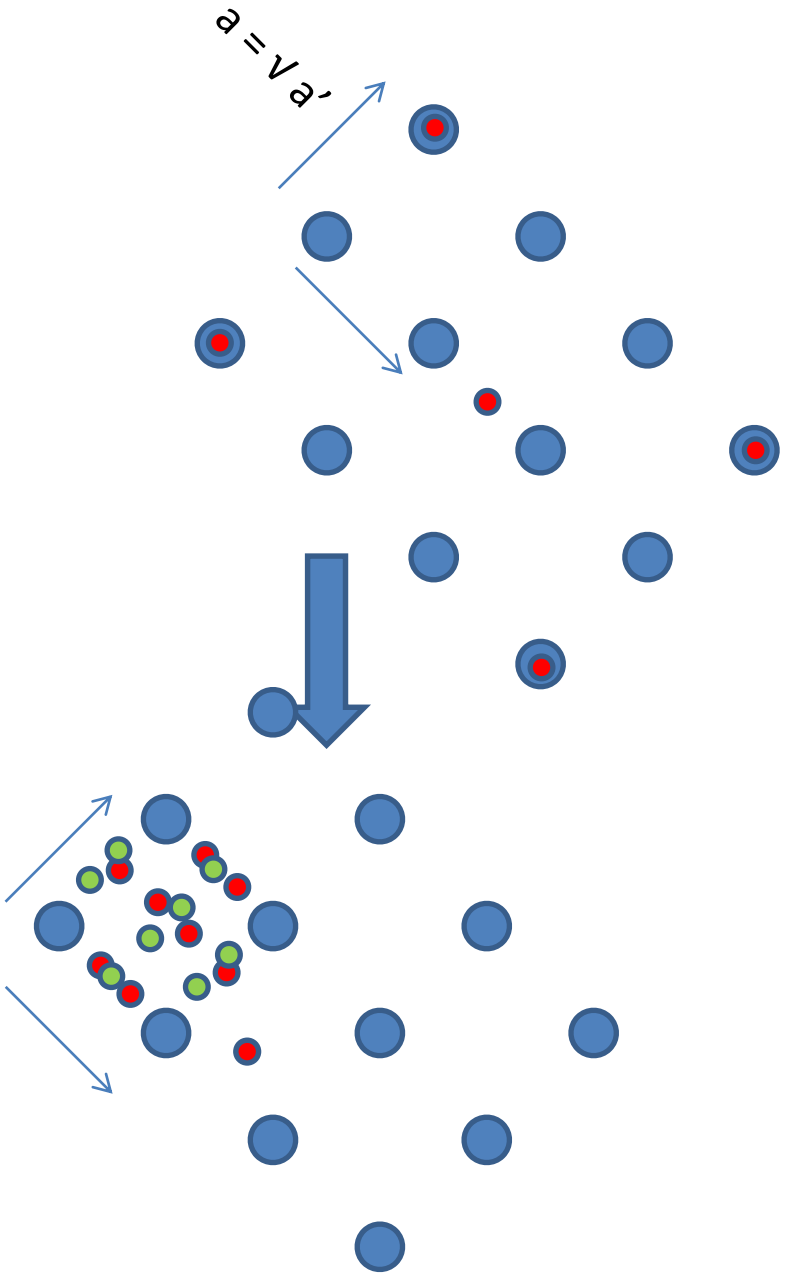
O1 = (3/2 a1 + a2)
O2 = (3/2 a1 – a2)

O1* = 1/3 b1 + ½ b2
O2* = 1/3 b1 – ½ b2



(c)

2 domain structure



Applications of LEED:

1. Surface order and cleanliness – most common
2. Surface atomic structure – need theory
3. Step density – get step height/density from angular beam profile (SPALLED)
4. Phase transition in overlayers - structure may undergo transition with change in coverage or T
5. Dynamics of ordering, disordering, growth, phase transitions - time evolution

Complications and other aspects of LEED:

1. Electron beam damage – sensitive molecular adsorbates
2. Domain structure

– if two domains with different structure coexist $\Rightarrow$ easy to distinguish

– sometimes difficulties exist (e.g., 3 domains of p(2x1) on fcc(111) = (2x2)

3. Transfer width (for real experimental system $\Delta\varphi$ ~0.01, ΔE~0.5eV)

- the dimensions of ordered regions on the surface are limited to the "transfer width" (Woodruff, p.36-37)

RHEED – Reflected High Energy Electron Diffraction

Elements of RHEED: high energy electrons (5-50keV); grazing incidence on crystalline sample; often in Molecular Beam Epitaxy (MBE) setups

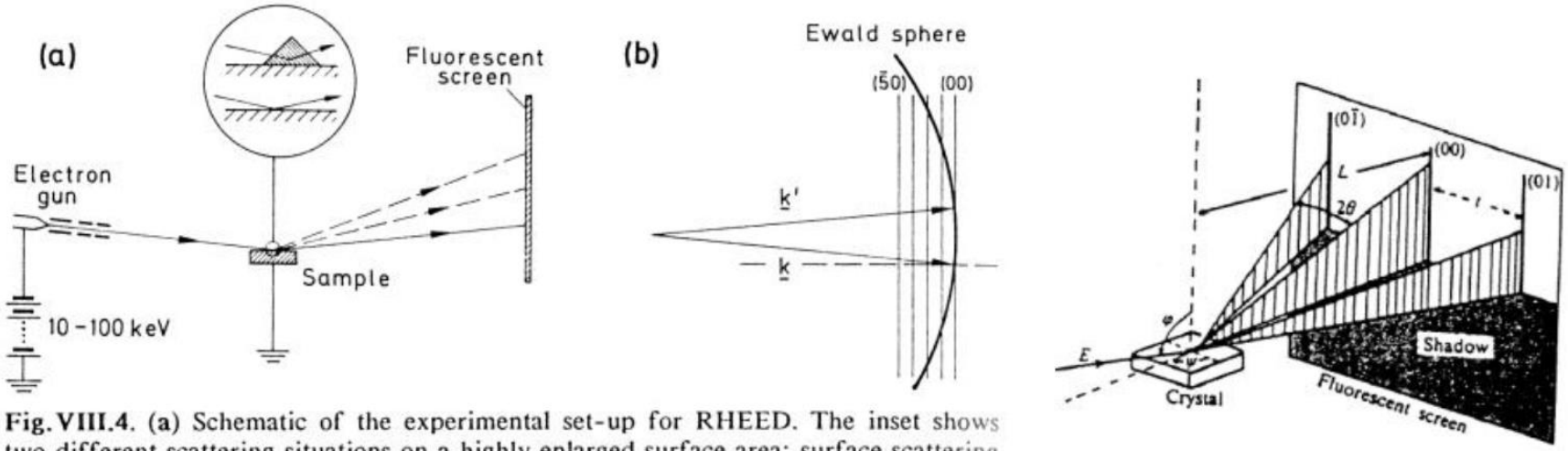


Fig. VIII.4. (a) Schematic of the experimental set-up for RHEED. The inset shows two different scattering situations on a highly enlarged surface area: surface scattering on a flat surface (below) and bulk scattering by a three-dimensional crystalline island on top of the surface (above). (b) The Ewald sphere construction for RHEED. k and k′ are primary and scattered wavevectors, respectively. The sphere radius k = k′ is much larger than the distance between the reciprocal lattice rods (hk). For more details, see Sect.4.2 and Figs.4.2,3

cf. Luth, pp.201-209

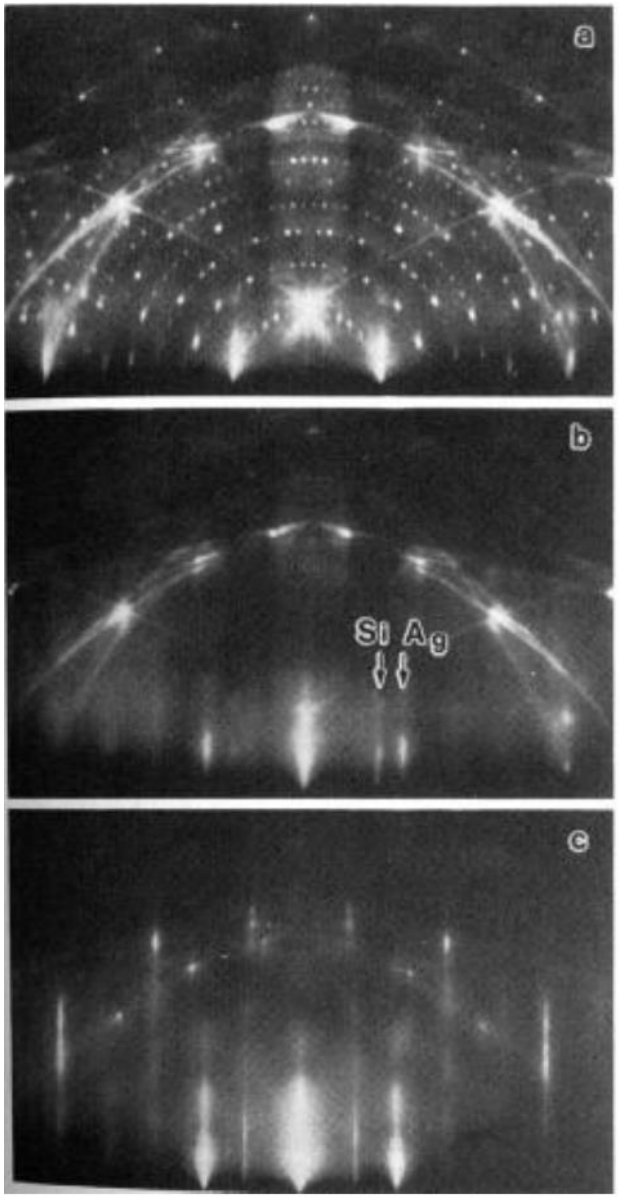
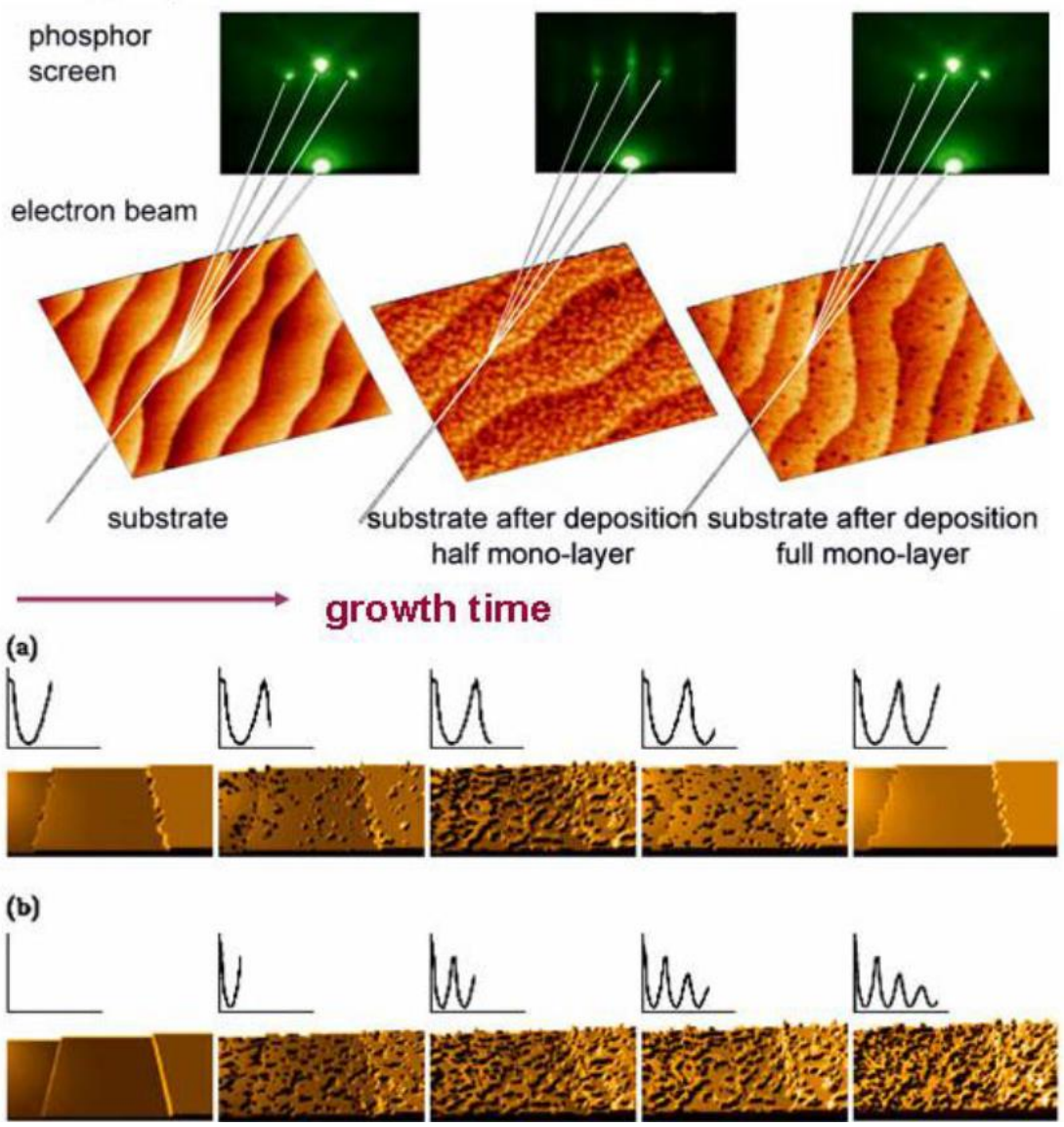


Fig. VIII.5a–c. RHEED patterns taken with a primary energy of E = 15 keV and a direction of incidence of [112] on a Si(111) surface: (**a**) Clean Si(111) surface with a (7×7) superstructure. (**b**) After deposition of nominally 1.5 monolayers (ML) of Ag streaks due to the Ag layers are seen on the blurred (7×7) structure. (**c**) After deposition of 3ML of Ag the texture structure due to the Ag layers develops in place of the (7×7) structure [VIII.3]

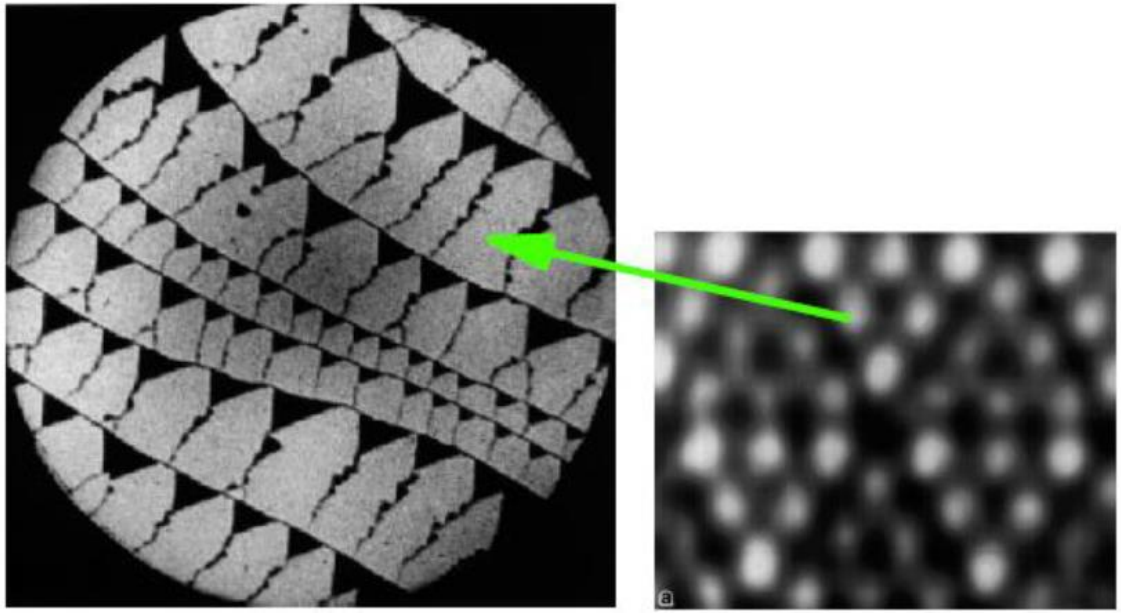

phosphor
screen
electron beam
substrate
substrate after deposition
half mono-layer
substrate after deposition
full mono-layer
growth time
(a)
(b)

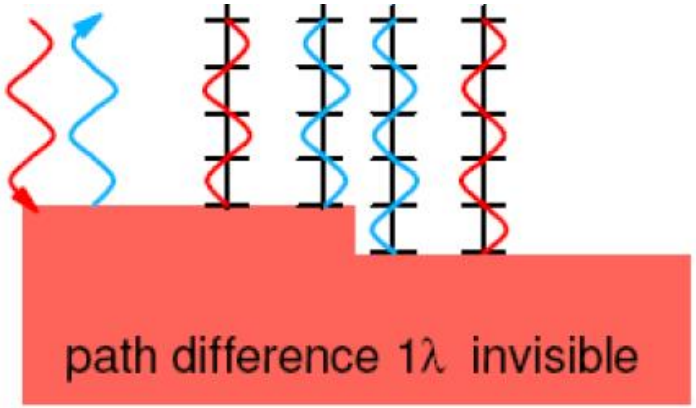
Comparison of Experimental Specs for LEED and RHEED

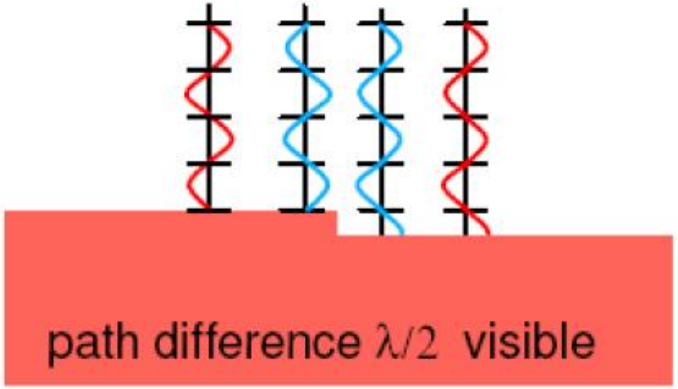
Range of elements:	all, but not element specific	both
Destructive:	no, except in special cases of electron-beam damage	both
Depth probed:	4-20Å (LEED) 2-100Å (RHEED)	
Detection limits:	0.1ML; atomic positions to 0.1Å	both
Resolving power:	typically 200Å; best systems 5μm	both
Lateral resolution:	typically 0.1mm; best systems ~10μm (LEED)	
	200μm x 4mm; best systems 0.3nm x 6 nm (RHEED)	
Imaging capability:	no; need special instruments – LEEM	
Main uses:	analysis of surface crystallography (LEED)	
	monitoring surface structure, in-situ growth (RHEED)	

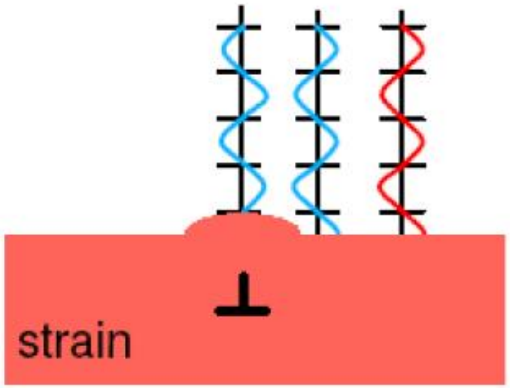
LEEM – Low Energy Electron Microscopy

- 1962 Invention by Ernst Bauer
- 1985 Operational LEEM instrument (Telieps and Bauer)
- 1991 IBM LEEM-I (Tromp and Reuter)
- 1998 IBM LEEM-II
- 2006 SPECS FE-LEEM P90

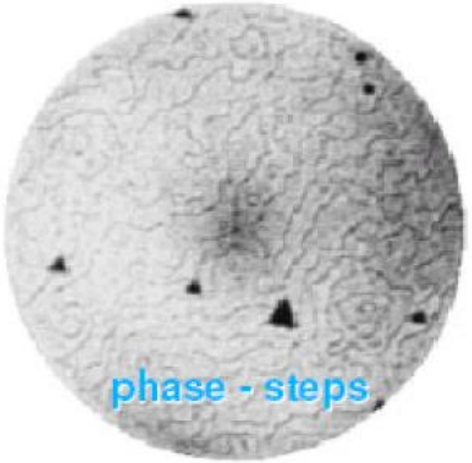




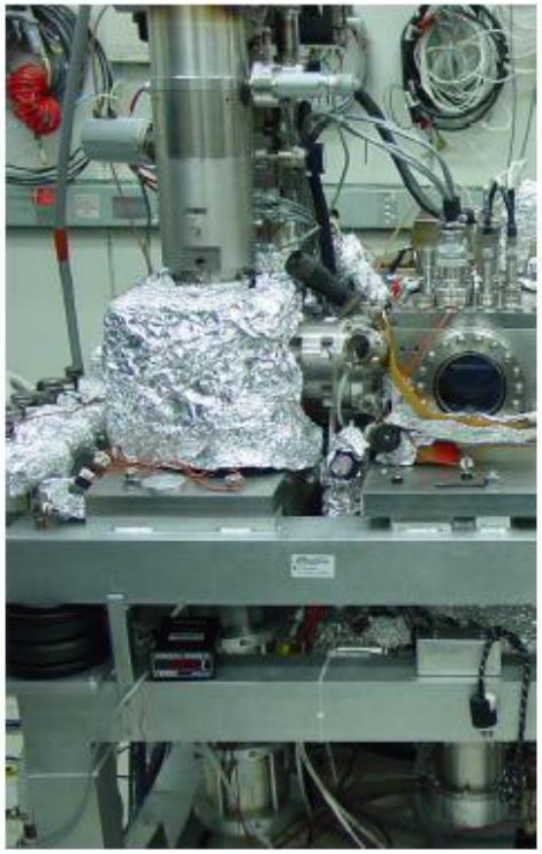


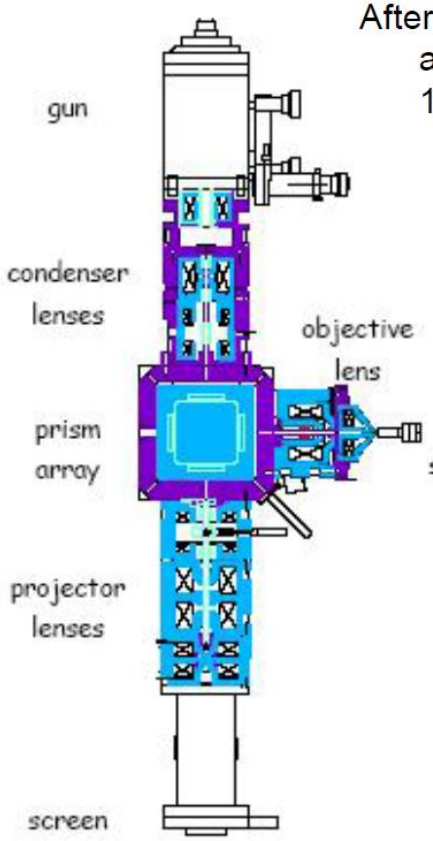


Si(111) CaF_2
Surface

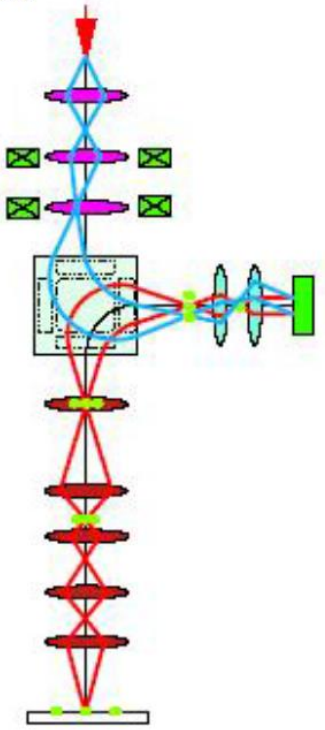


Si(111) CaF_2
Interface





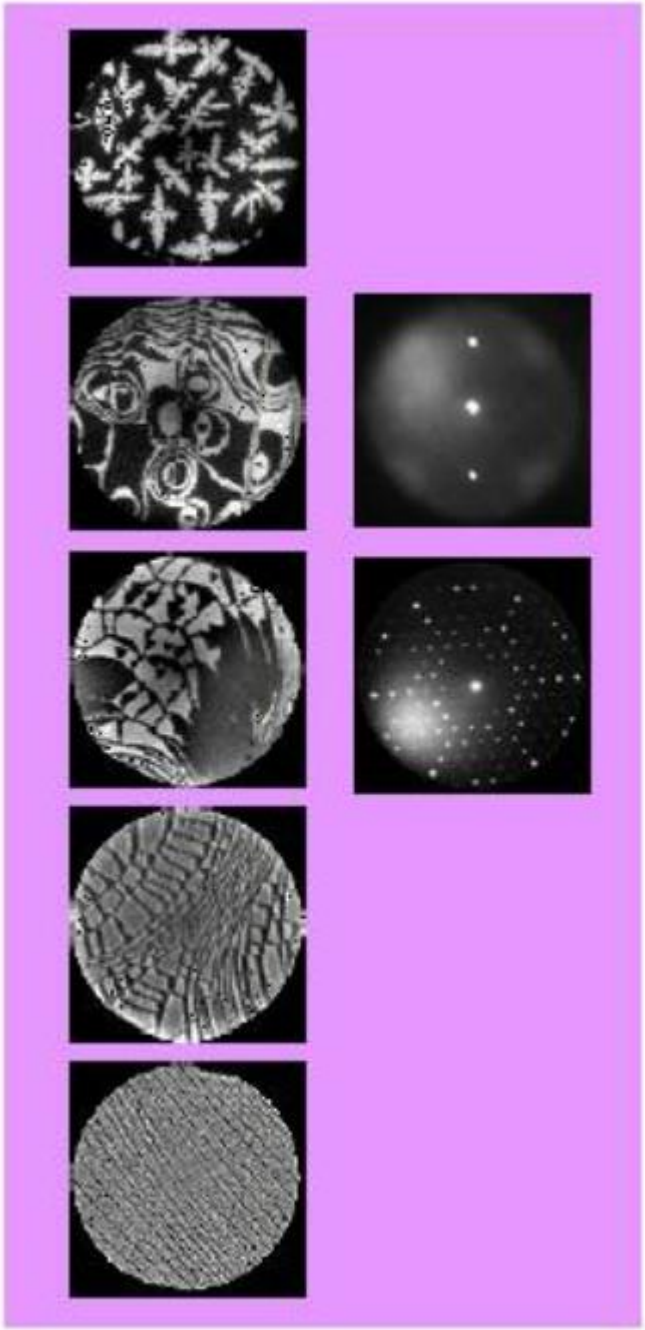
After diffraction, electrons are accelerated from ~ 1 eV to ~ 10,000 eV



Surf. Reviews and Lett. 5 (1998) 1189

- 0 - 100 eV electron energy
- field of view 1 - 100 µm
- 5 nm resolution in plane
- vertical resolution: atomic steps, 0.1 nm
- in situ growth, etching
- RT – 1200°C

⇒ extremely useful tool to study crystal growth in situ

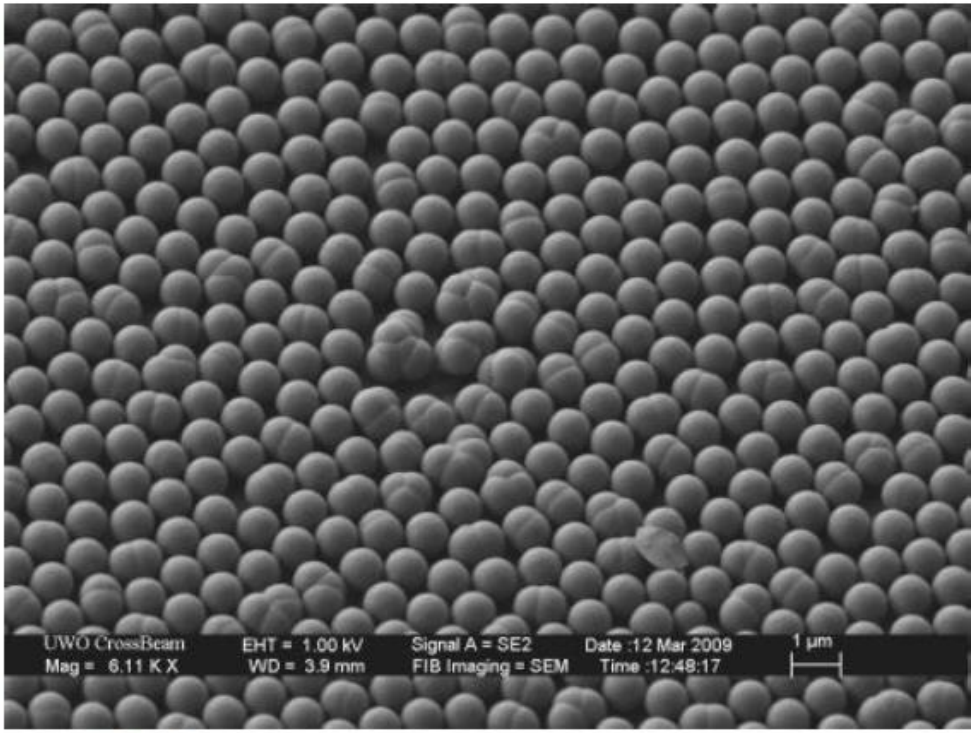


http://www.research.ibm.com/leem/

Scanning electron microscopy (SEM)

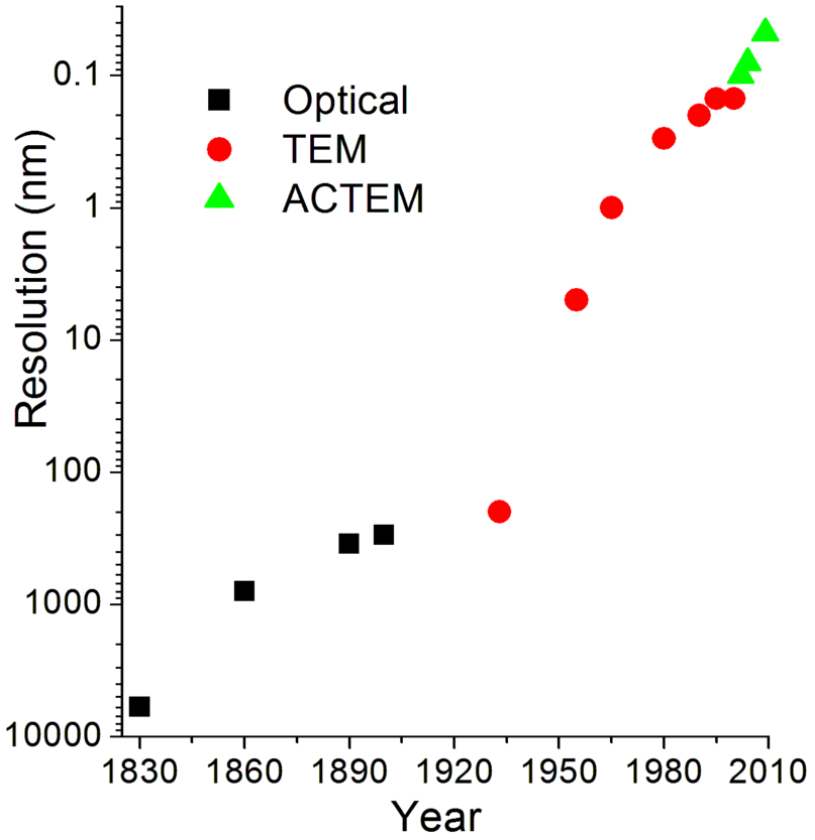
- topology, morphology, chemical information (BSE and EDX)

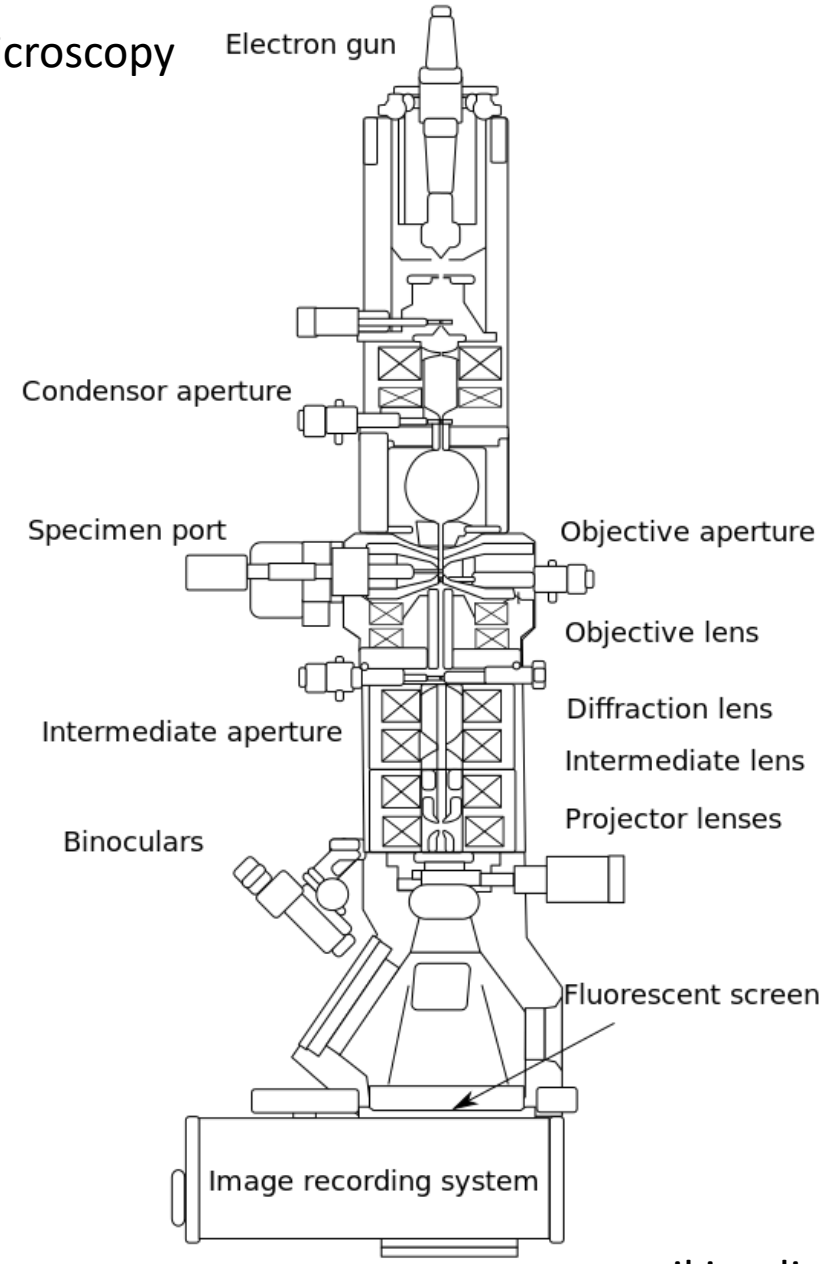
- 0.5-1000keV electron energy
- field of view 0.1 - 100 μm
- 5 nm resolution in plane
- Magnification 10x – 300,000x
- Typical operating pressure <1atms
- Non-destructive nature: though sometimes electron beam irradiation can cause sample damage



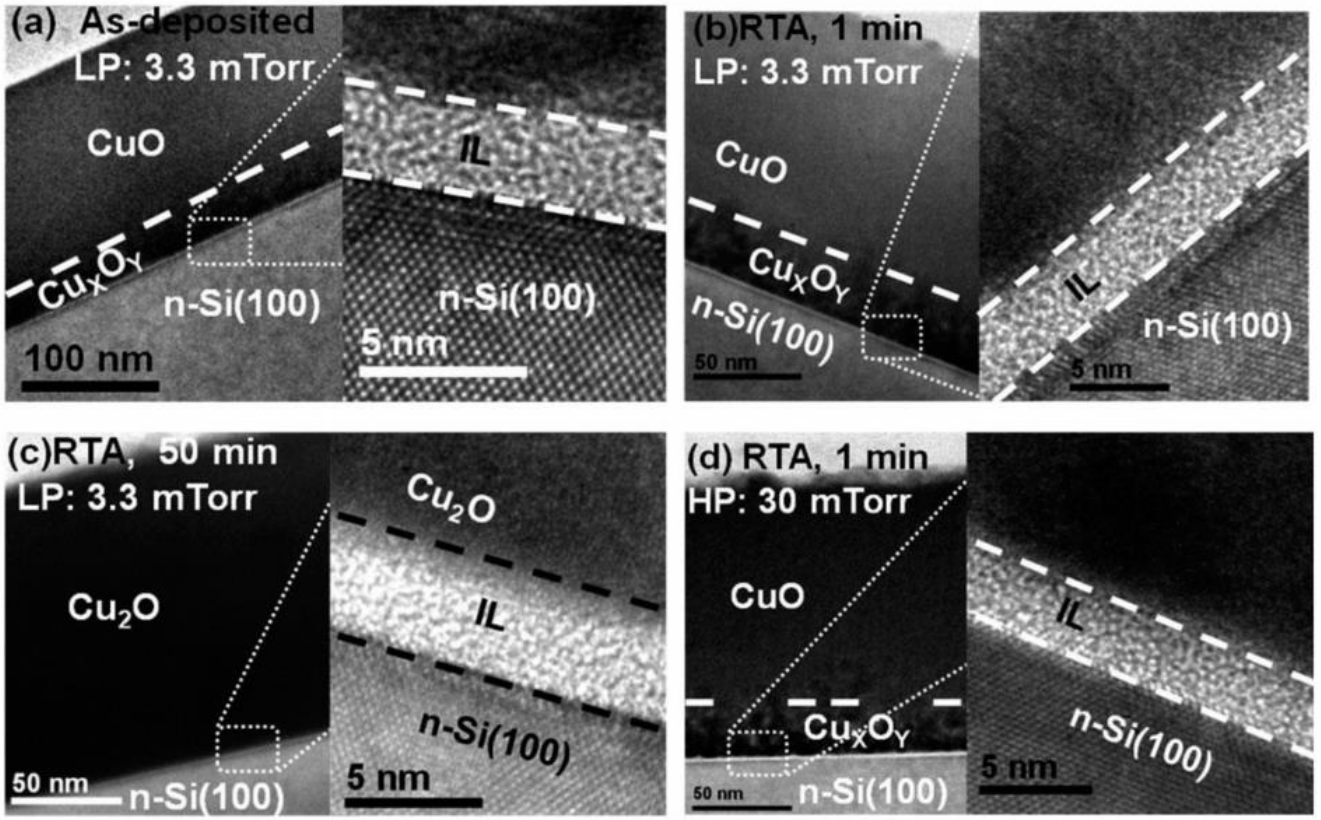
by Eric Barbagiovanni

TEM – Transmission Electron Microscopy

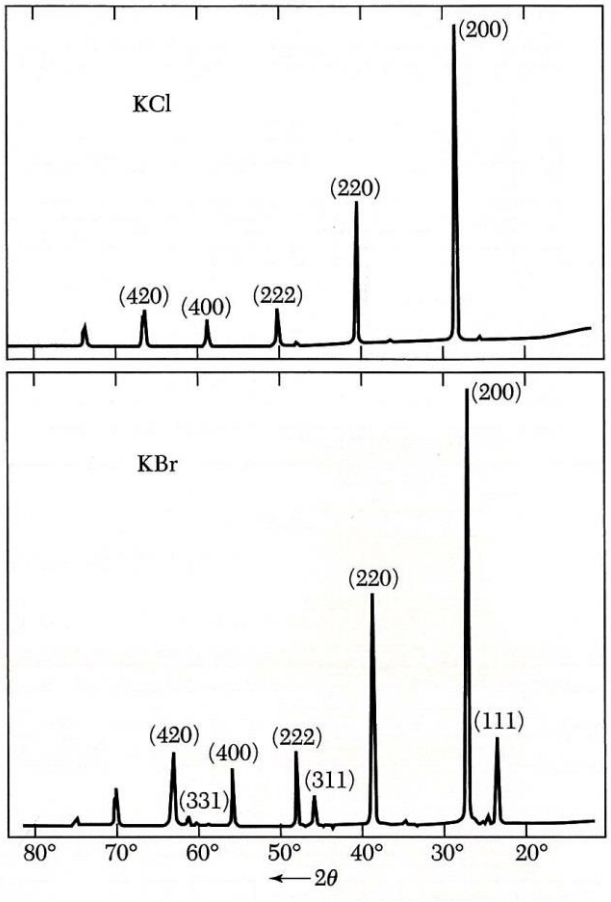




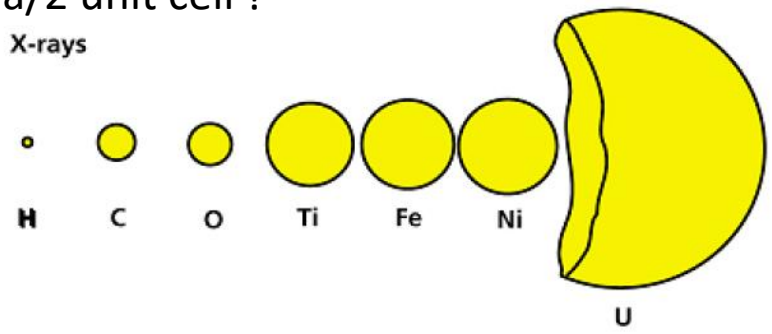
wikipedia


(a) As-deposited
LP: 3.3 mTorr
CuO
Cu_xO_Y
n-Si(100)
100 nm
IL
n-Si(100)
5 nm
(b)RTA, 1 min
LP: 3.3 mTorr
CuO
Cu_xO_Y
n-Si(100)
50 nm
IL
n-Si(100)
5 nm
(c)RTA, 50 min
LP: 3.3 mTorr
Cu_2O
50 nm
n-Si(100)
Cu_2O
IL
n-Si(100)
5 nm
(d) RTA, 1 min
HP: 30 mTorr
CuO
Cu_xO_Y
50 nm
n-Si(100)
IL
n-Si(100)
5 nm

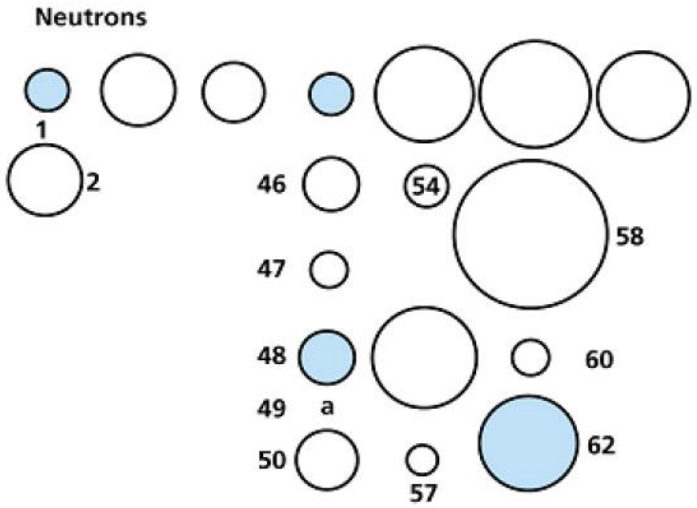
XRay Scattering (see previous lectures)
vs.
Neutron Scattering



Looks like sc with a/2 unit cell !



Looks like fcc !



Wavelength of Neutrons

Room Temperature Neutrons

$K_{translation} = \frac{1}{2} mv^2 = 3/2\ kT = 6 \times 10^{-21} J$ (@T= 293K)

$v = 2.7 \times 10^3$ m/s

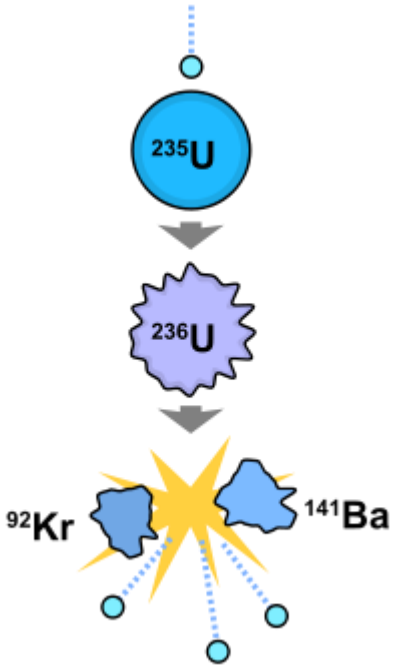
$p = mv = 4.5 \times 10^{-24}$ kg m / s

de Broglie Wavelength

$\lambda = h/p = 0.147$ nm

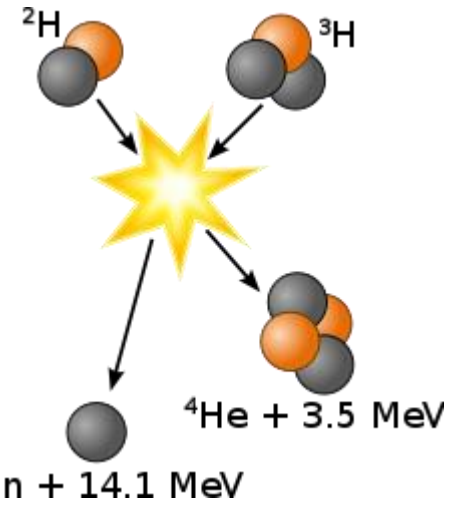
Neutron Source

Nuclear Fission

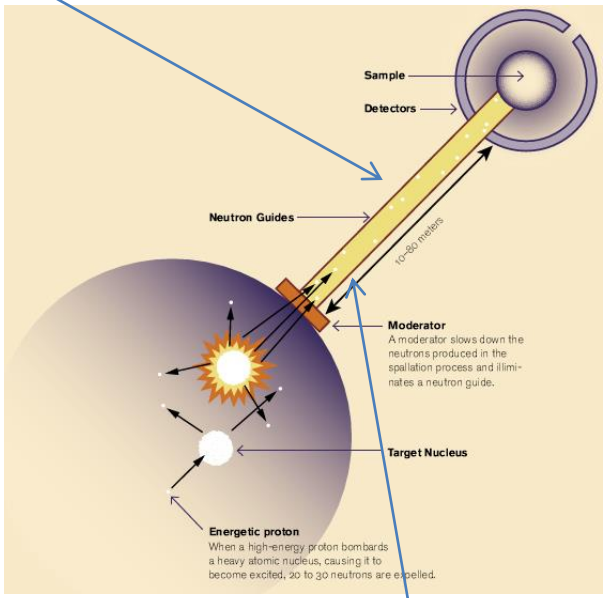


(a) pulsed source
=> time correlates with v

Nuclear Fusion



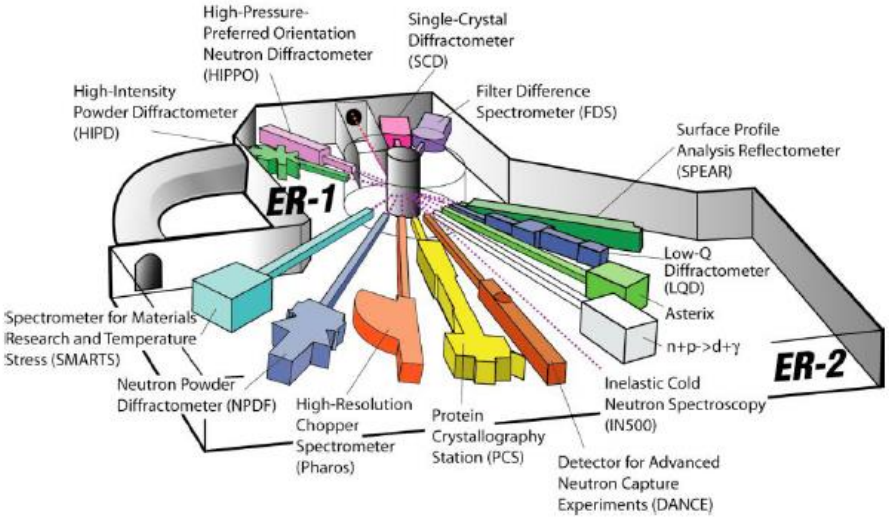
Spallation Source



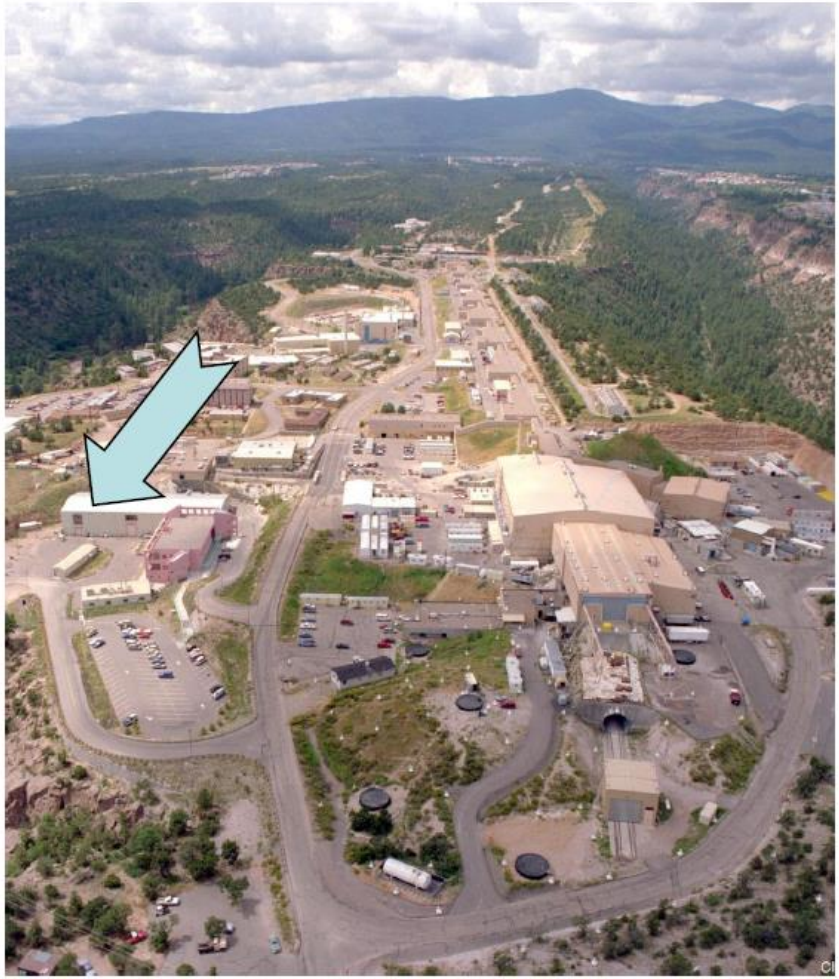
(b) scattering at crystal
$\Rightarrow$ Bragg Reflection to select wavelength

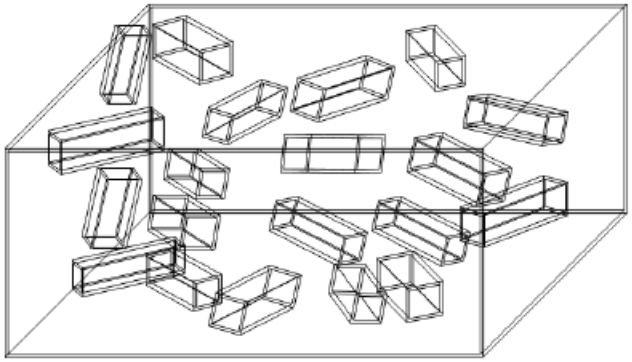
Los Alamos
NATIONAL LABORATORY
EST. 1943

Operated by the Los Alamos National Security, LLC for the DOE/NNSA

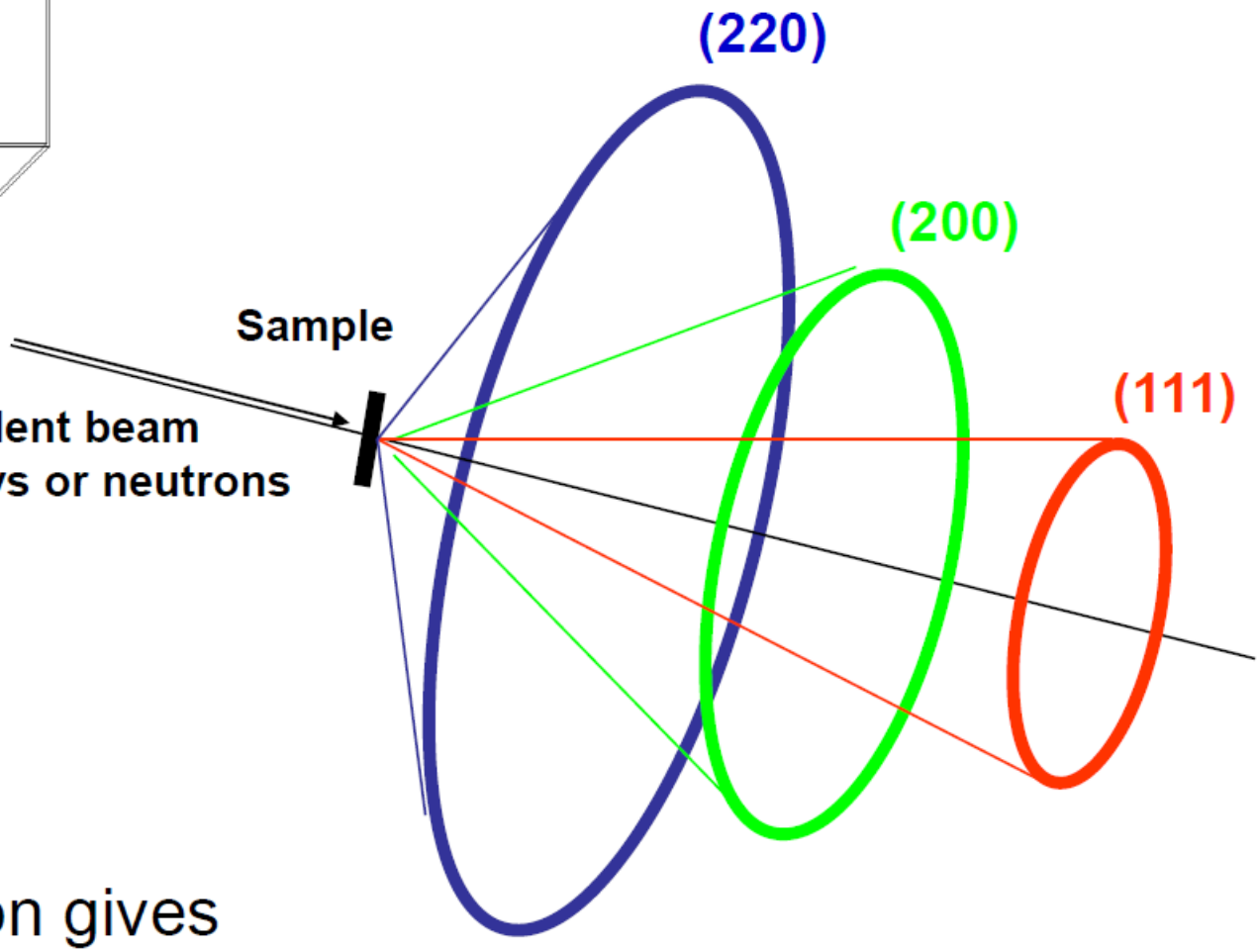


NPDF
Flightpath 1

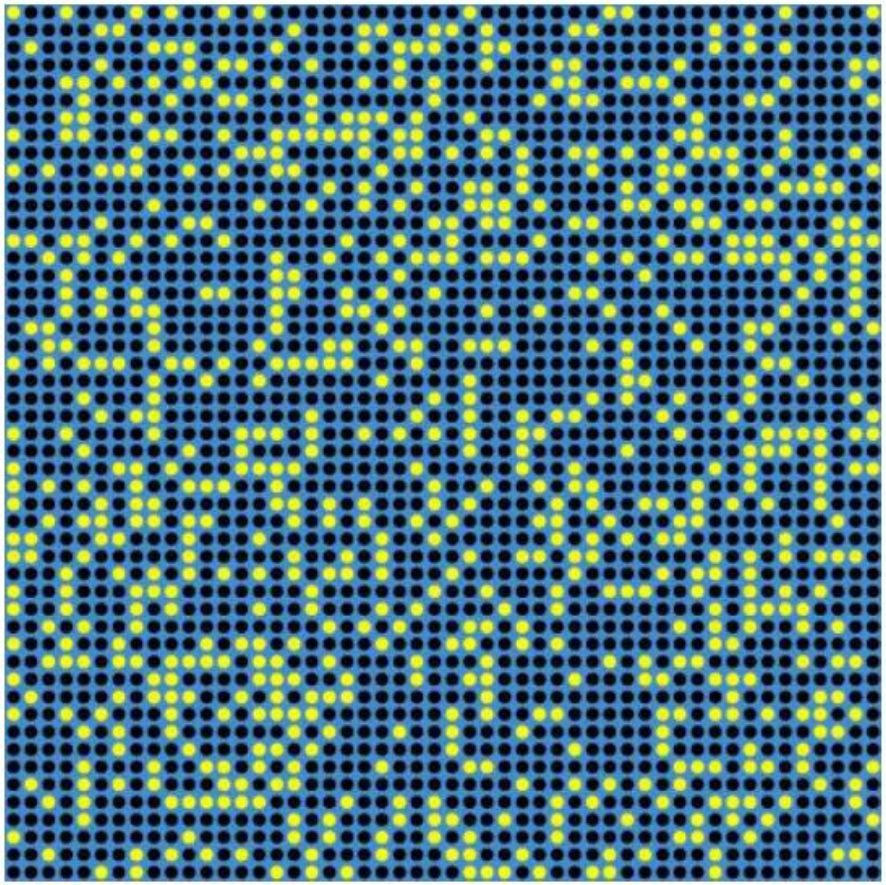


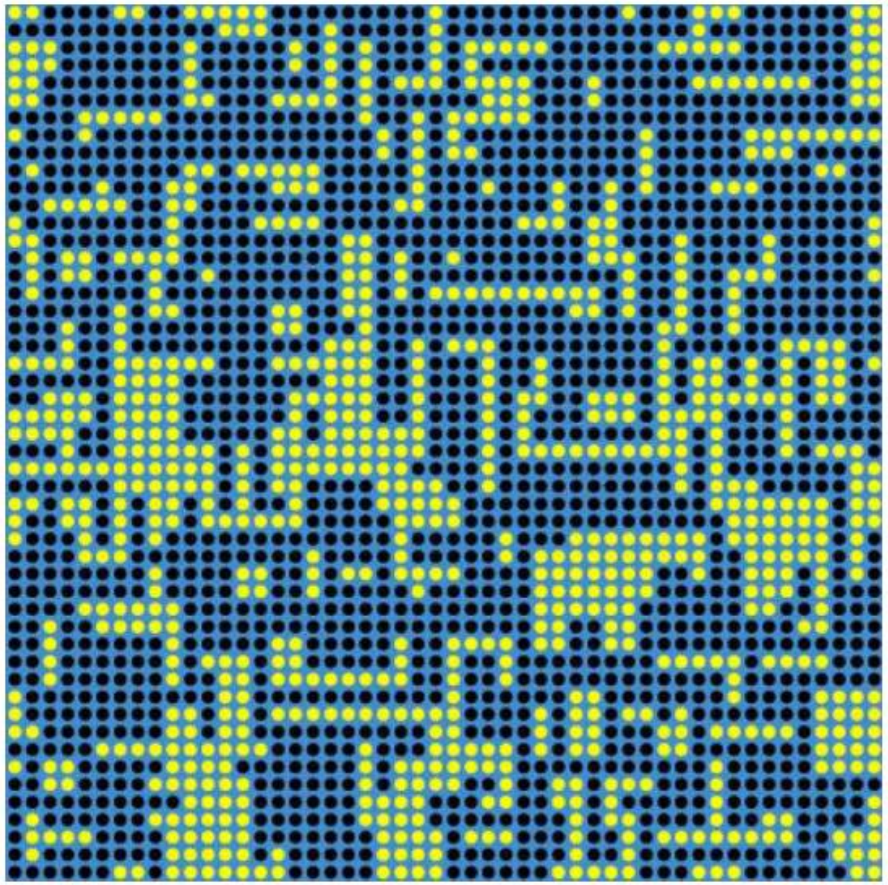


All orientations of crystallites possible.



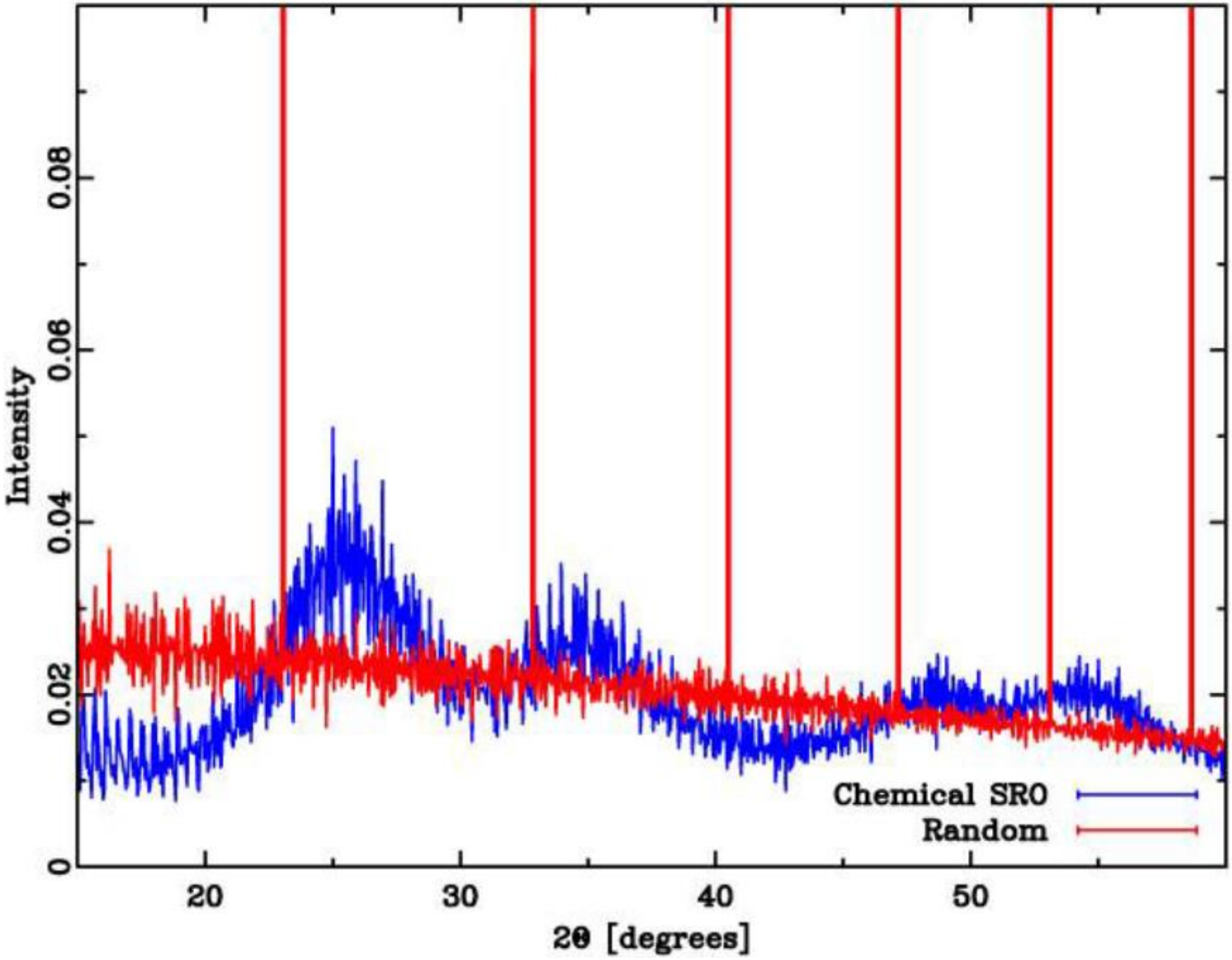
- Powder Diffraction gives
- Scattering on Debye-Scherrer Cones

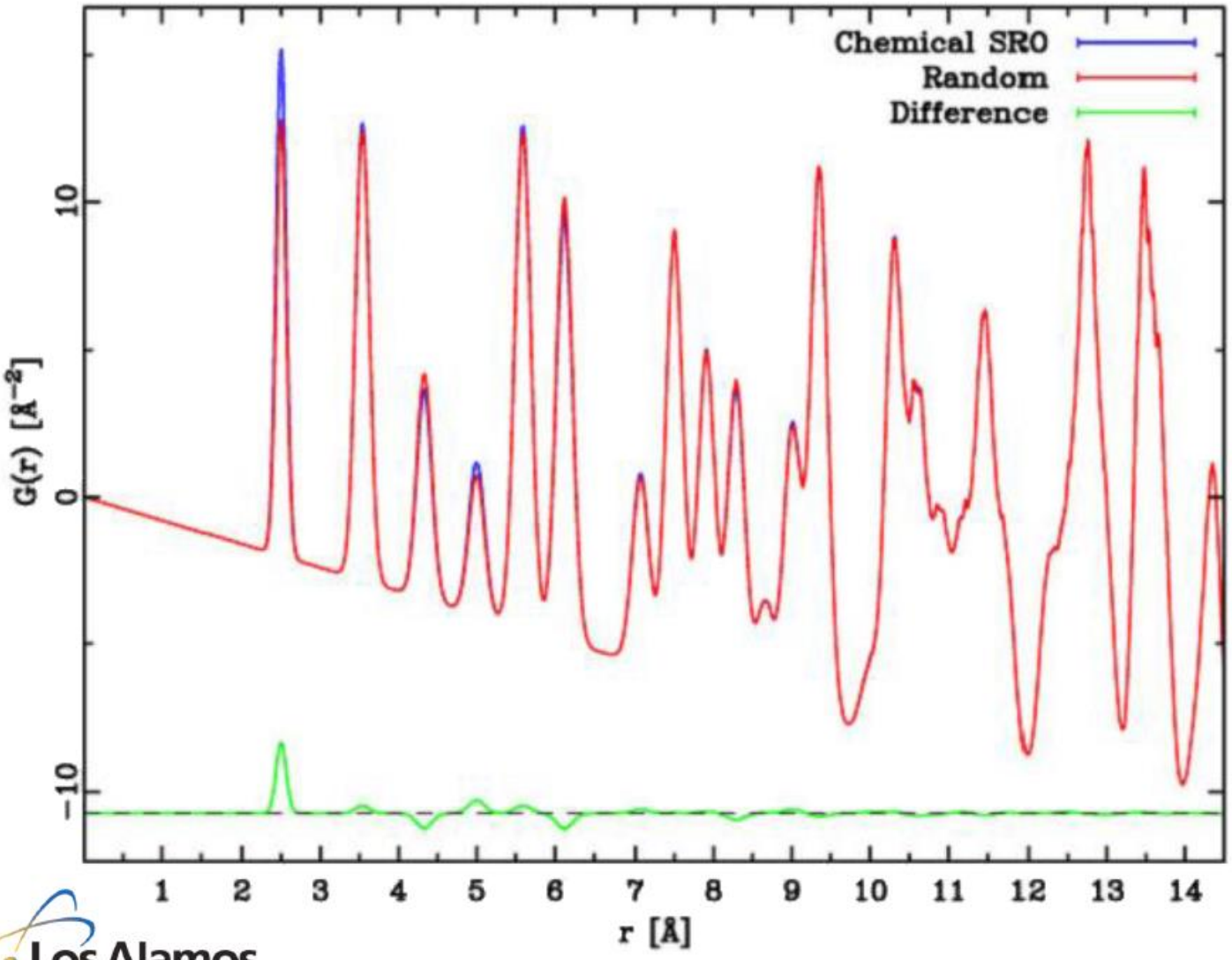




Cross section of 50x50x50 u.c. model crystal consisting of 70% black atoms and 30% *vacancies* !

Properties might depend on vacancy ordering !!


Intensity
0
0.02
0.04
0.06
0.08
20
30
40
50
2θ [degrees]
Chemical SRO
Random

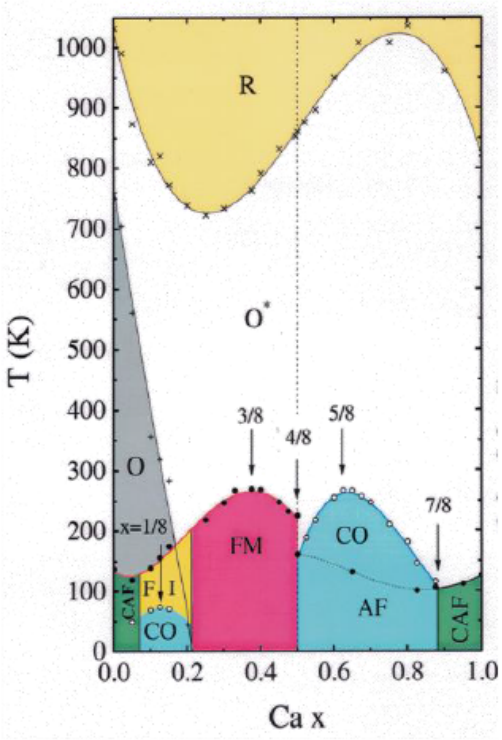


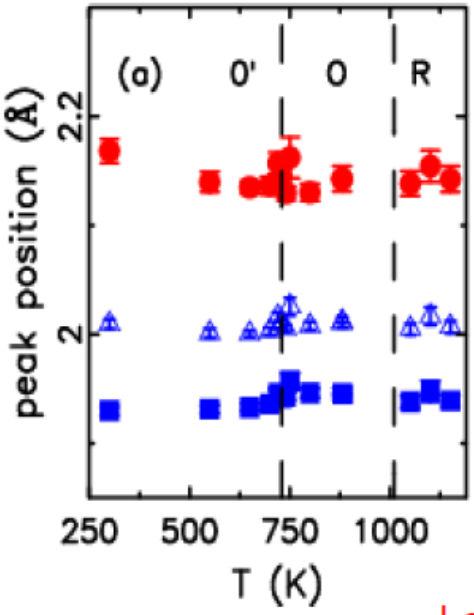
The PDF is the Fourier transform of the total scattering diffraction pattern !

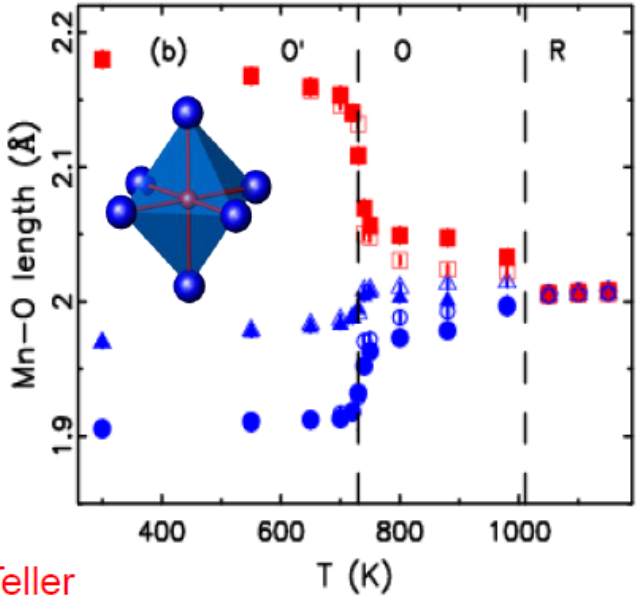
Proffen, *Z. Krist*, **215**, 661 (2000)

Los Alamos

$LaMnO_3$: Jahn-Teller distortion







Jahn Teller
Long Mn-O bond

Local structure

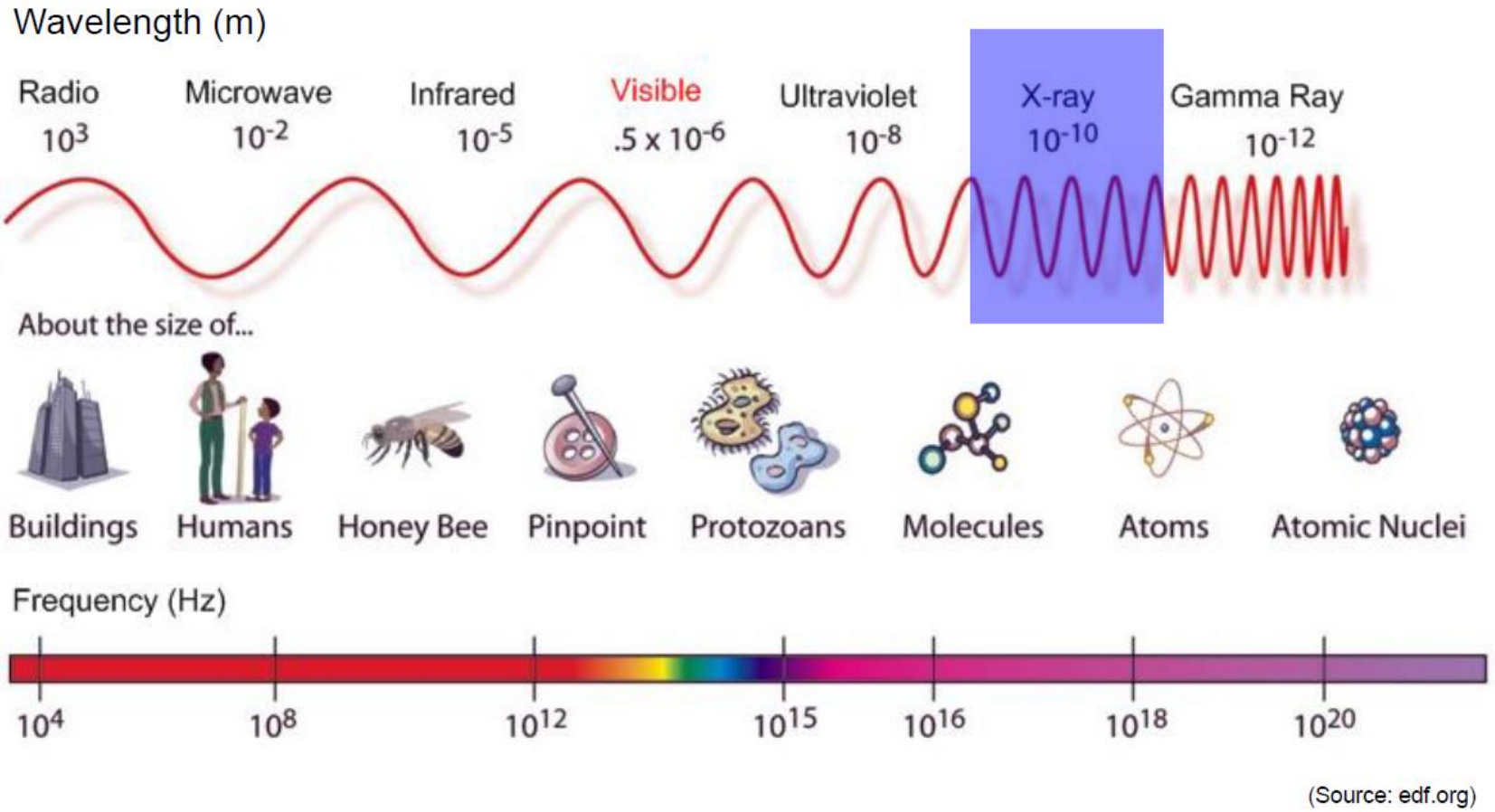
Average structure

- Mn-O bond lengths are invariant with temperature, right up into the R-phase
- JT distortions persist locally in the pseudocubic phase
- Agrees with XAFS result: M. C. Sanchez et al., PRL (2003).

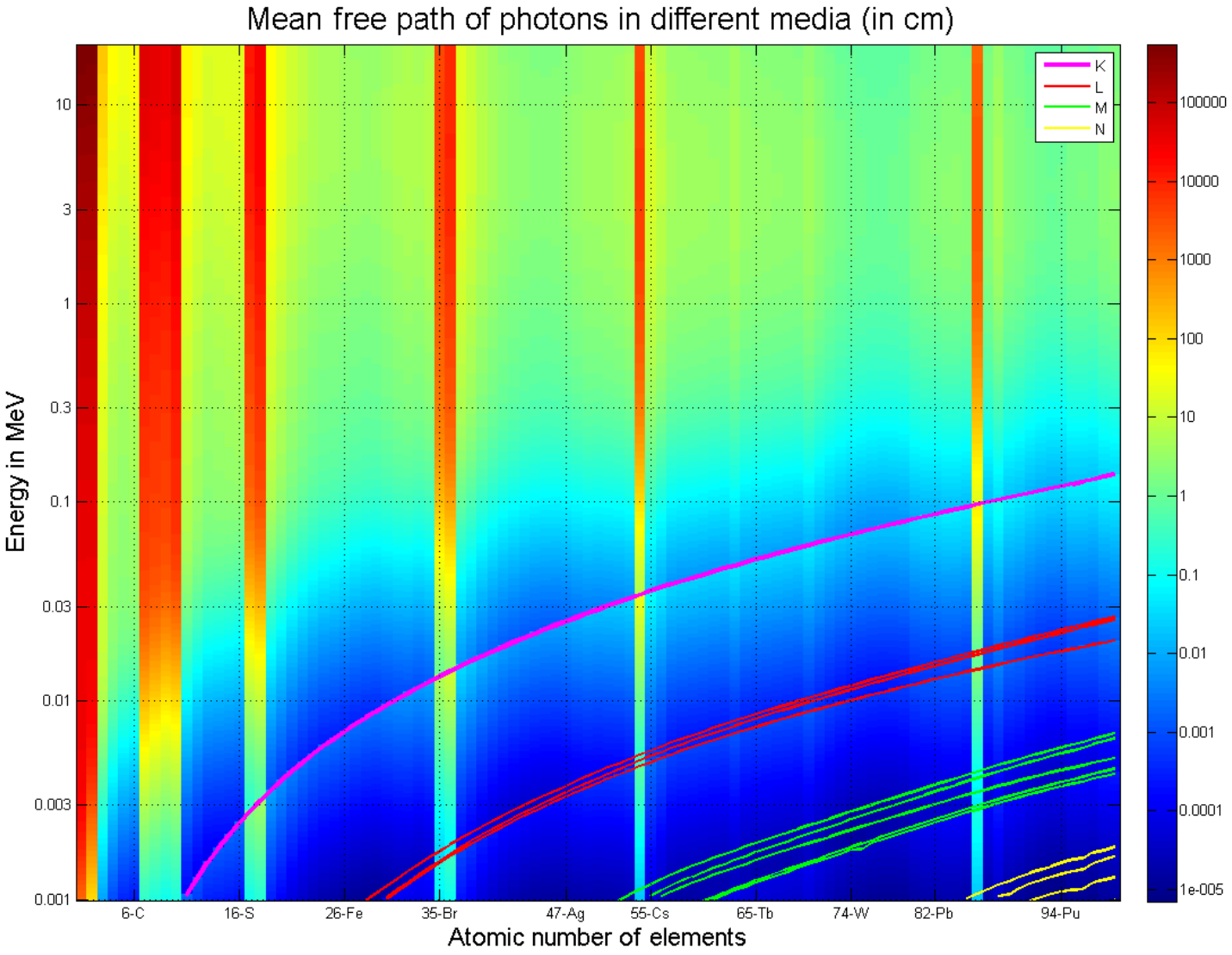
Last but not least

Neutrons have a magnetic moment – and can image magnetic ordering

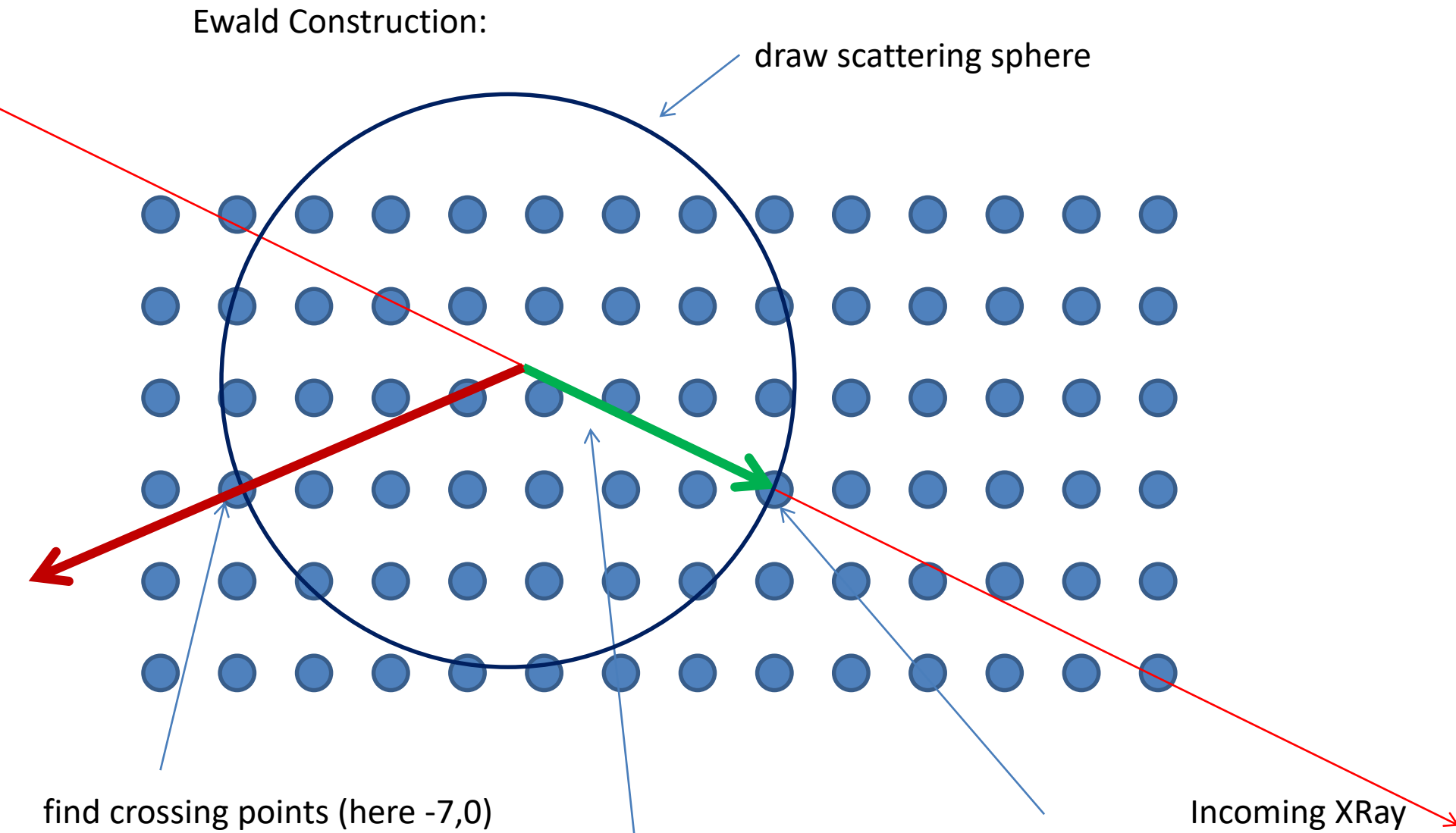
Let us go back to XRay Scattering



(Source: edf.org)

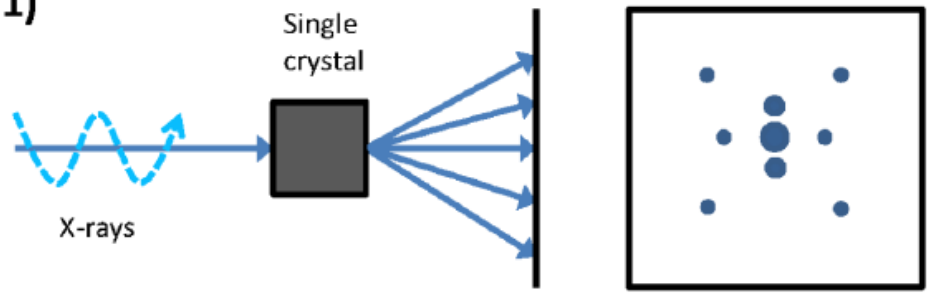

Mean free path of photons in different media (in cm)
Energy in MeV
10
3
1
0.3
0.1
0.03
0.01
0.003
0.001
6-C
16-S
26-Fe
35-Br
47-Ag
55-Cs
65-Tb
74-W
82-Pb
94-Pu
Atomic number of elements
K
L
M
N
100000
10000
1000
100
10
1
0.1
0.01
0.001
0.0001
1e-005

Ewald Construction:

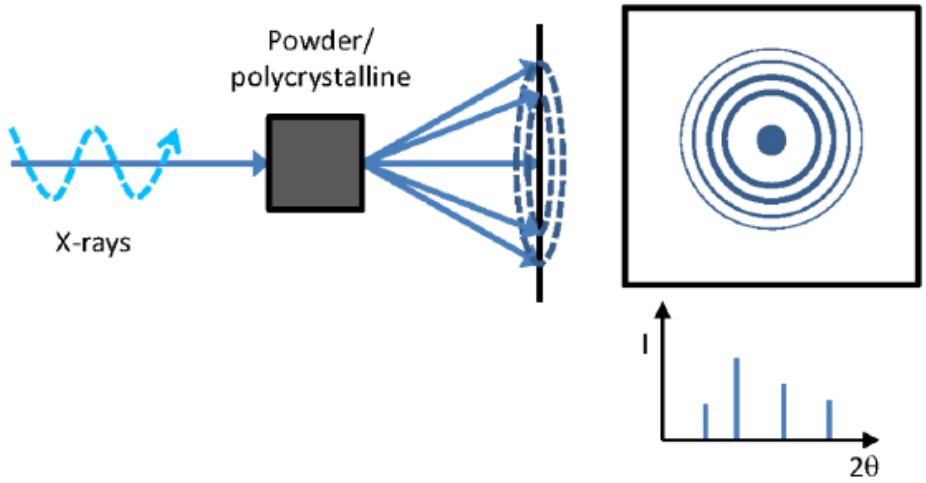


Problem: Not many crossing points can be found !

1)



2)

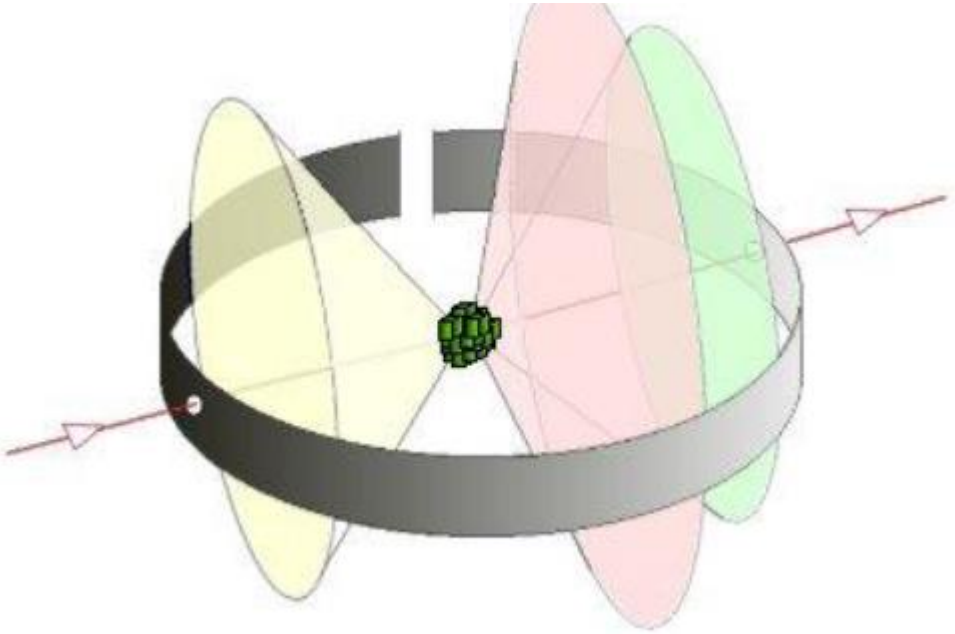


Single crystals

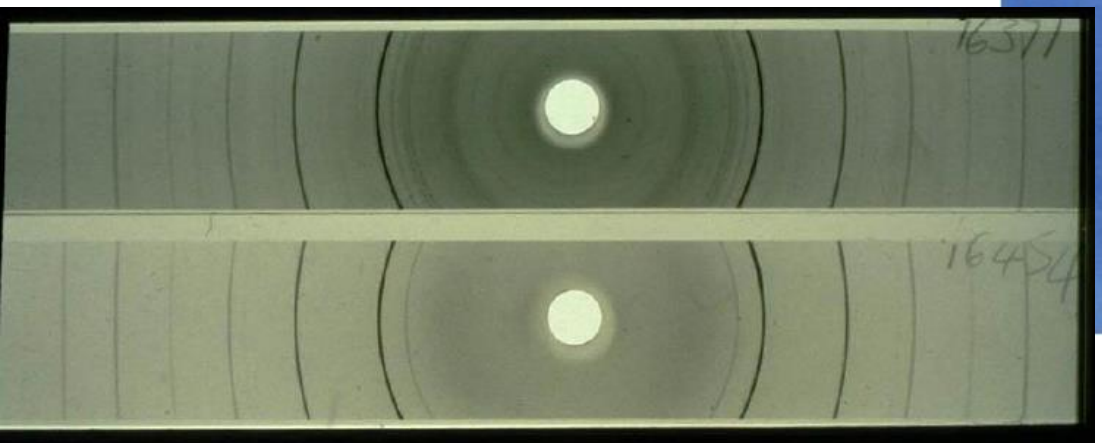
- X-rays diffracted from a single crystal produce single spots which are well resolved
- due to the orientation effects reflections are missing from lattice planes which are not in reflection condition (Bragg´s Law)

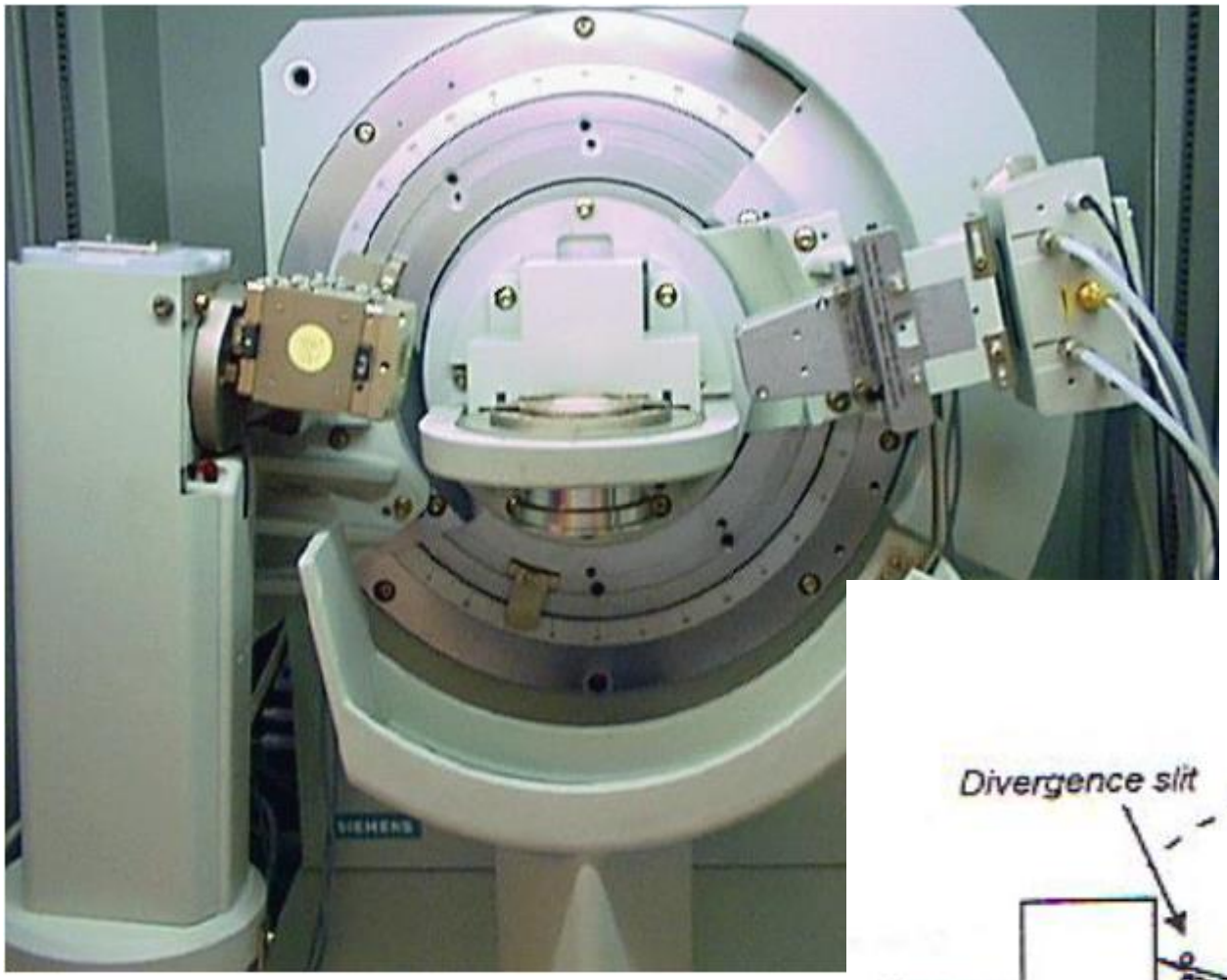
Polycrystalline powder

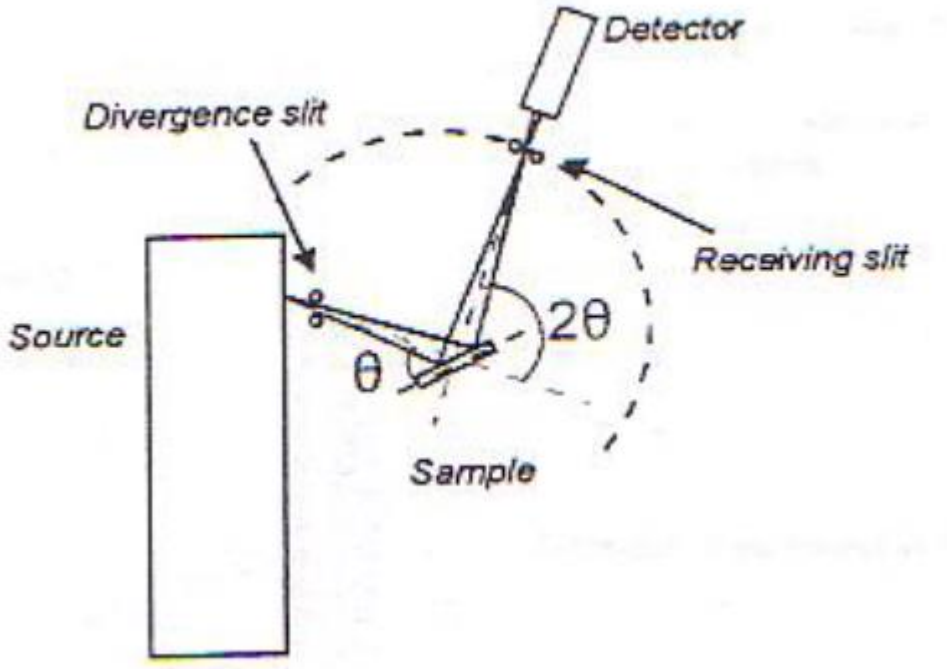
- all orientations present -> continous „Debye“ diffraction rings
- spots are not resolved and superimposed



Debye-Scherrer camera

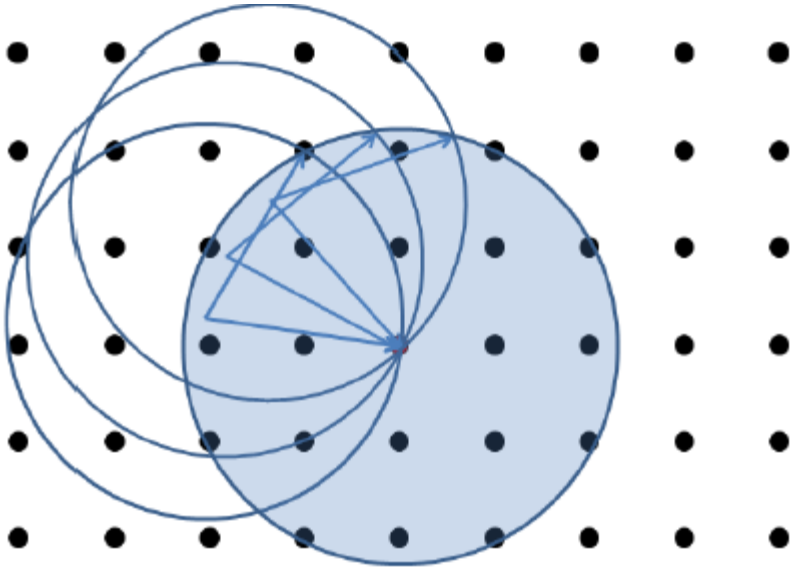


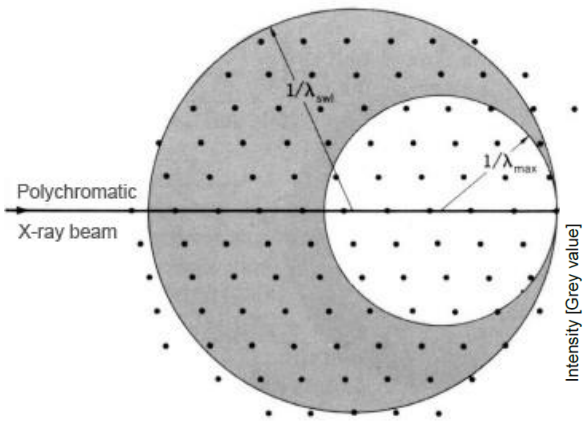


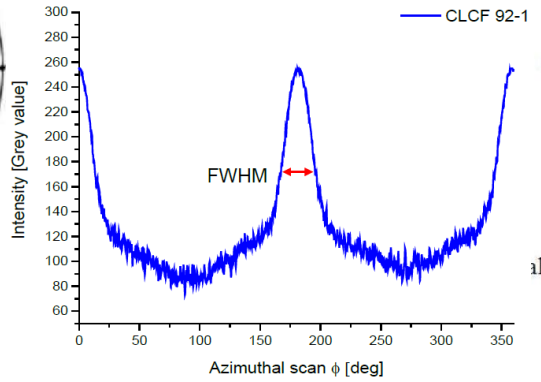


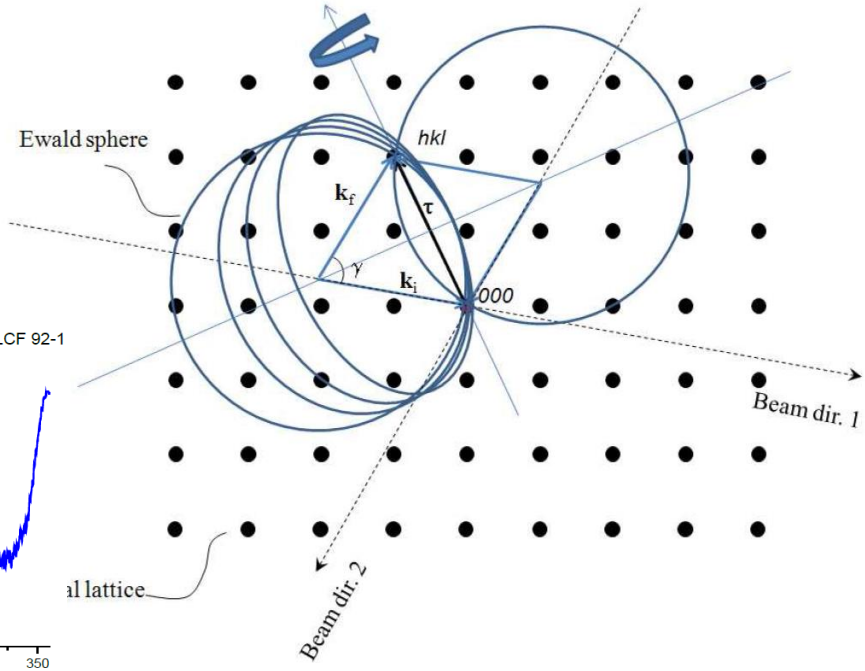
Powder Diffractometer

- Rotate Sample in plane
- Rotate Sample along a scattering axis (azimuthal scan)
- Use a wavelength range (Laue method)



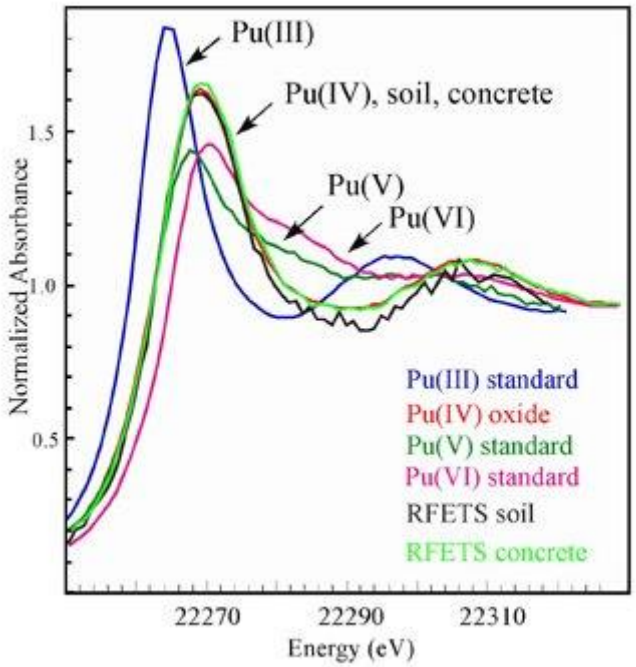




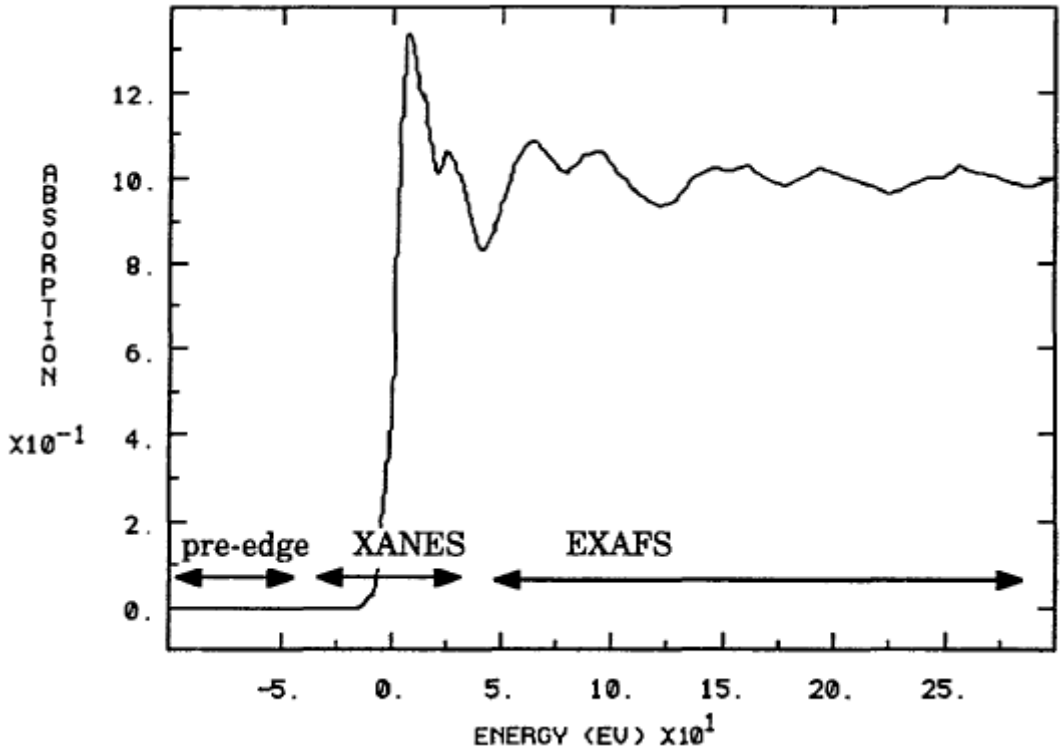


EXAFS - edge X-ray absorption fine structure

NEXAFS - near edge X-ray absorption fine structure /
XANES - X-ray absorption near edge structure



wikipedia



Chapter 3

X-Ray Absorption Spectroscopy: EXAFS and XANES - A Versatile Tool to Study the Atomic and Electronic Structure of Materials

E. E. Alp, S. M. Mini, and M. Ramanathan

EXAFS

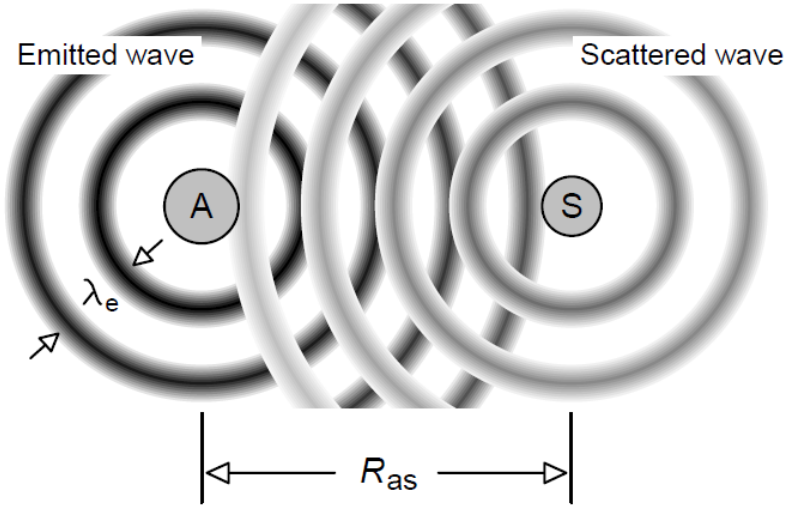


Figure 1.3 A photoelectron wave emitted from the absorbing atom (A) is back-scattered by a scattering atom (S). The back-scattered wave modifies the final-state wavefunction at the absorber. If the emitted and back-scattered waves are in phase, the wavefunction is increased. If the emitted and back-scattered waves are out of phase, the wavefunction is decreased.