Low Angle X-ray Scattering (LAXS) for Tissue Characterization

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Statement of Problem

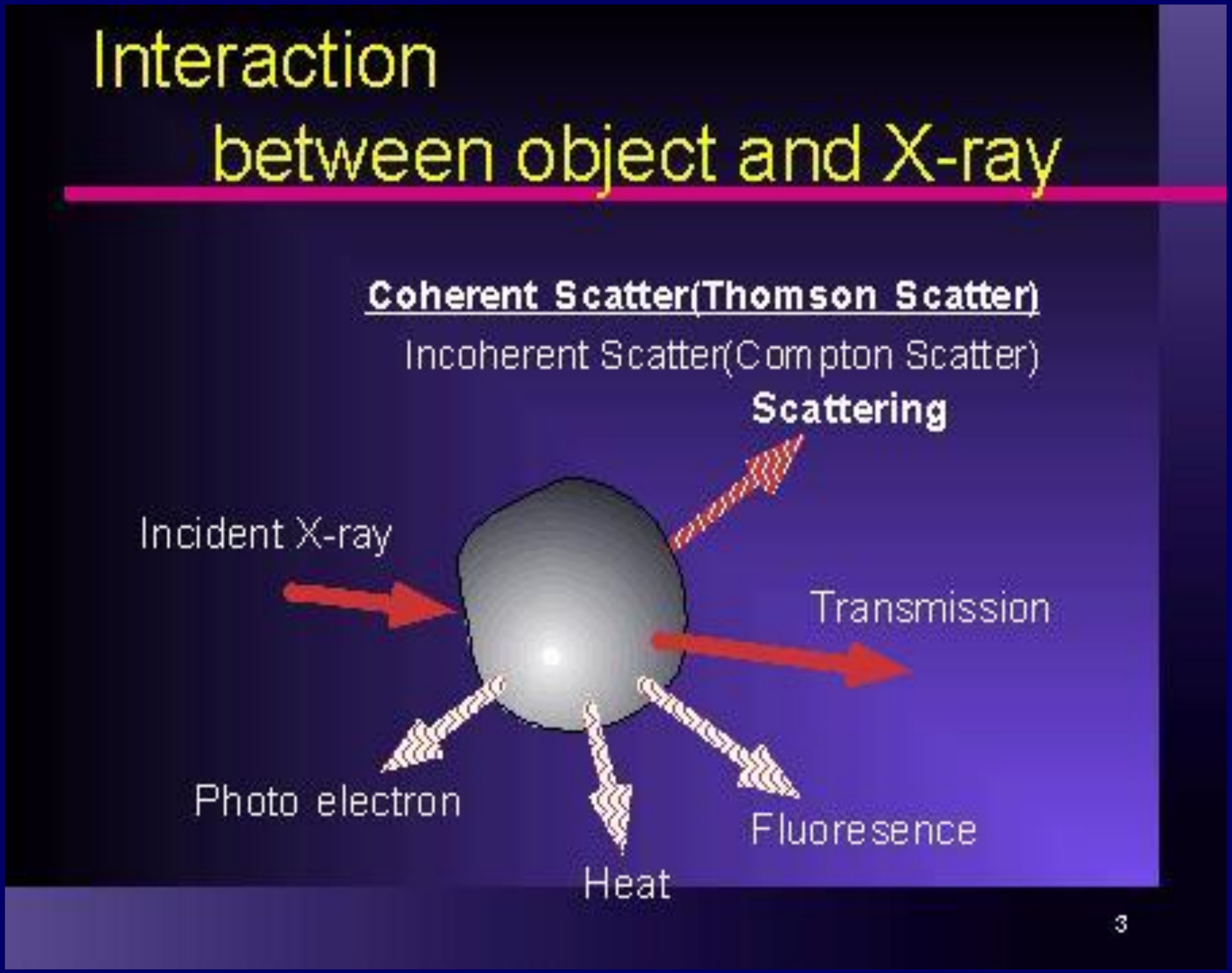
Deficiencies of the Current Imaging Techniques

- Poor contrast between healthy and diseased soft tissues (eg; Breast tissues)
- Presence of scatter, which further degrades the contrast
- Low Specificity in Mammography (50%)
- No molecular and cellular changes is possible in early stages
- Only Bulk changes are visible
- Types of materials consisted in a specific tissue are not accessible

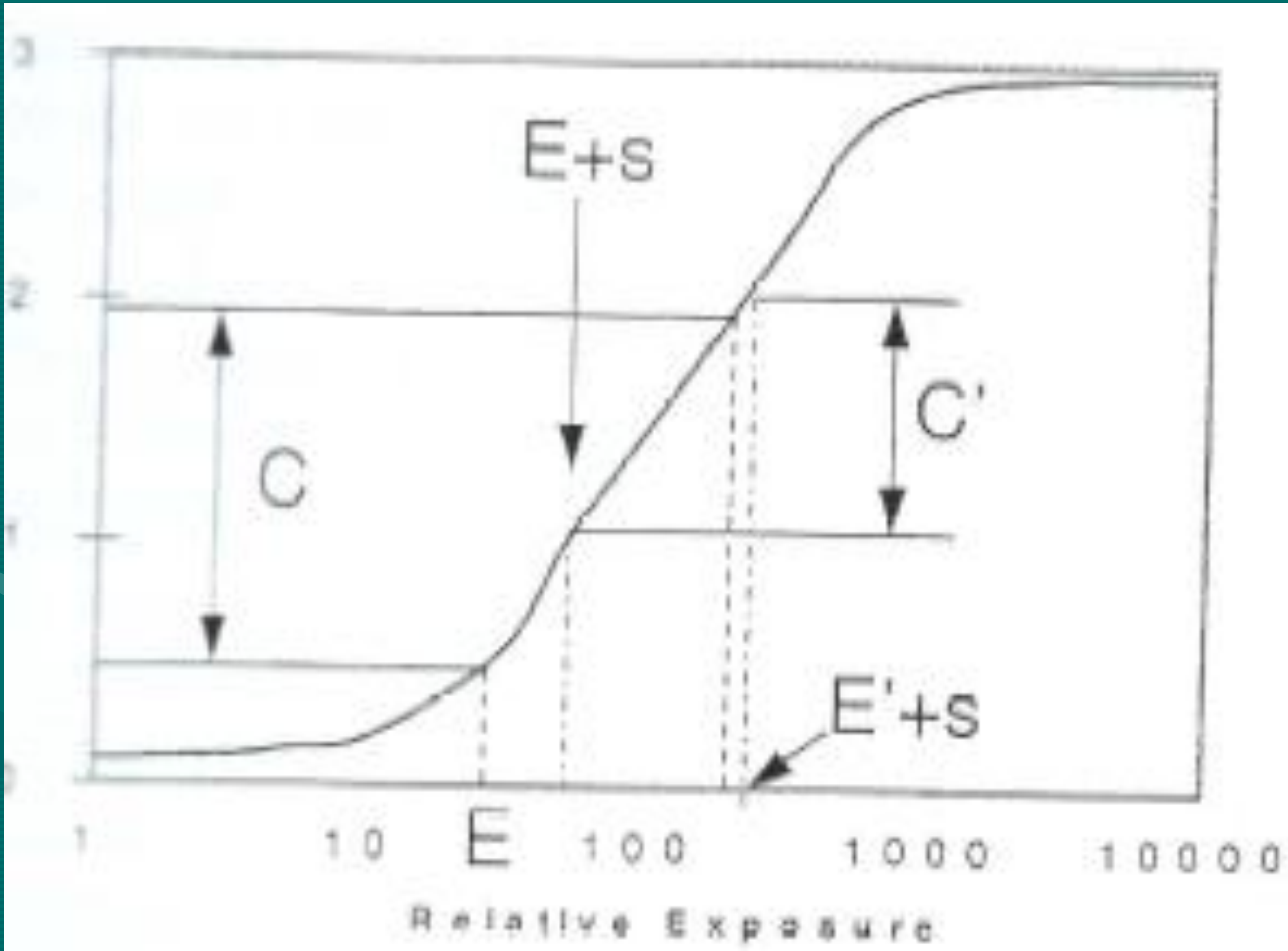
What is the SOLUTION?

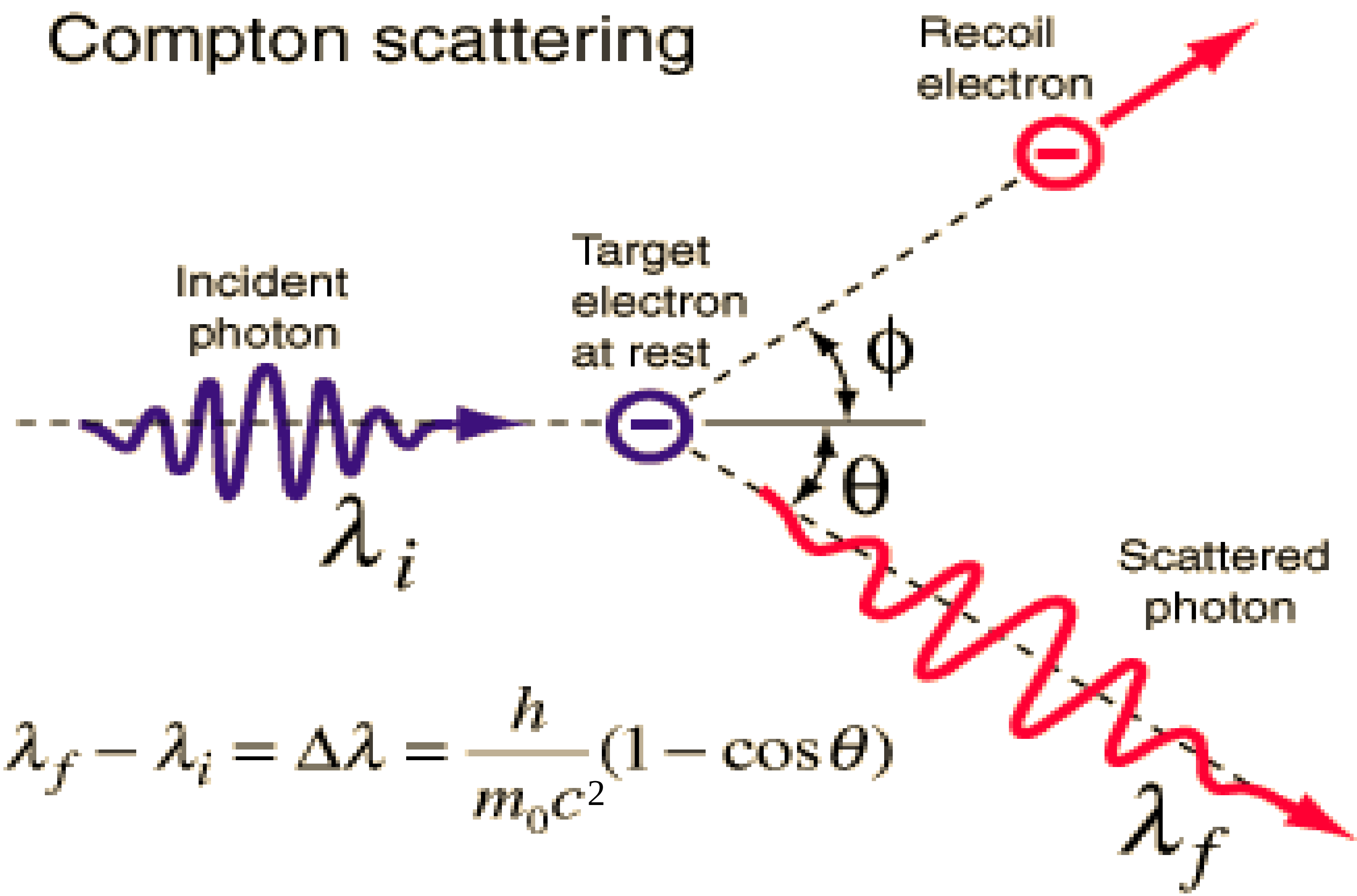
- Refractive/*interference effects is about 1000 times larger than* absorption

- If interference-related effects of scattering is properly exploited, much more intense information is obtained


Interaction
between object and X-ray
Coherent Scatter(Thomson Scatter)
Incoherent Scatter(Compton Scatter)
Scattering
Incident X-ray
Transmission
Photo electron
Heat
Fluoresence
3

Characteristic curve for a tissue contract, C without scatter, C’ with scatter




Compton scattering
Recoil electron
Incident photon
Target electron at rest
ϕ
θ
λ_i
Scattered photon
λ_f
$\lambda_f - \lambda_i = \Delta\lambda = \frac{h}{m_0 c^2}(1 - \cos\theta)$

Differential Thomson Cross Section per electron for Elastic Scattering

Scattering from a single electron (regarded as a point charge) is defined as:

$$\frac{d\sigma_T}{d\Omega} = \frac{r_e^2}{2}(1 + Cos^2\theta)$$

Coherent (Rayleigh) Differential Scatter Cross Section for Atomic Species

When Photons excite more than one electron, Coherent Scatter from different electrons demonstrate interference effects:

$$\frac{d\sigma_{Coh}}{d\Omega} = \frac{d\sigma_T}{d\Omega}(\theta)\, f^2(x, Z)$$

$f^2(x,Z)$ is Atomic form Factor, x is momentum transfer, Z atomic Number

What is Atomic form factor?

- **Atomic form factor**, or atomic scattering factor, is a measure of the amplitude of a wave scattered from an isolated atom (scattering amplitude).
- x-rays are scattered by the electron cloud of the atom and hence the scattering power of x-rays increases with the atomic number of the atoms in a sample.
- The x-ray form factor is defined as the Fourier transform of the electron charge density of scaterer.

Coherent Differential Scattering Cross section of Condensed Material

- Atomic form factor gives a good description of scattering when phase relationship from different atoms is not constant (eg in gaseous samples)

- In Condensed state of Matters, the atomic form factor should be modified, to include the interference effects from neighboring atoms:

$$\frac{d\sigma_{Coh}}{d\Omega} = \frac{d\sigma_T}{d\Omega}(\theta)F_m^2(x,Z)$$

Molecular Form factor

$$F^2(x)=f^2(x)(1+H(x))$$

- $f(x)$ is the IAM (independent atomic model) form factor
- $H(x)$ an oscillatory structure function which accounts for the interference effect.

- For amorphous materials and liquids, $H(x)$ shows a damped behavior around zero and vanishes for values of x>4-5 nm^{-1}.

Form-factor of Multi-element materials

- Structure function data can be taken from experimental measurements.
- *If x* ranges from about 4-5 to 10^{10} nm^{-1}, IAM is valid, and each atom is assumed to scatter independent of the others, therefore the Sum rule is applied:

$$f^2(\chi) = M \sum_i [(w_i / A_i) f_i^2(\chi)]$$

- w_i is Mass fraction, and A_i is Atomic Mass of ith element, M: molecular weight
- Incoherent contribution is always considered in the IAM frame, that is:

$$S(\chi) = M \sum_i [(w_i / A_i) S_i(\chi)]$$

- S_i and f_i can be found from the extensive tabulation from the existing literature for all elements

Form-factor of an amorphous material

The form-factor for an amorphous material is given by:

$$\left|F_R(x)\right|^2 = H(x)\sum_i w_i \left| f_{Ri}(x)\right|^2$$

W_i is atom fraction and

$f_{Ri}(x)$ is Atomic form-factor of the ith element in the material.

H(x) is a structure function that accounts for diffraction effects

Rayleigh differential cross-section of an amorphous material

$$\frac{d\sigma_R}{d\Omega} = \pi r_0^2 (1 + \cos^2\theta) \left| F_R(x) \right|^2$$

r_0 is the classical electron radius,

θ is the scattering angle,

$F_R(x)$ is the form-factor

$x = \sin(\theta/2)/\lambda$ is the momentum transfer.

Cross-section for Crystal material (Bragg cross-section)

cross-section for Bragg scattering from a crystal:

$$\sigma_B = \frac{r_0^2 \lambda^2}{2NV} \sum_i \left(\frac{1+\cos^2\theta}{2} \right) m_i d_i \left| f_i \right|^2$$

λ is the X-ray wavelength,

N is the number of atoms in the crystal unit cell,

V is the unit crystal volume,

m_i, multiplicity,

d_i, atomic plane spacing

f_i , Structure factor (form-factor) of the plane i.

Total Linear differential Coefficient for Mono-molecular material

Linear differential scattering coefficient which is the probability of a photon being scattered per unit length of beam path, and has unit of m^{-1} sr^{-1}:

$$\mu_S(E, \chi) = \frac{N_A \rho}{M} \left\{ \frac{d\sigma_T(\theta)}{d\Omega} F^2(\chi) + \frac{d\sigma_{KN}(E, \theta)}{d\Omega} S(\chi) \right\}$$

M: molecular weight

NA: Avogadro number

ρ: density of the material.

F (*x*): Molecular form factor of sample material referring to coherent (Rayleigh) scattering

S(*x*): incoherent (Compton) scattering function

x: Momentum transfer $x = \sin(\theta/2)/\lambda$

Bragg Diffraction

- Diffraction is a phenomenon of reinforced Coherent scattering.
- Coherent Scattering from all atoms in a material undergo reinforcement in a certain direction where they are in phase (Constructive interference),
- And cancel each other in other directions , where they are out of phase (Destructive interference)
- Diffraction can easily observed in material with Crystalline structure, because the atoms are rigidly fixed to one another

Bragg's Law

- When constructive interference occurs, we get diffracted beams in specific directions

- These directions are defined by the wavelength λ of the incident radiation and the nature of the crystalline sample (ie d)

- Bragg's law relates the wavelength of the x-rays to the spacing of the atomic planes and scattering angle

$$n\lambda=2d\sin(\Theta/2)$$

n:an integral number

λ:wavelength

d:interplanar spacing

Θ:angle between the incident wave & atomic planes

Bragg's law and Form factor of Crystal

Bragg's law states that scattering can only occur when $d = 1/2x$ Therefore:

$$\sigma_B = \frac{r_0^2}{4} \sum_i \left(\frac{(1+\cos^2\theta)\sin^2(\theta/2)}{2} \right) |F_B(x)|^2$$

where:

$$|F_B(x)|^2 = \sum_i \frac{m_i |f_i|^2}{NVx^3} \delta(x - x_i)$$

$\delta(x)$ is the Dirac delta function

$x_i = 1/(2d_i)$ is momentum exchange corresponding to plane i.

$x = \sin(\theta/2)/\lambda$

cross-sections and form-factors of mixed crystalline and amorphous materials

For both Rayleigh scattering from amorphous materials and Bragg scattering from crystals, the total scattering cross-section of a mixture is:

$$\sigma(E) = \sum_i \alpha_i \sigma_i(E)$$

E is the photon energy

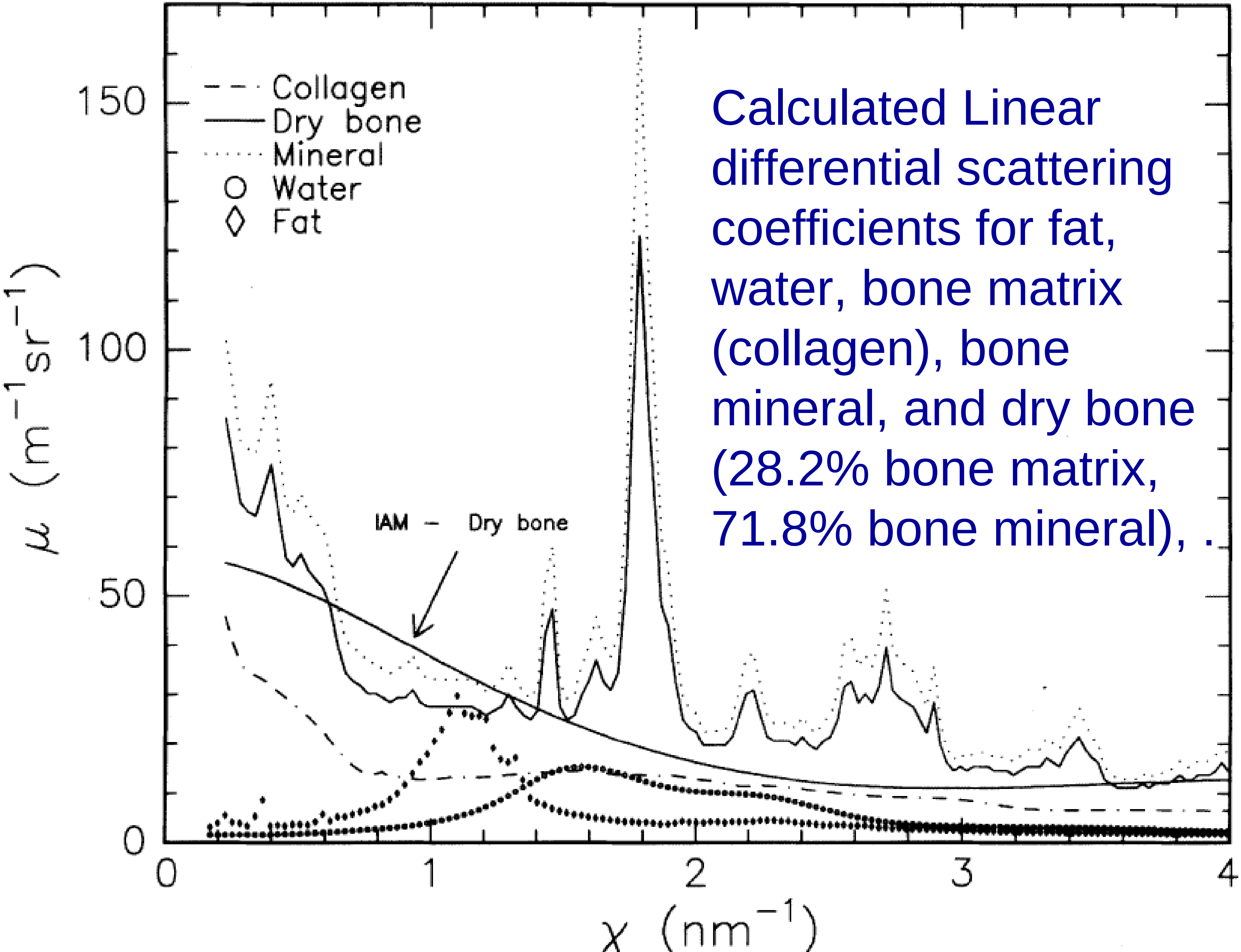
α_i is the mass fraction

σ_i is either the Rayleigh or Bragg cross-section of material i in the mixture.

Similarly, the Rayleigh and Bragg form factors of a mixture are given by:

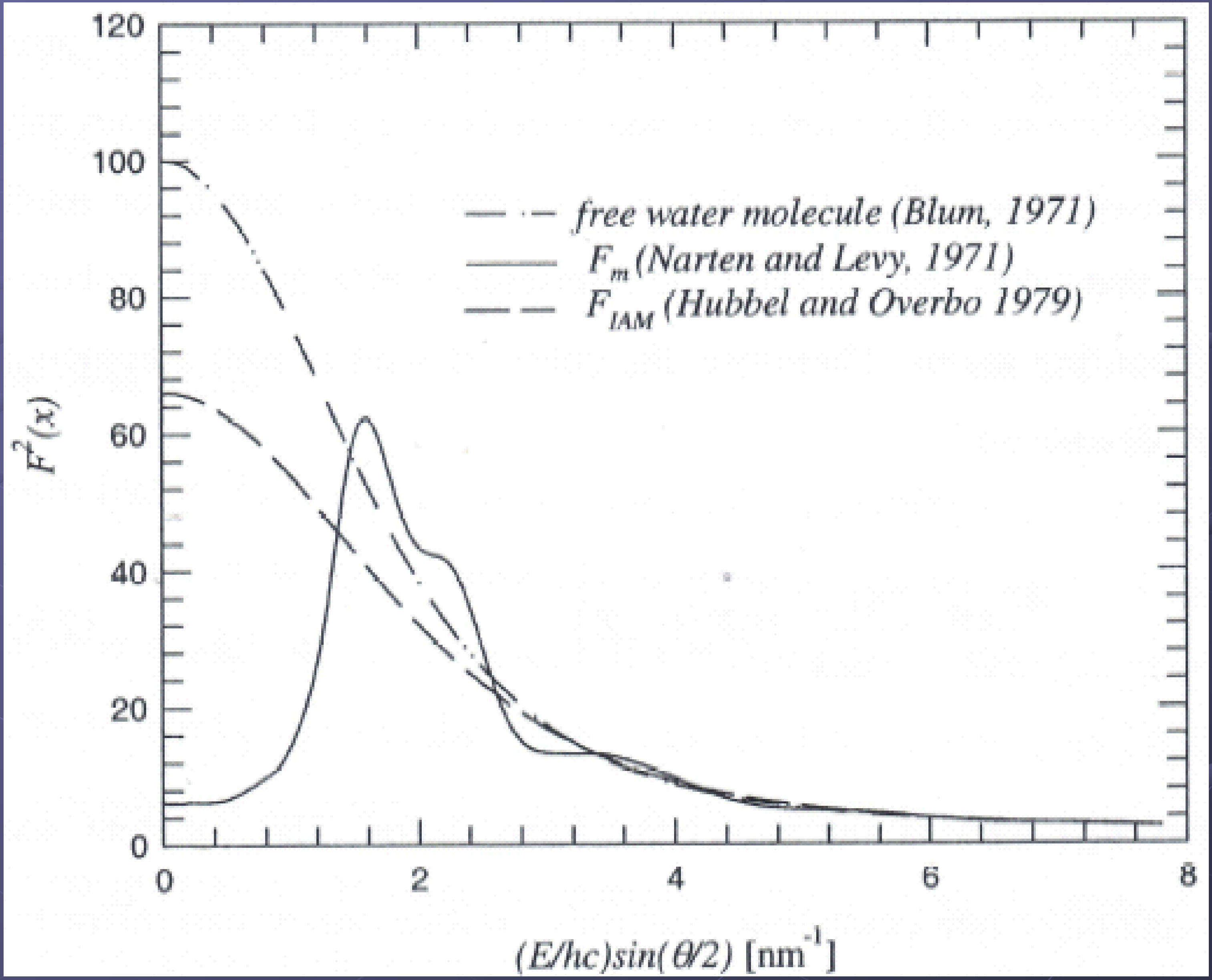
$$|F(x)|^2 = \sum_i \alpha_i |F_i(x)|^2$$

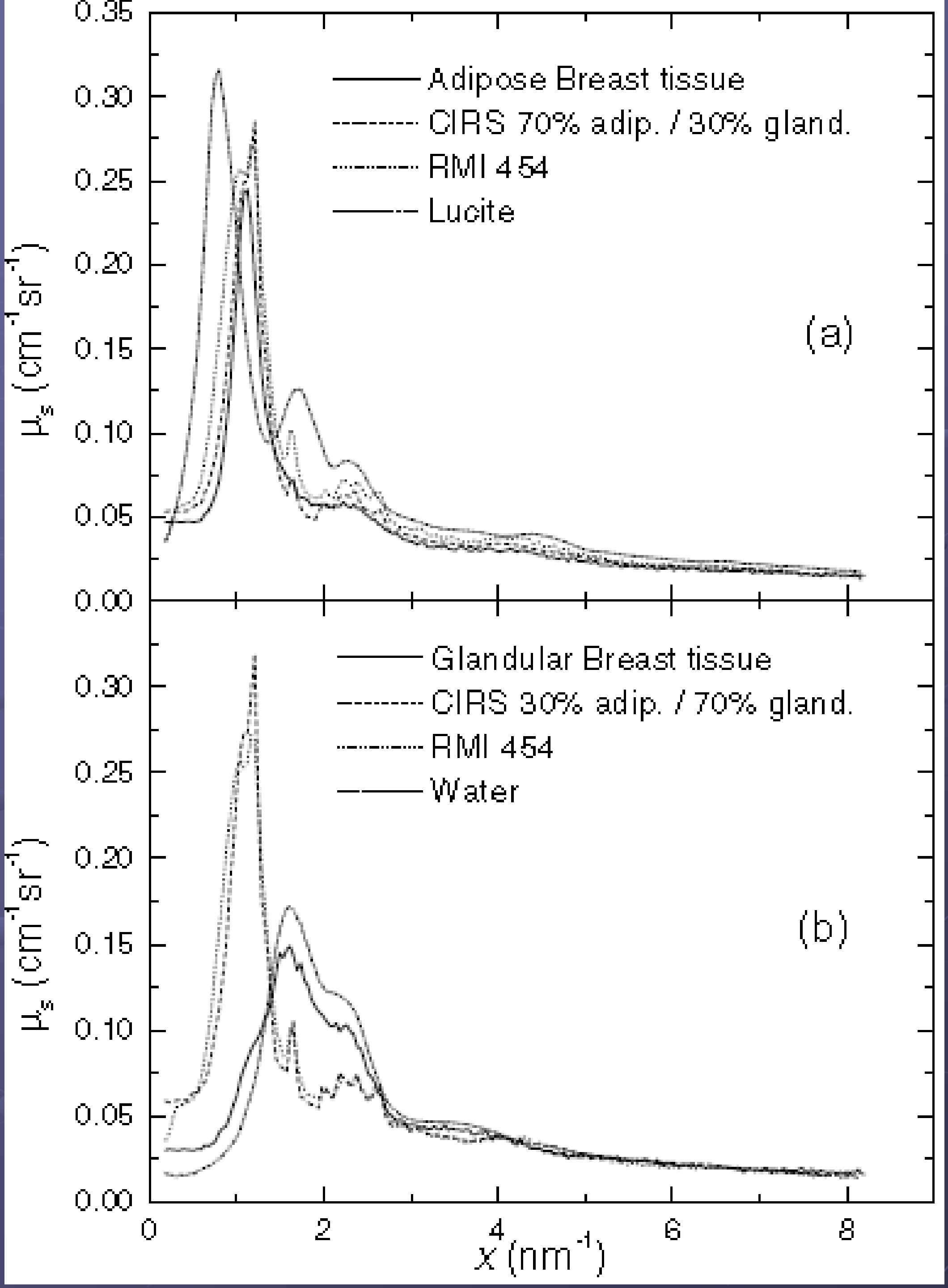
$F_i(x)$ is the Rayleigh or Bragg form factor of the ith material.



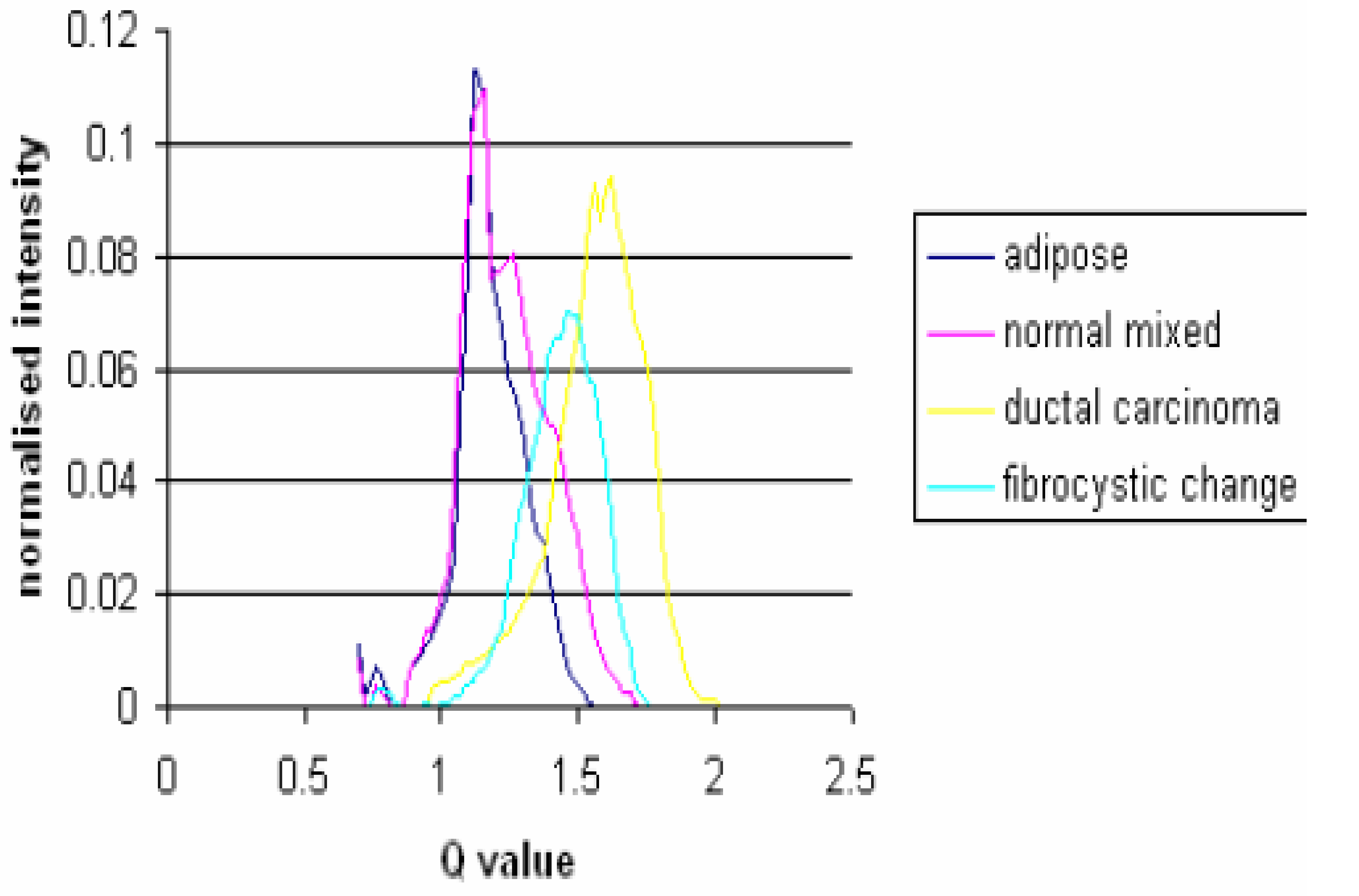
Calculated Linear differential scattering coefficients for fat, water, bone matrix (collagen), bone mineral, and dry bone (28.2% bone matrix, 71.8% bone mineral), .

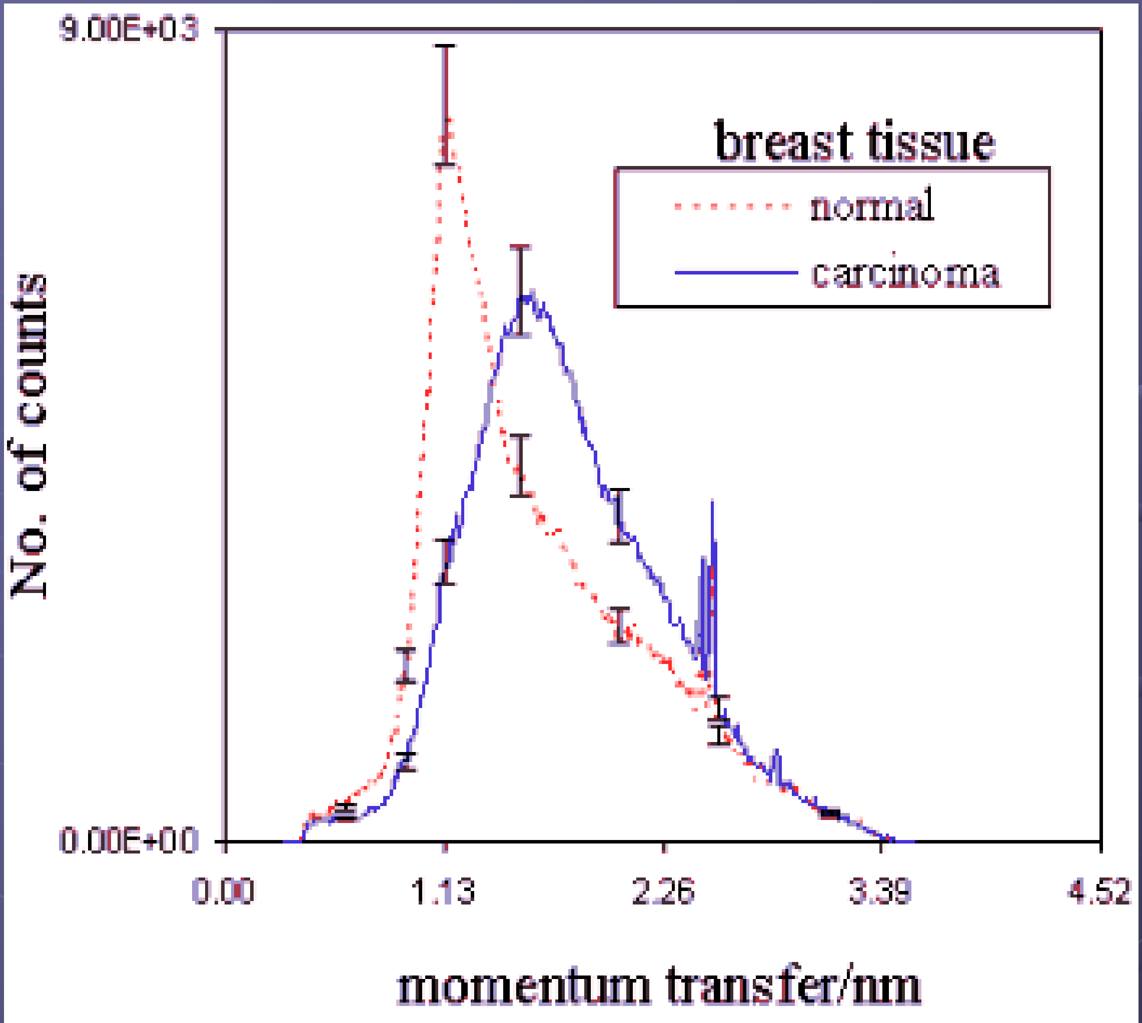
Diffraction patterns of free molecule, Independent free Atom, and Molecular form factor (condensed molecules)





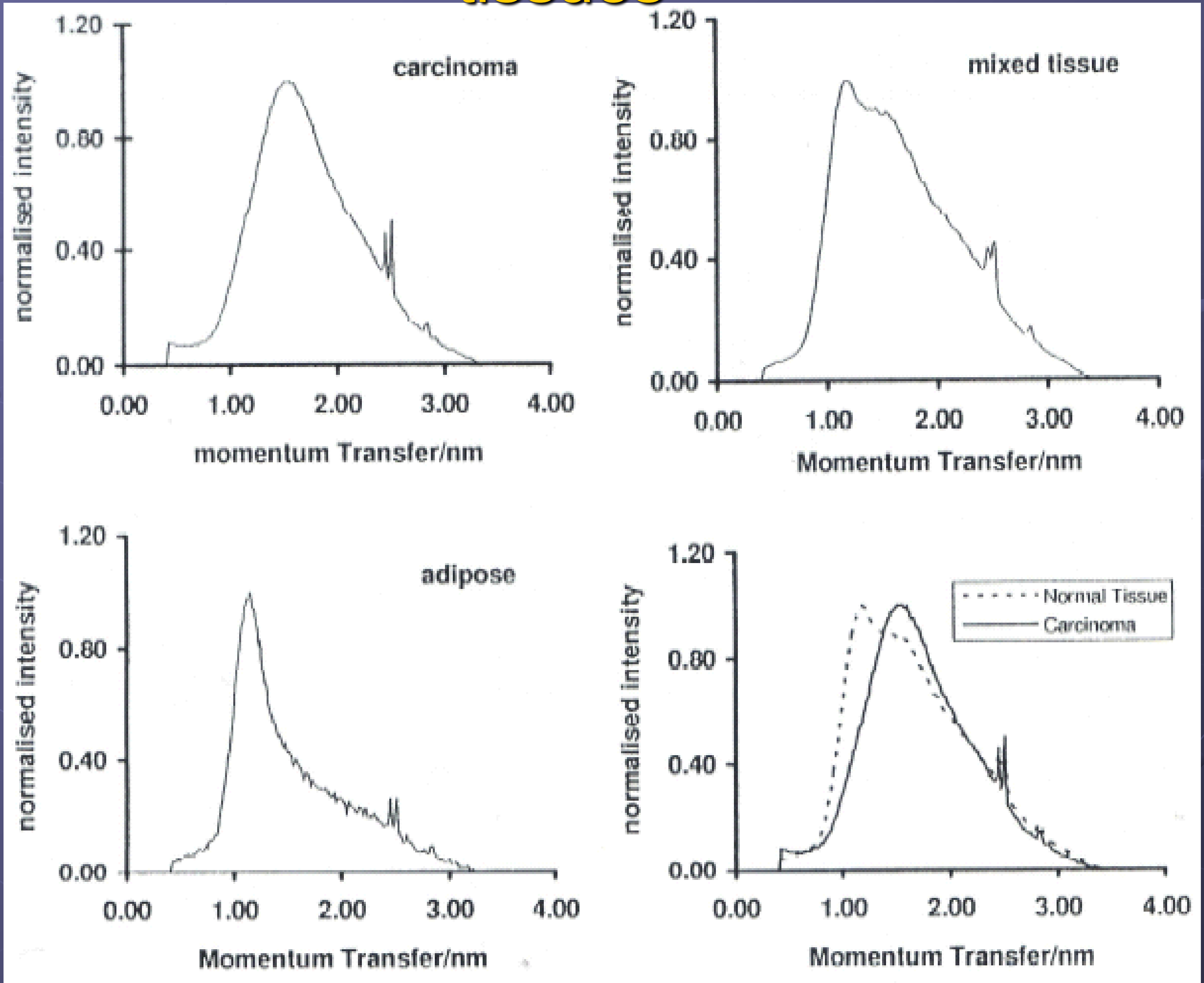
Adipose Breast tissue
CIRS 70% adip. / 30% gland.
RMI 454
Lucite
(a)
Glandular Breast tissue
CIRS 30% adip. / 70% gland.
RMI 454
Water
(b)
μ_s (cm^{-1}sr^{-1})
x (nm^{-1})
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
0
2
4
6
8


0.12
0.1
0.08
0.06
0.04
0.02
0
normalised intensity
0
0.5
1
1.5
2
2.5
Q value
adipose
normal mixed
ductal carcinoma
fibrocystic change

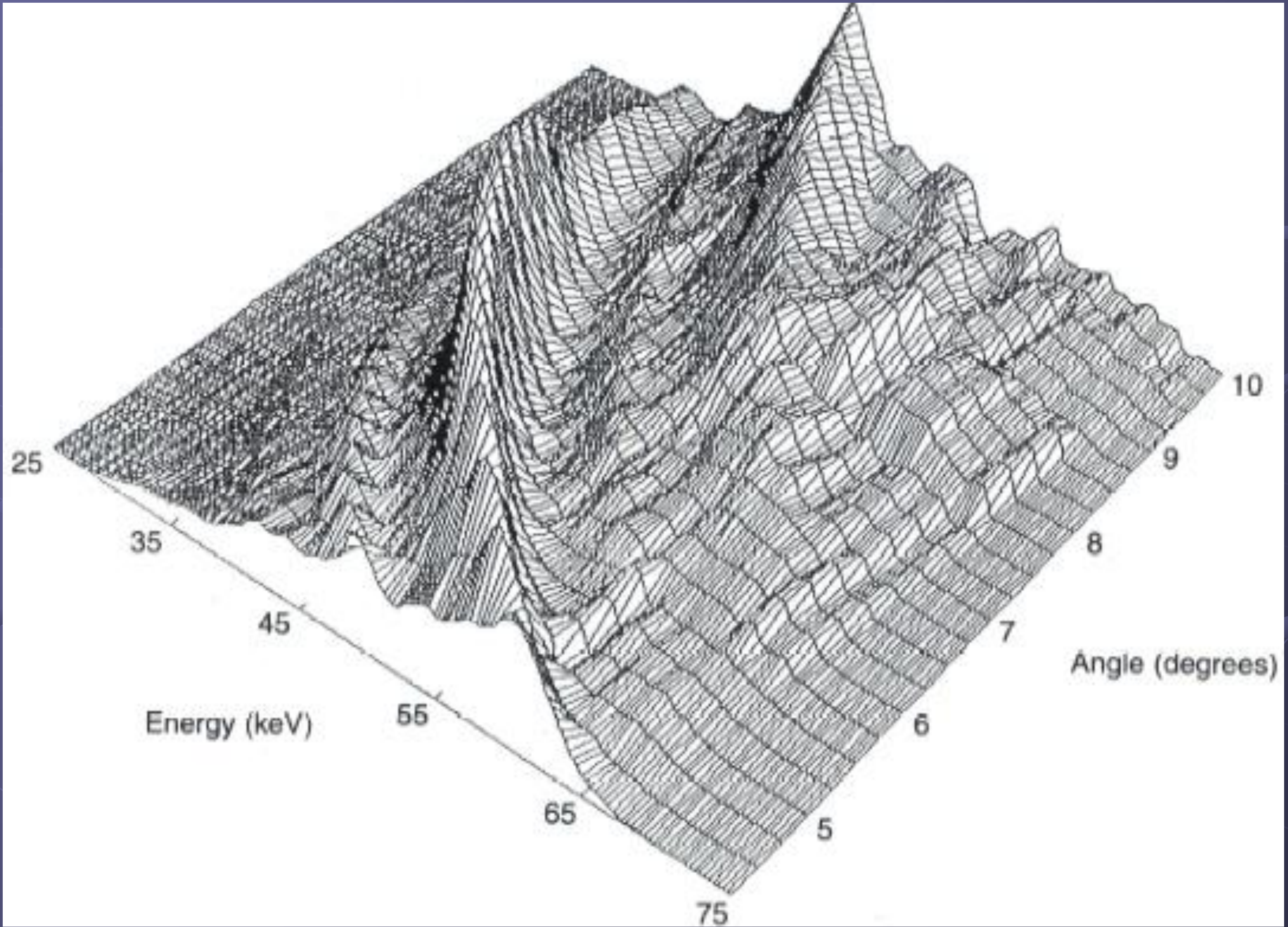


Low Angle X-ray Scattering Signatures of carcinoma and normal breast tissue

Diffraction Profile for different Amorphous tissues

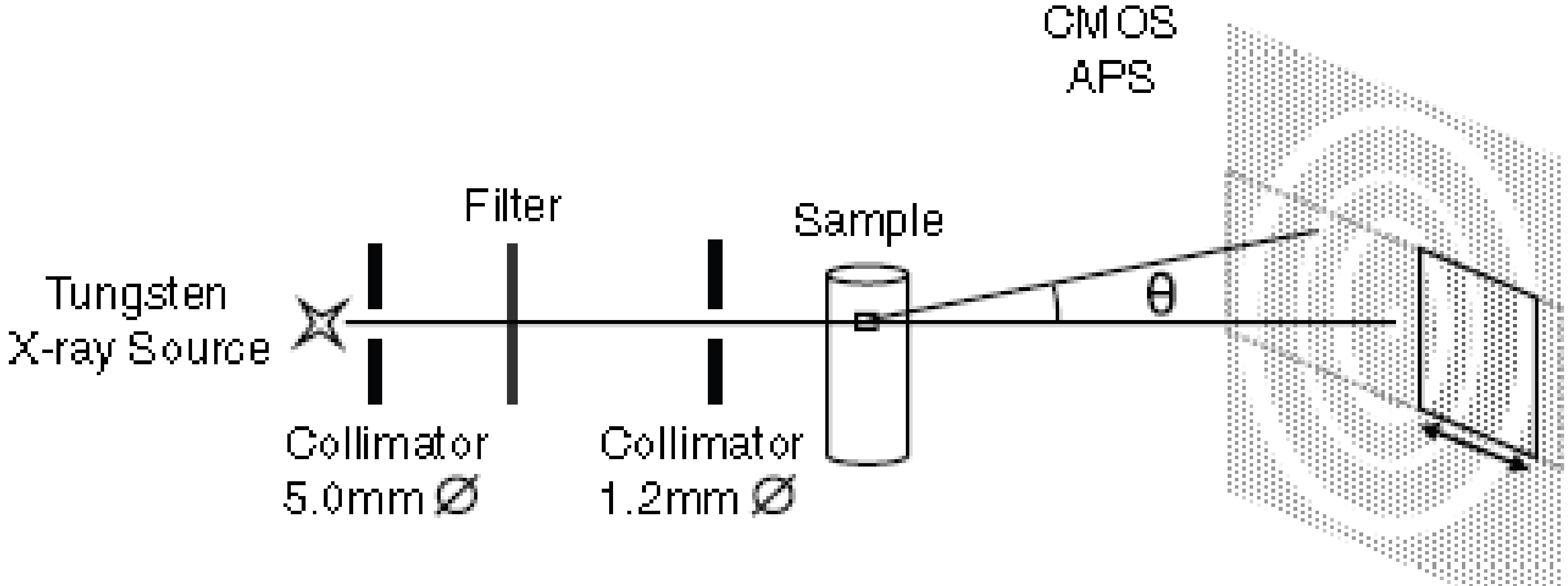


Diffraction profile for Hydroxiapatite over scattering angle from 4 to 10 degrees

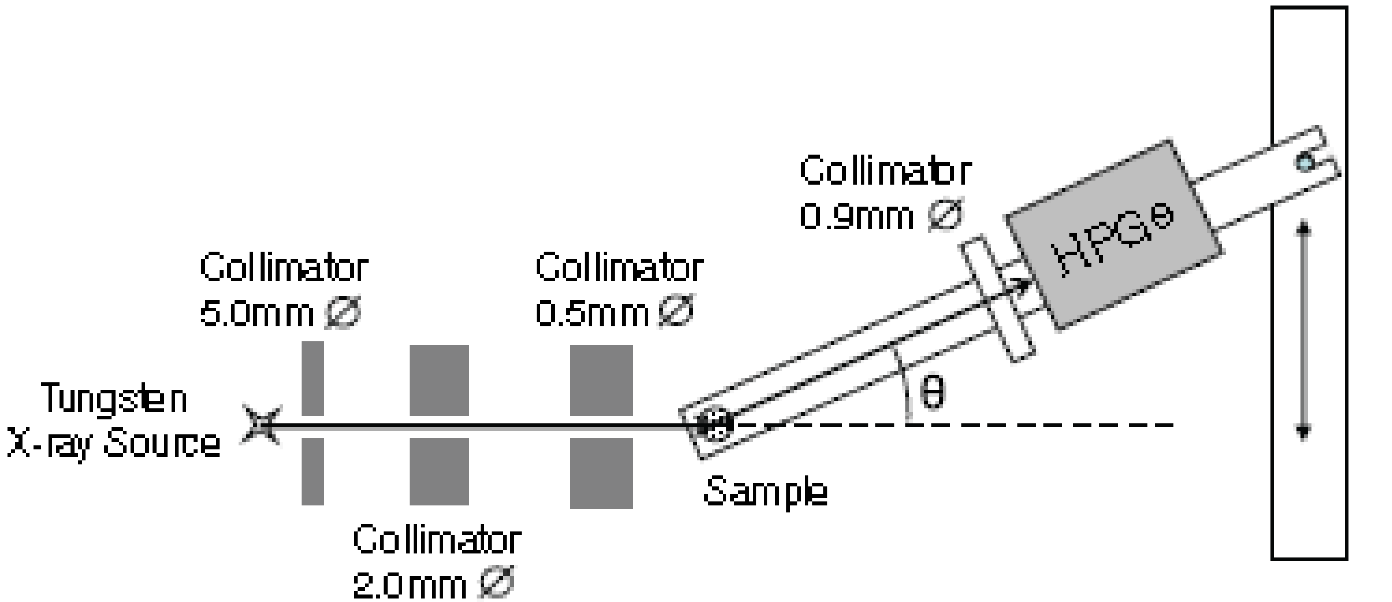


Low Angle x-ray Scattering (LAXS or SAXS)

- Interference effects occurring among the Low angle coherently scattered photons from a material due to the electron distribution
- This type of scattering leads to materials characterization



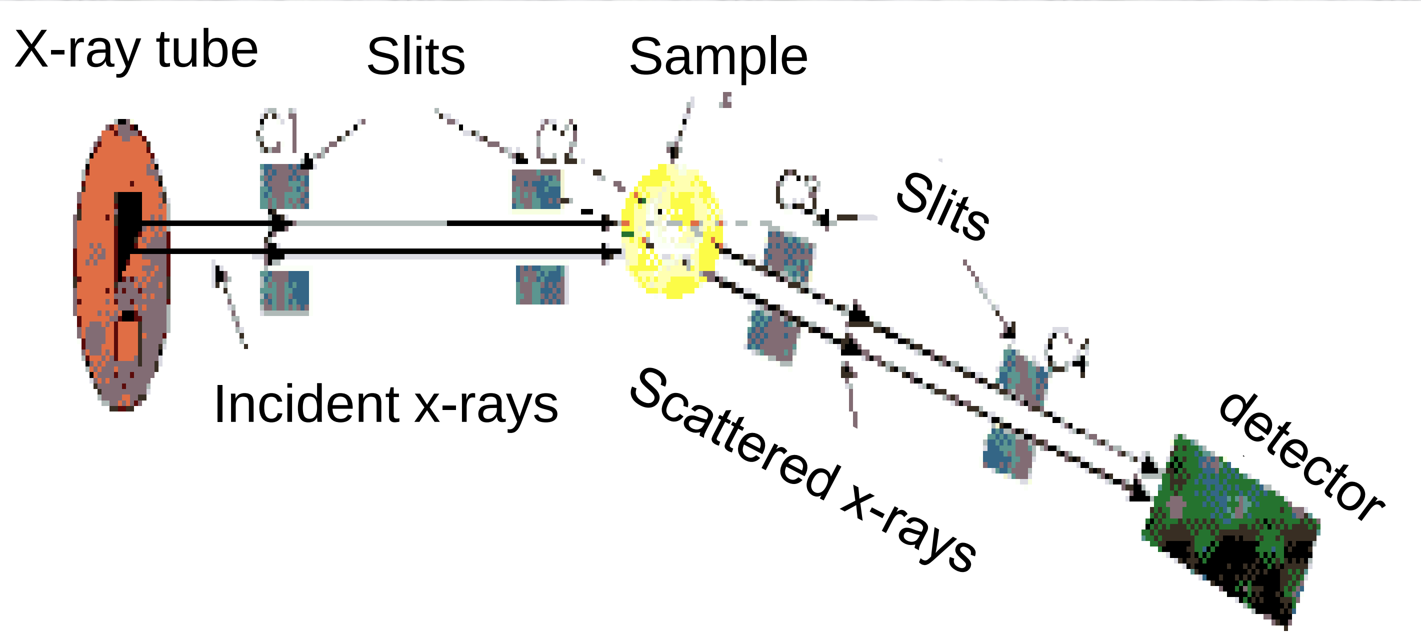
(a) Angle Dispersive Diffraction setup with APS detector



(b) Energy and Angle Dispersive Diffraction setup with HPGe detector

LAXS SET UP

- X-ray tube
- Primary collimator
- Sample
- Secondary collimator
- HP GE detector
- Amplifire
- MCA



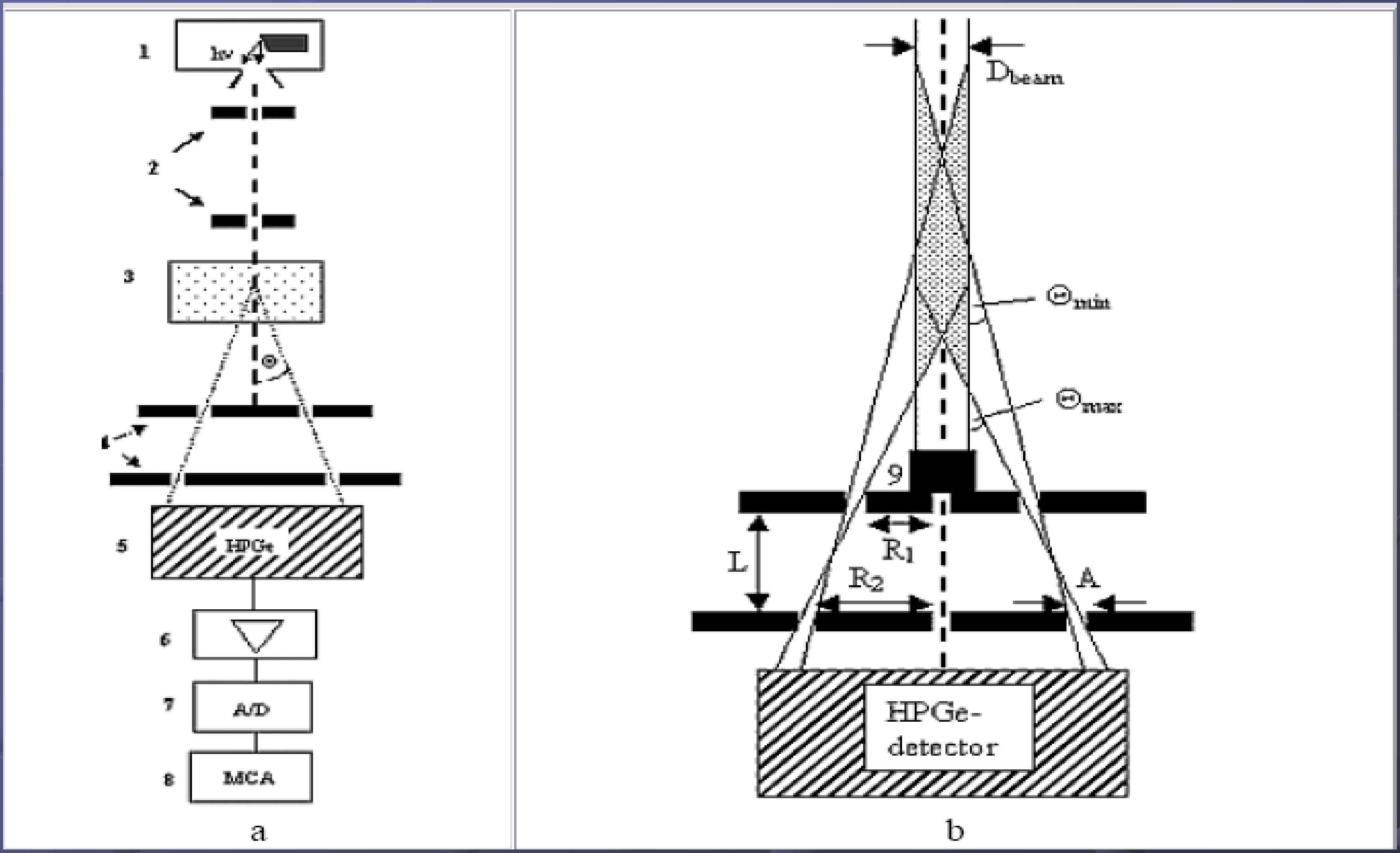
The physical lay out of the LAXS experimental set up

Experiment System

9ch HPGe detector

Full view of the experiment system
(A) 9ch HPGe detector
(B) Target on the X-Y-θ stage
(C) Ionization chamber

Coherent X-Ray Scatter for Non-Destructive



Dual Detector system for Breast Imaging