A Tunable X-ray Diffractometer for the Quantitative Determination of Metal Distribution and Morphology in Bone

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Problem: Bone density loss under prolonged exposure to microgravity

Supports the *Human Health and Performance* component of the Exploration Systems Mission directorate.

Currently,

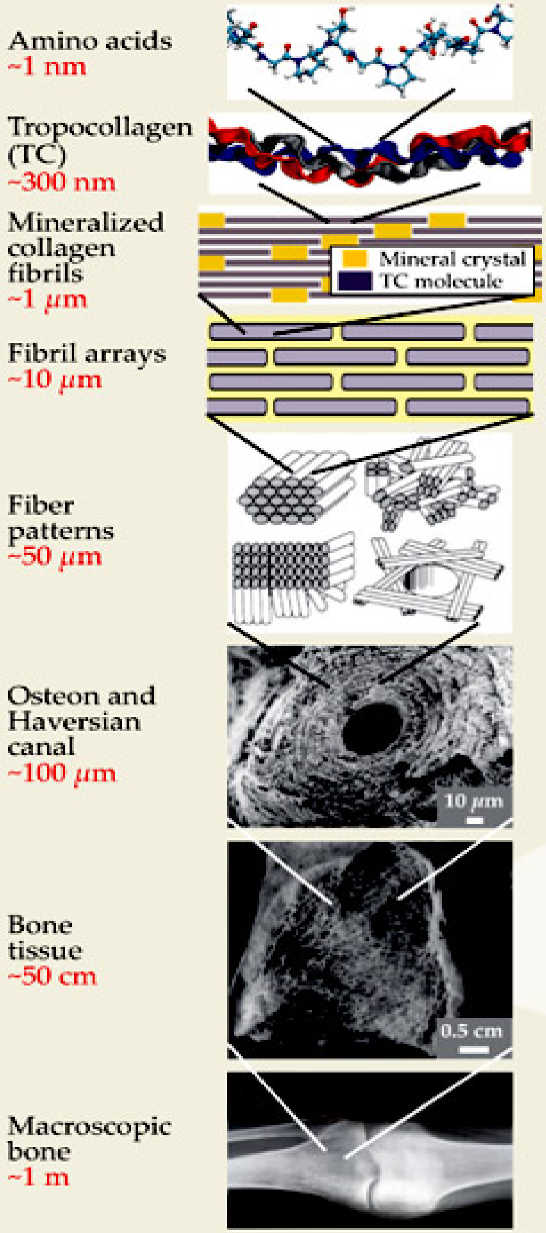
exercise routines
preventive medicine strategies

Want to learn:

The processes involved in the progression of osteoporosis.
Long-term effects of medicinal strategies

Benefits:

Ensure there are no serious drawbacks to the short-term benefits.
Allows tailored physical health programs for exploration crews.

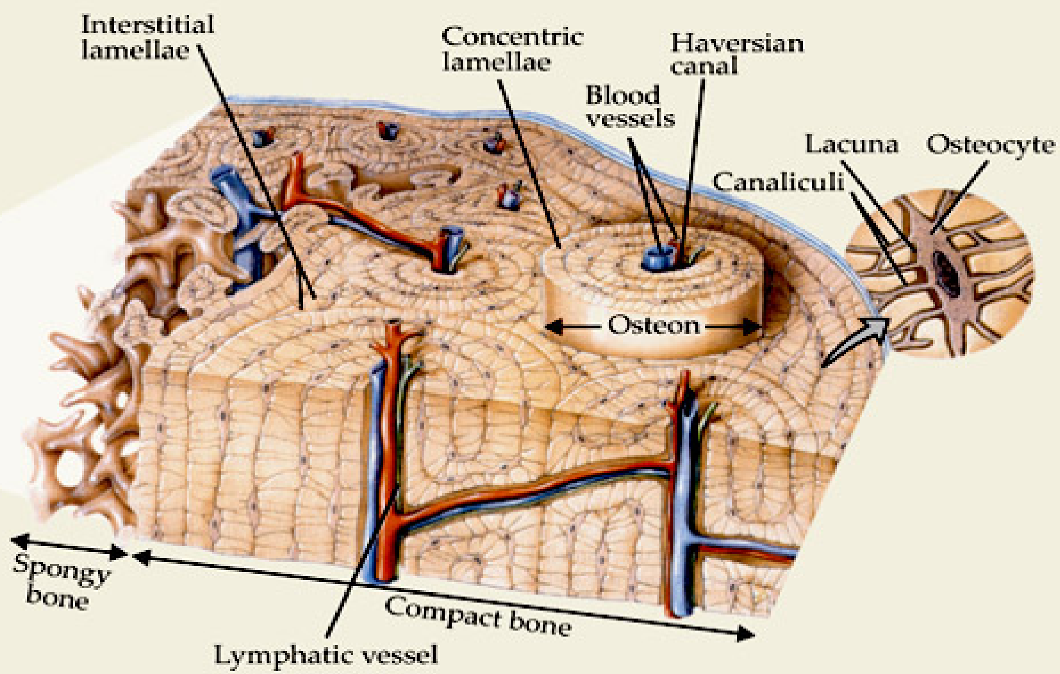


Bones

-provide structural rigidity to vertebrates
-house blood production
-help to regulate bodily pH.

The Osseous tissue

Composed of collagen molecules reinforced by hydroxyapatite

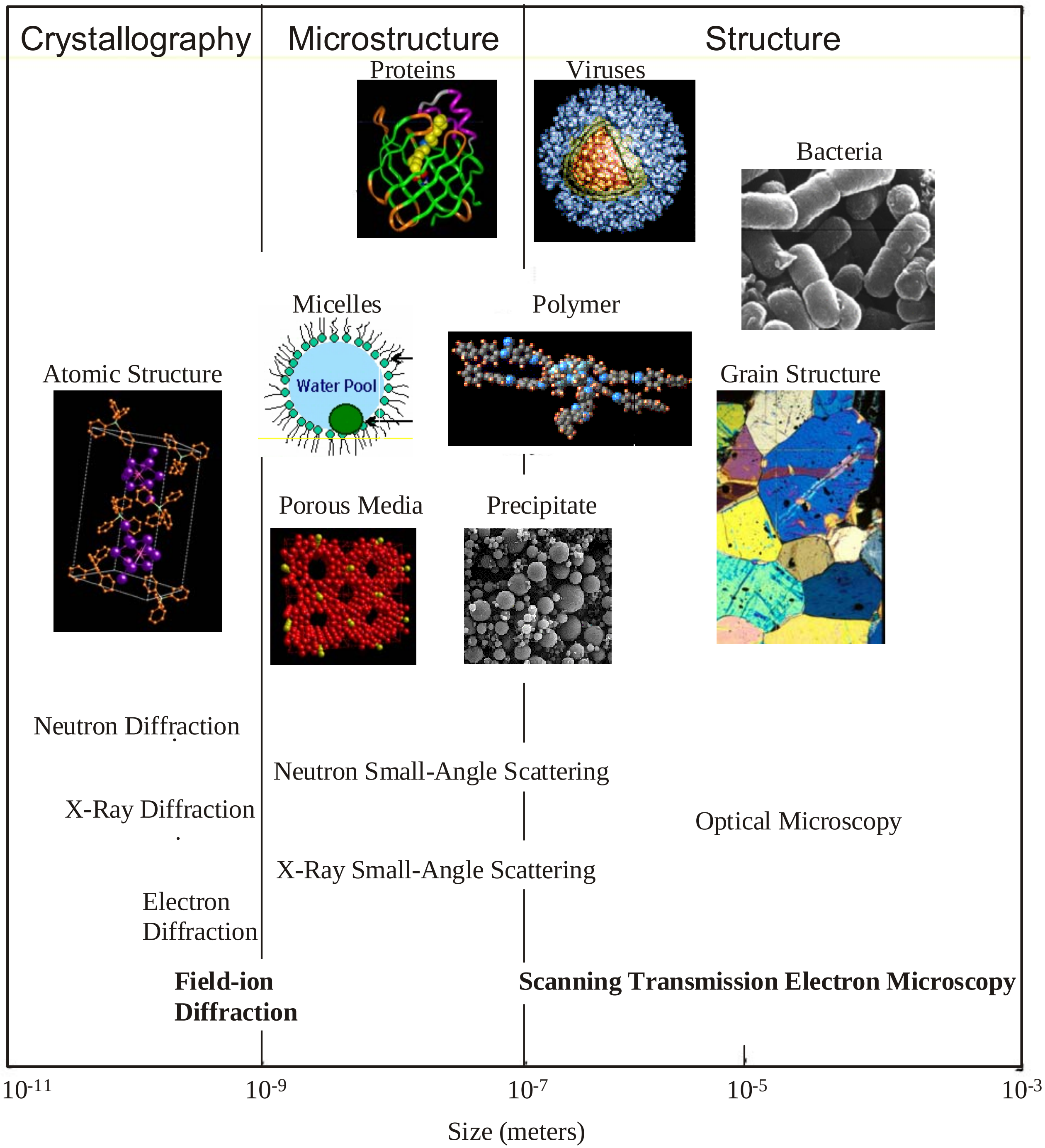


Ritchie, Buehler, Hansma. Phys. Today. June 2009. Weiner and Wagner, Annu. Rev. Mater. Sci. **28**, 271 (1998). G. J. Tortora, *Principles of Human Anatomy*, Wiley, New York, 2002.

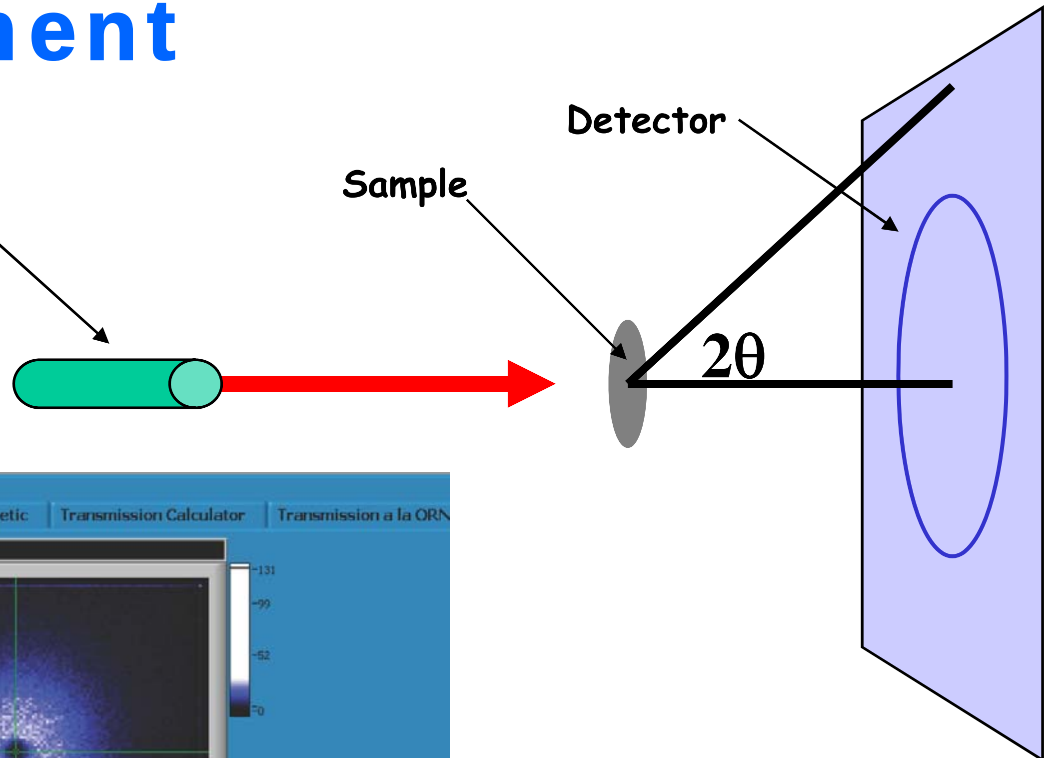
Small Angle X-ray Scattering probes structure

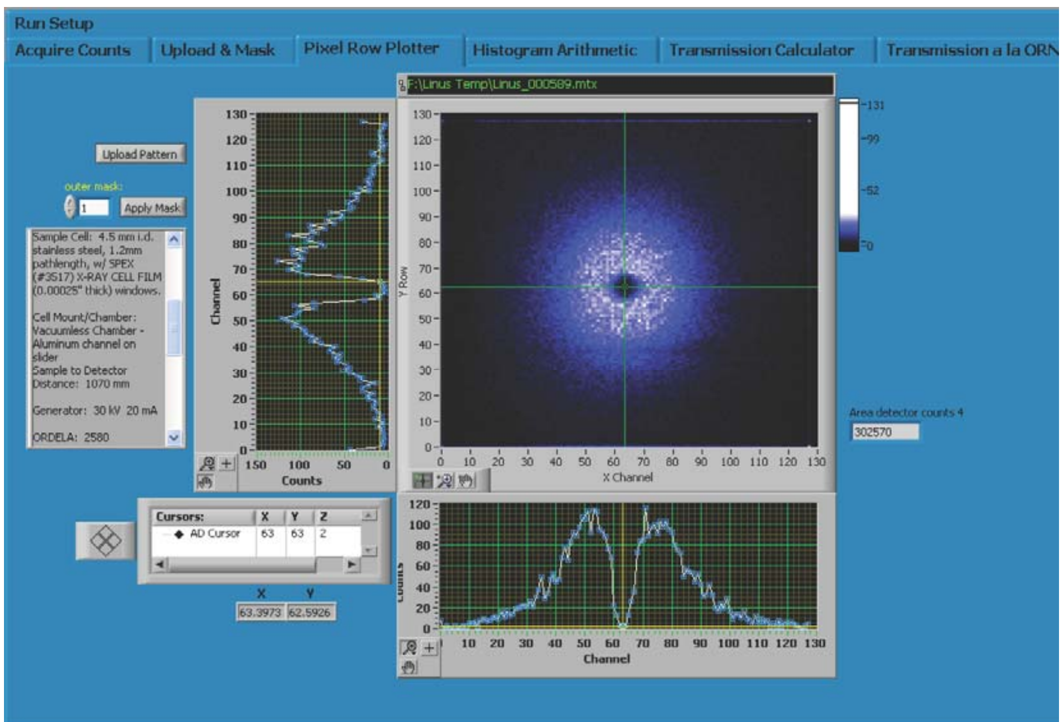
Learn:

- Size
- Density
- Distribution
- Shape
- Composition

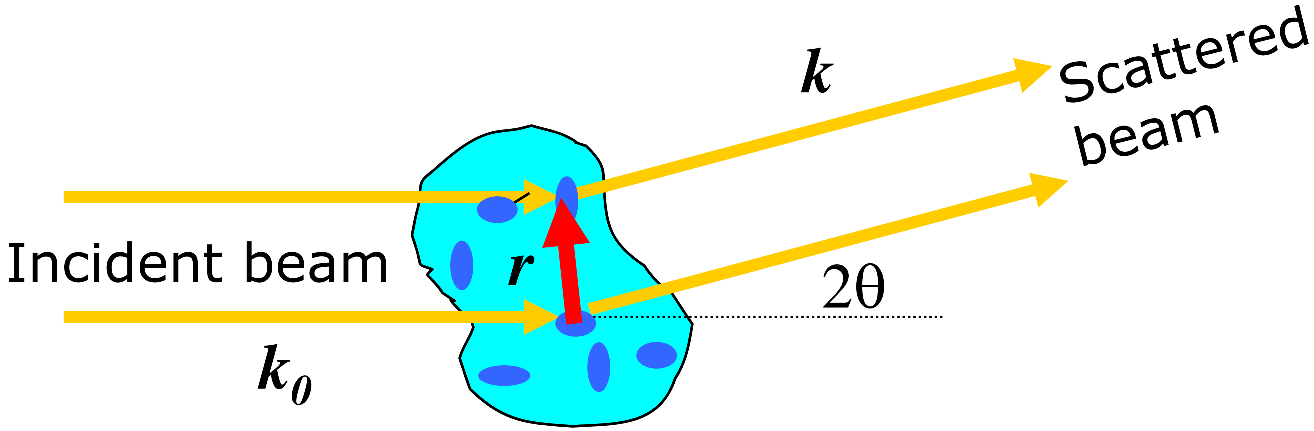


Small Angle Scattering -The Experiment





A Scattering Overview



$$\vec{Q} = \vec{k} - \vec{k}_0 \longrightarrow Q = \frac{4\pi}{\lambda}\sin\theta$$

We measure scattering intensity $I(Q)$ as a function of Q.

$$r \sim \frac{2\pi}{Q} \sim \frac{\lambda}{2\sin\theta}$$

Q: 0.005 – 0.8 $Å^{-1}$

r:10 – 1300 Å

Scattering Contains Information

differential scattering cross section per unit volume (cm^{-1}):

$$I(Q) \propto \frac{d\Sigma}{d\Omega}(Q) = N\Delta\rho^2 V^2 S(Q)P(Q)$$

N	particle density per unit volume (cm^{-3})
V	particle volume (cm^{3})
$\Delta\rho$	electron density contrast (cm^{-2})
S(Q)	particle interactions
P(Q)	morphology and size of scatterer

The Use of Energy for Contrast

In general, higher energy photons are absorbed less by matter.

However, every element has a unique set of absorption edges.

An x-ray absorption edge for an element is the threshold energy at which inner orbital electronic transitions occur.

Incoming radiation induces these transitions resulting in a steep increase in absorption at that energy.

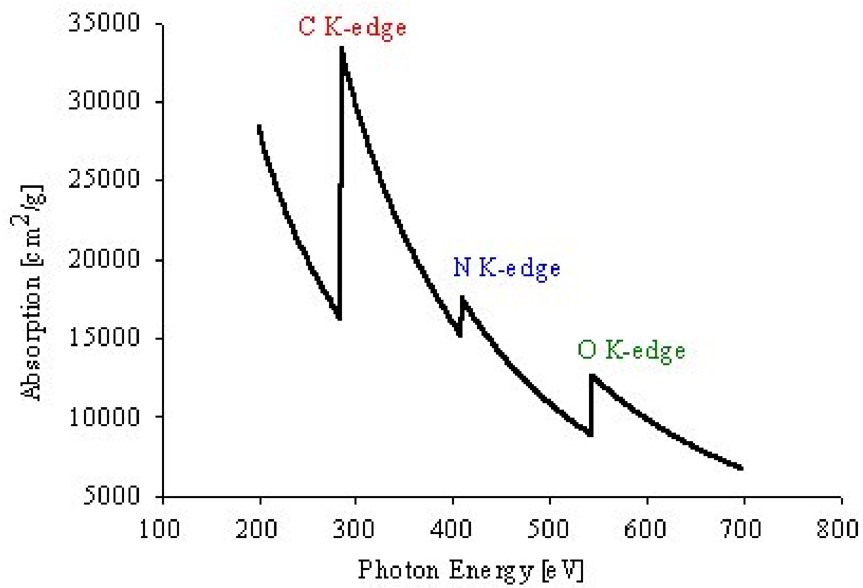
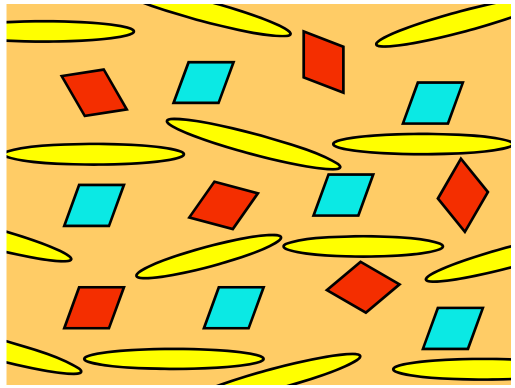
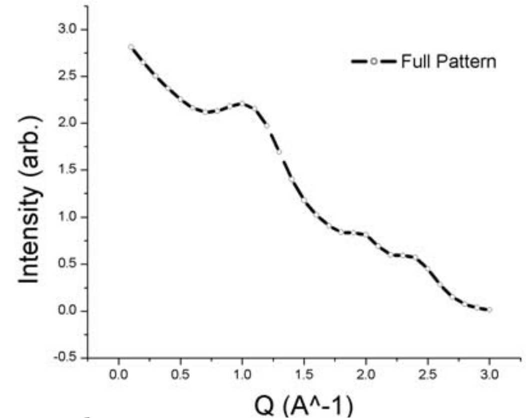


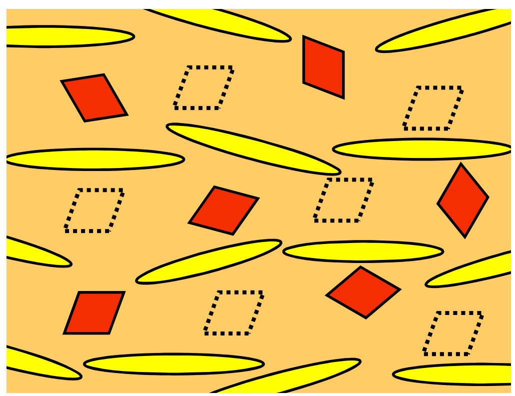
Fig. 1 X-ray absorption edges of carbon, nitrogen and oxygen of a composition typical of a polymer. A rapid increase of the absorption occurs at the threshold of energy required to excite electrons from these inner shells.

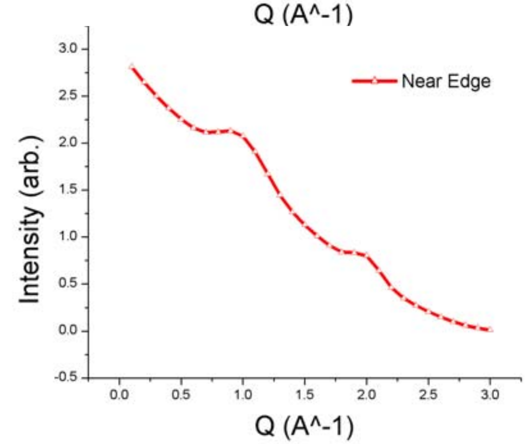
The Use of Energy for Contrast



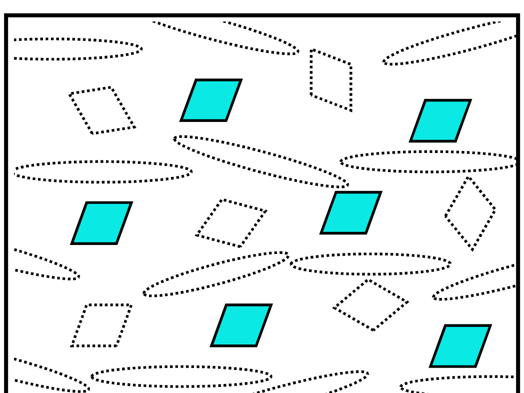


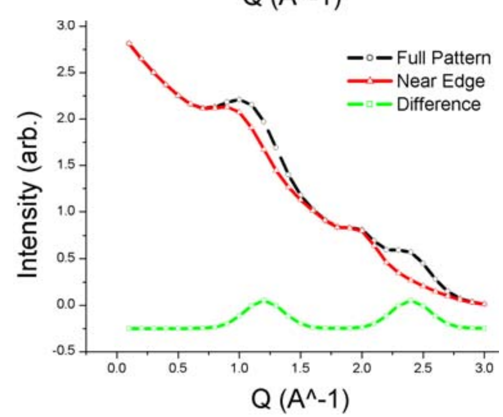
Full Pattern





Near Edge



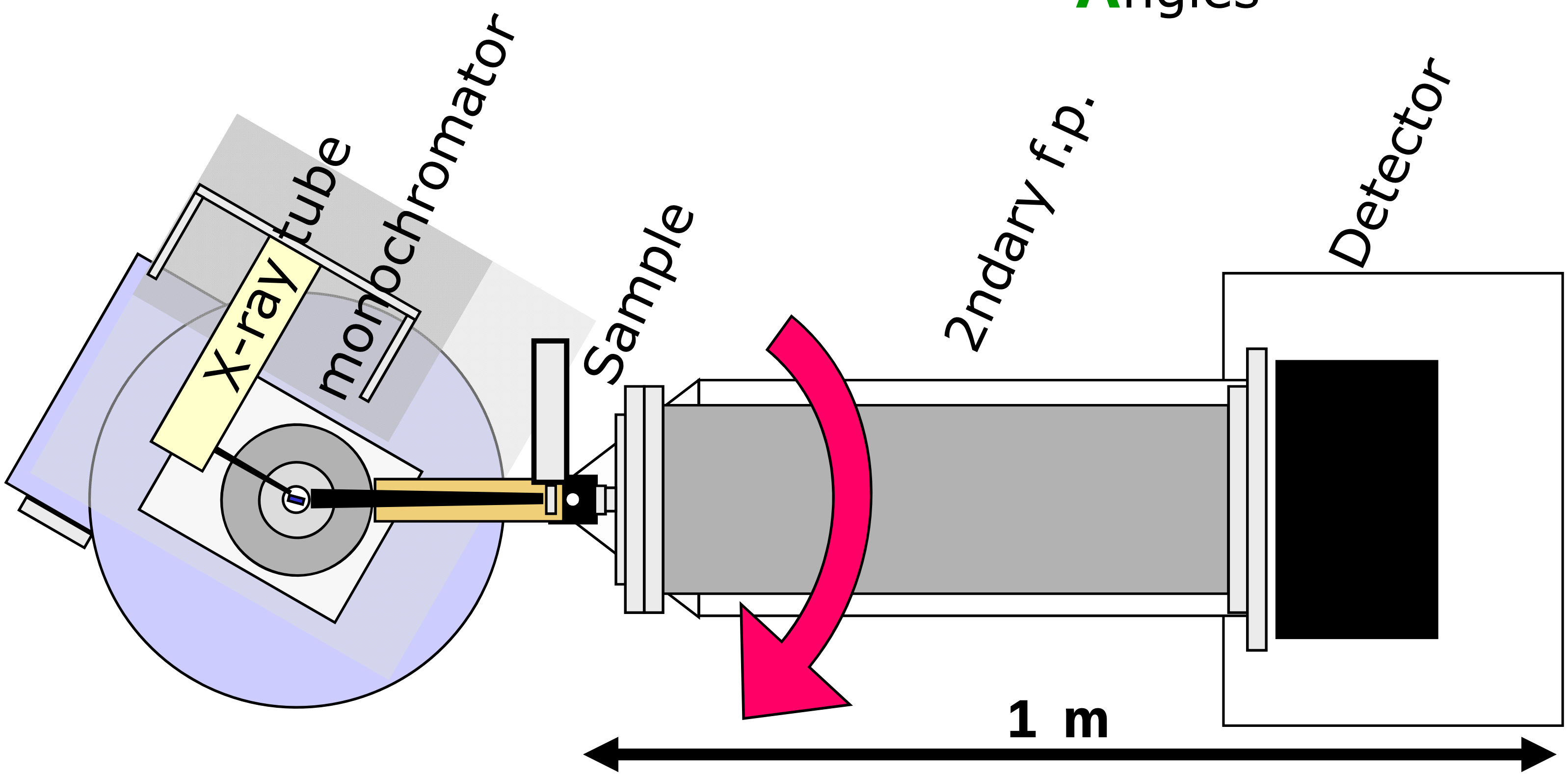


Difference (green)

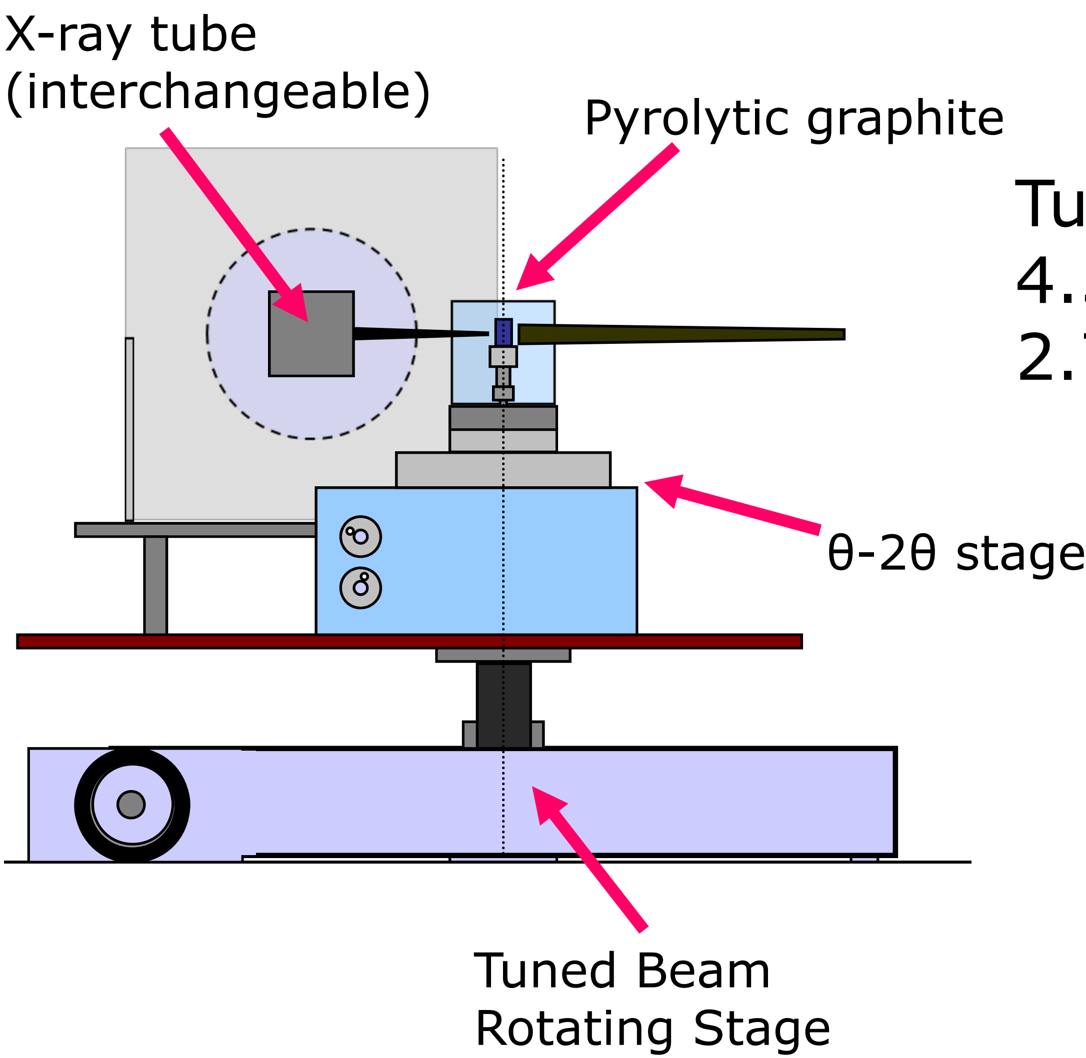
Tunable
Energy
X-ray
Anomalous
Scattering diffractometer

OR,

Multiple
Energy
Diffractometer
Using
Small & intermediate
Angles



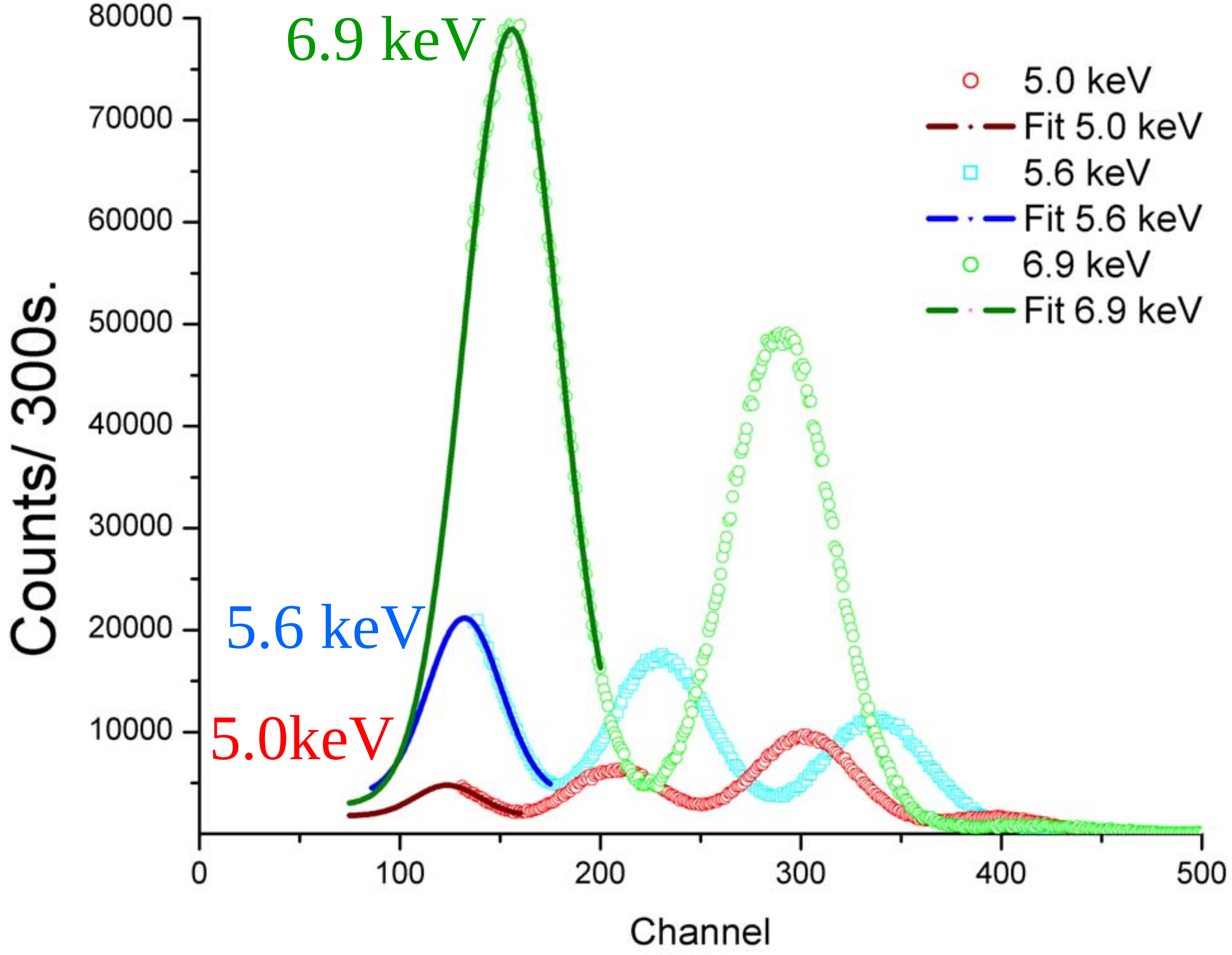
The Tunable Source



Tunable:
4.5 keV – 40 keV
2.76 Å – 0.31 Å

Source Spectrum at Different Tunings

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



E(keV)	Intg. Cts.
6.9	4,547,173
5.6	798,509
5.0	120,666

Conclusions

The new instrument introduces great flexibility to perform standard SAXS investigations, but also more complex techniques:

- -ASAXS
- -high resolution intermediate and wide angle diffraction
- -Versatility allows source to service more than one instrument

Higher order reflections must be addressed:

- -Investigate detector sensitivity as a function of applied voltage
- -Insertion of optic element at source end, e.g. grazing incidence surface to eliminate unwanted reflections

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