Last time we defined a crystal as a solid containing translational symmetry.

The directions of translation can be used to from a unit cell.

A primitive unit cell is on in which there is no translational symmetry within the cell. This is the smallest volume.

Since we now have some idea what a crystal is we need to consider x-rays.

X-Rays

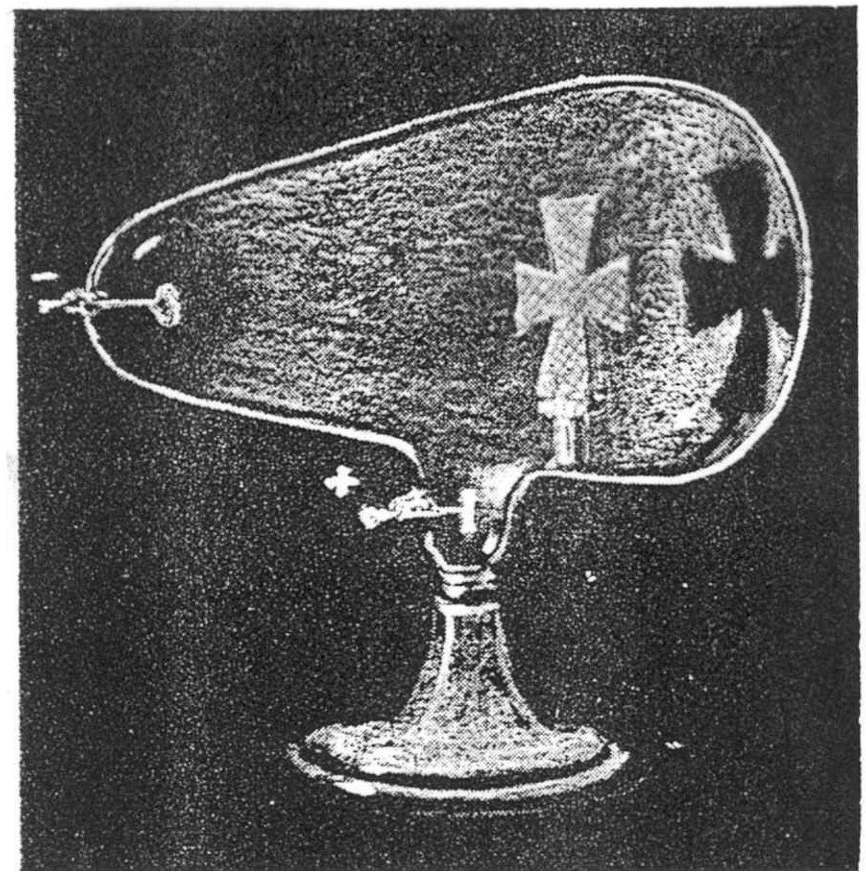
What are they?
How are they produced?

How do x-rays interact with matter?

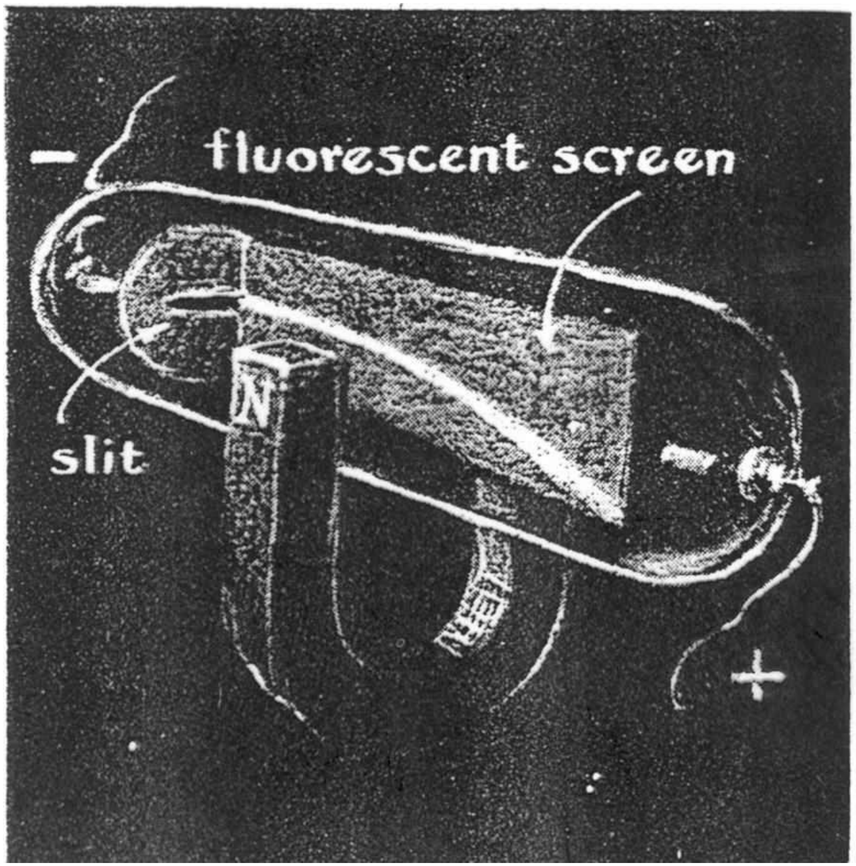
How does the nature of the crystal effect that interaction?

Wilhelm Röntgen (1845-1923)

Crook's Tubes



Crook's Tubes



Crooks Tubes

Produced cathode rays
Cathode rays were particles
Cathode rays did not penetrate matter—they were not observed outside the tube.
Cathode rays were charged.

The Discovery of X-rays in 1895

- Röntgen was working in a very dark lab with a Crook's tube.
- Across the room was a watch glass containing $Ba[Pt(CN)_4]$
- Whenever the Crook's tube was turned on the watch glass glowed.
- These were a new mysterious ray
- Named x-rays

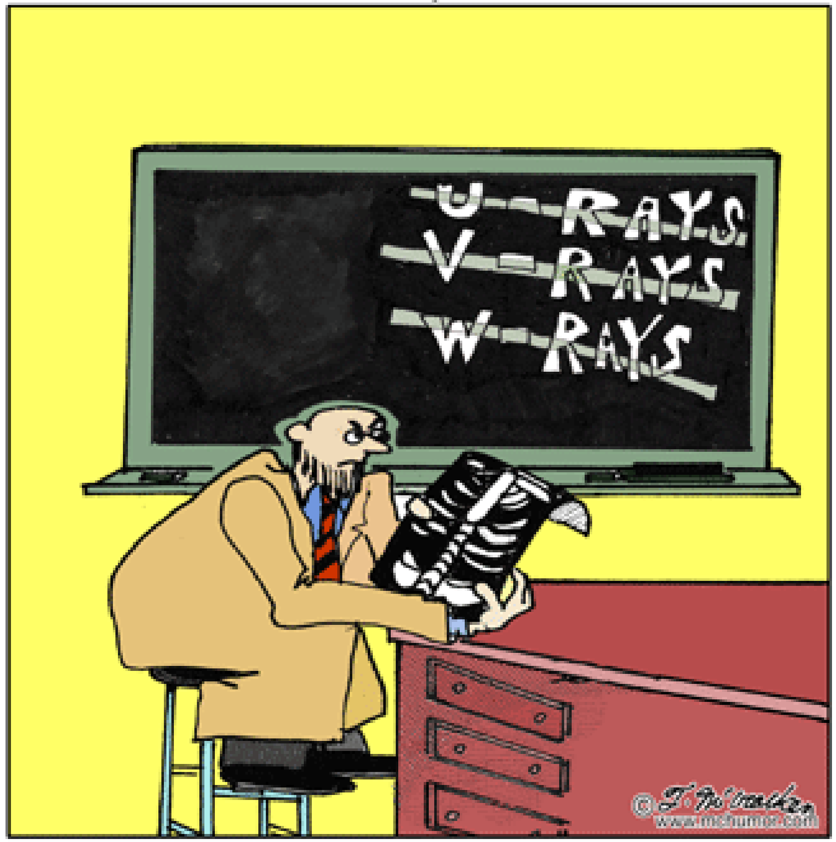
What could you do with X-rays?

WILHELM RÖNTGEN'S FIRST ATTEMPT AT X-RAYS:
SHINING A BRIGHT LIGHT THROUGH MADAME RÖNTGEN

What were x-rays?

- Were they waves or particles?
- What was their wavelength (energy)?
- How were they produced?
- What more could be done with them?
- A question that wasn't asked until much later is how safe are they?

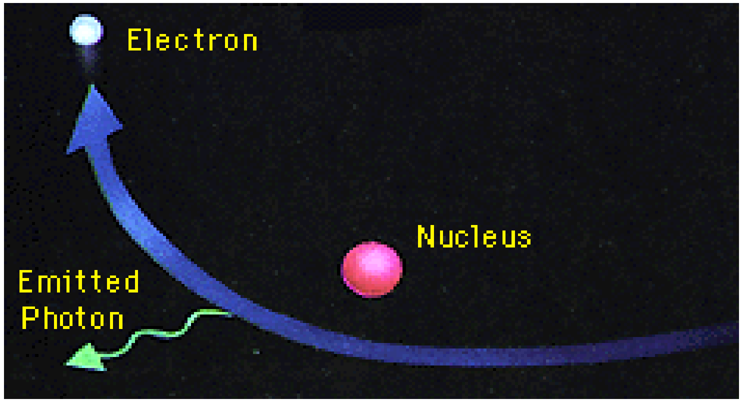
MCHUMOR.com by T. McCracken



Roentgen tries to figure
out what he's discovered.

- X-rays are produced whenever an energetic electron beam interacts with matter.
- The cathode rays were producing x-rays from the elements in the glass.
- X-rays come off the target in all directions.

There are two types of x-rays

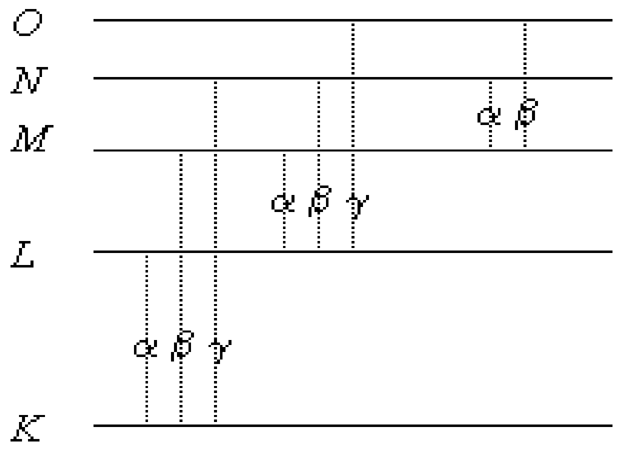


This deceleration of a high energy electron produces white radiation called Bremsstrahlung.

This is a process not described by quantum mechanics

If the energy of the electron is too low it is simply repelled.

Discrete Lines

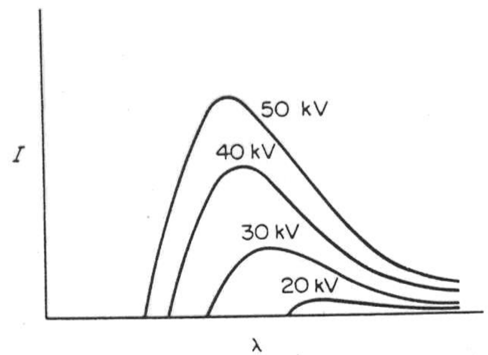


Obviously this energy spectrum differs for each element. Thus, different elements have different x-ray spectra. By firing an electron beam into a solid and analyzing the x-rays produced the elements present can be determined (usually F and greater).

How does this happen?

- The most intense line is the Kα line.
- Do the incoming electrons knock out a 1S electron? Not likely.
- Consider the electron cloud to be like the nucleus with many quantum states.
- When an electron is added to the cloud, the cloud becomes unstable and kicks out radiation to return to the ground state.

X-rays



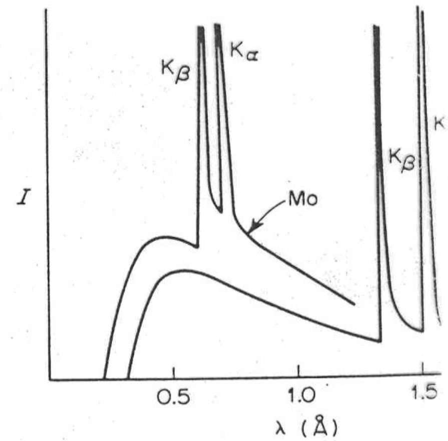
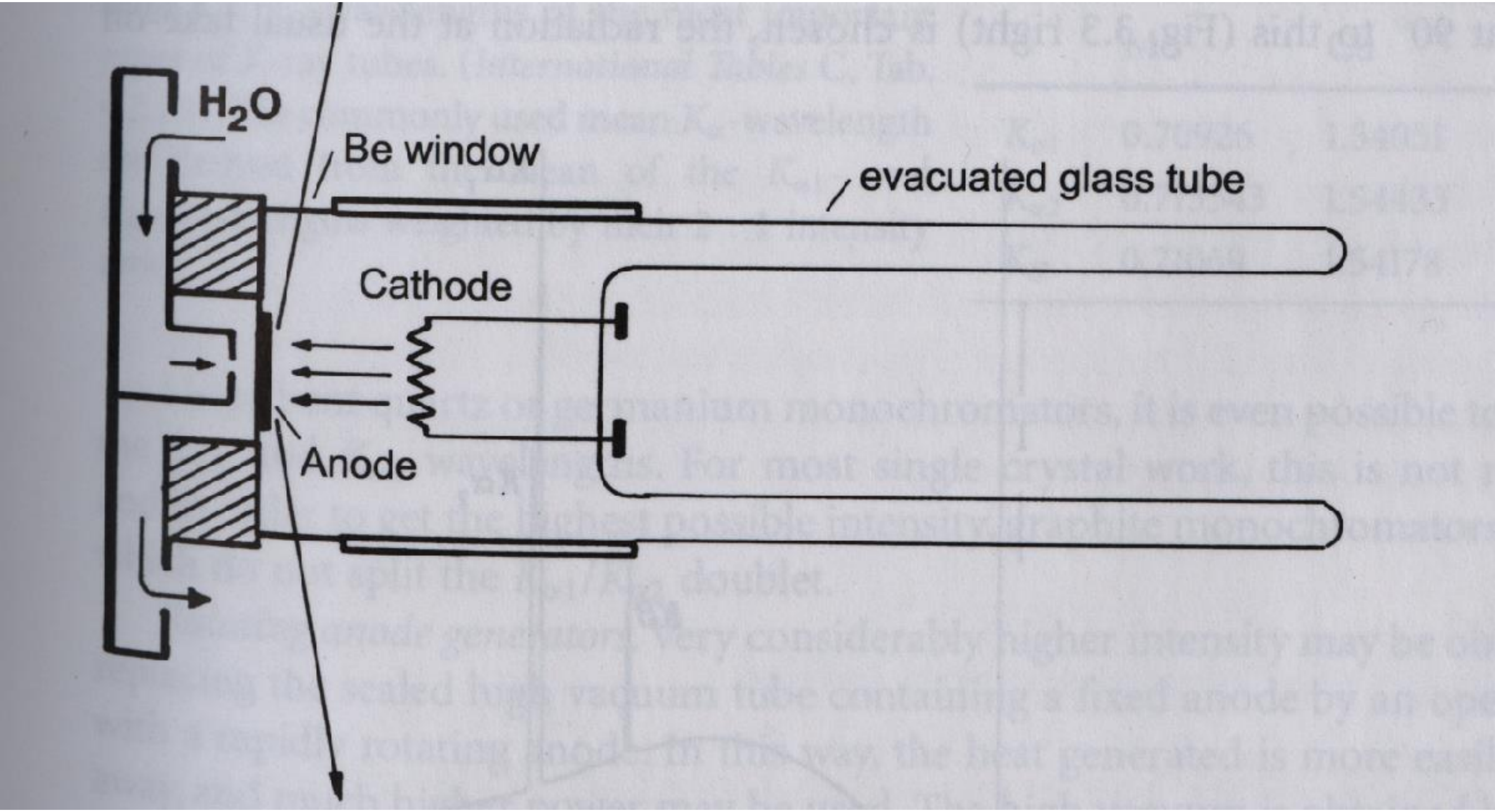


TABLE 1.1 Target Materials and Associated Constants

	Cr	Fe	Cu	Mo
Z	24	26	29	42
α_1 (Å)	2.2896	1.9360	1.5405	0.70926
α_2 (Å)	2.2935	1.9399	1.5443	0.71354
$\langle\alpha\rangle^a$ (Å)	2.2909	1.9373	1.5418	0.71069
β_1 (Å)	2.0848	1.7565	1.3922	0.63225
β filt	V, 0.4 mil[b]	Mn, 0.4 mil	Ni, 0.6 mil	Nb, 3 mils
α filt	Ti	Cr	Co	Y
Resolution (Å)	1.15	0.95	0.75	0.35
Critical potential (kV)	5.99	7.11	8.98	20.0

[a] $\langle\alpha\rangle$ is the intensity-weighted average of α_1 and α_2 and is the figure usually used for the wavelength when the two lines are not resolved.
[b] 1 mil = 0.001 in. = 0.025 mm.

Modern X-ray Tube



Problems

- Most of the electrons are simply conducted by the target. This produces a huge amount of heat in a small area.
- For example, a power supply might provide 20ma at 50Kv or 1Kw of power. Of this ~97% will become heat. For a small beam a small target is required. Target melting.
- Obviously it is important that there be a good vacuum between the filament and the anode or there will be arcing.

One Solution to the heat Problem

- We can better dissipate the heat if we spin the target
- This is a rotating anode generator
- In this case the vacuum must be kept by pumps
- Need a seal to hold $1x10^{-8}$mm vacuum and allow anode to spin at 3000-6000 rpm.

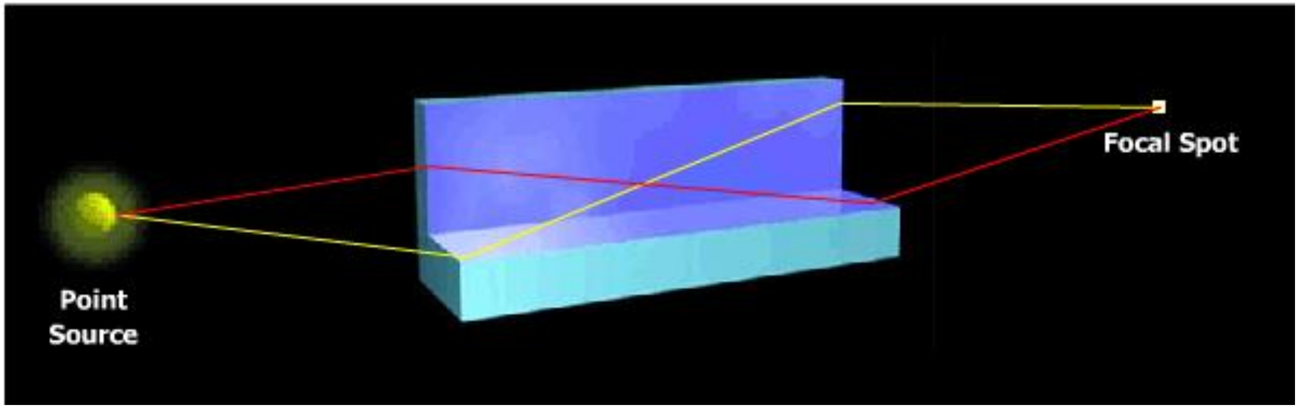
Rotating Anodes

- Expensive to purchase
- Expensive to maintain
- ~12 fold increase in beam intensity
- Various beam diameters are possible

Focusing Optics

A multilayer optic is produced by depositing alternating layers of light-element- and heavy-element-containing materials onto a substrate. The layer thickness acts like the d spacing in a crystal in the sense that X-rays impinging on a multilayer optic at the proper θ angle will produce a monochromatic diffracted X-ray beam. If the layer thickness is varied across a pre-curved substrate, a graded optic can be produced that captures a larger angle of X-rays from the source and produces either a focused or parallel X-ray beam.

X-ray Optics



Rigaku MM002+

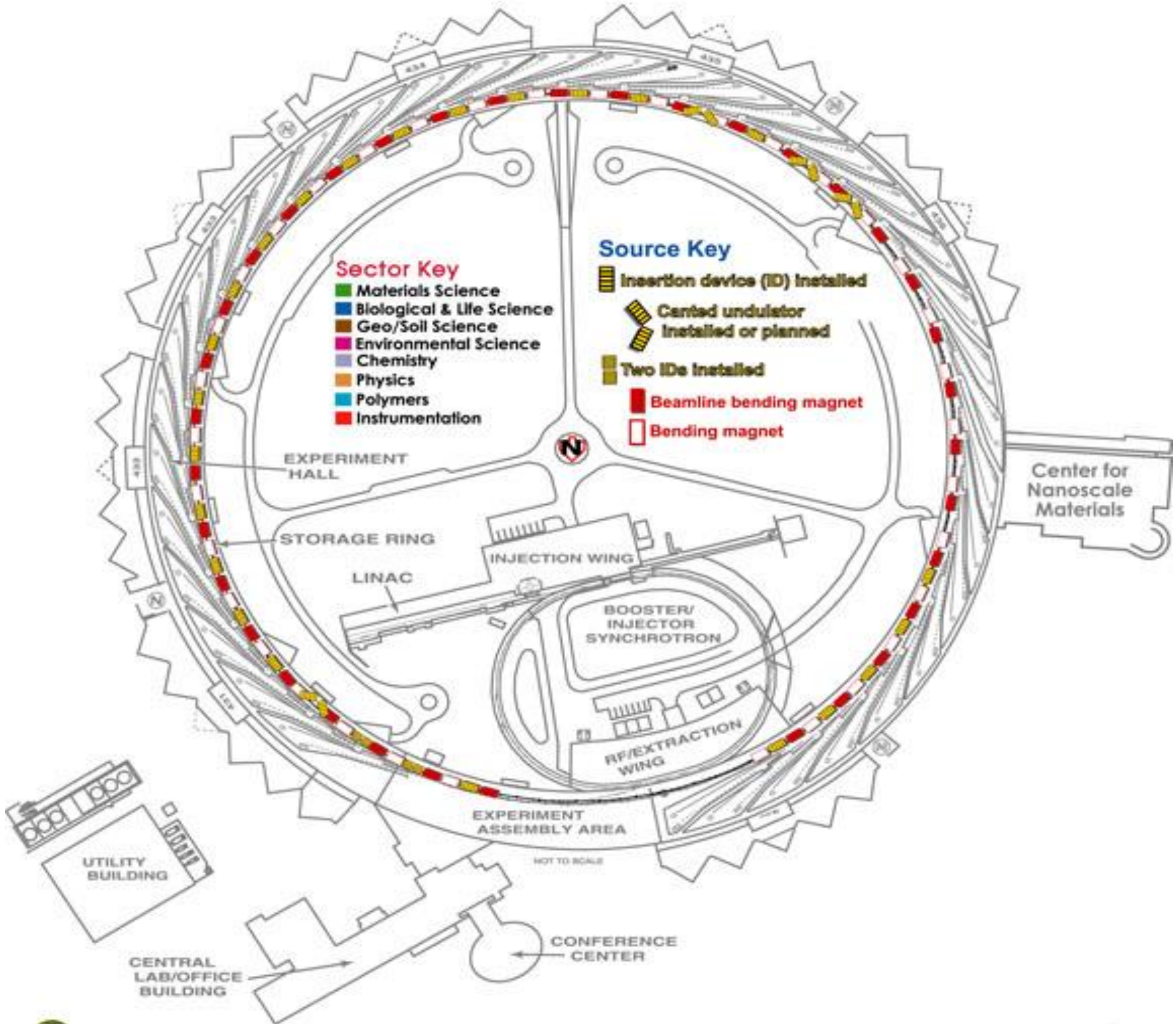
- Uses a Copper target.
- The electron beam is focused using magnets to produce a small size.
- The x-rays go through an optics system
- Current 0.88ma Voltage 45Kv vs for a regular tube 20ma and 50Kv.
- Intensity is roughly 5 times greater than tube.
- Spot size 0.1 mm vs 0.4 mm
- The unit uses 110v and plugs into a standard outlet.

Need Even More Intensity

- Want 2 to 3 orders of magnitude or more.
- Want tunable wavelength
- Want very small beam size
- Use a synchrotron.
- Accelerate electrons to near the speed of light and have them circle around a large circle
- Only standing waves of the circle diameter will be allowed

The Advanced Photon Source

The ADVANCED PHOTON SOURCE @ Argonne National Laboratory



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Which Wavelength to Use

- Generally use Cu 1.5418Å or Mo 0.71073Å
- The longer the wavelength the farther apart the diffraction spots are in space. For large unit cells like macromolecules use Cu. As the distance between spots is given by Bragg's law.
- Cu produces more x-rays and the detectors have a higher efficiency in measuring them.
- Mo is not as absorbed as Cu. Best for heavy element problems.
- Move back to copper lately.

Medical Xrays vs Crystallography

- Medicine needs penetrating x-rays—so short wavelength.
- The power loading on the target is limited by its melting point—want high melting metal
- Medical x-rays use a tungsten target—0.15Å
- Since the x-rays are on for less than a second do not need to worry about variations in the beam.