Production of X-rays
2007 ACA Summer School
Illinois Institute of Technology

T. I. Morrison
Physics Department, Center for Synchrotron Radiation Research and Instrumentation,
IIT
Modified 2007 by Andy Howard

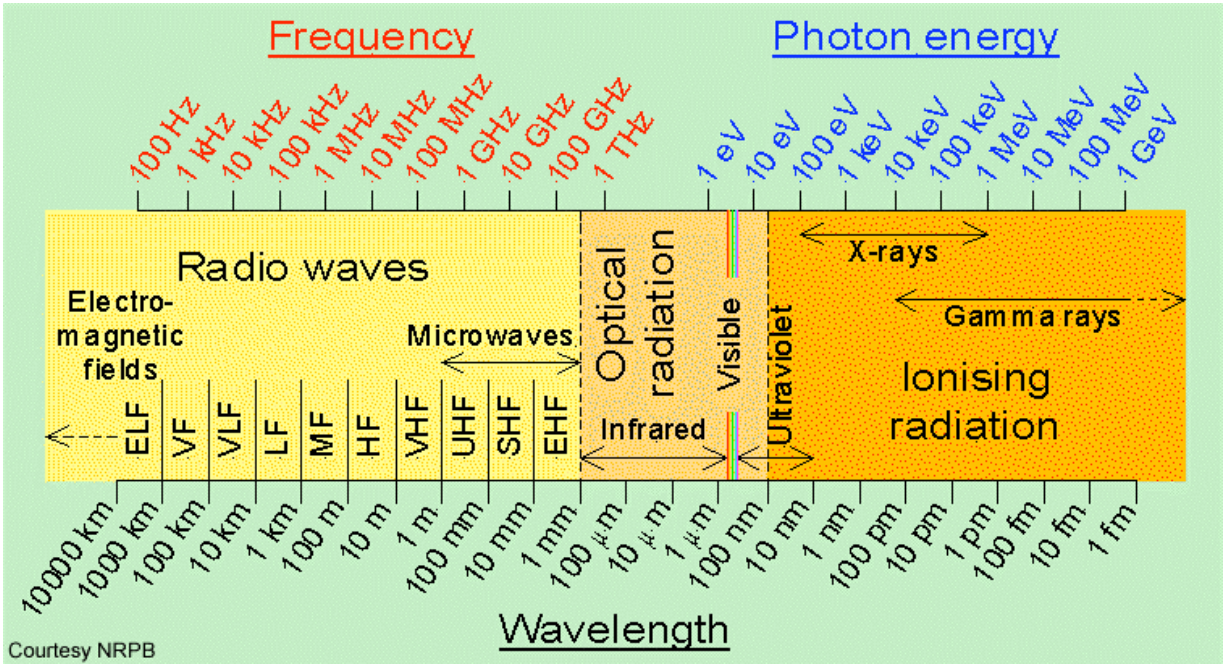
Historical Background

Wilhelm Conrad Roentgen

- was German
- discovered X-rays in 1895
- is currently dead

http://www.nobel.se/physics/laureates/1901/rontgen-bio.html

X-rays are electromagnetic radiation over a range of energies or wavelengths; the specific range depends on the author



http://images.google.com/imgres?imgurl=www.srp-uk.org/gif/emspectrum1.gif&imgrefurl=http://www.srp-uk.org/spectrum.html&h=409&w=755&prev=/images%3Fq%3Delectromagnetic%2Bspectrum%26start%3D40%26svnum%3D10%26hl%3Den%26lr%3D%26ie%3DUTF-8%26oe%3DUTF-8%26safe%3Doff%26sa%3DN

For this author, the range is from about 1.2 KeV (soft X-rays) to about 1,020KeV (pair production)

$$E=h\nu = hc/\lambda$$

In practical terms,
E (keV) =12.3984/ λ (Angstroms)

Origins of electromagnetic radiation:

Acceleration (deceleration) of a charged particle

Transitions between electronic (or molecular) states
(also interpretable as a change in momentum)

Consequence of the constancy of the speed of light: it takes a finite amount of time for the information that a charged particle has changed its velocity to get to another point, thus changing the electric field density at that point. This causes a "pulse" in the em field; a series of pulses makes up a wave train

Deceleration of a charged particle

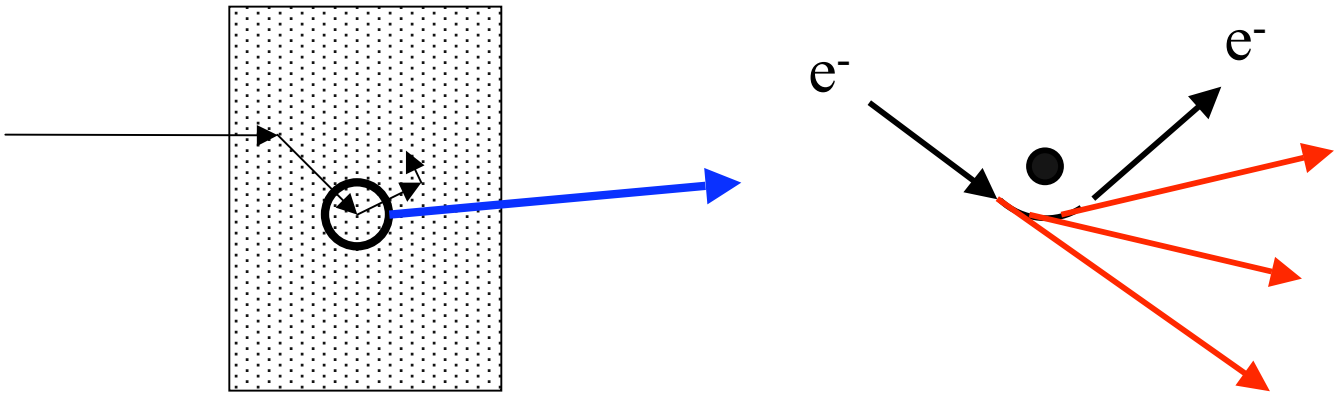
~~Brehmsstralung~~

~~Bremsstrhalung~~

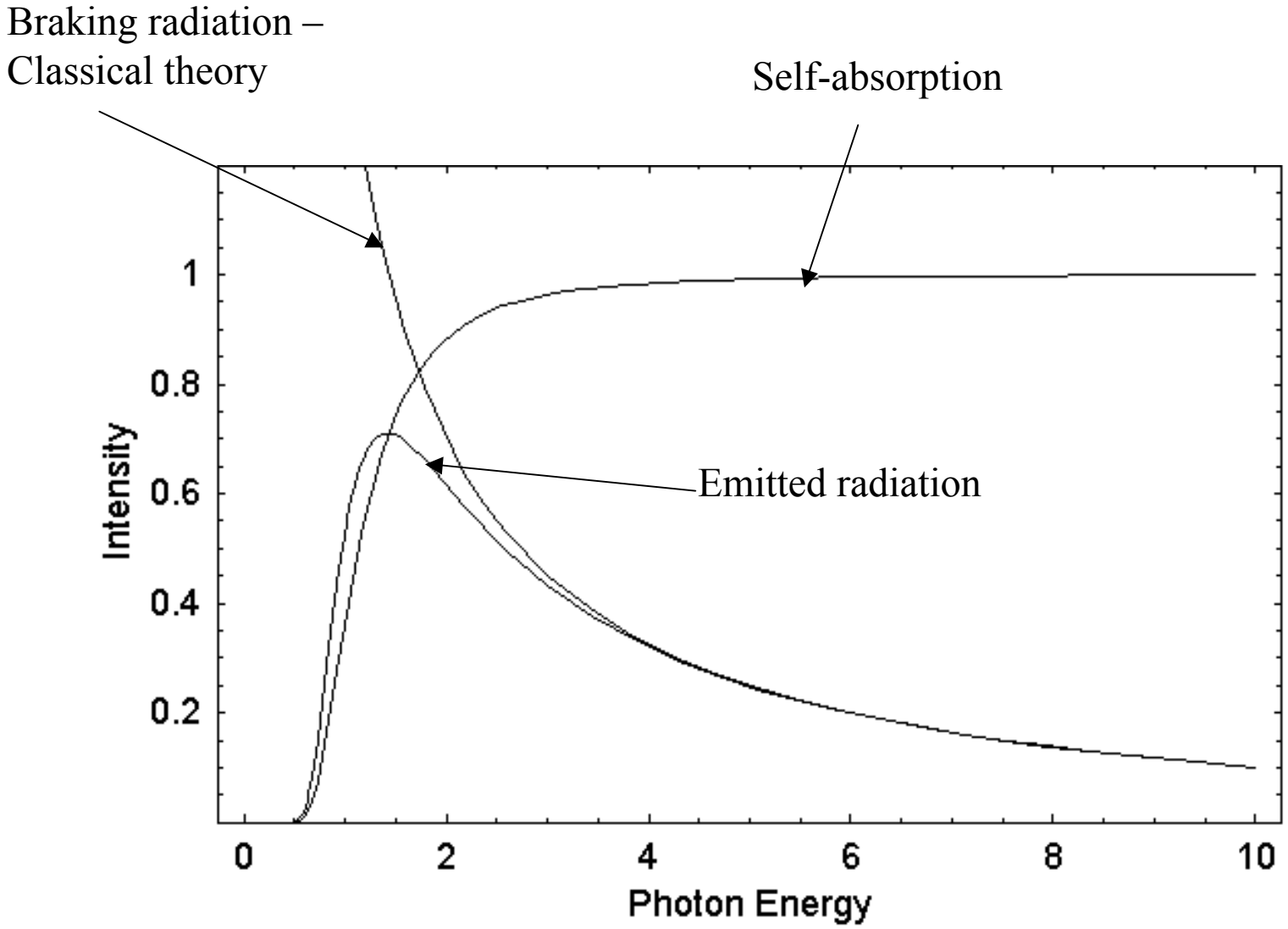
~~Brhemsstrahlung~~

Bremsstrahlung: "Braking radiation"

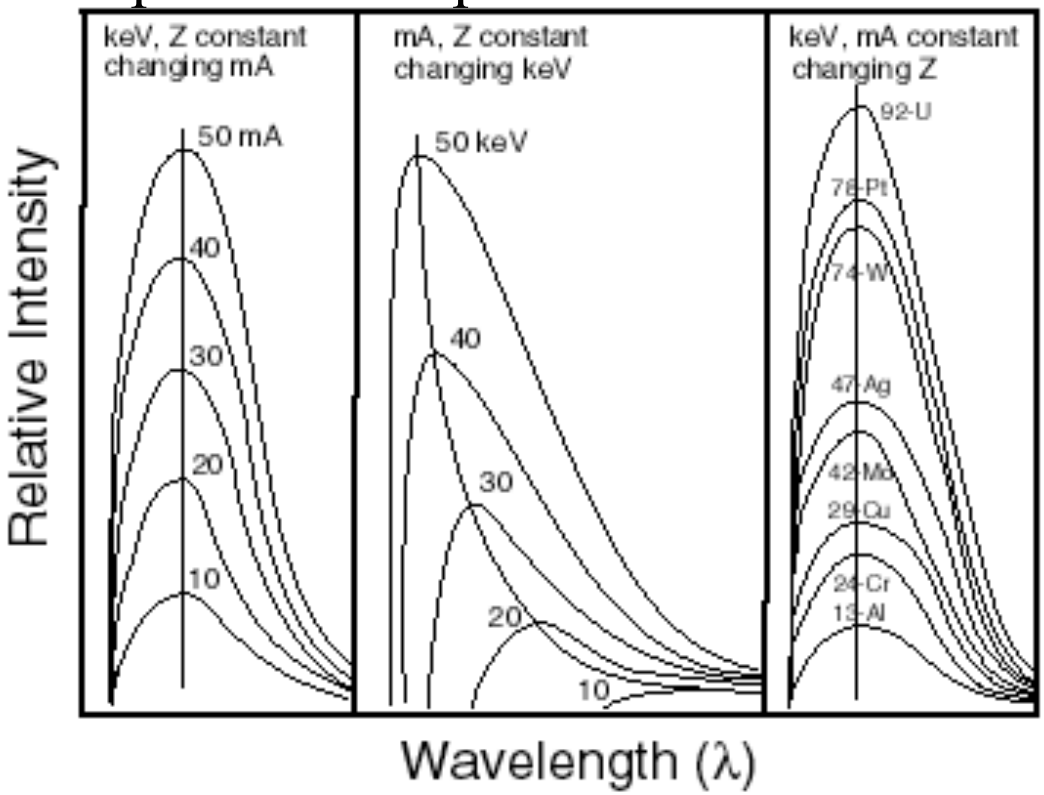
Deceleration of a multi-keV electron in a metal target:



Bremsstrahlung spectral output



Bremsstrahlung: dependencies on experimental options

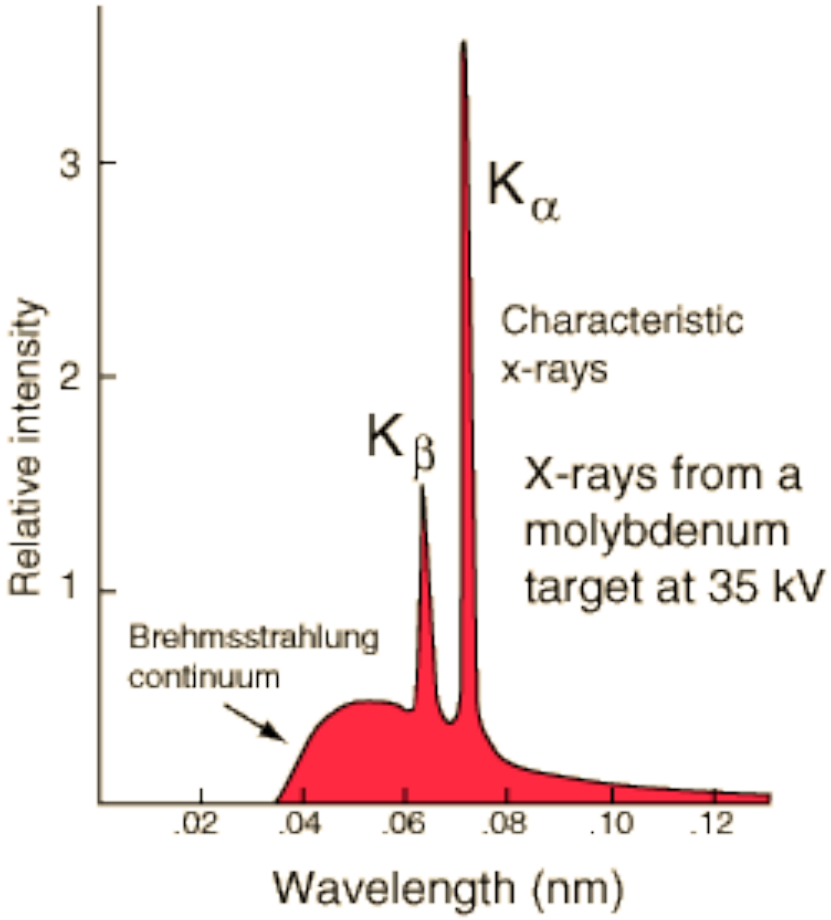


http://jan.ucc.nau.edu/~wittke/Microprobe/Xray-Continuum.html

From Kramer (1923)

$I_{continuum} \cong (const.)\ i_{beam} Z_{target} (E_{accel} - E)/E$

Transitions between electronic states: Characteristic lines

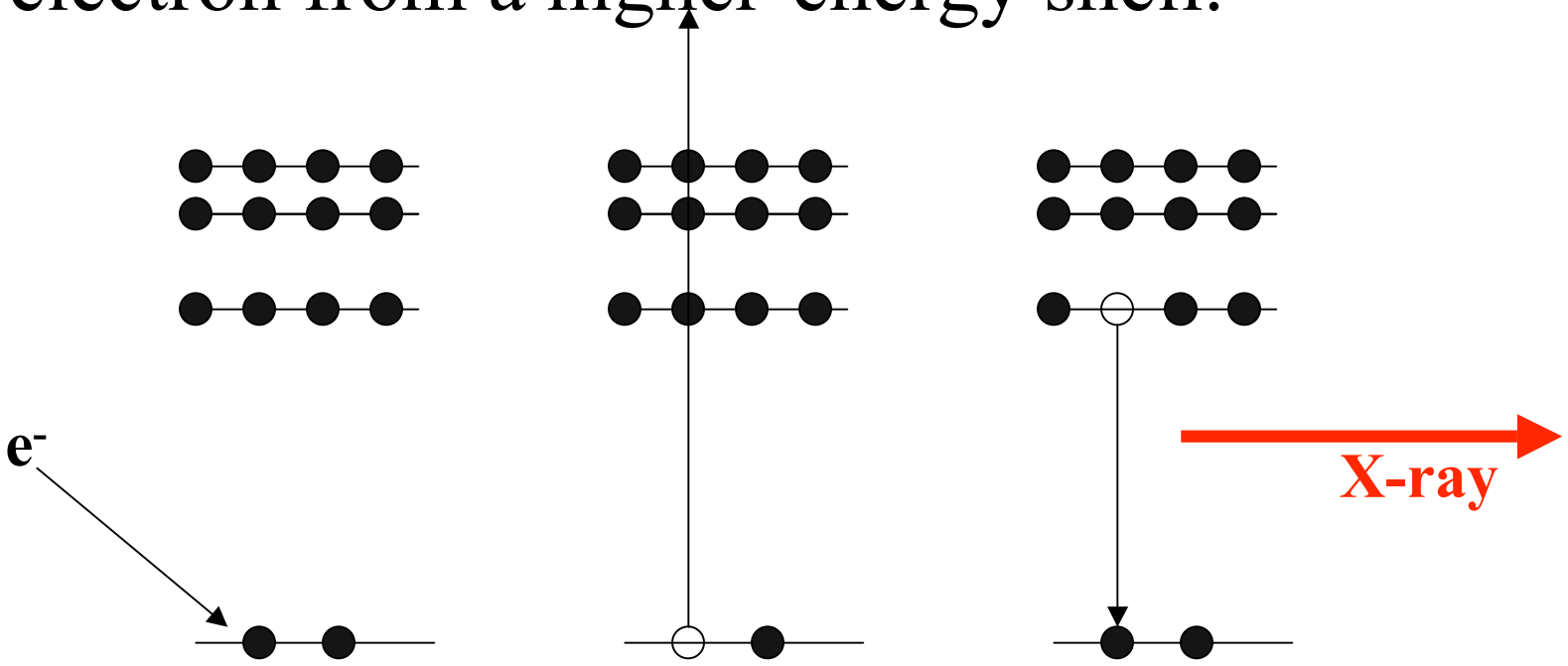


http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/xrayc.html#c1

Characteristic lines

Characteristic lines are unique to each element.

They are caused by decay processes in which a "hole" in a core-level shell is filled by an electron from a higher-energy shell.



Intensities of Characteristic lines

Can be understood as product of hole formation probability times relaxation cross-section:

$$|\langle e^{ikr}|e\mathbf{r}|\psi_{1s1}\rangle|^2 * |\langle \psi_{1s2}|e\mathbf{r}|\psi_{2p(hole)}\rangle|^2$$

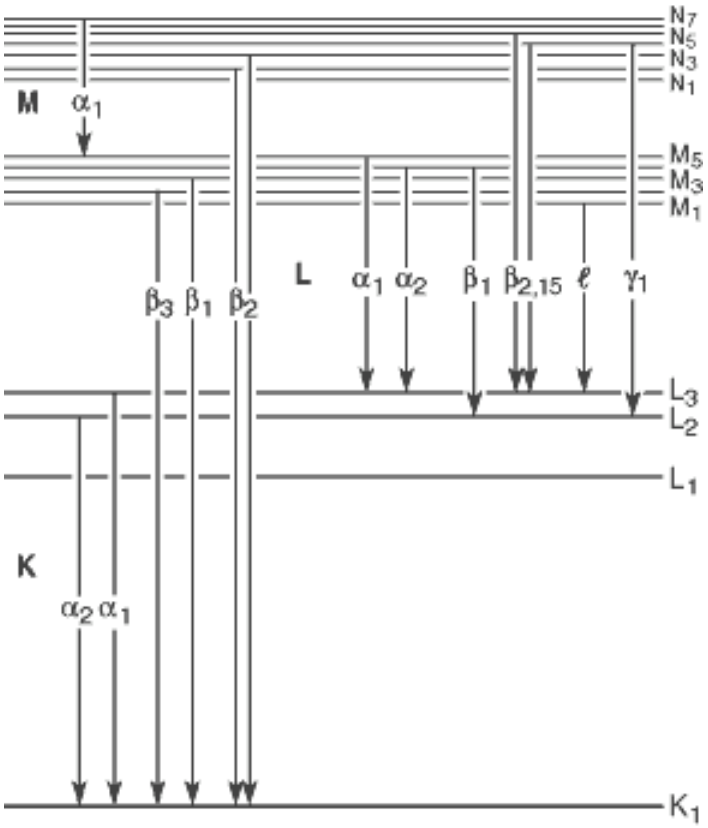
$I = (f(Z))\ i_{electron\ beam}(E_0 - E_c)^p$
where $p \sim 1.7$ for $E_0 < 1.7\ E_c$ (and smaller for higher values of E_0)

http://jan.ucc.nau.edu/~wittke/Microprobe/Xray-LineIntensities.html

Transitions:

2p -> 1s:	K_α
3p -> 1s:	K_β
3p -> 2s:	L_α
4p -> 2s:	L_β

Characteristic X-ray Emission Lines: Atomic Energy Level Transitions



http://xdb.lbl.gov/Section1/Sec_1-2.html

X-Ray Emission Lines

K-level and *L*-level emission lines in KeV

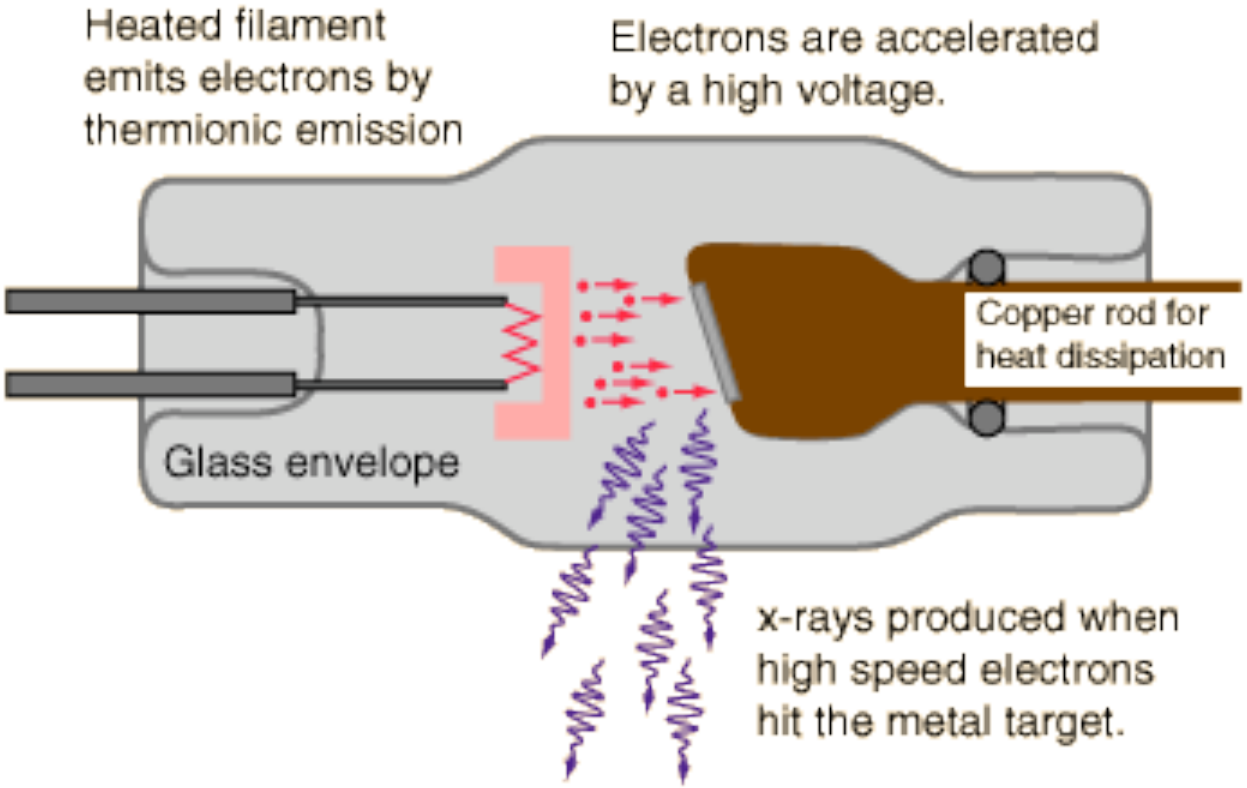
No.	Element	Ka1	Ka2	Kb1	La1	La2	Lb1	Lb2	Lg1
26	Fe	6.40384	6.39084	7.05798	0.7050	0.7050	0.7185		
27	Co	6.93032	6.91530	7.64943	0.7762	0.7762	0.7914		
28	Ni	7.47815	7.46089	8.26466	0.8515	0.8515	0.8688		
29	Cu	8.04778	8.02783	8.90529	0.9297	0.9297	0.9498		
30	Zn	8.63886	8.61578	9.5720	1.0117	1.0117	1.0347		
33	As	10.54372	10.50799	11.7262	1.2820	1.2820	1.3170		
34	Se	11.2224	11.1814	12.4959	1.37910	1.37910	1.41923		
35	Br	11.9242	11.8776	13.2914	1.48043	1.48043	1.52590		
42	Mo	17.47934	17.3743	19.6083	2.29316	2.28985	2.39481	2.5183	2.6235
43	Tc	18.3671	18.2508	20.619	2.4240	-	2.5368	-	-
44	Ru	19.2792	19.1504	21.6568	2.55855	2.55431	2.68323	2.8360	2.9645
45	Rh	20.2161	20.0737	22.7236	2.69674	2.69205	2.83441	3.0013	3.1438
46	Pd	21.1771	21.0201	23.8187	2.83861	2.83325	2.99022	3.17179	3.3287
47	Ag	22.16292	21.9903	24.9424	2.98431	2.97821	3.15094	3.34781	3.51959
53	I	28.6120	28.3172	32.2947	3.93765	3.92604	4.22072	4.5075	4.8009
73	Ta	57.532	56.277	65.223	8.1461	8.0879	9.3431	9.6518	10.8952
74	W	59.31824	57.9817	67.2443	8.3976	8.3352	9.67235	9.9615	11.2859
77	Ir	64.8956	63.2867	73.5608	9.1751	9.0995	10.7083	10.9203	12.5126
78	Pt	66.832	65.112	75.748	9.4423	9.3618	11.0707	11.2505	12.9420
79	Au	68.8037	66.9895	77.984	9.7133	9.6280	11.4423	11.5847	13.3817
82	Pb	74.9694	72.8042	84.936	10.5515	10.4495	12.6137	12.6226	14.7644

Values are from J. A. Bearden, "X-Ray Wavelengths", *Review of Modern Physics*, (January 1967) pp. 86-99, unless otherwise noted.

So far, so what?

How are X-ray *really* produced?

Here is the general idea:



But it isn't quite this simple.

http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/xtube.html#c1

For most diffraction studies, the X-ray source should be

- **Intense**
- **A point**
- **Monochromatic**

Oh. ***Anything else?***

Intensity

More photons on sample => shorter acquisition times => more publications/unit time => decreased rate of funding cuts

X-ray generation is **EXTREMELY** inefficient

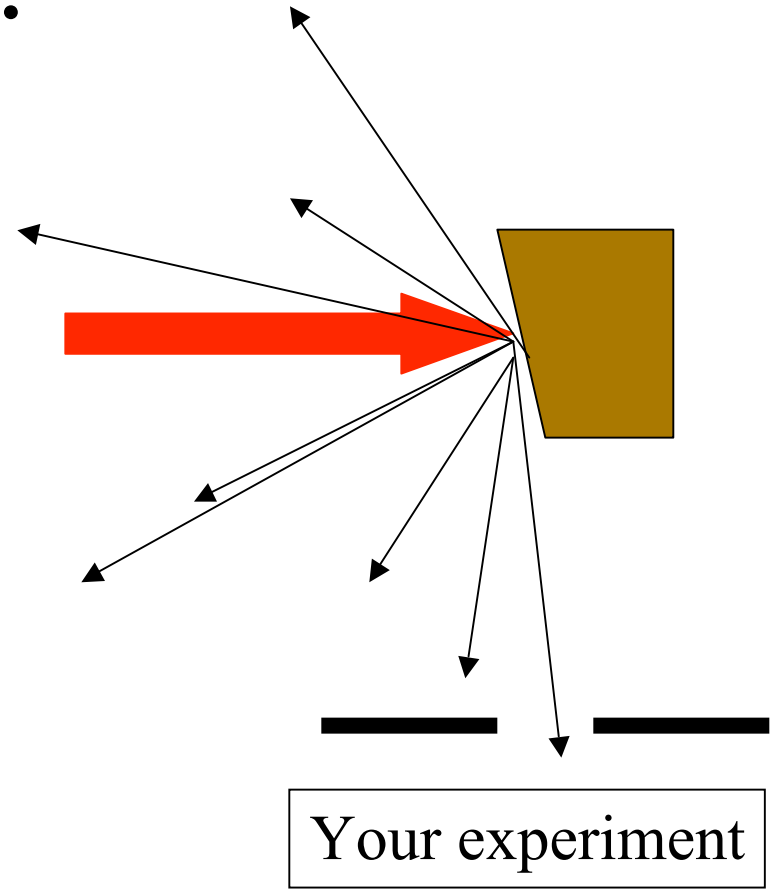
Total power ~ accelerating potential x electron beam current

~ 99% of total power goes into heat production

$$I_{continuum} \cong (const.)\ i_{electron\ beam}\ Z_{target}(E_{accel}-E)/E$$

$$I_{characteristic} \cong (f(Z))\ i_{electron\ beam}(E_{accel} - E_c)^p$$

It gets worse:



X-rays are produced nearly isotropically; very few go where you would like them

How bad is is REALLY?

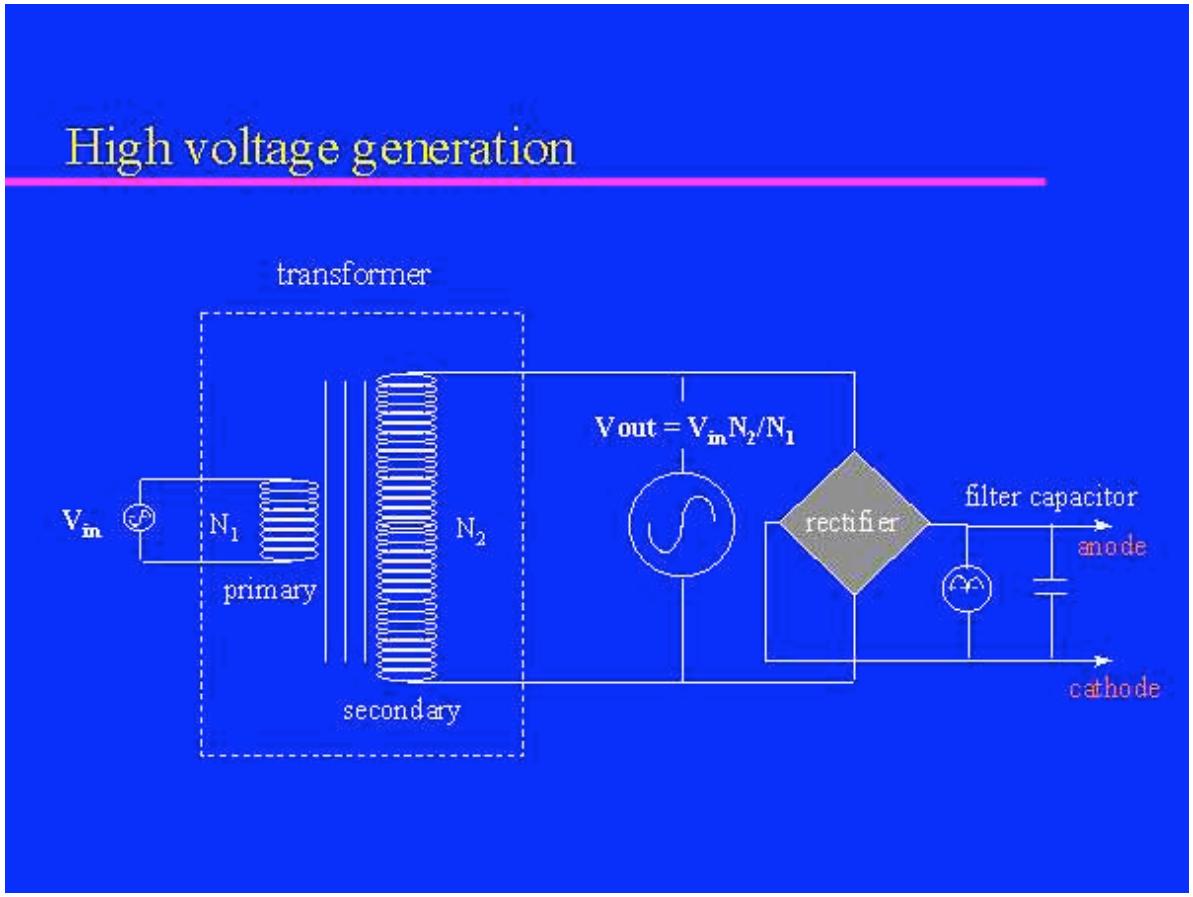
An example:

3 kW X-ray source
1.54 Å radiation (8.05 keV)
10^7 photons/sec

$(10^7 * 8.05 * 10^3 * 1.6 * 10^{-19})/(3*10^3) \sim 0$

$(=4*10^{-12})$

Power supplies:



Virtually always the anode floats at 20-80KV; the cathode is grounded

This has typically meant big, heavy supplies with big, heavy transformers

http://www.rigaku.com/protein/ruh3r.html

18 KW
60 KV
300 mA

which will eventually be replaced by small, lightweight HF supplies

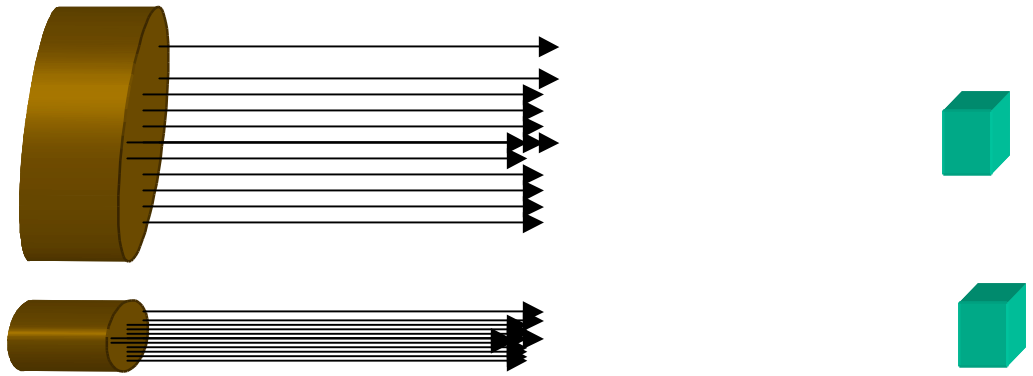
20 KW
200 KV
100 mA

http://www.voltronics.com/products/index.html

Point sources

Stipulate the need for high intensities

Smaller source puts more X-rays on sample



=> More difficulties: high heat loads

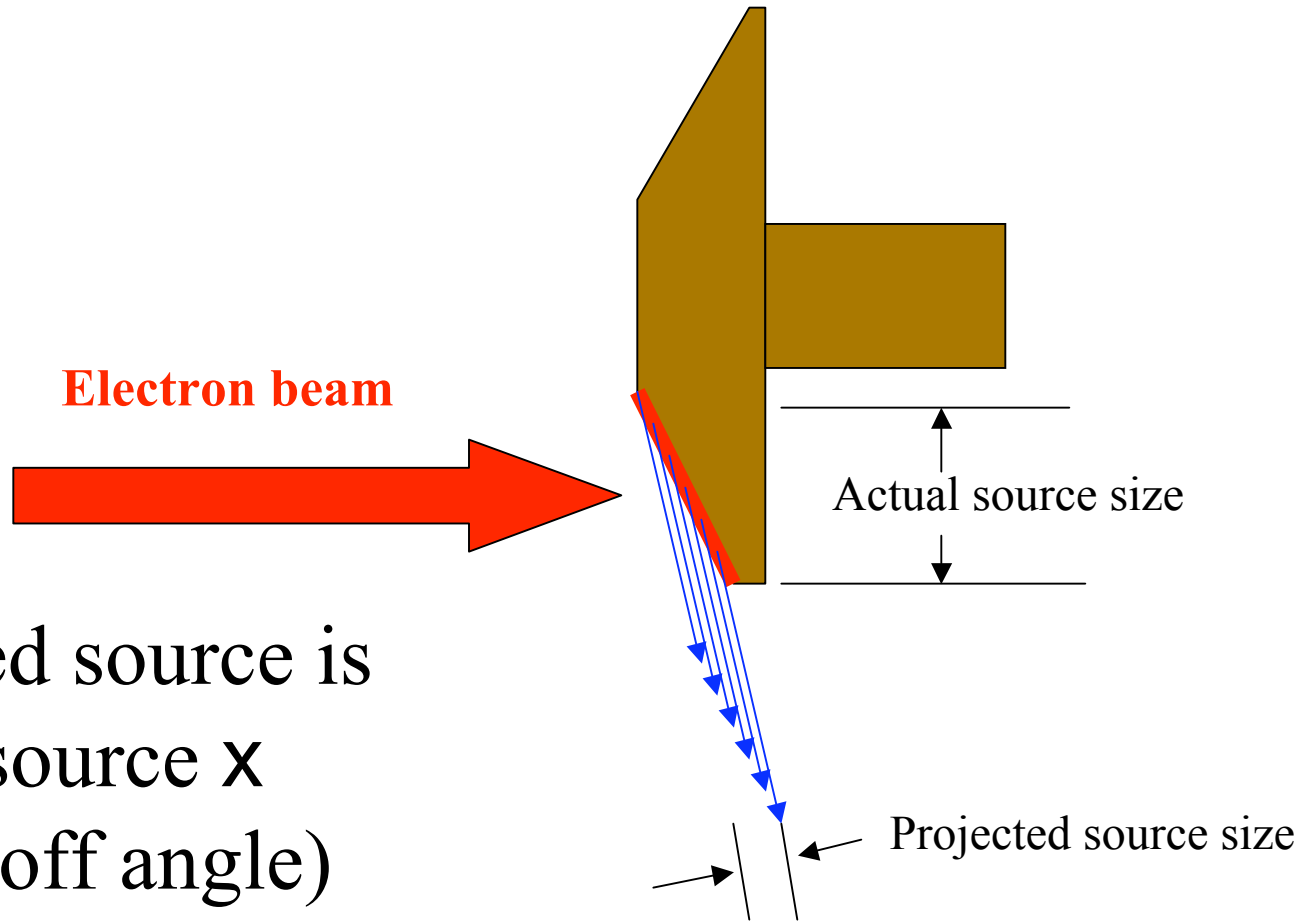
Typically acceptable source size ~ 1mm x 1mm

3kW/mm^2 exceeds most materials capabilities

Multiple approaches required:

- Spread beam out
- Active water cooling
- Move beam along target (or equivalent)

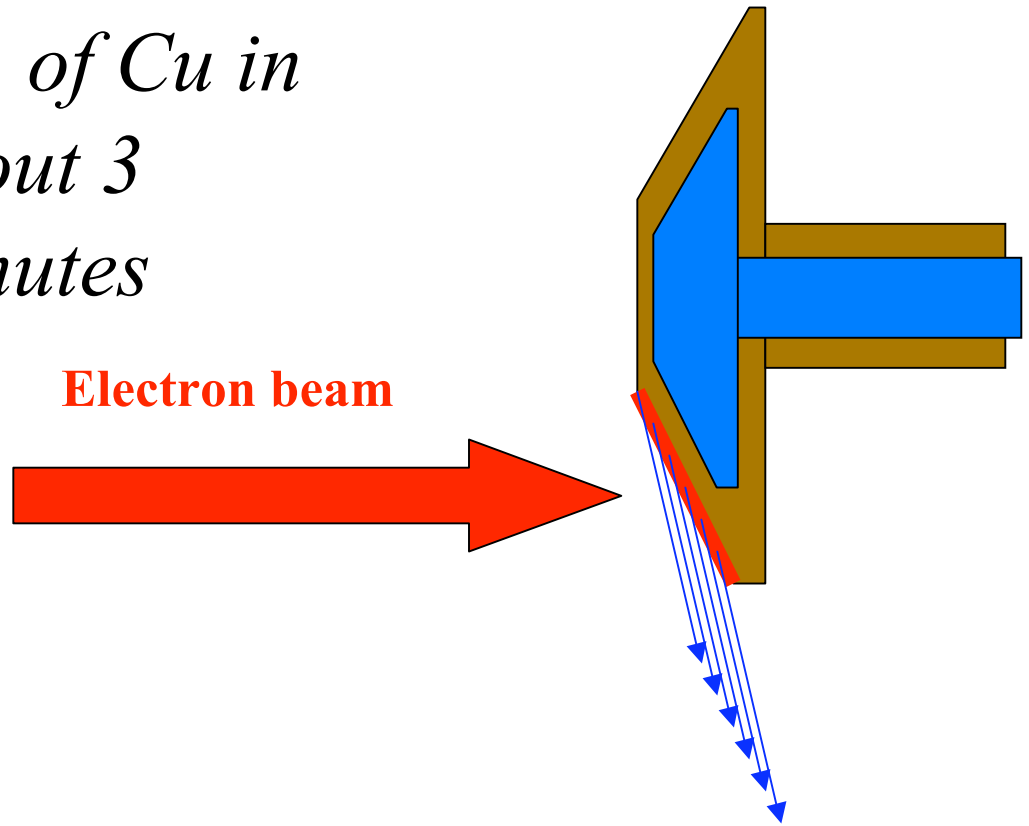
Spreading the beam reduces power density

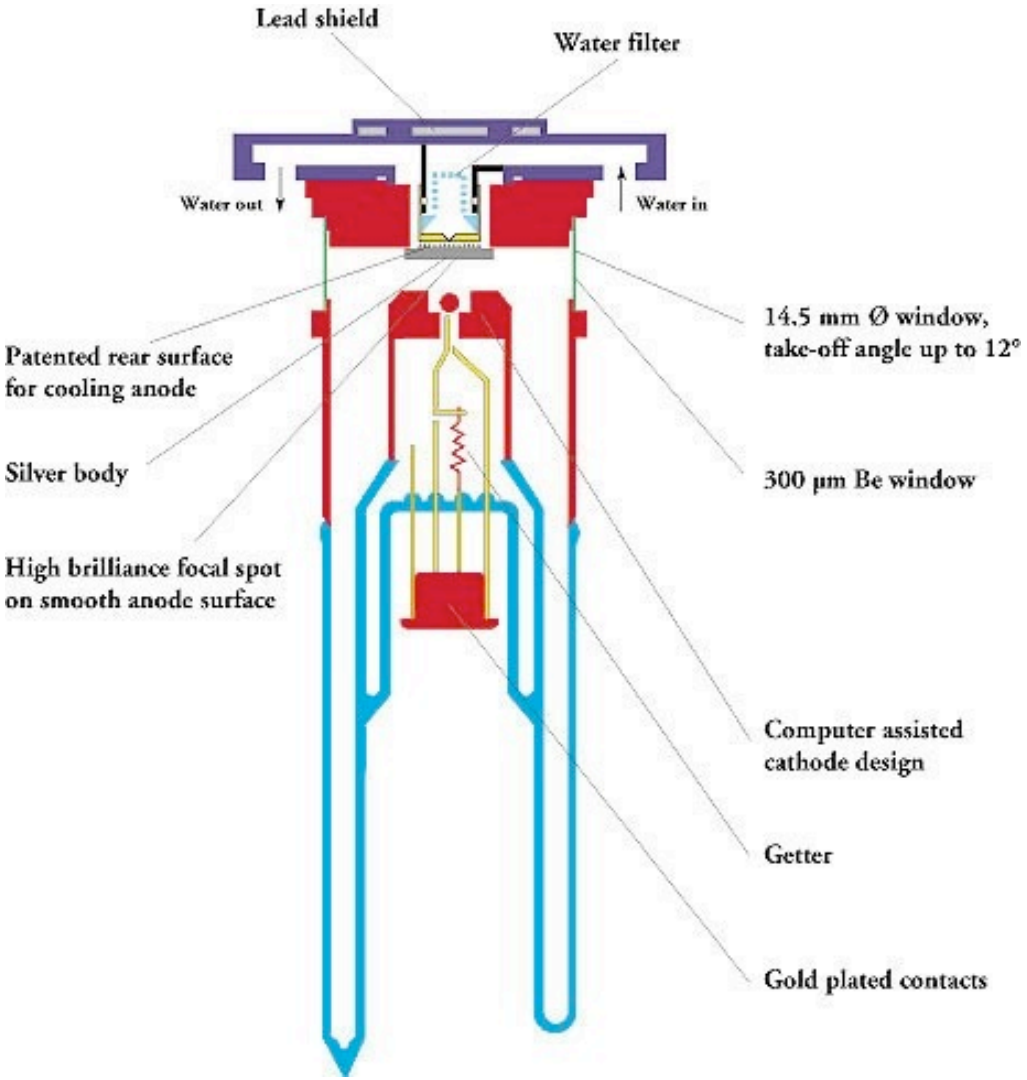


Projected source is
Actual source x
sin(takeoff angle)

Active water cooling removes heat load

3kW heat load would melt 1 kG of Cu in about 3 minutes





http://www.panalytical.com/images/products/xrdgp.jpg

Details of a typical “sealed” tube

Maximum practical thermal loads

$dQ/dt_{max} \sim 80kW$

$\Delta T_{reasonable} \sim 80K$

$C_p(water) = 4190\ J/kg\ K$

$m_{water}/time \sim .02kg/sec$

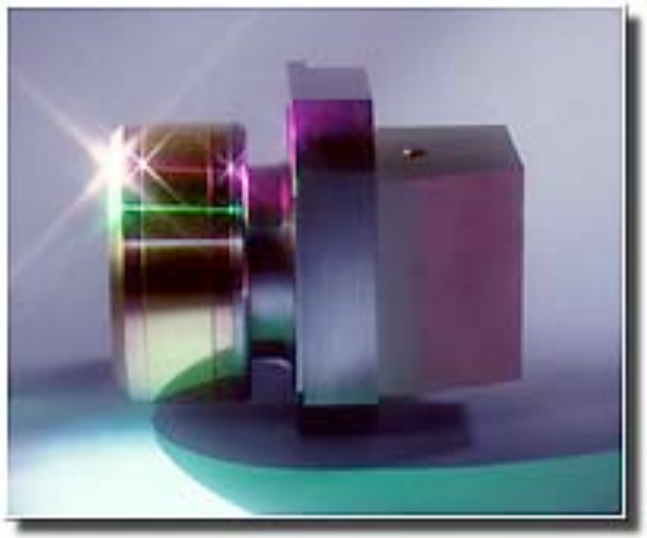
But: 3 kW/10mm^2 exceeds thermal transport capabilities of most materials!

Move beam along target (or equivalent)

i.e. rotate target *very quickly* under electron beam

How quickly?

~6000 rpm for 3-12 kW operation

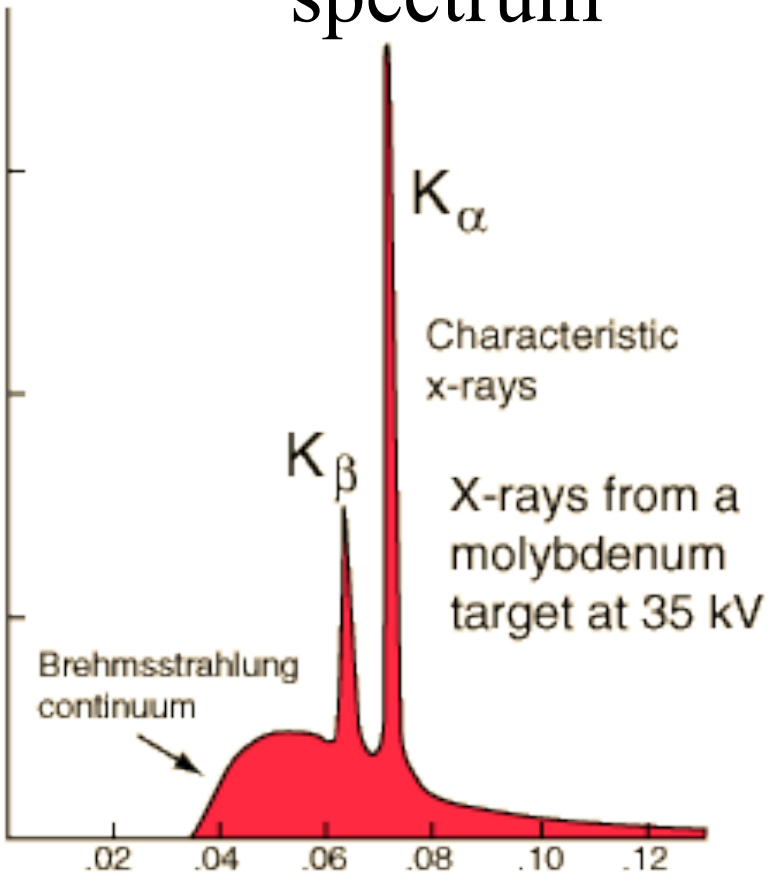


http://www.nonius.com/products/gen/fr591/anode.jpg

Monochromatic

$$n\lambda = 12.4n/E = 2\,d\,\sin\theta$$

=> Take a narrow, bright slice out of emitted spectrum



http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/xrayc.html#c1

How? Crystal monochromator.

How wide a slice (bandwidth)?

Dunno – depends on experiment.

What crystal monochromator to use?

Dunno – depends on the bandwidth

$$n\lambda = 12.4n/E = 2\,d\,\sin\theta \Rightarrow$$

$$\Delta E/E = \cot\theta\,\Delta\theta$$

and $\Delta\theta <$ experimental diffraction linewidth

Thus, experimental needs will dictate desired energy and *desired* energy and angular bandwidths.

Materials properties dictate what you *can have*.

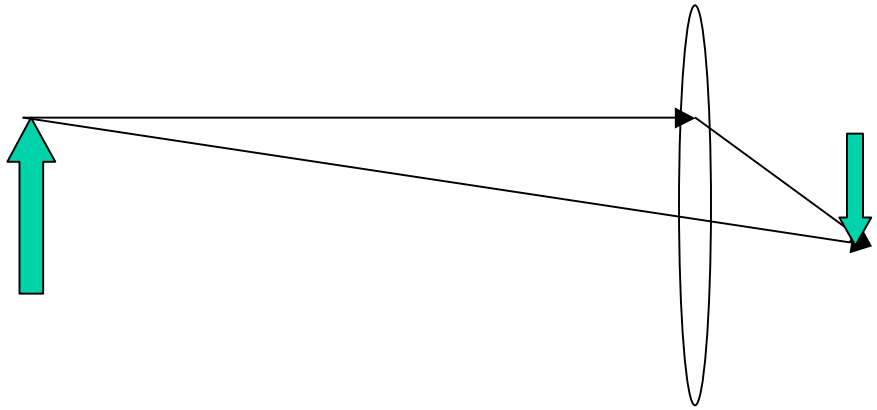
	K-alpha energy (KeV)	K-alpha wavelength (Angstroms)	Melting Point (K)	Thermal Conductivity (J/(m-sec-K))	Heat capacity (J/(g-K))
Iron	6.4	1.94	1808	73	0.44
Cobalt	6.93	1.79	1768	100	0.42
Nickel	7.48	1.66	1726	91	0.44
Copper	8.05	1.54	1357	401	0.38
Molybdenum	17.48	0.71	2890	138	0.25
Silver	22.16	0.56	1235	429	0.24
Tungsten	59.31	0.21	3683	173	0.13

Beam focusing: Size, angle, and phase space

X-rays can be focused using

- Diffraction
  - Bragg
  - Laue
- Mirrors (specular reflection)

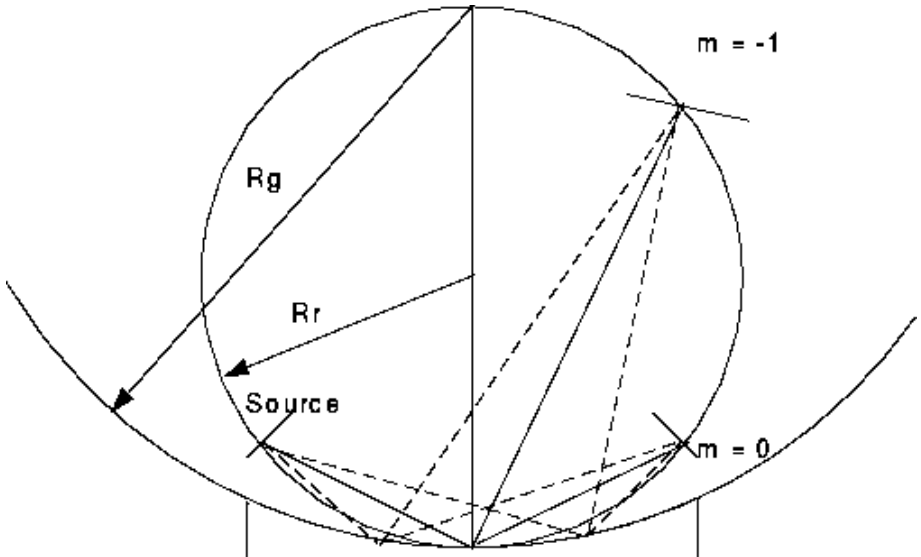
However, beam size and convergence angle must be conserved



Smaller beam, greater convergence angle. Sorry.

$(\cos^2\theta/p) - 2(\cos\theta)/R_c + (\cos^2\theta/q) = 0$

$R_c/2$ = radius of Rowland circle, on which object, optic and image lie



http://www.nanotech.wisc.edu/shadow/SHADOW_Primer/figure711.gif

Rowland Circle Geometry

For bent crystal optics:

Meridional radius

$$R_m = (2/\sin\theta_B)[pq/(p+q)]$$

Sagittal radius

$$R_s = R_m \sin^2\theta_B$$

For specular reflection optics:

$\theta_c = \arcsin[\lambda(e^2\rho_e/m_o c^2\pi)^{1/2}] \sim$ few milliradians where θ_c is the critical angle for total external reflection

So: for small angles

Meridional radius

$$R_m = (2/\theta_B)[pq/(p+q)]$$

Sagittal radius

$$R_s = R_m\ \theta_B^2$$

Thus, we have a system comprising:

- **A 12-60kW transformer**
- **A vacuum on the order of 10^{-7} torr**
- **A heated metal target rotating at 6000 rpm**
- **An electron filament at ~20 – 60KVP above ground**
- **Ionizing radiation everywhere**
- **A water flow rate from .05 – 1 l/sec**
- **Optical components aligned to fractions of milliradians**
- **An efficiency of ~4×10^{-12}**

Nonetheless:

- **Bragg's Law necessitates reflections of x-rays from crystals**
- **Relatively few photons are necessary to define the location of a crystal reflection**
- **Sources and cooling schemes continue to provide higher brilliances from rotating anode systems**
- **Higher-power generators continue to be developed**
- **Detector technology continues to advance**
- **It *is* possible to determine 3-dimensional structural information at the atomic level using x-ray crystallographic techniques**