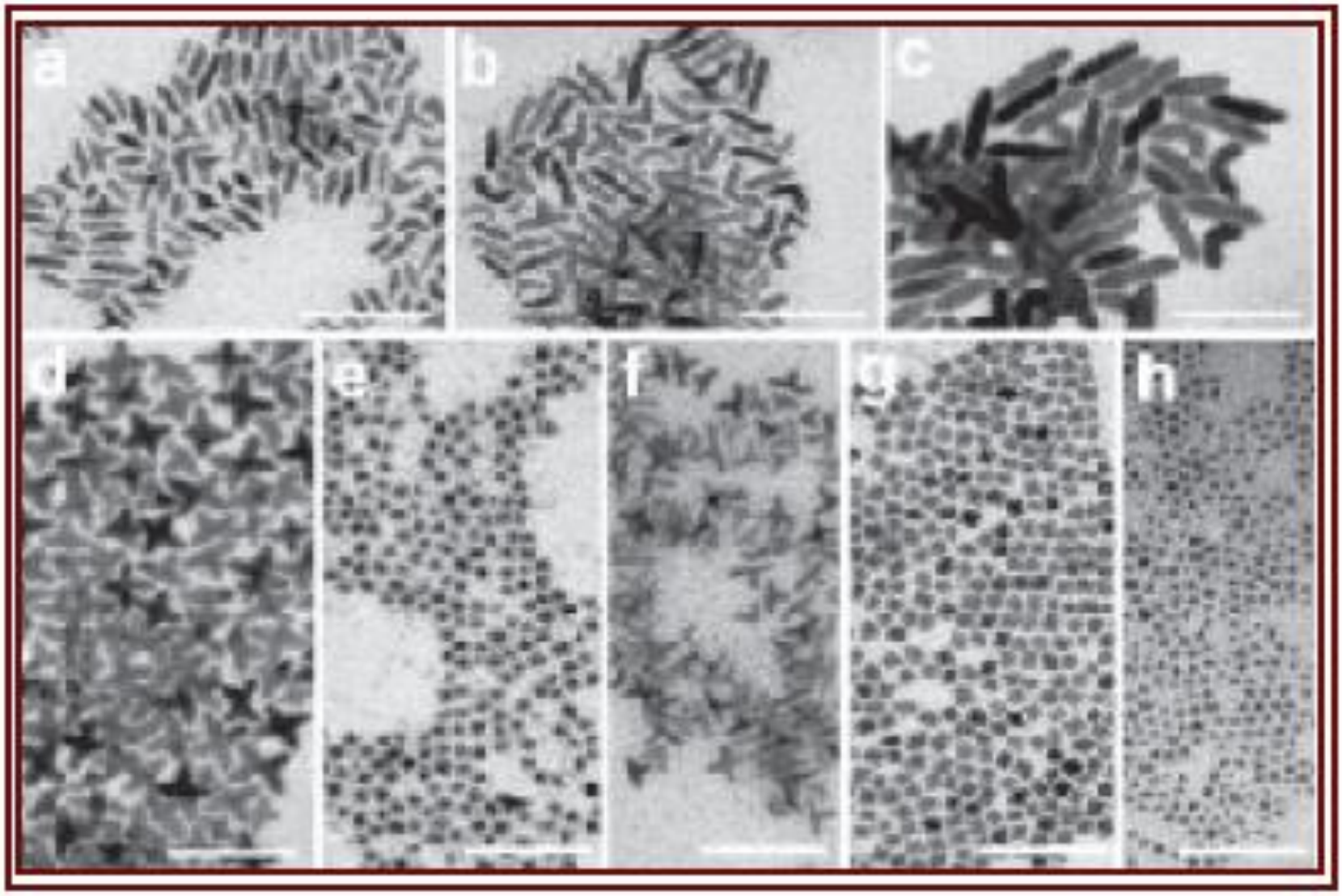
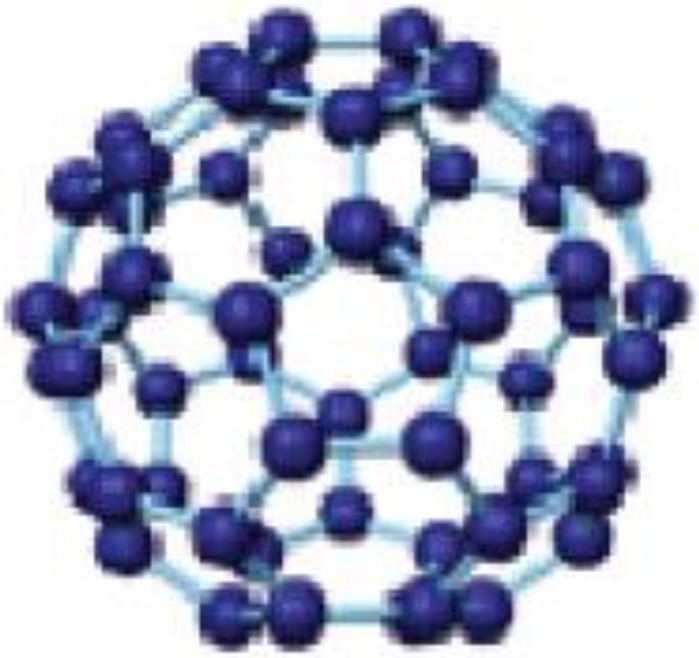
الخواص الفيزيائية للمواد النانوية

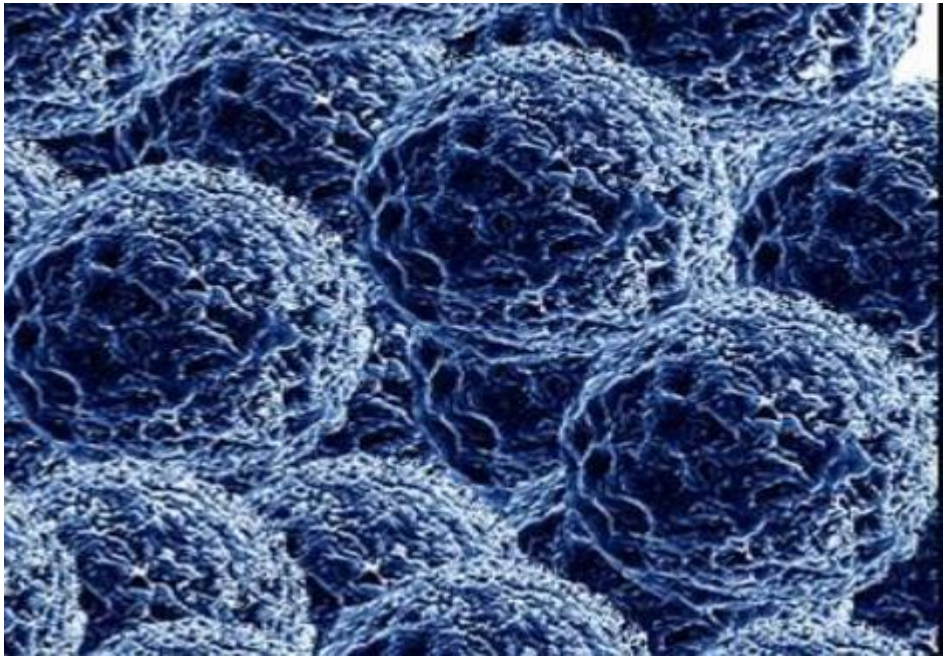
الخصائص الشكل مورفولوجيا

Figure 1: Echelle



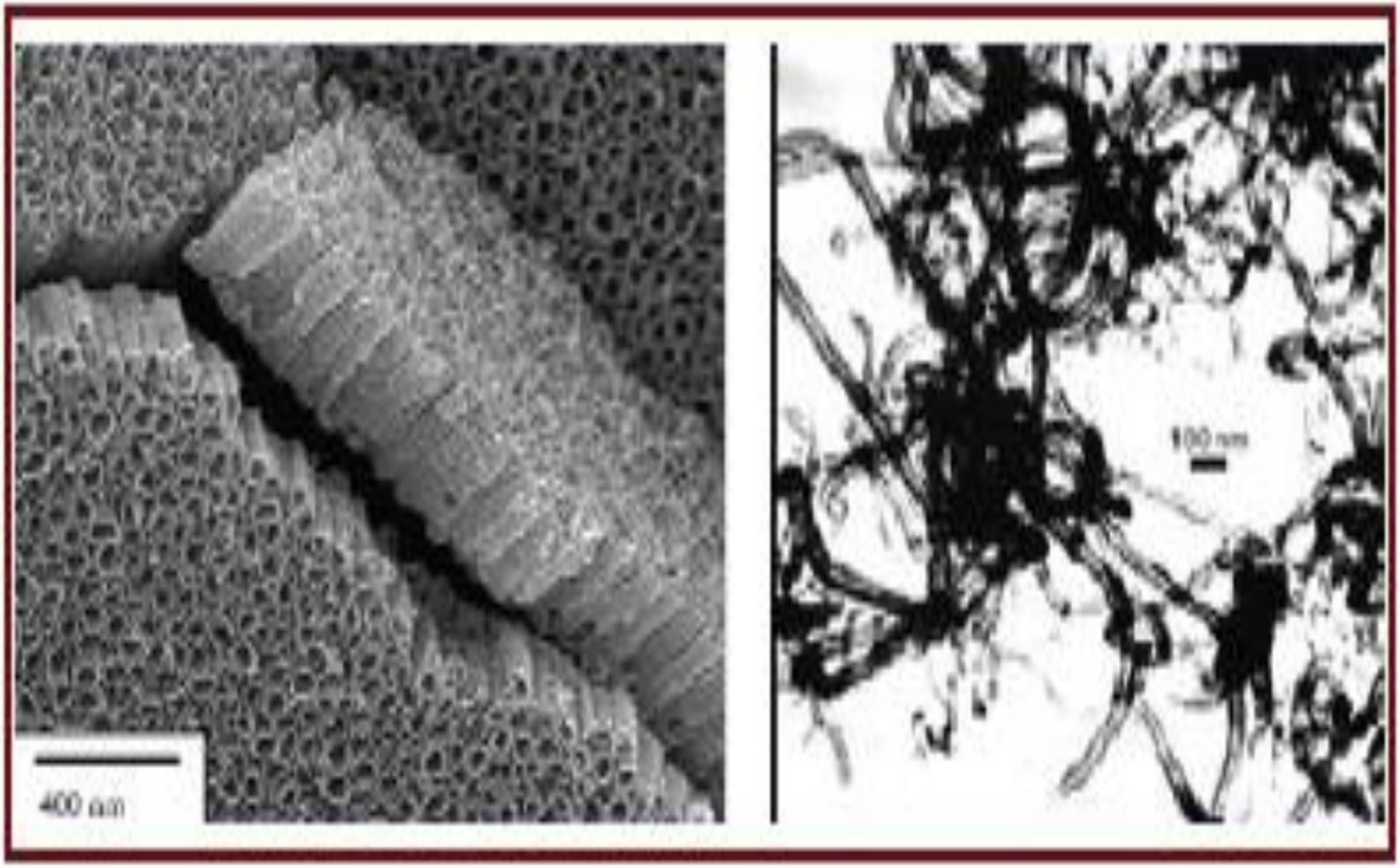
أحجام وأشكال مختلفة (مكعب، نجمي، كروي) لحبيبات نانو مصنوعة من PbSe



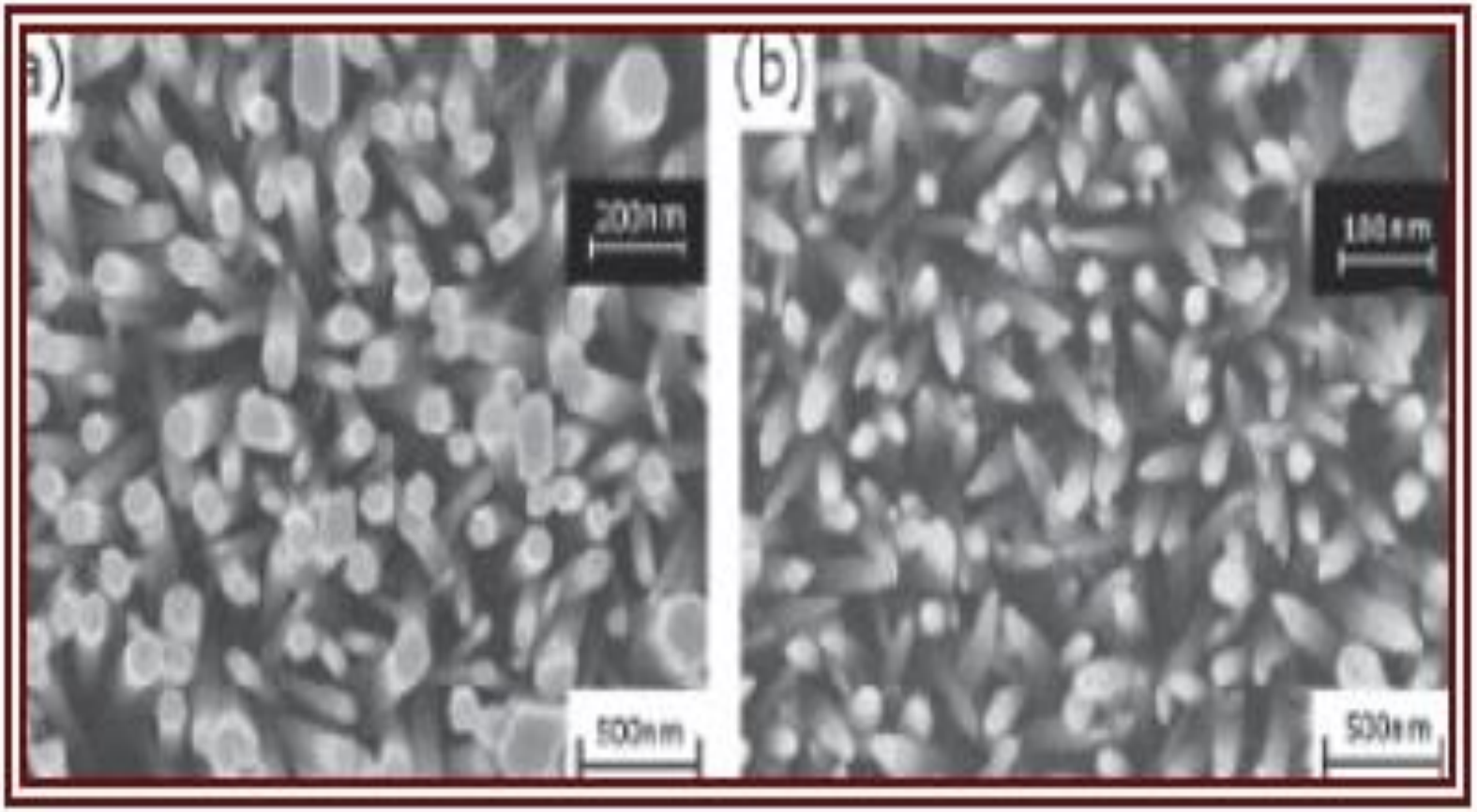


الفلورين Fullerene مكون من 60 ذرة كربون

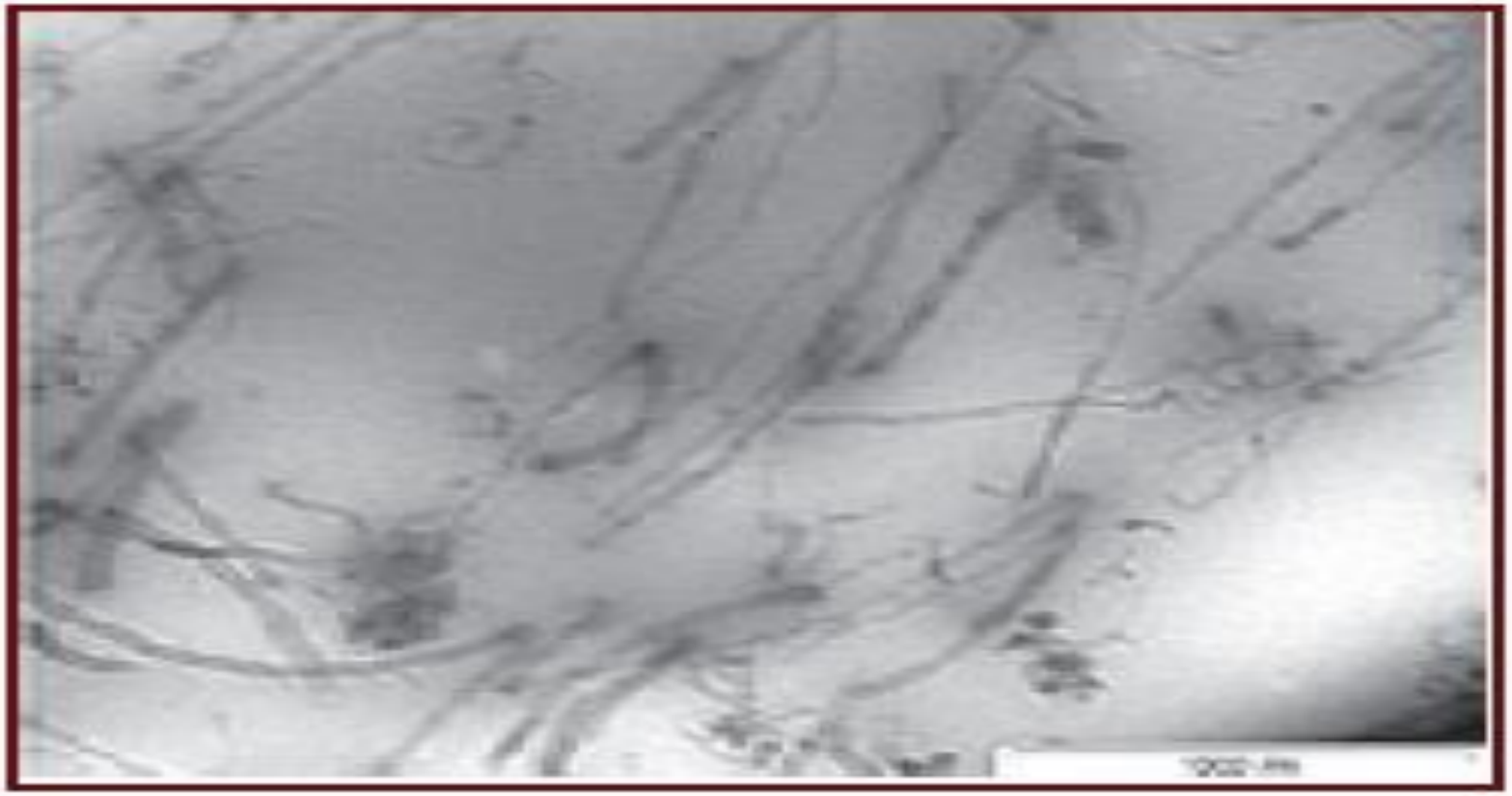
الأنابيب النانوية



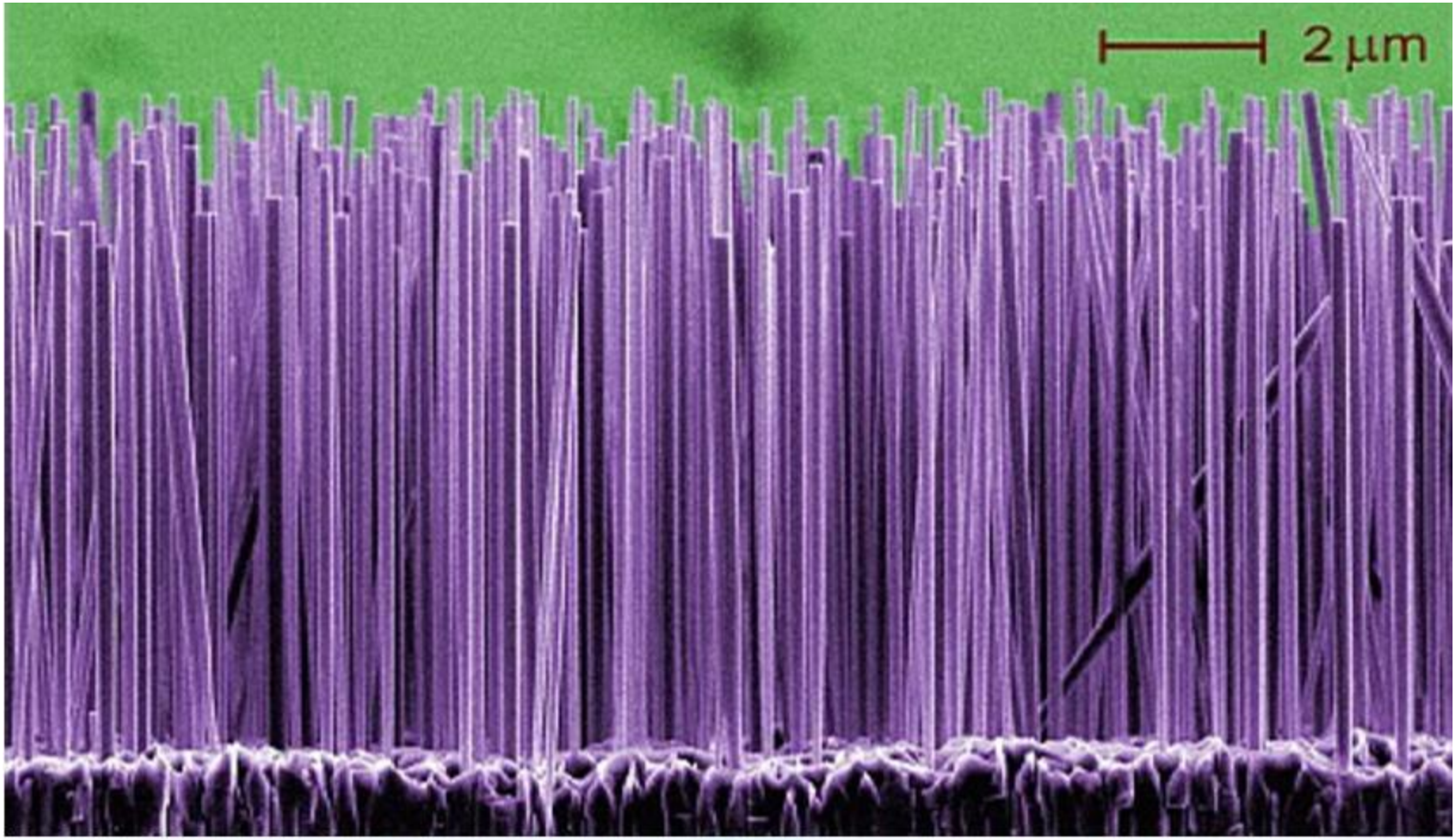
أنابيب الكربون نانوية(يمين) وأيضا أنابيب النانو مصنوعة من أوكسيد التيتانيوم(يسار) ويلاحظ أن قطر أنبوب النانو أقل من 100 نانومتر أما الطول فيصل إلى الميكرمتر.



عينة لأعمدة نانو nanorodes مصنوعة من أوكسيد الزنك ZnO ويلاحظ أن أعمدة النانو مصمتة بخلاف أنابيب النانو تكون مجوفة



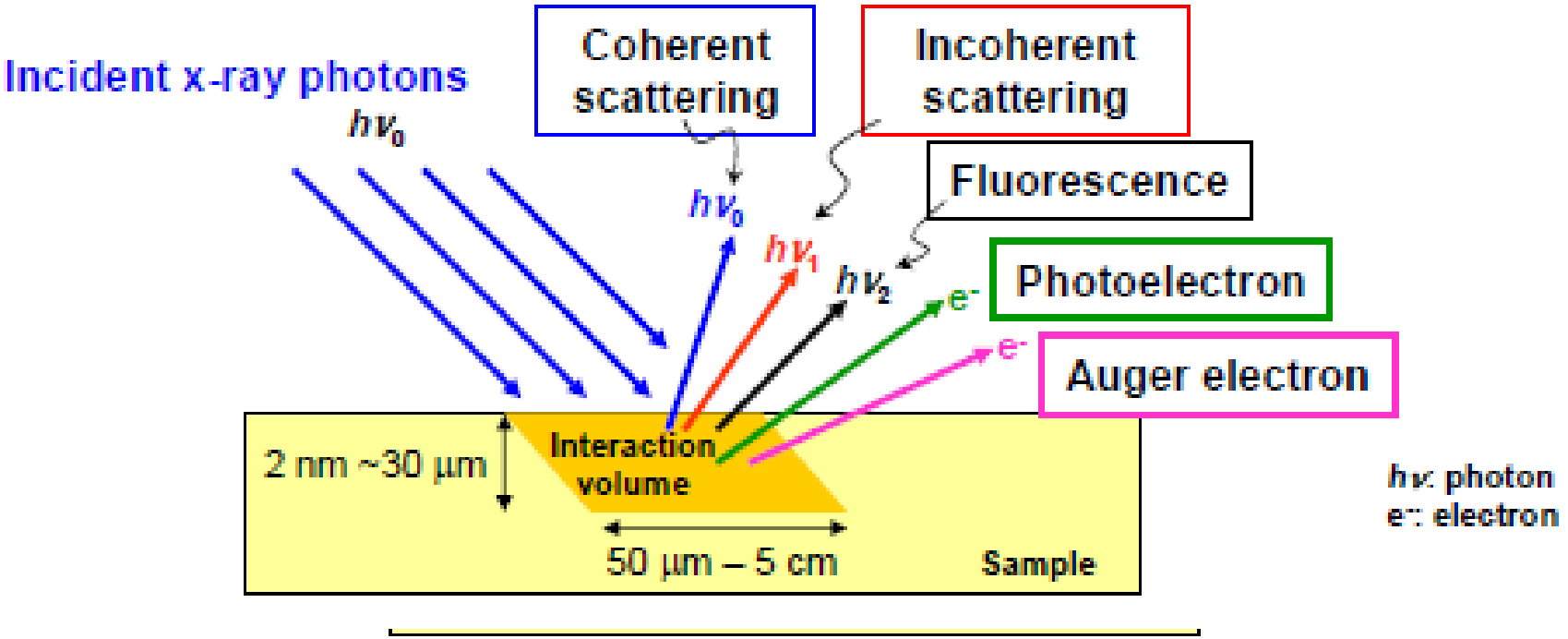
مركب من مواد النانو nanocomposite مكون من أنابيب كربون نانوية (المادة السوداء)ومادة المطاط الطبيعي (المادة البيضاء).



الأسلاك النانوية

الخصائص البنيوية

X-ray interactions with matter



Coherent scattering (Thompson scattering / diffraction): incident photon $h\nu_0$ interacts with e⁻ with no energy loss and no phase change

Incoherent scattering (Compton scattering): (a) e⁻ absorbs incident energy $h\nu_0$ (excited photoelectron); (b) part of the energy is emitted at different energy $h\nu_1$ and different phase.

Fluorescence: (a) K/L shell e⁻ absorb incident energy $h\nu_0$; (b) outer shell e⁻ "cascade" down filling the "holes" causing secondary photons emission ($h\nu_2$).

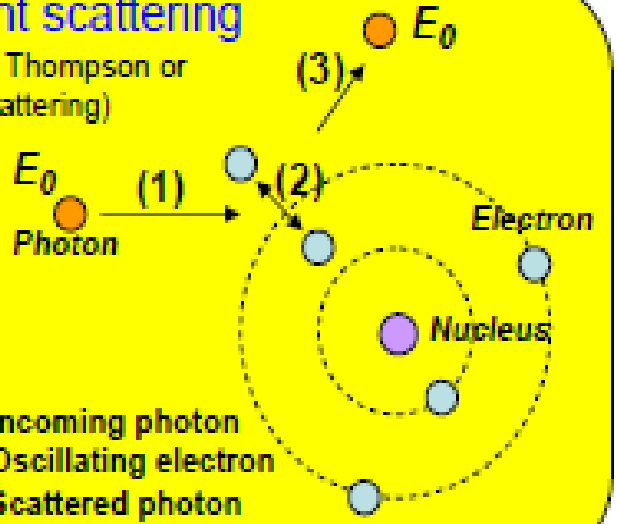
Photoelectron emission: $h\nu_0$ energy is used to eject electron e⁻ with kinetic energy = $h\nu_0$ – B.E.(binding energy).

Auger electron emission: (a) incident $h\nu_0$ used to eject e⁻ from atom; (b) 2nd e⁻ "drops" to lower levels to fill the "hole" and a photon is emitted; (c) the emitted photon is absorbed by valance e⁻, which ionizes and leaves the atom.

X-ray interactions with matter

Coherent scattering

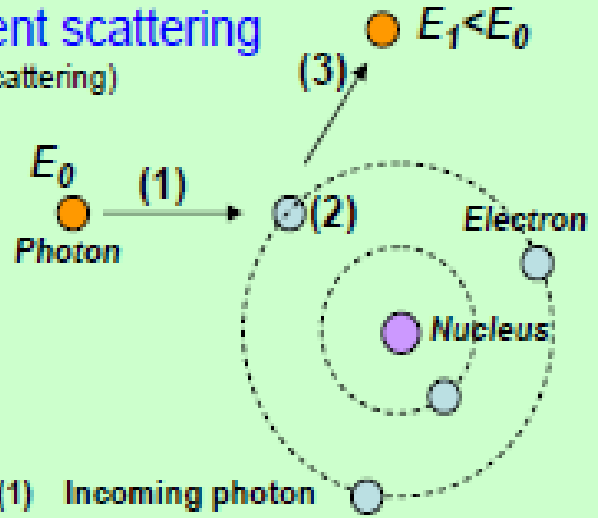
(Diffraction, Thompson or Rayleigh scattering)



(1) Incoming photon
(2) Oscillating electron
(3) Scattered photon
No loss of energy.

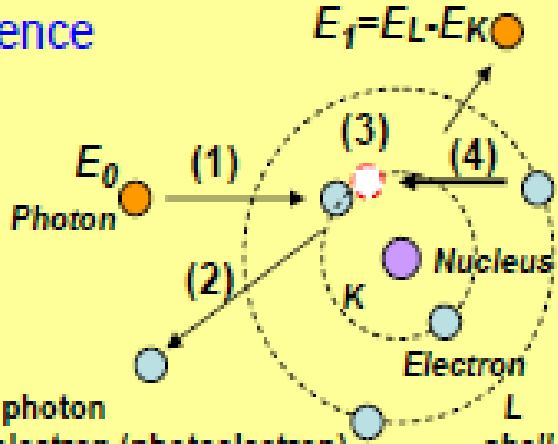
Incoherent scattering

(Compton scattering)



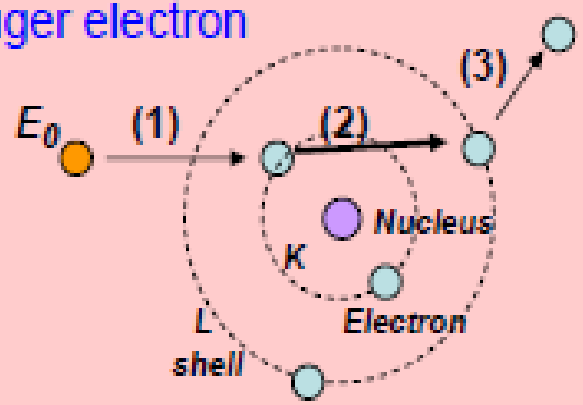
(1) Incoming photon
(2) Energy is partially transferred to electron
(3) Scattered photon (energy loss).

Fluorescence



(1) Incoming photon
(2) Expelled electron (photoelectron)
(3) Hole is created in the shell
(4) Outer shell electron moves to the inner shell hole
(5) Energy excess emitted as characteristic photon.

Auger electron



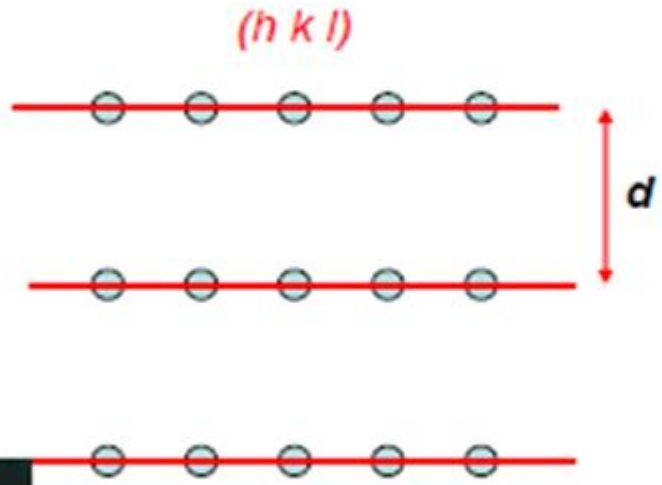
(1) Incoming photon excites inner shell electron
(2) Excitation energy is transferred to outer electron
(3) Electron ejected from atom (Auger electron)

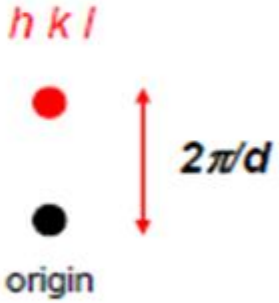
Fundaments of diffraction

"Real" space
Set of planes

$\mathcal{F}$

Reciprocal space
Point



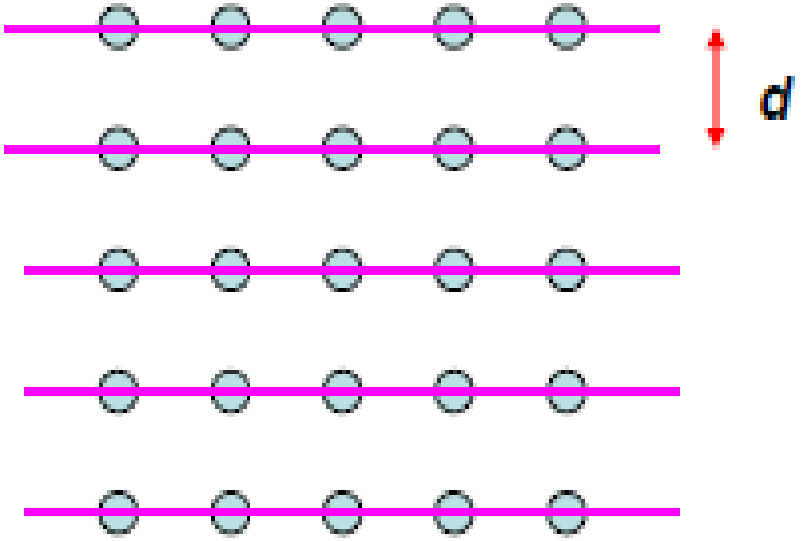


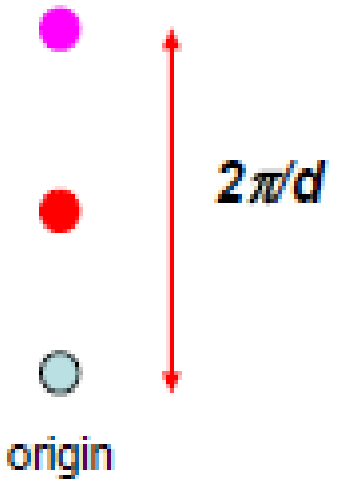
M. von Laue 1879-1960
X-rays from crystals, 1912.

"Real" space

$\mathcal{F}$

Reciprocal space

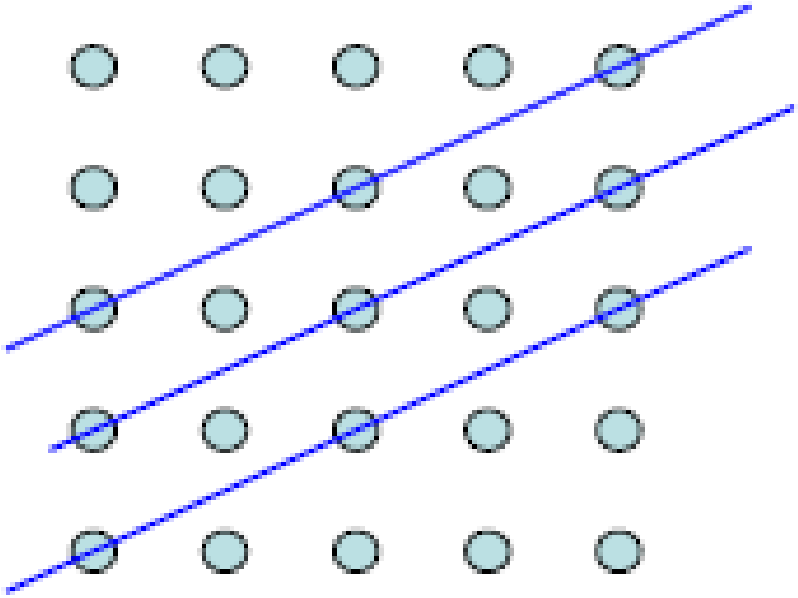


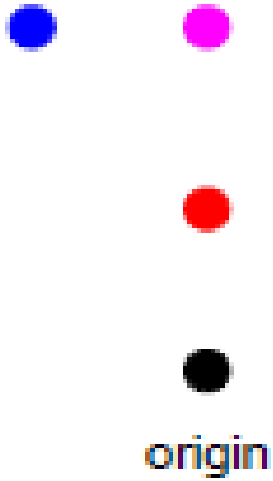


"Real" space

$\mathcal{F}$

Reciprocal space





Fundaments of diffraction

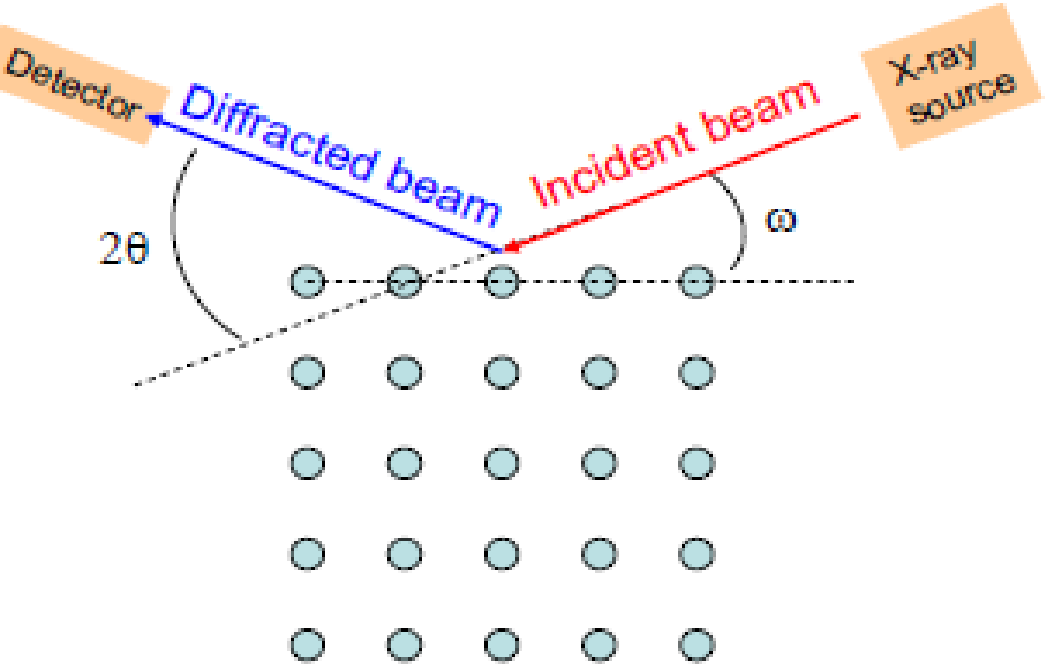
"Real" space

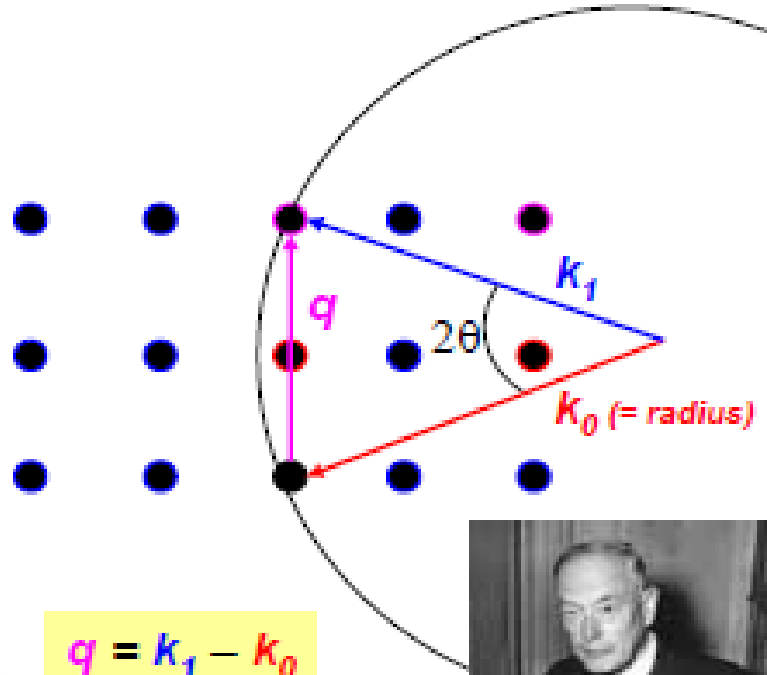
$\mathcal{F}$

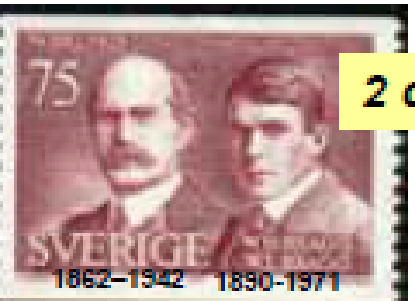
Reciprocal space

Bragg's law

Ewald's sphere







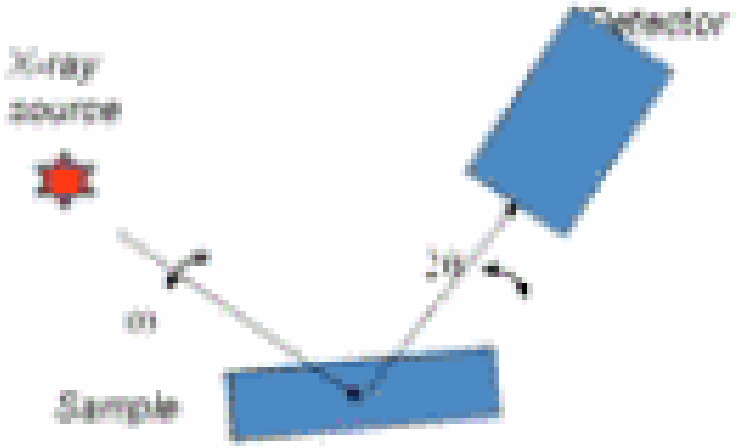
$2\,d\,\sin\theta = n\,\lambda$

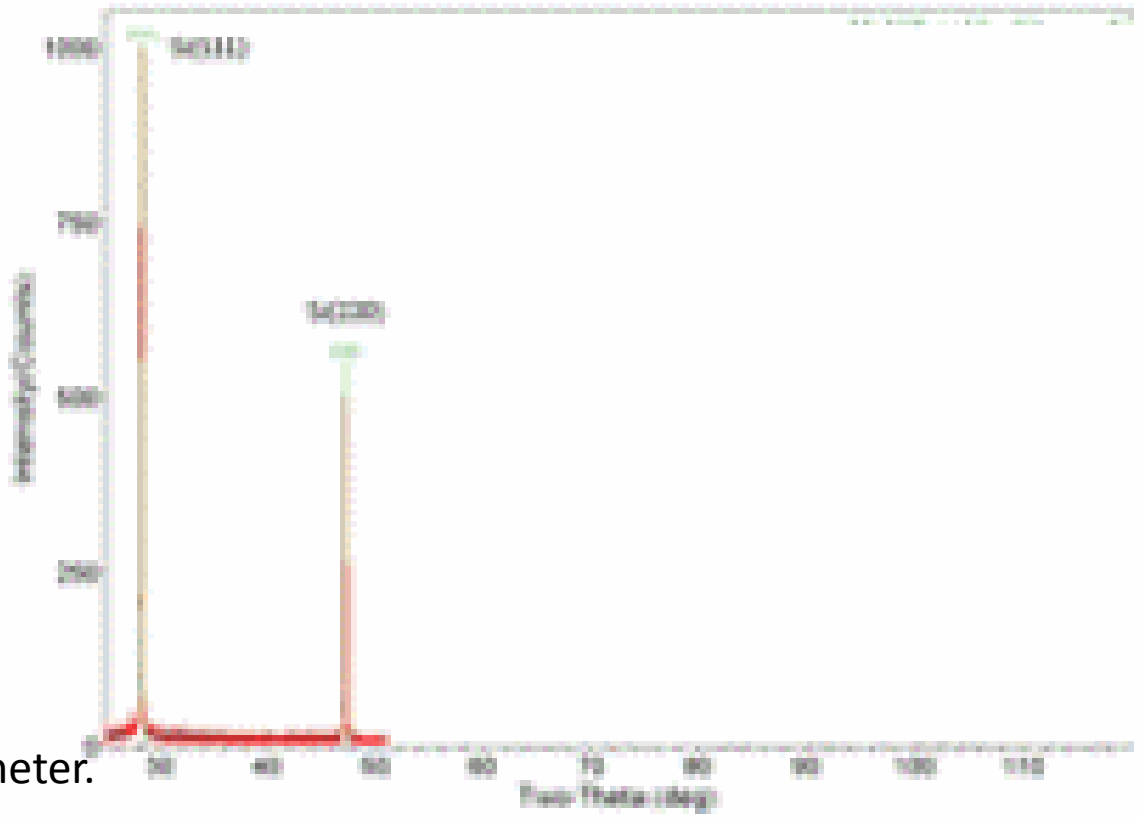
Elastic (Thompson's) scattering

$q = k_1 - k_0$

q: scattering vector
$q = (4\,\pi/\lambda)\,\sin\theta$

Information contents in the XRD pattern





Peak position

Identification, struture, lattice parameter.

Peak width

Crytalline size,strain, defects

Peak area or height ratio

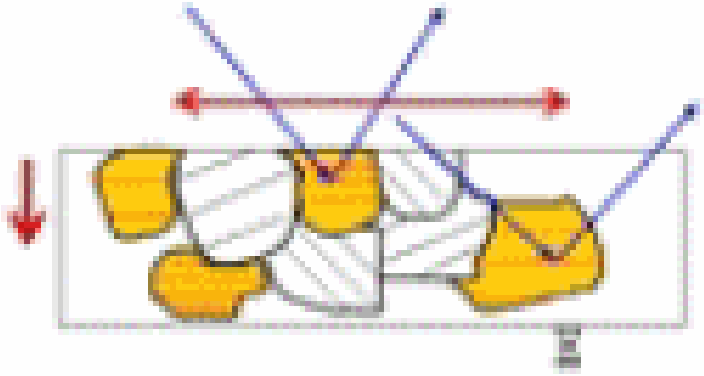
Preferred orientation

Peak tails

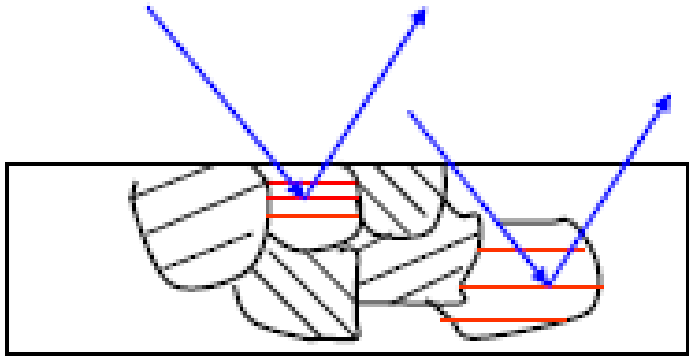
Diffuse scattering point defects

Background

Amorphous contents



Powder diffraction methods



Crystalline? Amorphous?

What elements, compounds, phases are present?

Structure? Lattice constants?

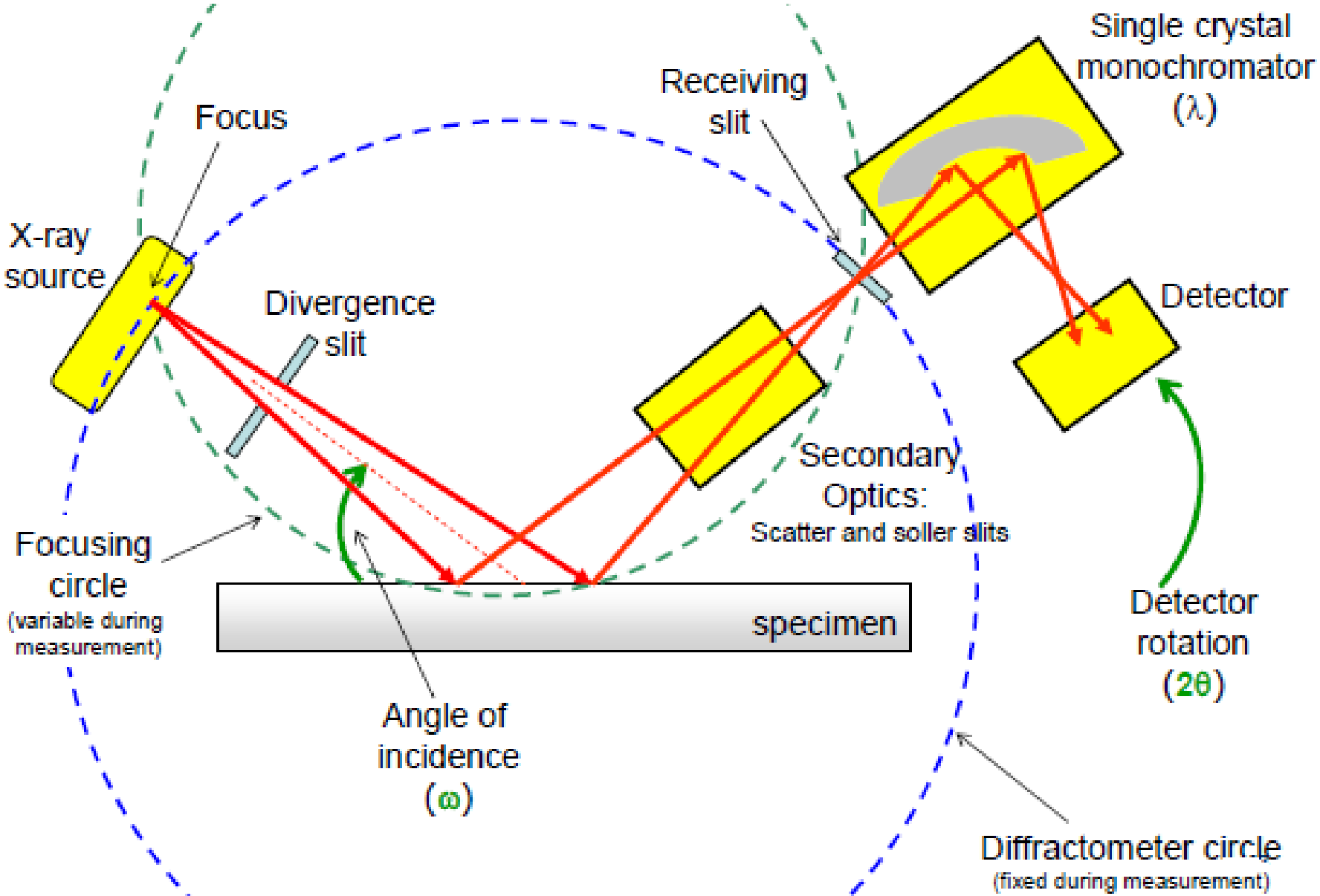
Strain?

Grain sizes? Grain orientations?

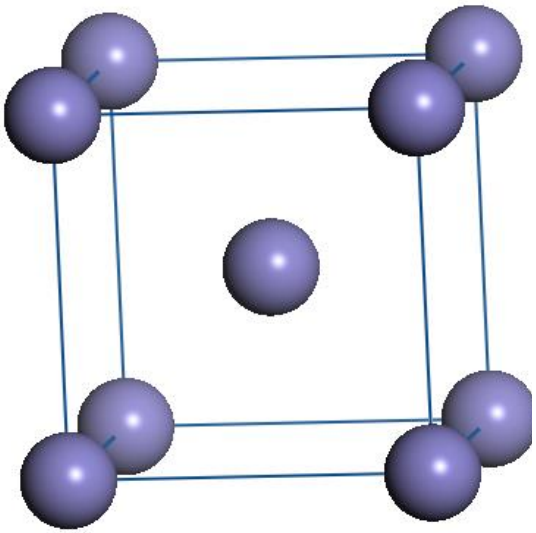
Is there a mixture? What % ?

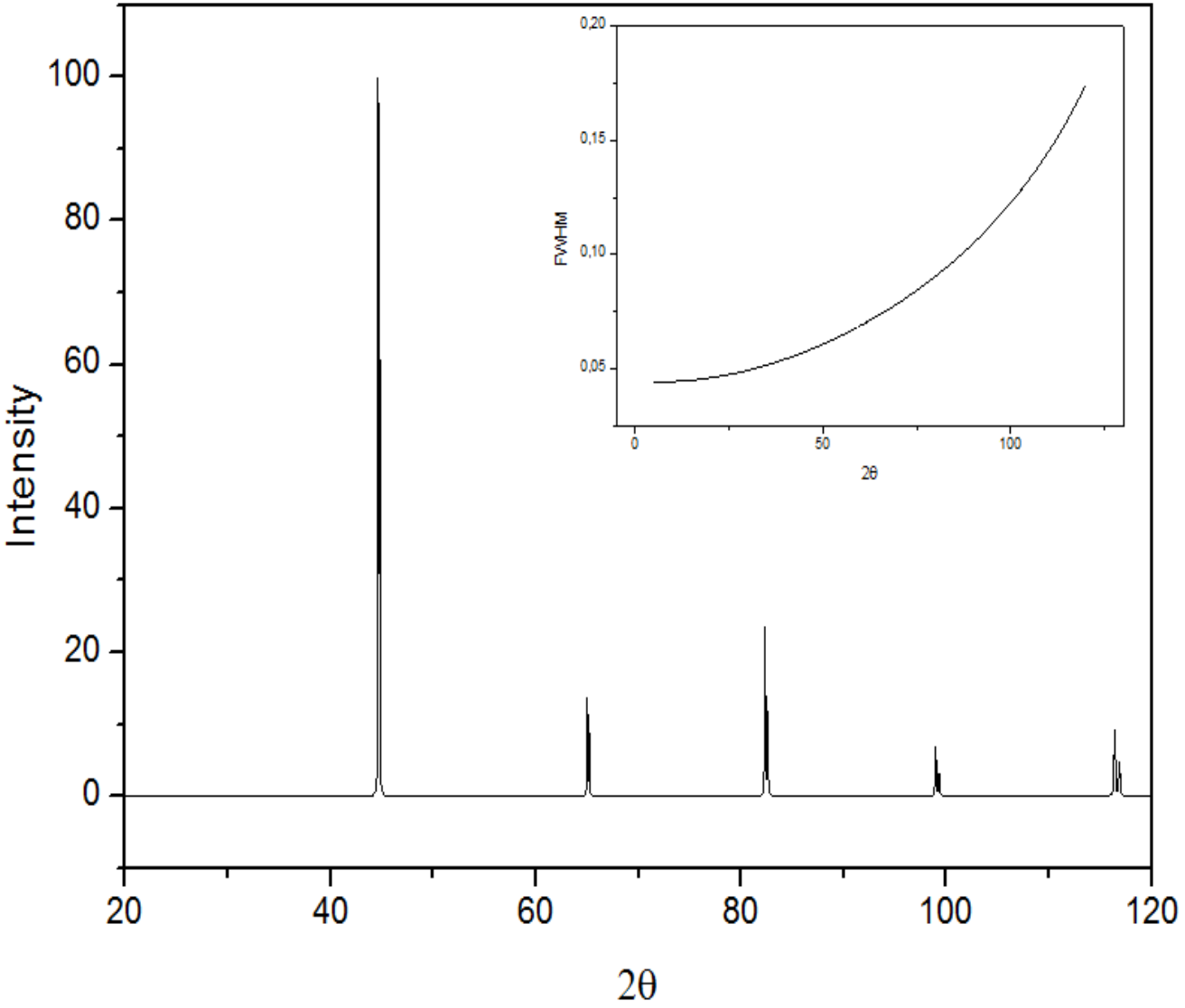
Powders, bulk materials, thin films, nanoparticles, soft materials.

Bragg –Brentano configuration

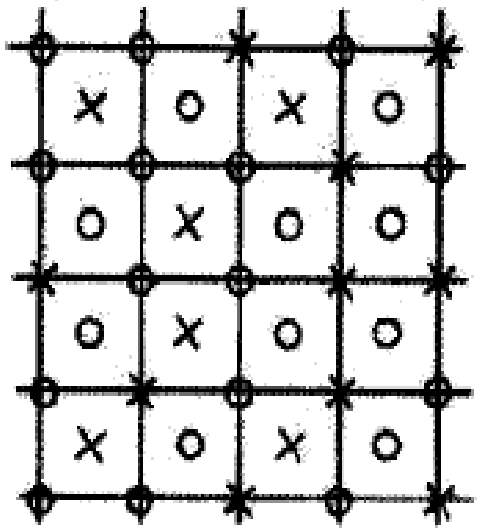


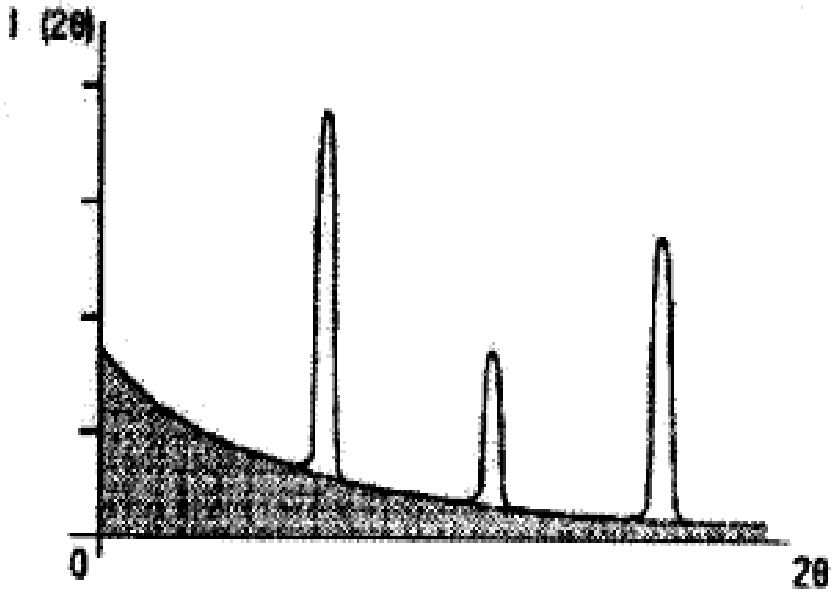
Perfect crystal



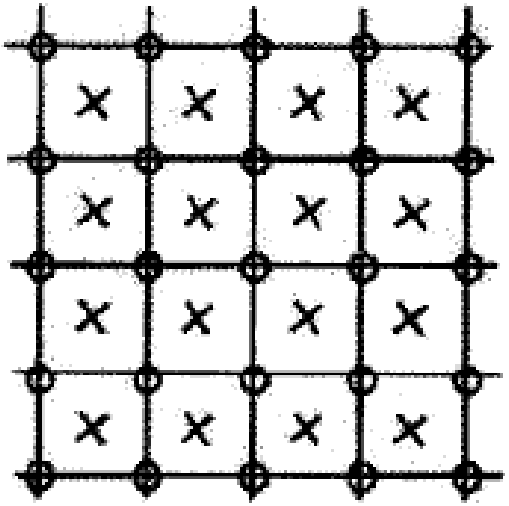


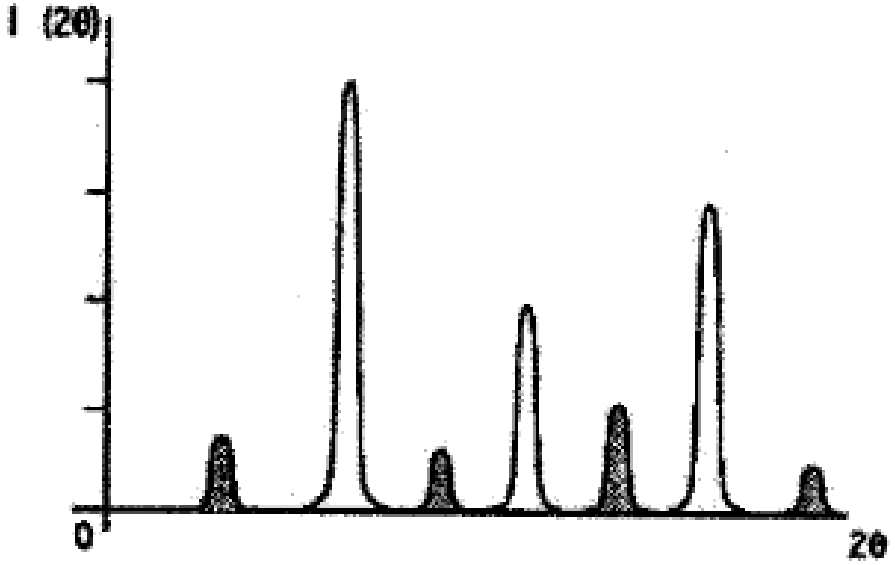
disorder in an alloy of composition AB



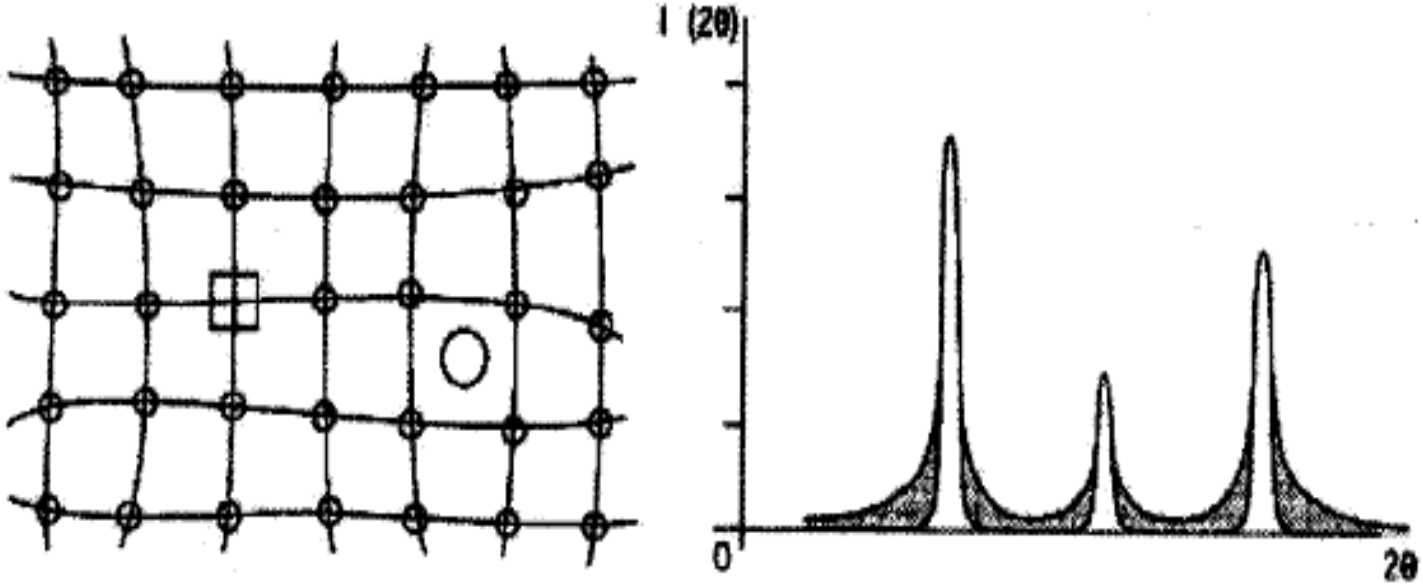


Ordered alloy AB





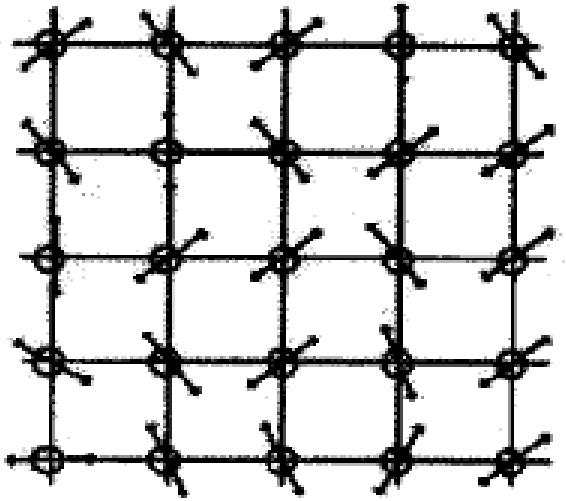
Disorder of position

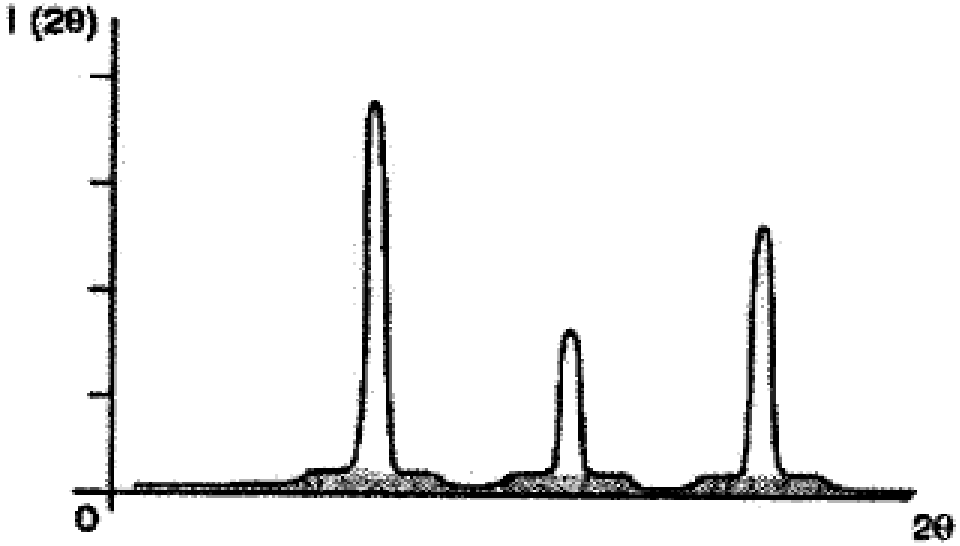


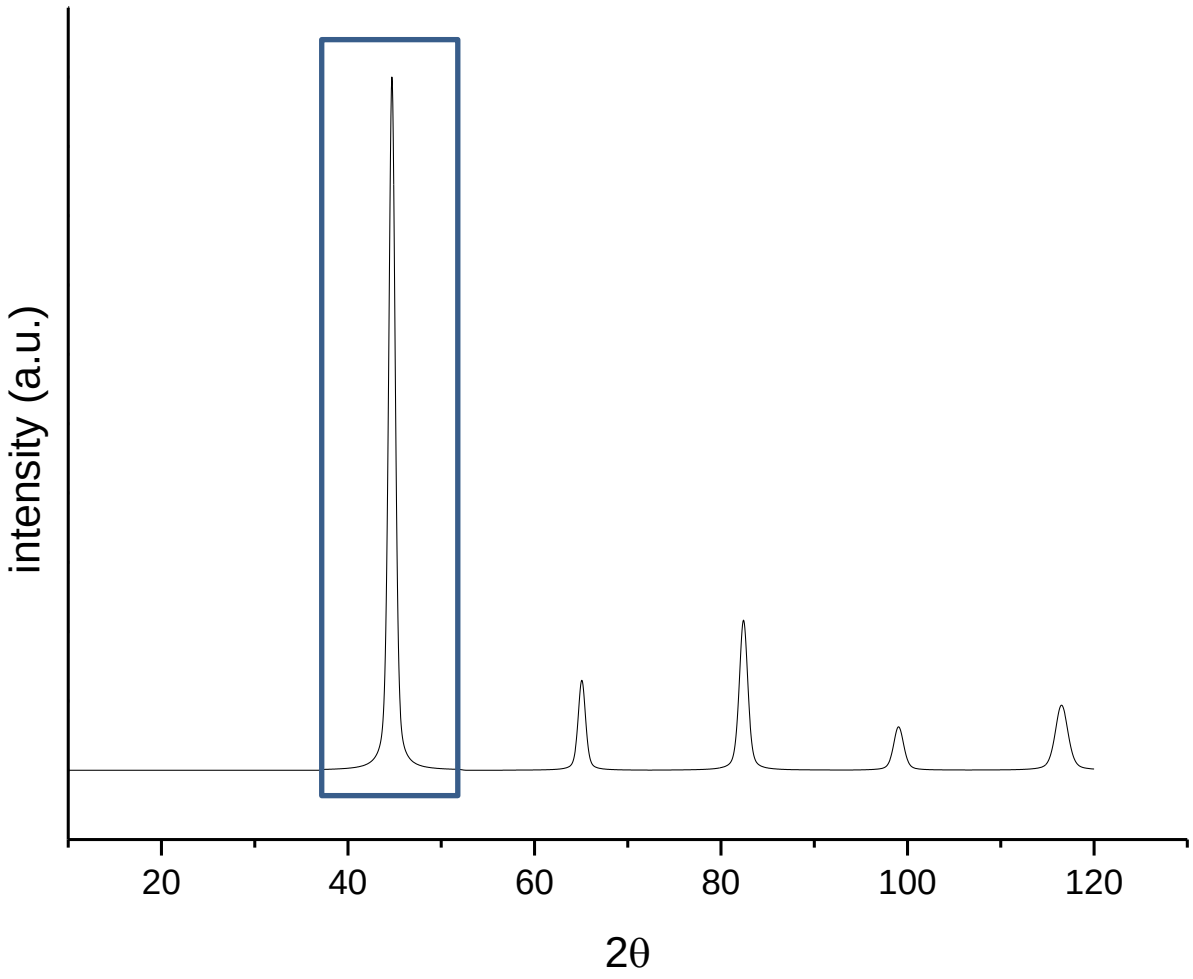
○ atom in position insersticielle

□ lacune

Thermal agitation






intensity (a.u.)
20
40
60
80
100
120
2θ

Crystallite size analysis

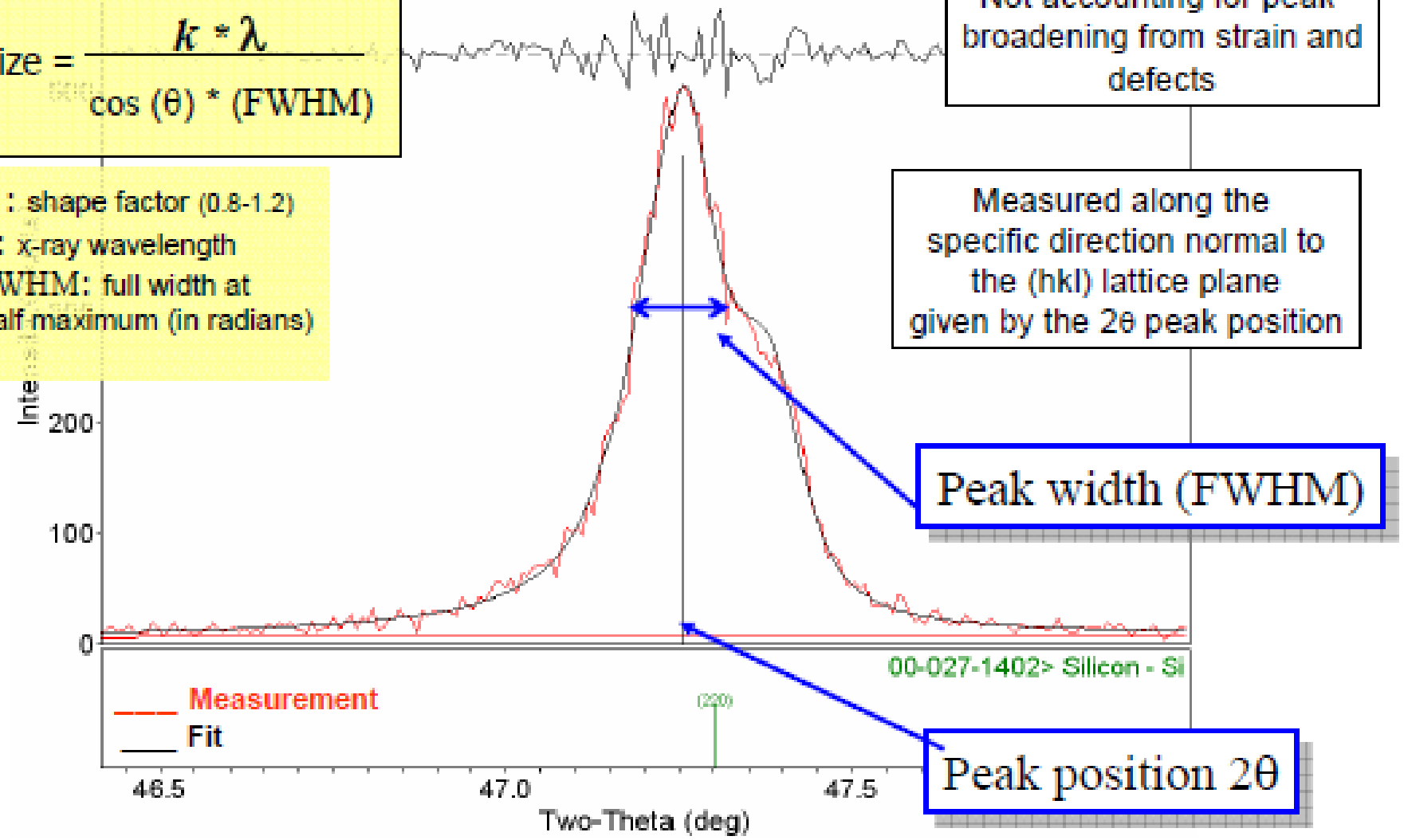
Scherrer's equation:

$$\text{Size} = \frac{k * \lambda}{\cos(\theta) * (\text{FWHM})}$$

k : shape factor (0.8-1.2)
λ: x-ray wavelength
FWHM: full width at half maximum (in radians)

Not accounting for peak broadening from strain and defects

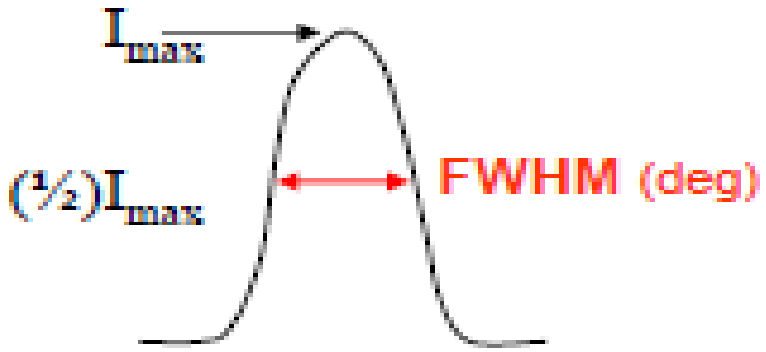
Measured along the specific direction normal to the (hkl) lattice plane given by the 2θ peak position

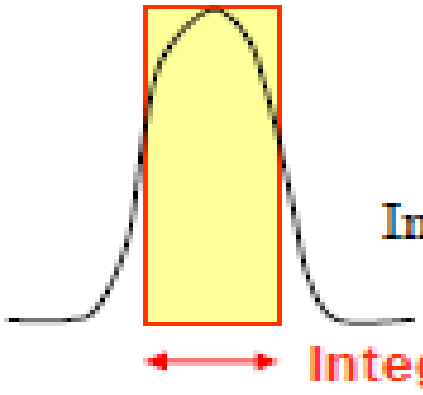


Peak width (FWHM)

Peak position 2θ

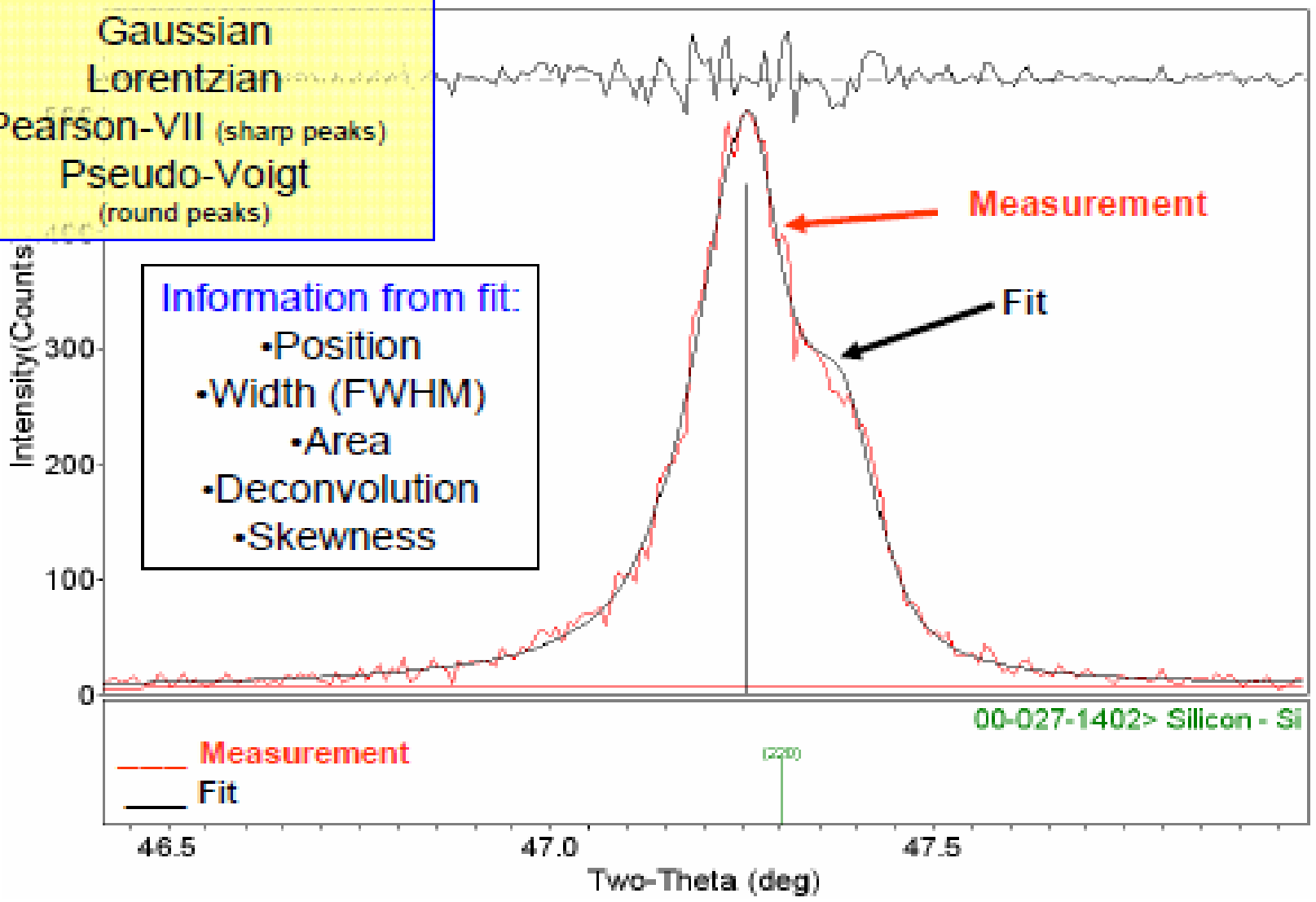
FWHM vs. integral breadth



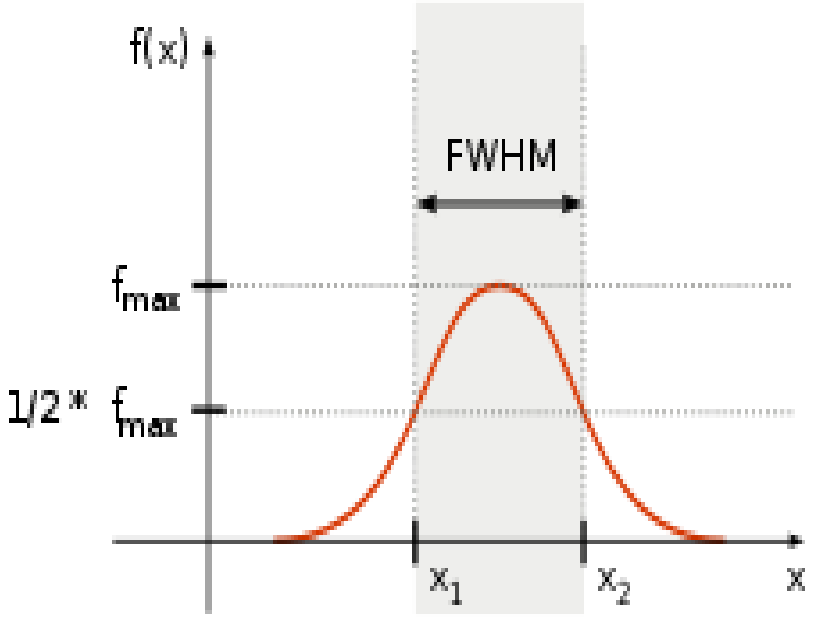


Peak shape analysis

Peak fit:
Gaussian
Lorentzian
Pearson-VII (sharp peaks)
Pseudo-Voigt
(round peaks)



If the considered function is the normal distribution of the form

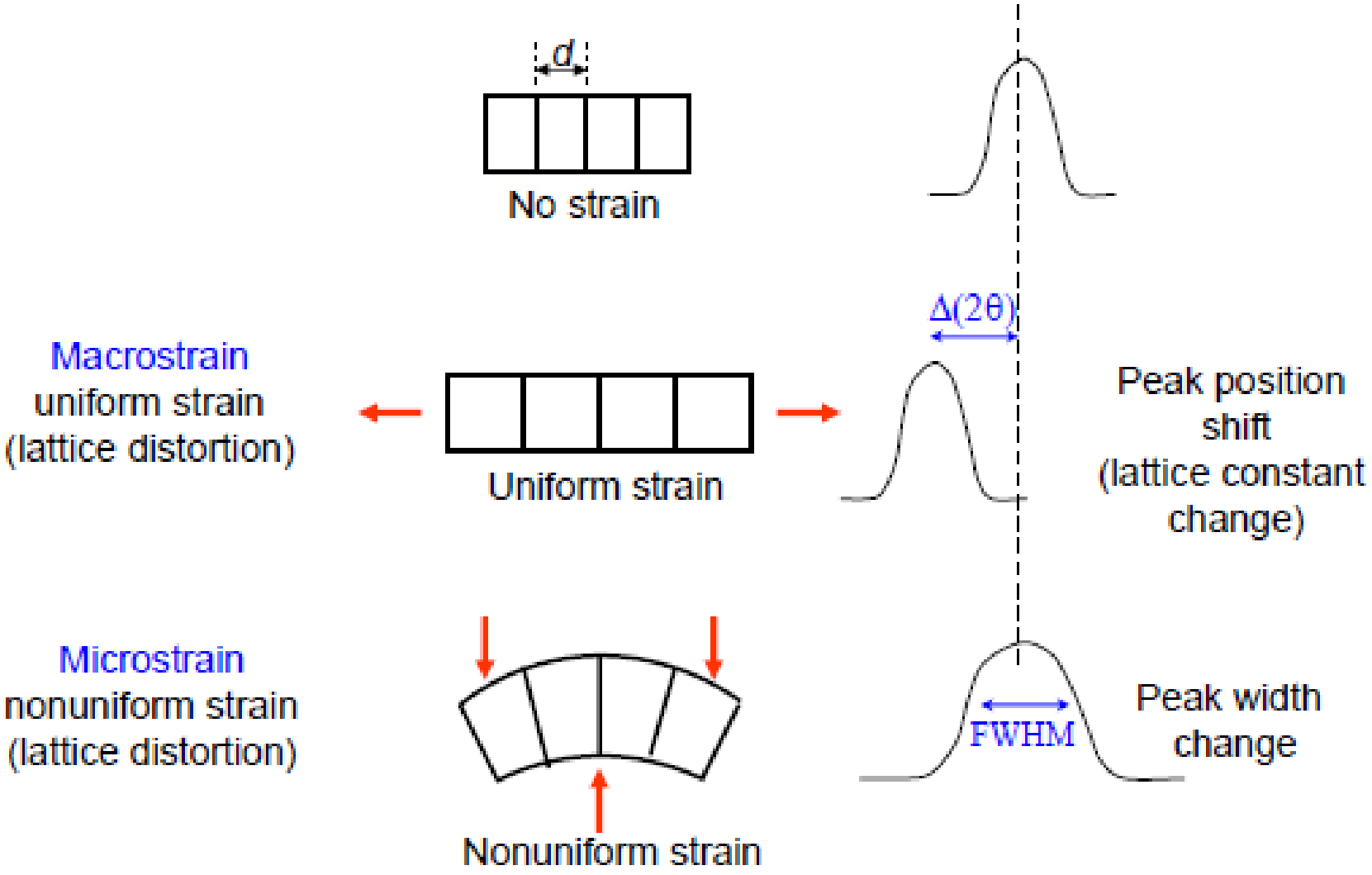


$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left[-\frac{(x - x_0)^2}{2\sigma^2}\right]$$

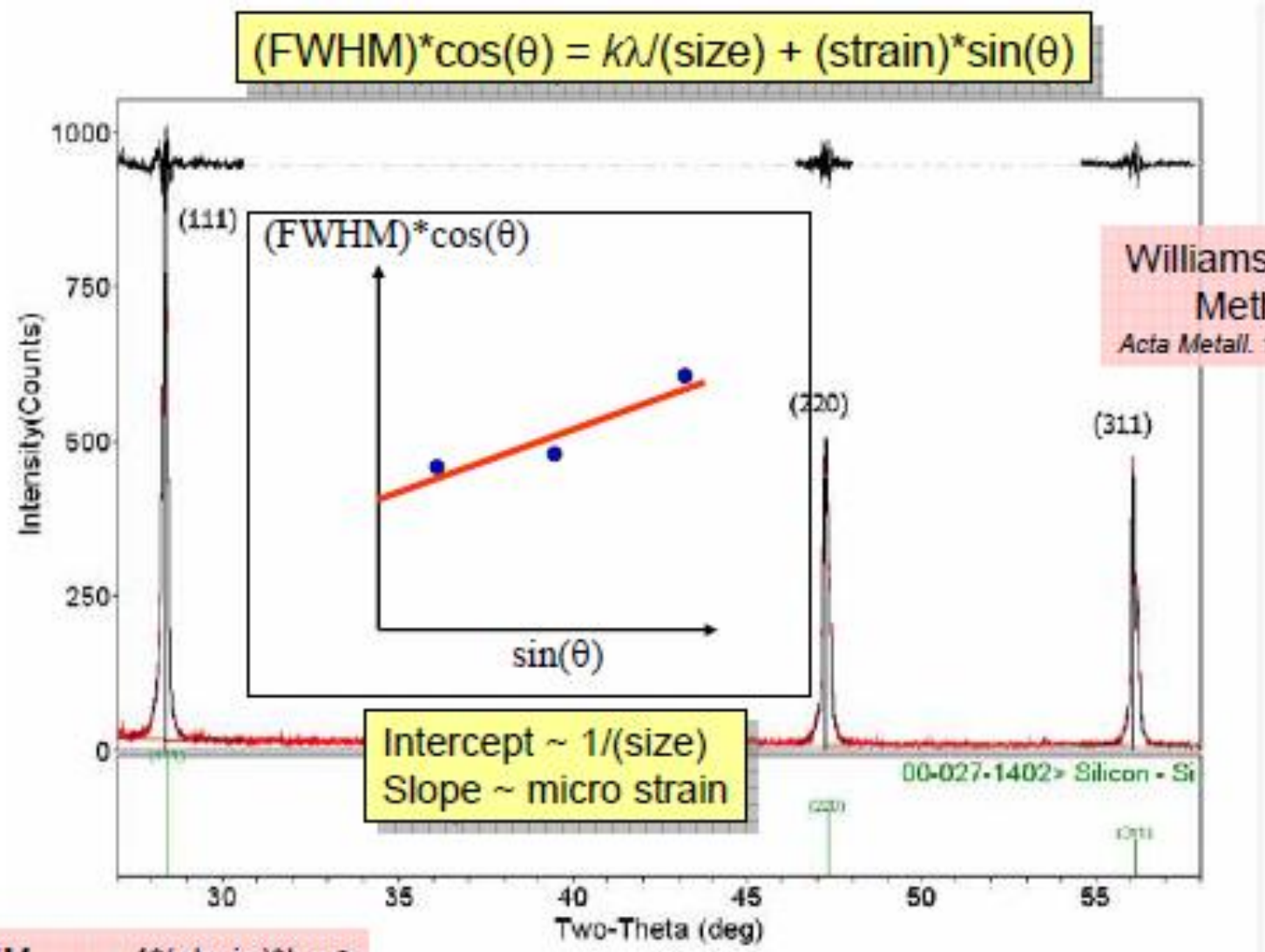
where σ is the standard deviation and then the relationship between FWHM and the standard deviation is

$$\mathrm{FWHM} = 2\sqrt{2\ln 2}\,\sigma \approx 2.355\,\sigma.$$

Strain effects in diffraction lines



Size and strain in peak shape analysis



$FWHM_{strain} = 4*(strain)*\tan\theta$