Experimental X-Ray Spectroscopy: Part 1

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Outline:

- **X-ray spectrometer optical design and capabilities:**
  - **Reflection crystals (Bragg)**
  - **Transmission crystals (Laue, Cauchois)**
- **Experiments at large laser and other facilities and example results.**

Science Motivation:

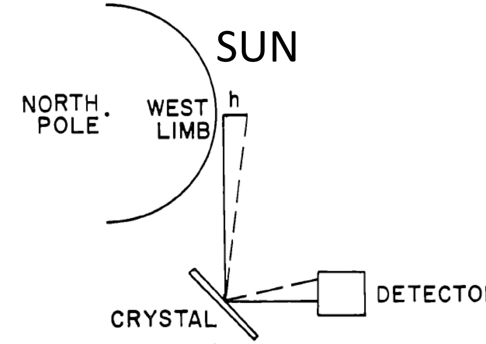
- **Atomic physics of inner-shell transitions in high atomic number atoms and highly charged ions.**
- **High-energy-density (HED) plasma diagnostics: temperature, density, ionization balance, opacity.**
- **Atomic physics code validation (FAC, HULLAC, FLYCHK, opacity, …)**
- **Atomic kinetics code validation (FLYCHK, NOMAD, …)**

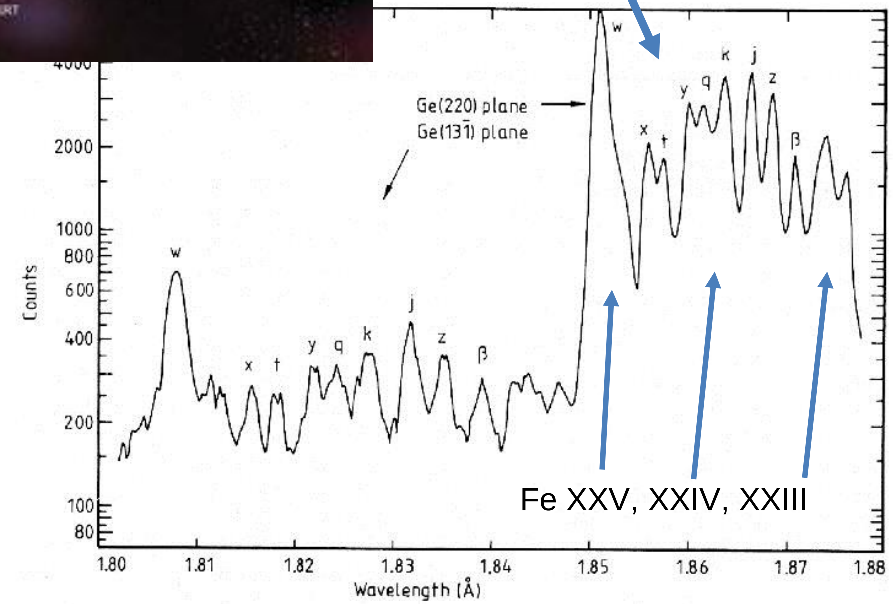
X-ray spectroscopic plasma diagnostics provide:

- **Identification of bound-bound transitions**
  - Measurement of transition energies (atomic physics code validation)
  - Determination of ionization balance (kinetics code validation)
- **Measurement of spectroscopic line ratios**
  - Electron temperature and density, opacity
- **Measurement of continuum emission**
  - Bound-free transition opacities; super-thermal electron energy component
- **Measurement of line widths, line shapes, energy shifts**
  - Doppler broadening, Stark broadening, opacity (requires high spectral resolution)
- **Spectra with temporal and/or spatial resolution**
  - Transient dynamics
- **Measurement of absolute intensities**
  - Source brightness, laser energy to x-ray conversion efficiency (Inertially Confined Fusion, ICF)
  - Density

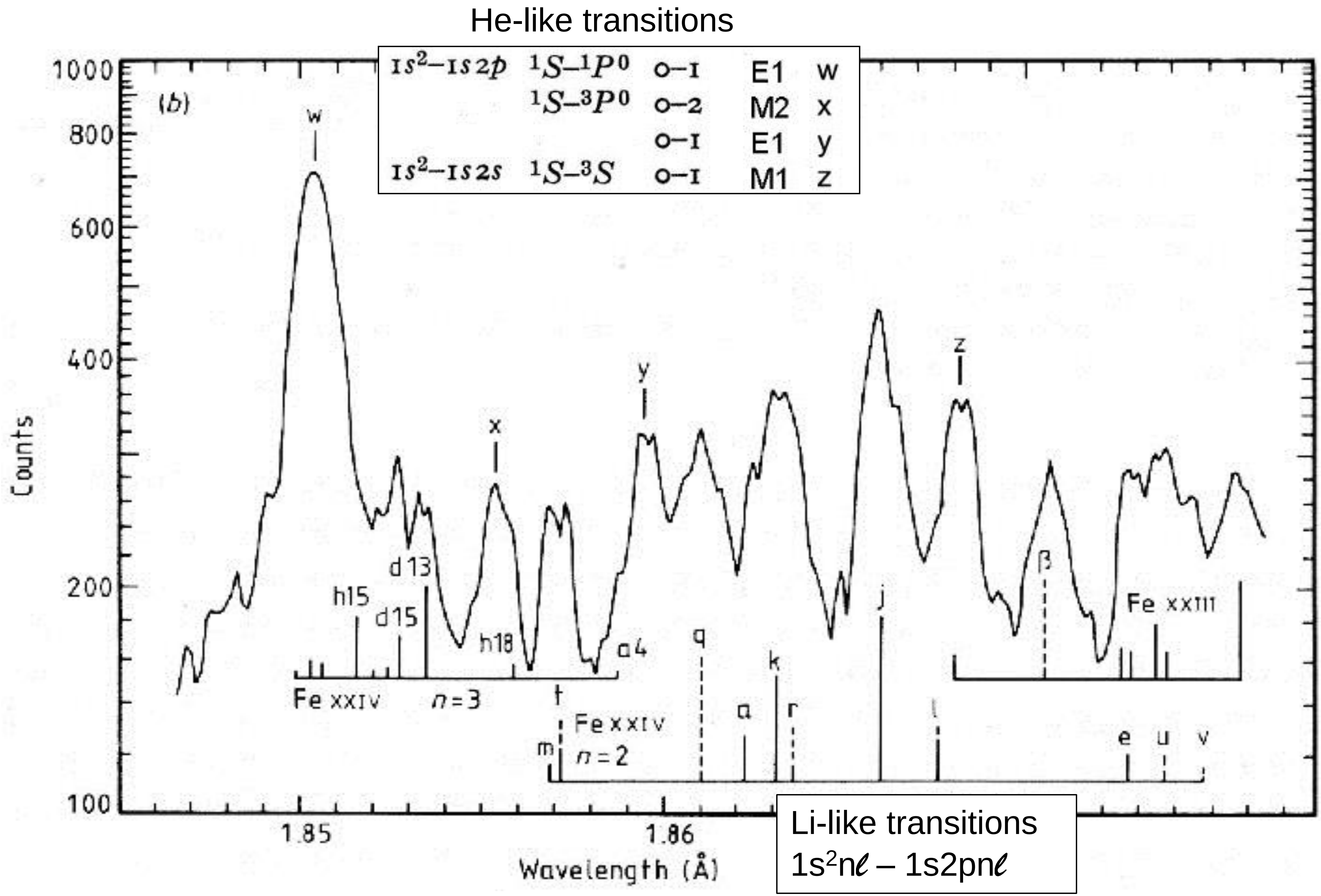
Many Sources of X-Rays

- Astrophysical
- Solar flares
- Low-density laboratory
  - Tokamaks
  - Electron Beam Ion Trap (EBIT)
- High-density laboratory
  - ***Long-pulse laser (ns)***
  - ***Short-pulse laser (ps and fs)***
  - ***Pulsed-power generators***
- X-ray free electron lasers (XFEL): FLASH, ***LCLS***, European XFEL, up to 25 keV)
- Laboratory testing and calibrations
  - ***Laboratory electron-bombarded anode (W, 300 kV at NIST)***
  - Radioactive sources (x-rays, gamma rays)



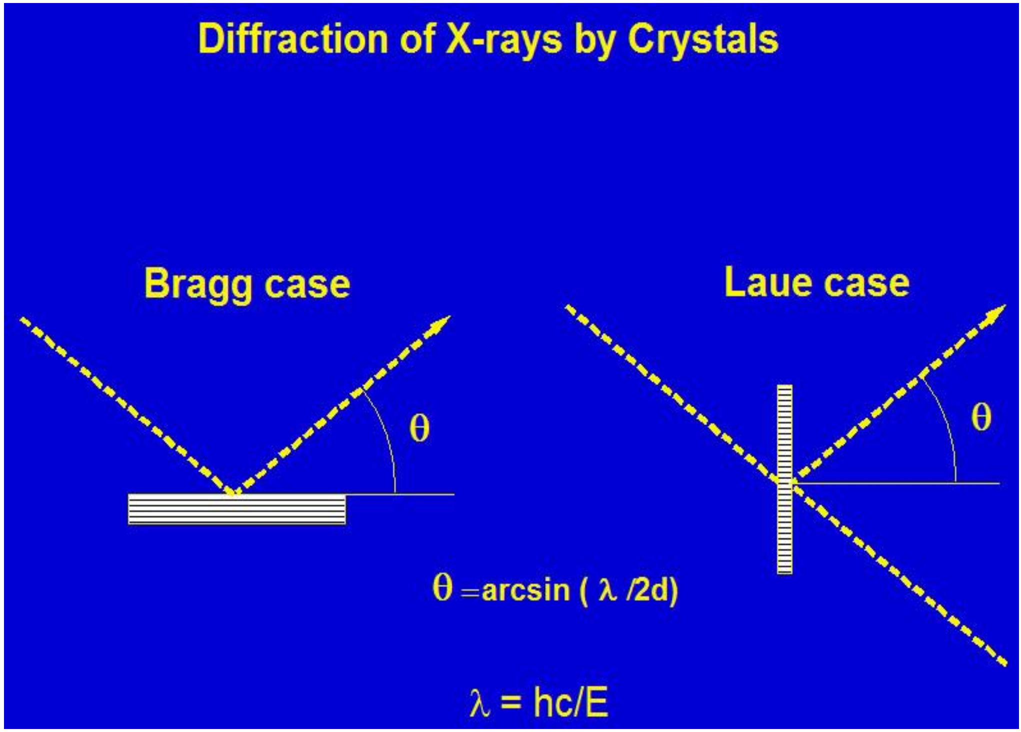


Solar Flare X-Ray Spectrum



Reflection and Transmission Crystal X-Ray Spectrometers

$n\lambda = 2d \sin\Theta$ (Bragg condition) where
n = diffraction order (usually n=1)
λ = wavelength ($E = hc/\lambda$, usually > 1 keV)
d = crystal lattice spacing (few nm)
= distance between diffracting planes
Θ = Bragg angle
= grazing angle to diffracting planes

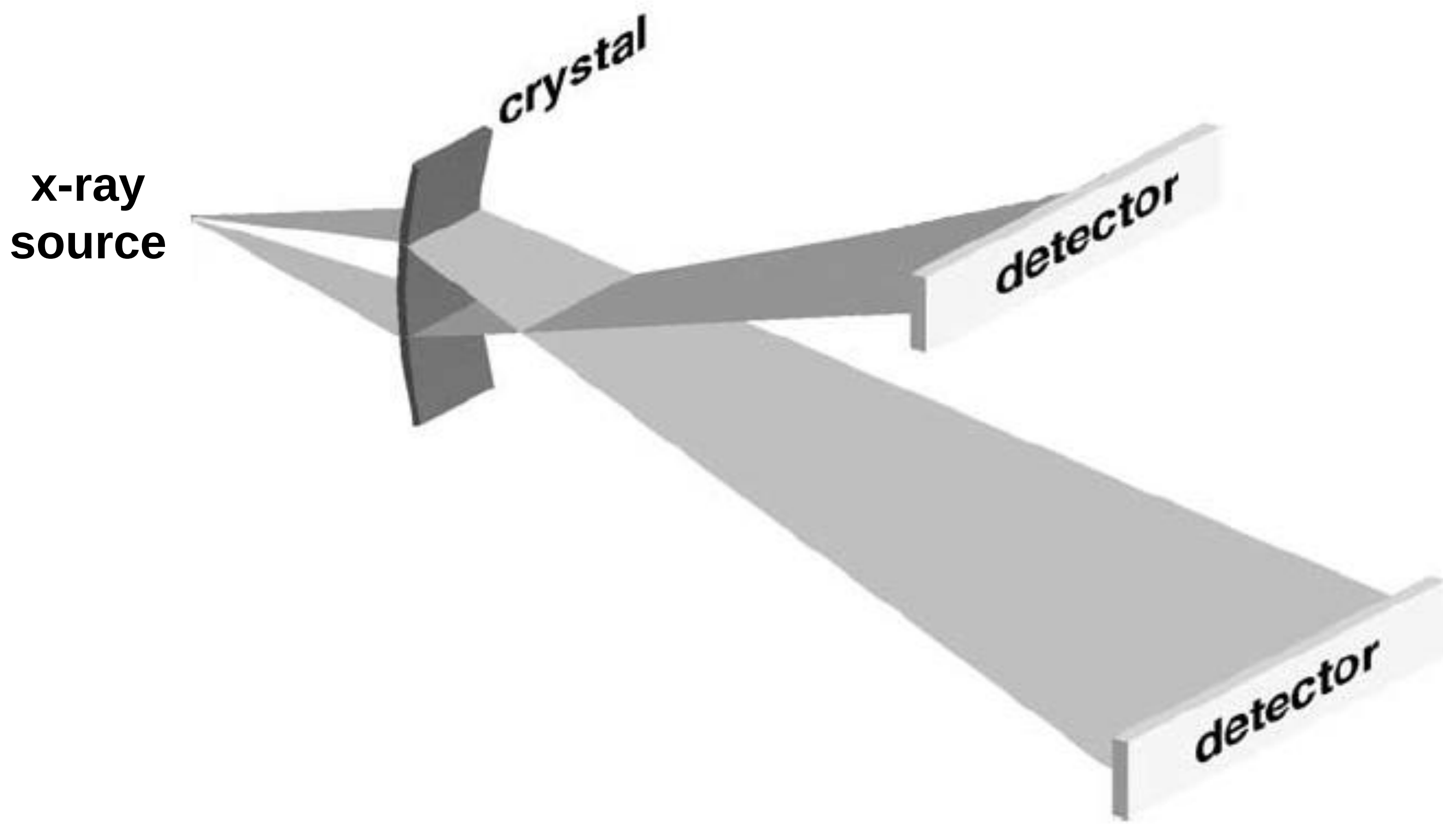


<u>Bragg case:</u>
Diffraction planes are parallel to crystal surface
Larger angles (>10 of deg)
Lower energies (< 10 keV)

<u>Laue case:</u>
Diffraction planes perpendicular to crystal surface.
Smaller angles (< 10 deg)
Higher energies (> 10 keV)

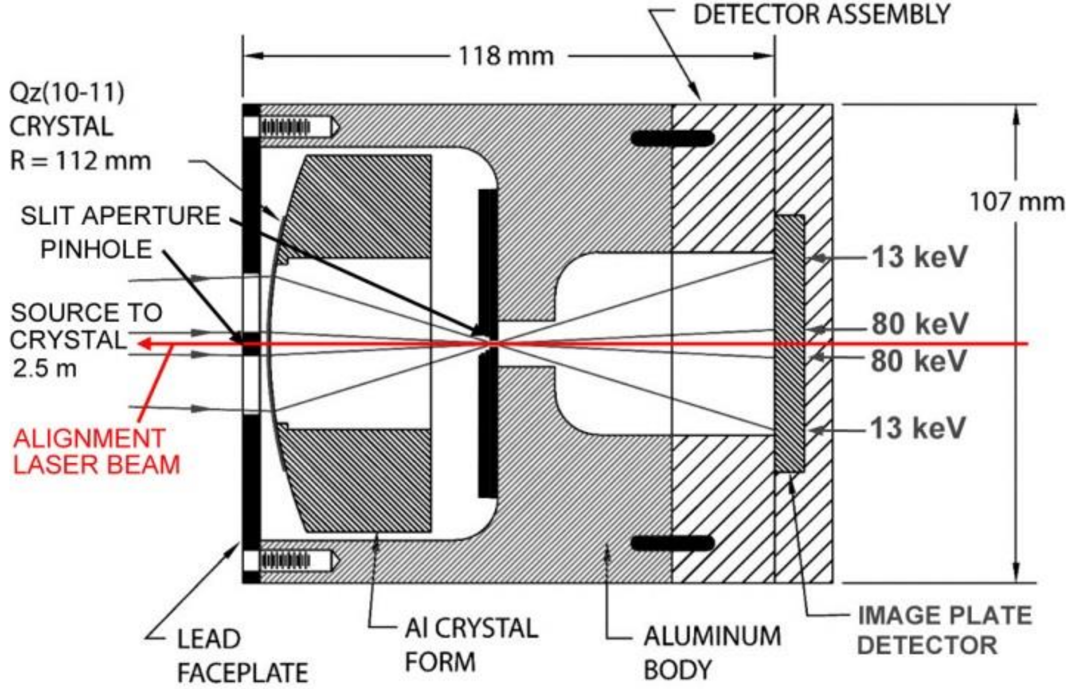
<u>Bending:</u>
- Concave facing the x-ray source (narrower angle and energy ranges, spatial resolution)
- Convex facing the x-ray source (broader angle and energy ranges)
- Single bending (e.g. cylindrical)
- Double bending (e.g. spherical, conical)

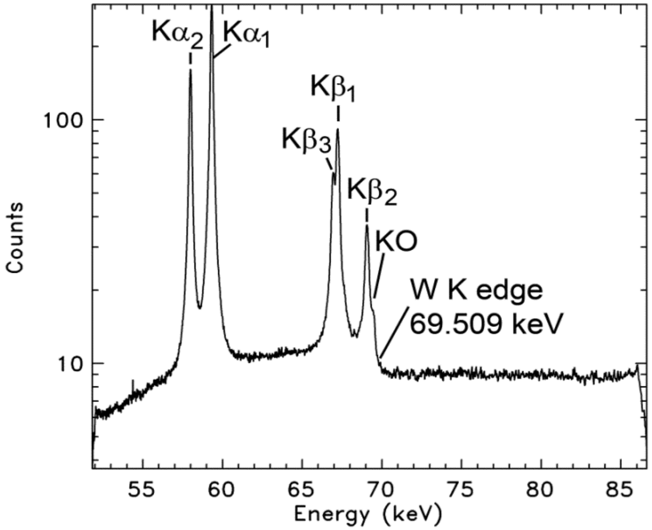
Transmission Crystal Spectrometer (Cauchois, 1932)



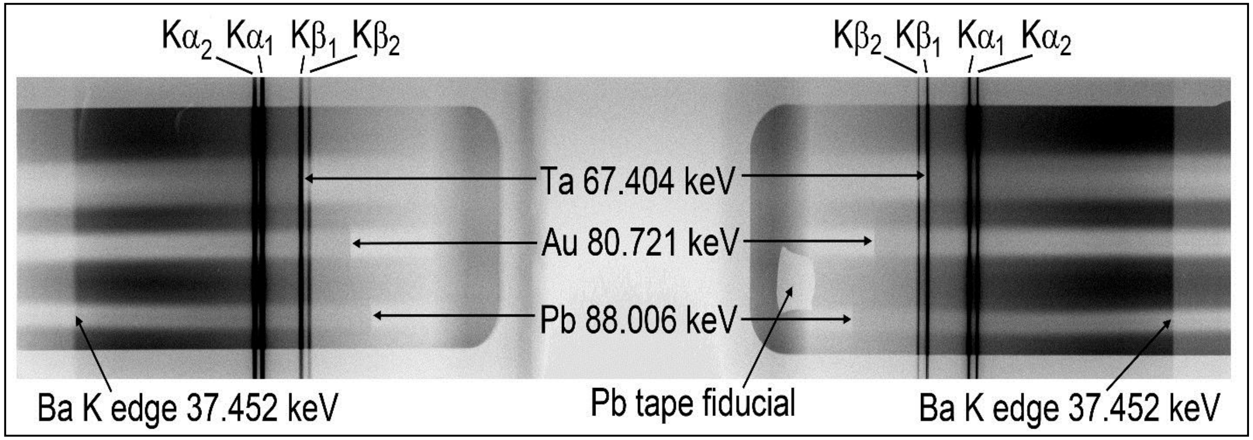
- Cylindrically bent crystal with convex side facing the x-ray source.
- All rays with the same energy and from an extended source are focused on the Rowland circle (diameter equal too the radius of the crystal). ***No source size broadening.***
- Rays with different energies are dispersed on the Rowland circle.

Transmission Crystal Hard X-Ray (> 10 keV) Spectrometer



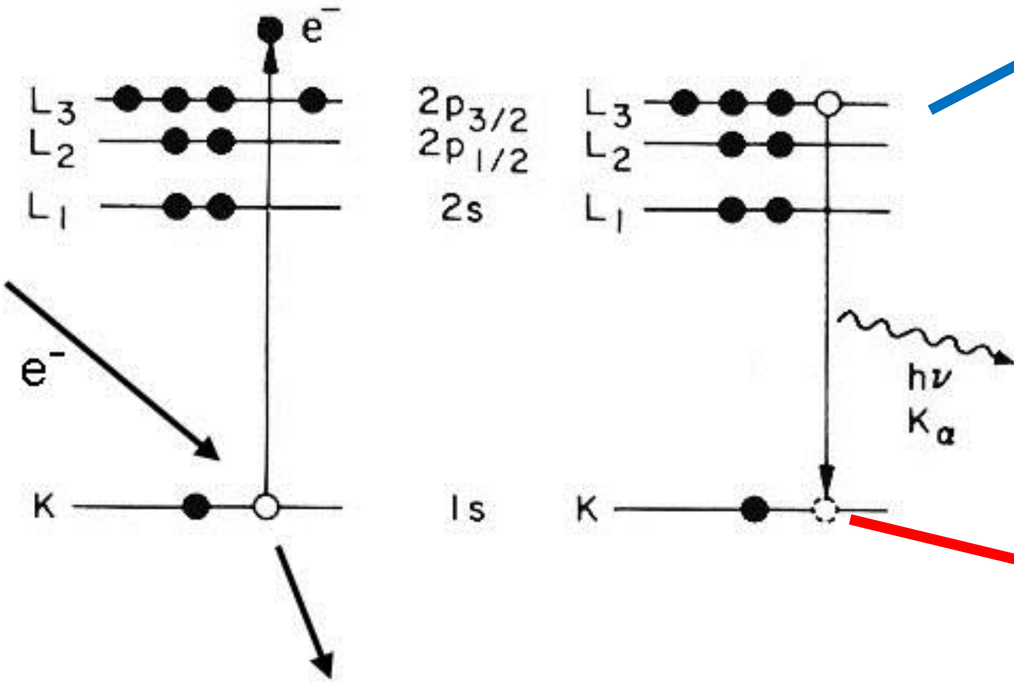


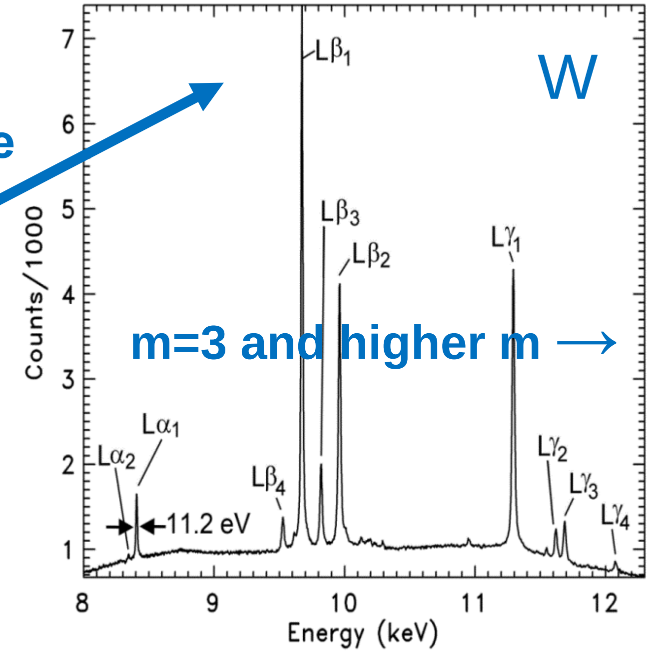
Spectrum from an electron-bombarded W anode



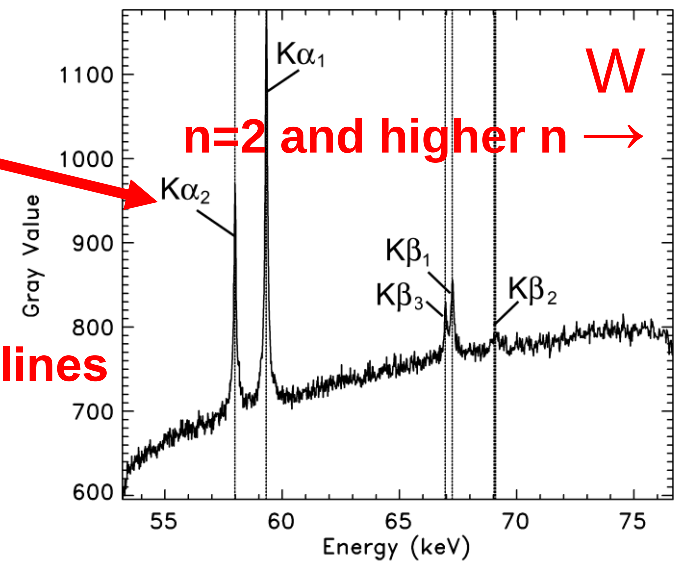
Energetic Electrons (and Photons) → 1s Vacancies → X-Ray Spectra

n = 2 vacancy **m→2 transition** **L spectral line**





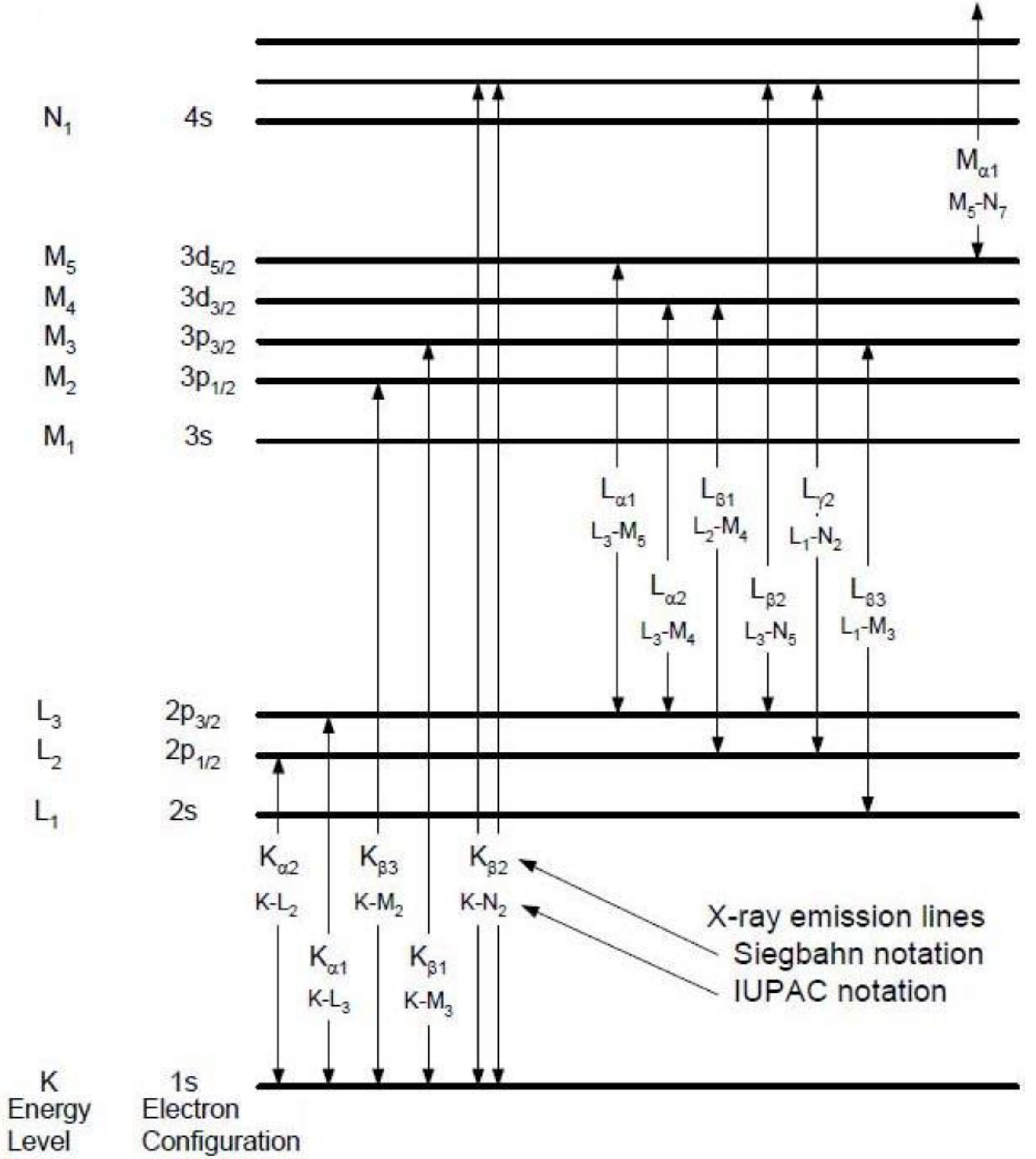
m=3 and higher m →



n=2 and higher n →

1s vacancy **n → 1s transition** **K spectral lines**

Designations of Characteristic X-Ray Lines



Energies and intensities of W L Lines

		W L Transitions		
Identification	Levels	Transition	Energy(eV)	Intensity
$L\alpha 2$	L3M4	2p3/2-3d3/2	8335.3	11.22
$L\alpha 1$	L3M5	2p3/2-3d5/2	8398.2	100.00
$L\eta$	L2M1	2p1/2-4s1/2	8724.4	1.17
$L\beta 4$	L1M2	2s1/2-3p1/2	9525.2	3.56
$L\beta 6$	L3N1	2p3/2-4s1/2	9608.2	1.10
$L\beta 1$	L2M4	2p1/2-3d3/2	9672.6	55.60
$L\beta 3$	L1M3	2s1/2-3p3/2	9818.9	5.05
$L\beta 2$	L3N5	2p3/2-4d5/2	9964.1	22.72
$L\beta 7$	L3O1	2p3/2-5s1/2	10129.2	1.61
$L\beta 5$	L3O5	2p3/2-5d5/2	10200.4	0.50
$L\beta 9$	L1M5	2s1/2-3d5/2	10290.7	0.10
$L\gamma 5$	L2N1	2p1/2-4s1/2	10948.9	0.10
$L\gamma 1$	L2N4	2p1/2-4d3/2	11286.0	10.45
$L\gamma 6$	L2O4	2p1/2-5d3/2	11538.7	0.40
$L\gamma 2$	L1N2	2s1/2-4p1/2	11610.5	1.10
$L\gamma 3$	L1N3	2s1/2-4p3/2	11680.5	1.61
$L\gamma 11$	L1N5	2s1/2-4d5/2	11861.9	0.10
$L\gamma 4$	L1O3	2s1/2-5p3/2	12063.4	0.10

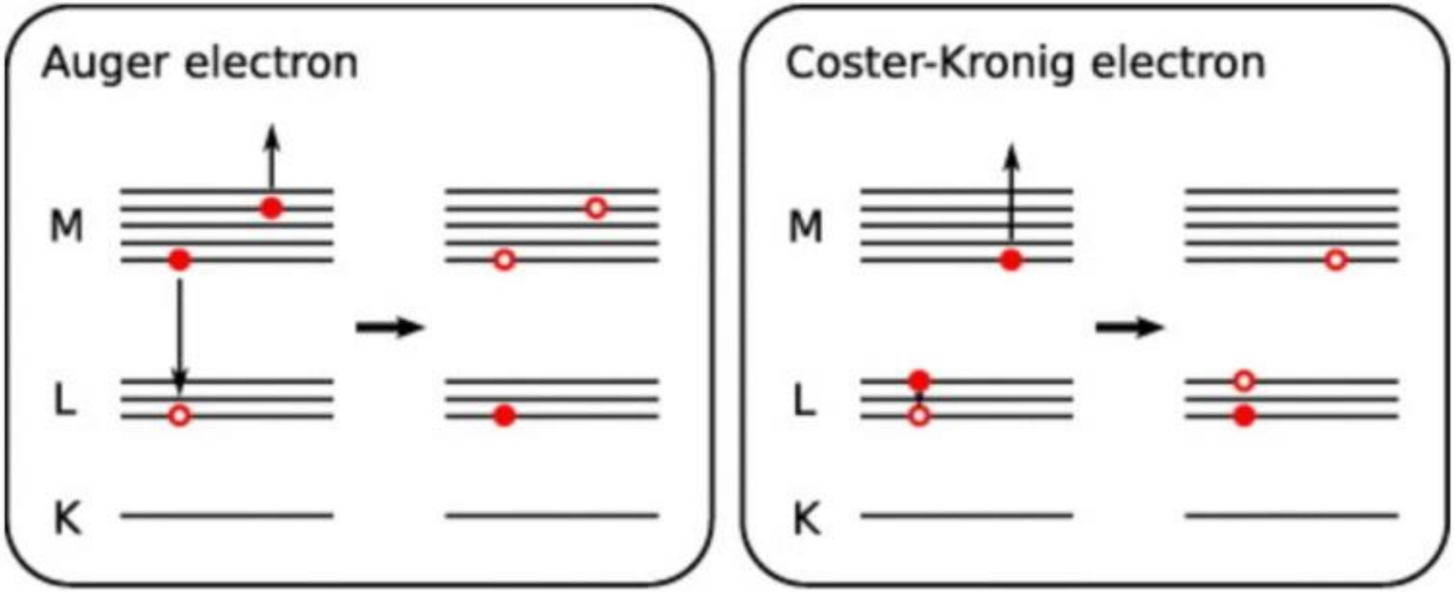
Energies of the characteristic x-ray transitions (type K, L, M, N) are very well know to a fraction of an eV (R. Deslattes, Rev. Mod. Phys. vol. 75, p. 35, 2003)

The lifetimes of the upper and lower levels contribute to the observed spectral lines widths (lifetime or natural widths).

Widths of the K transitions are dominated by the radiative decay rates: $\Delta E = (h/2\pi)\ A$

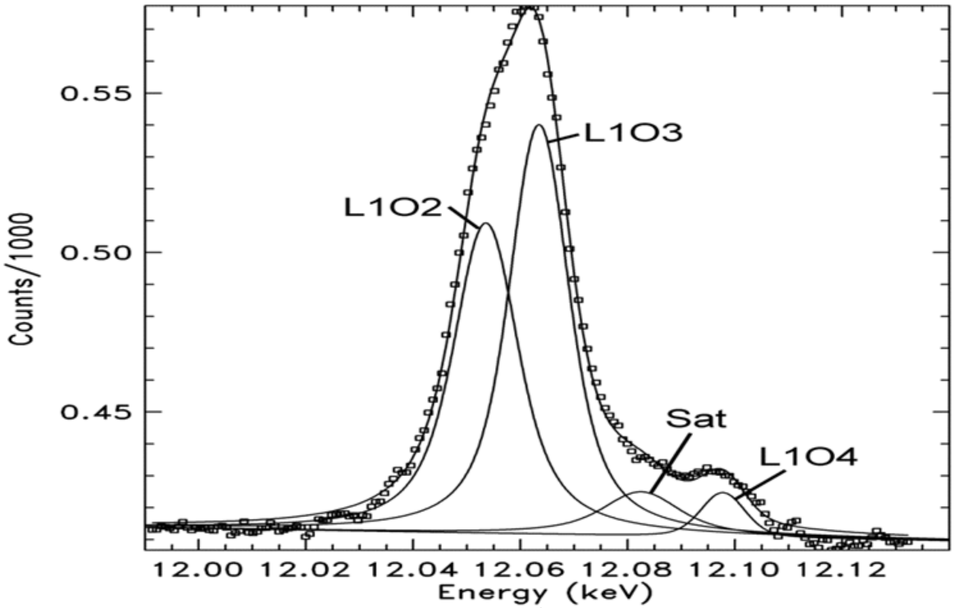
Widths of the upper levels of the L transitions are dominated by non-radiative rates:

Auger and Coster-Kronig



Line Widths are Measured by Fitting Voigt Profiles to the Lγ4 Transition

Convolution of Gaussian and Lorentzian profiles.

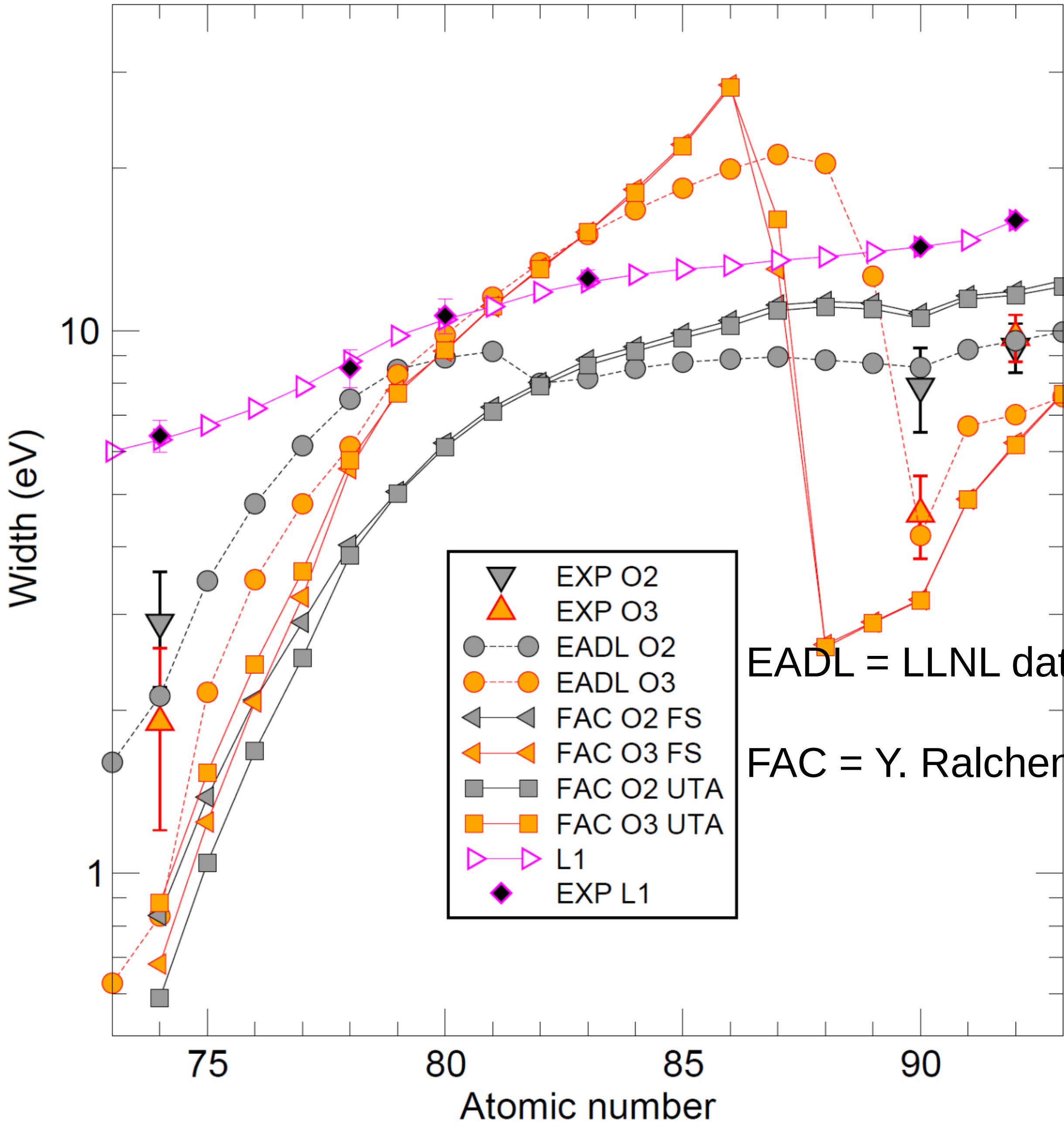


	L1O2 (2s1/2 - 5p1/2)		L1O2 (2s1/2 - 5p3/2)	
	Gaussian (eV)	**Lorentzian (eV)**	**Gaussian (eV)**	**Lorentzian (eV)**
Bent crystal broadening	7.6 ± 0.5		7.6 ± 0.5	
Detector resolution	2.8 ± 0.5		2.8 ± 0.5	
Experimental width		9.3 ± 0.3		8.3 ± 0.3
L1 (2s1/2) natural width		6.4 ± 0.4		6.4 ± 0.4
Coster-Kronig width		2.9 ± 0.3, ± 0.4		1.9 ± 0.3, ± 0.4

Coster-Kronig rates are determined from the widths.

Coster-Kronig process		**O2O3O4**		**O3O4O5**
Lifetime		0.23 fs		0.35 fs
Rate		4.4e15 1/s		2.9e15 1/s

O2 ($5p_{1/2}$) and O3 ($5p_{3/2}$) Level Widths

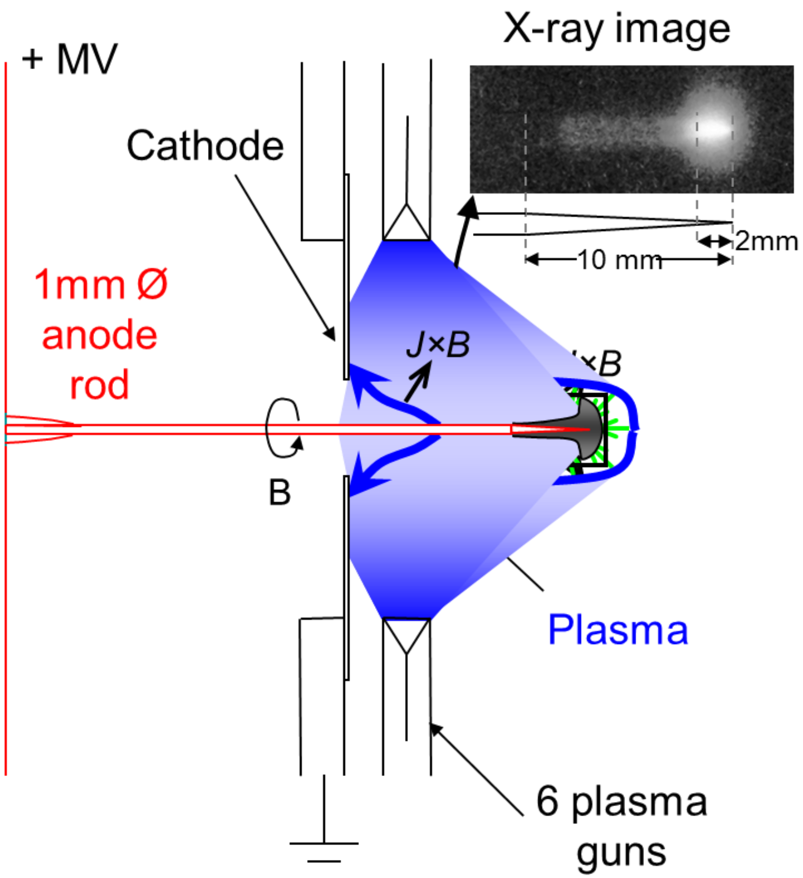


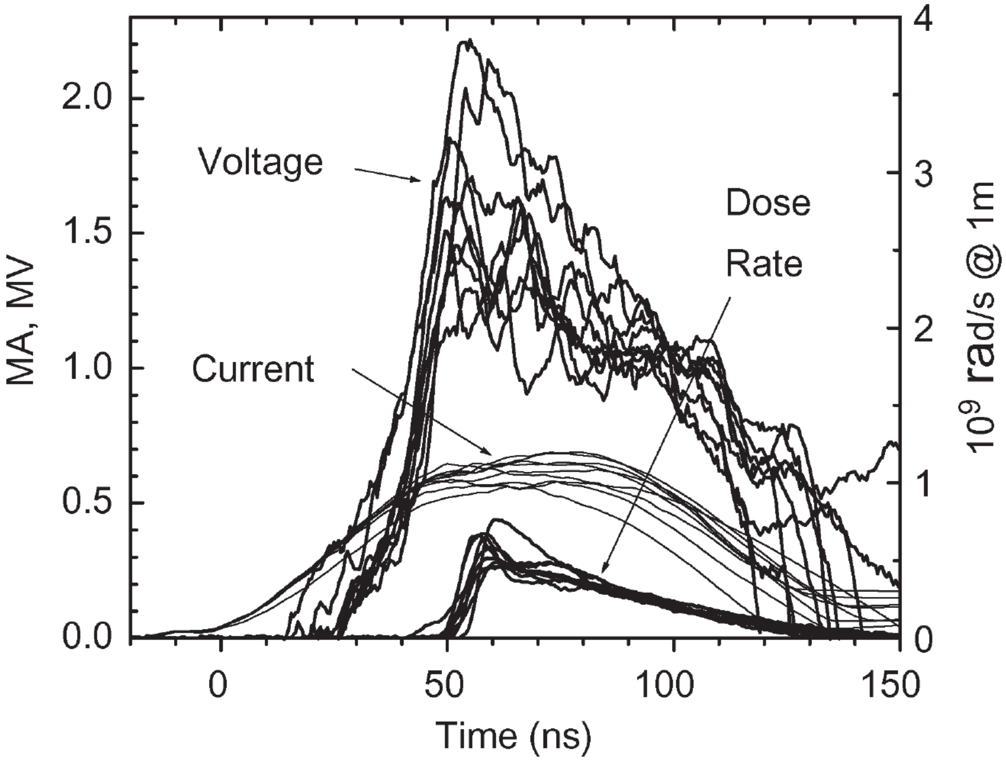
EADL = LLNL database

FAC = Y. Ralchenko

Pulsed Power X-Ray Generator of Warm Dense Plasma

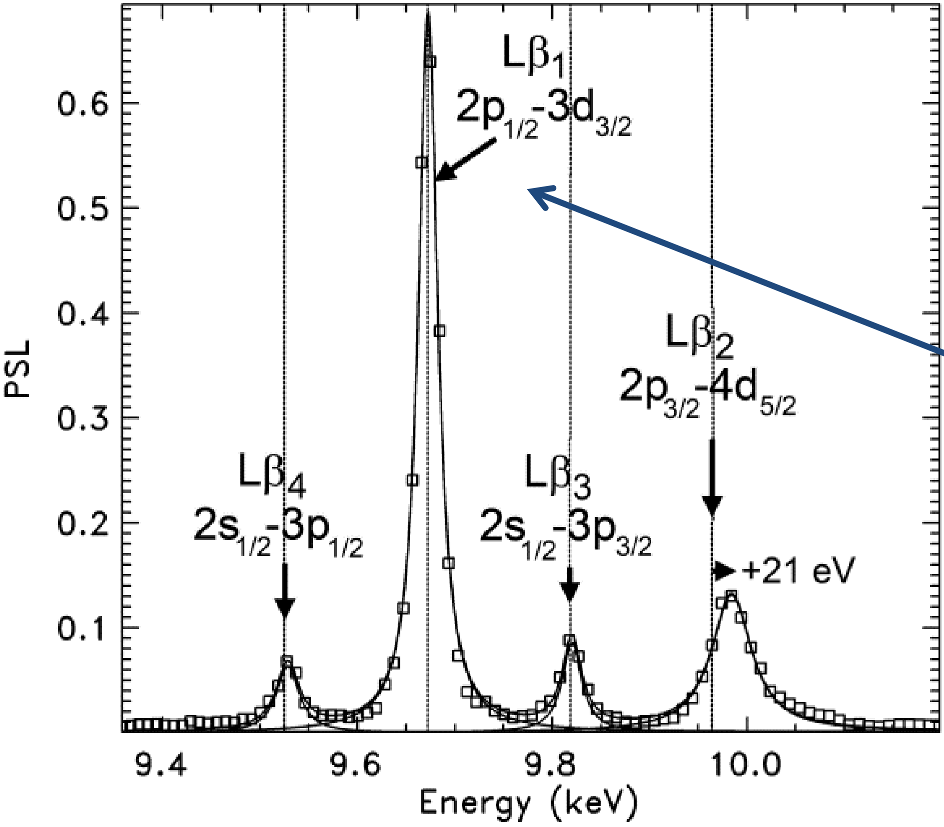
Electron current: 2 MeV, 0.6 MA, 50 ns

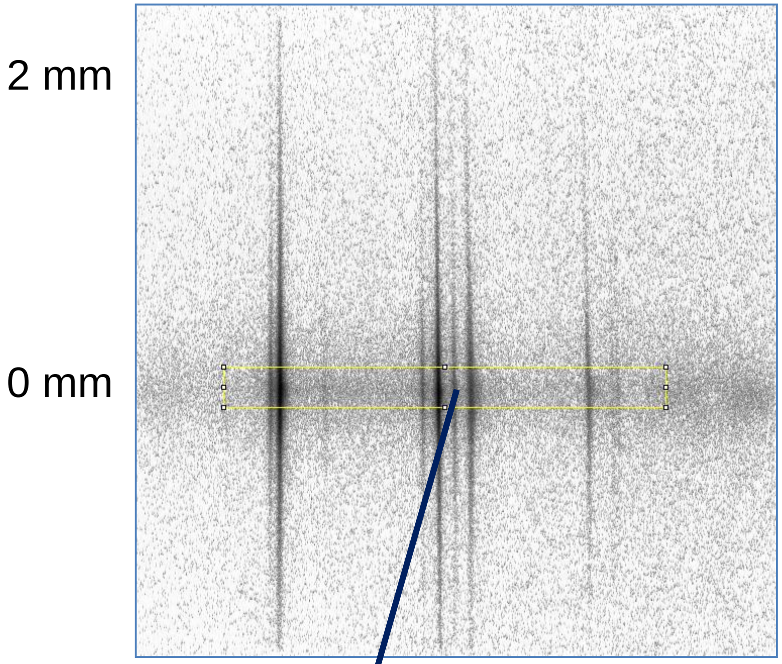


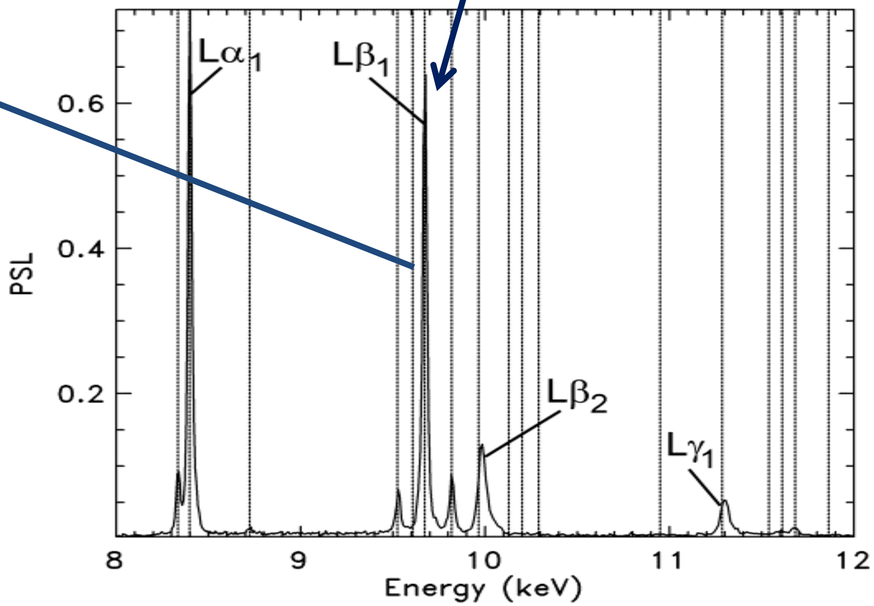


W Lβ$_2$ line is broad, asymmetric, and shifted to higher energy by ionization

Vertical lines are characteristic transition energies:







$L\beta_2$ Transition is Shifted by Outer-Shell Ionization

- Ionization of the outer $6s^2$, $5d^4$, $5p^6$, $5s^2$, and $4f^{14}$, up to the +28 charge state and approaching the $4d^{10}$ Kr-like closed shell.
- $L\beta_2$ transition having $4d_{5/2}$ upper level is perturbed to higher energy.
- Other nearby $L\beta$ transitions from more tightly-bound n=3 levels are essentially unperturbed.

Identification	Levels	W L Transitions Transition	Energy(eV)	Intensity
Lα2	L3M4	2p3/2-3d3/2	8335.3	11.22
Lα1	L3M5	2p3/2-3d5/2	8398.2	100.00
Lη	L2M1	2p1/2-4s1/2	8724.4	1.17
Lβ4	L1M2	2s1/2-3p1/2	9525.2	3.56
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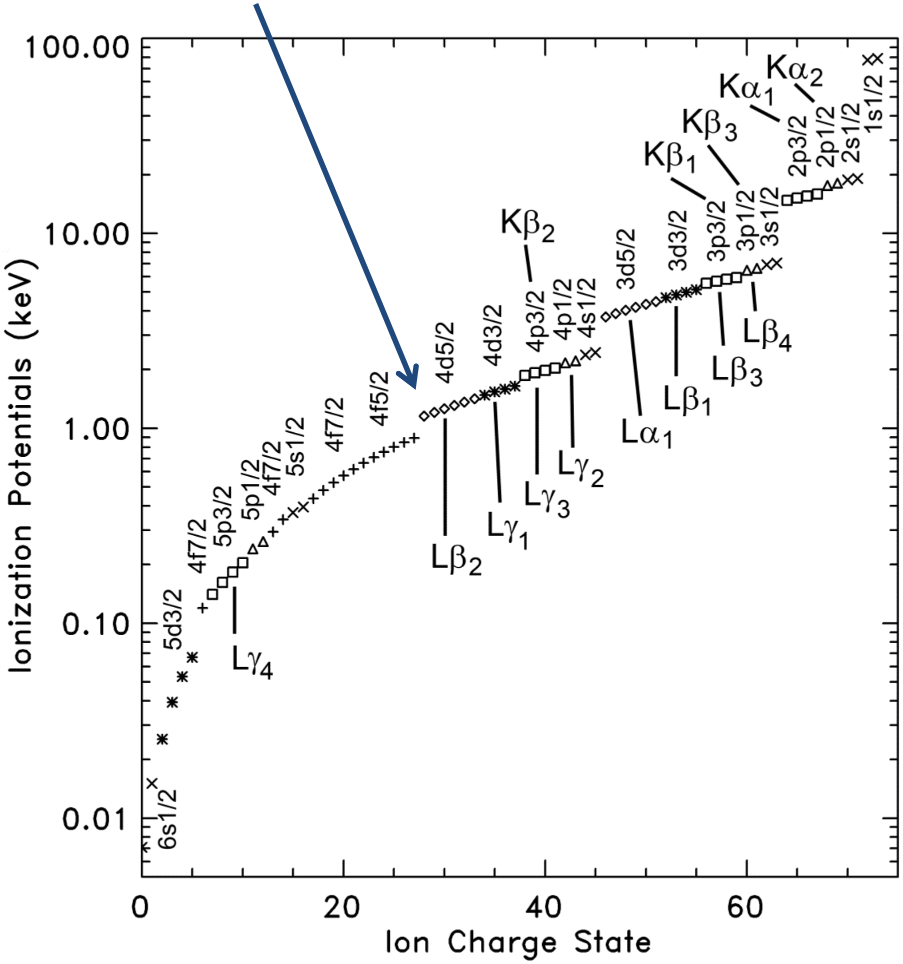
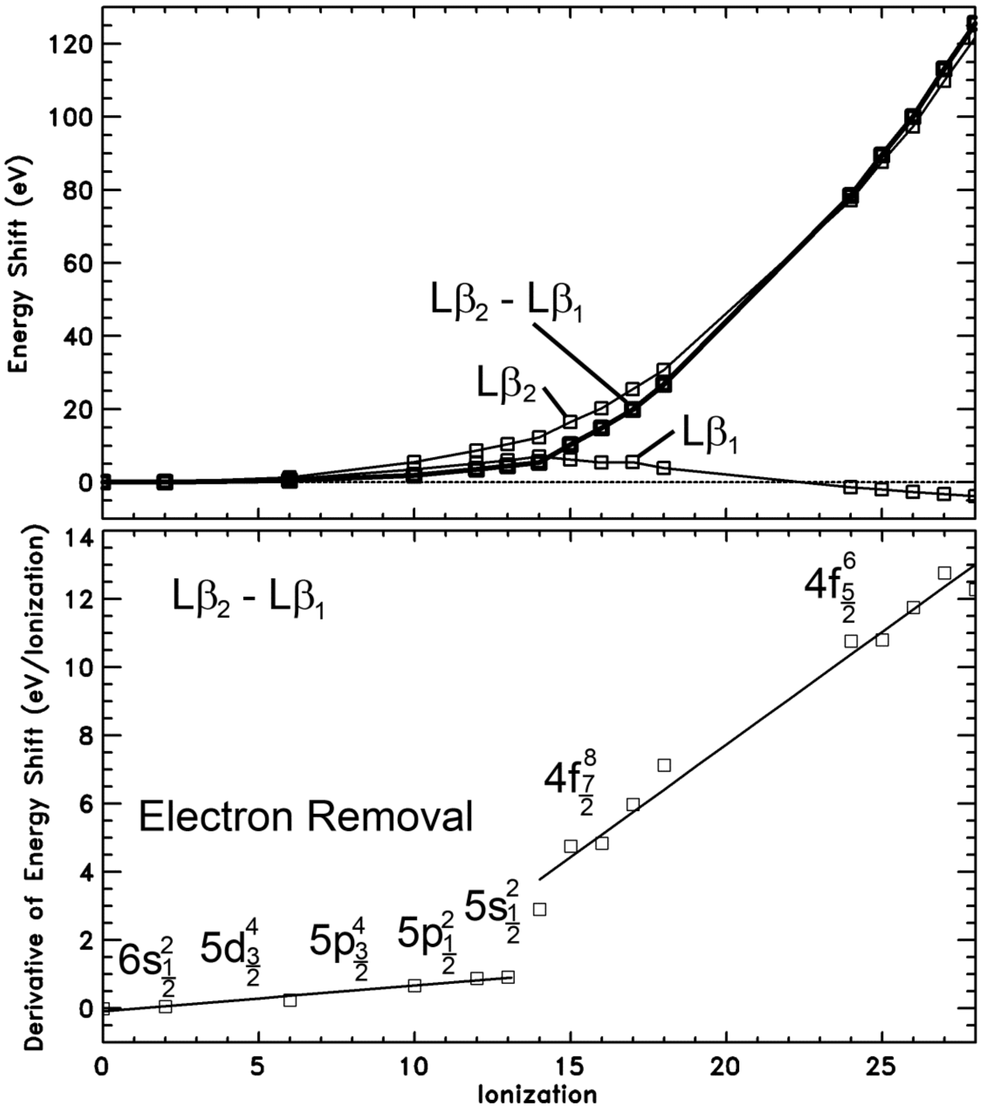
Lβ7	L3O1	2p3/2-5s1/2	10129.2	1.61
Lβ5	L3O5	2p3/2-5d5/2	10200.4	0.50
Lβ9	L1M5	2s1/2-3d5/2	10290.7	0.10
Lγ5	L2N1	2p1/2-4s1/2	10948.9	0.10
Lγ1	L2N4	2p1/2-4d3/2	11286.0	10.45
Lγ6	L2O4	2p1/2-5d3/2	11538.7	0.40
Lγ2	L1N2	2s1/2-4p1/2	11610.5	1.10
Lγ3	L1N3	2s1/2-4p3/2	11680.5	1.61
Lγ11	L1N5	2s1/2-4d5/2	11861.9	0.10
Lγ4	L1O3	2s1/2-5p3/2	12063.4	0.10

Ionization potential jump at the $[Kr]4d^{10}$ closed shell, Z=28

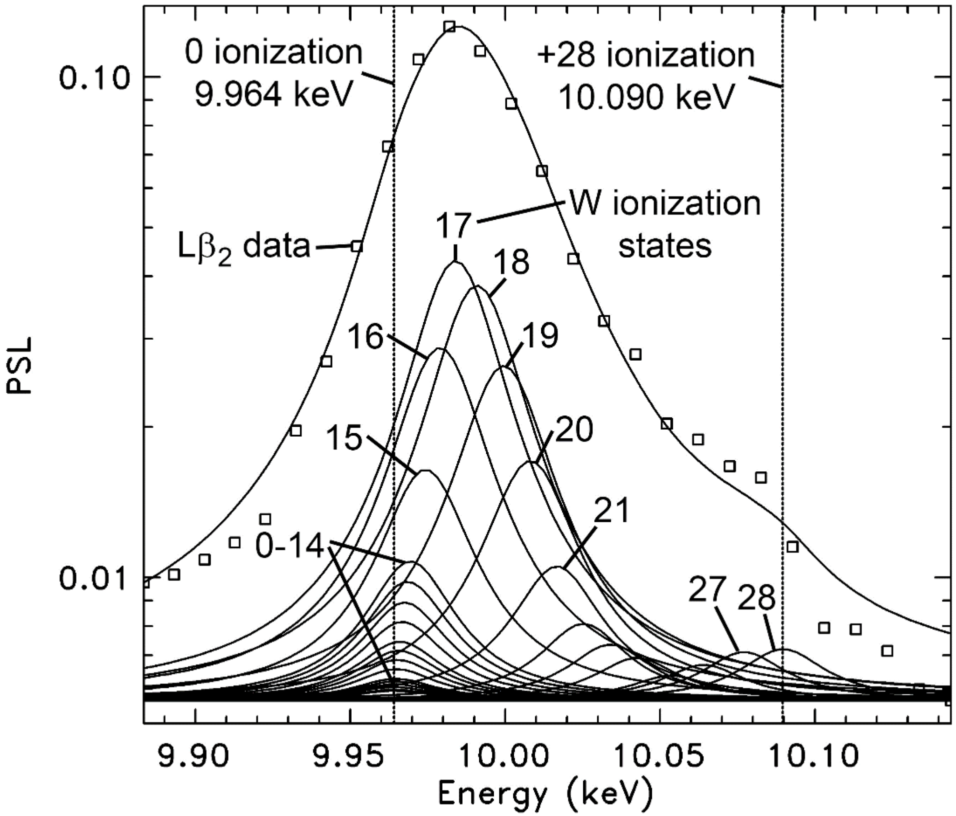


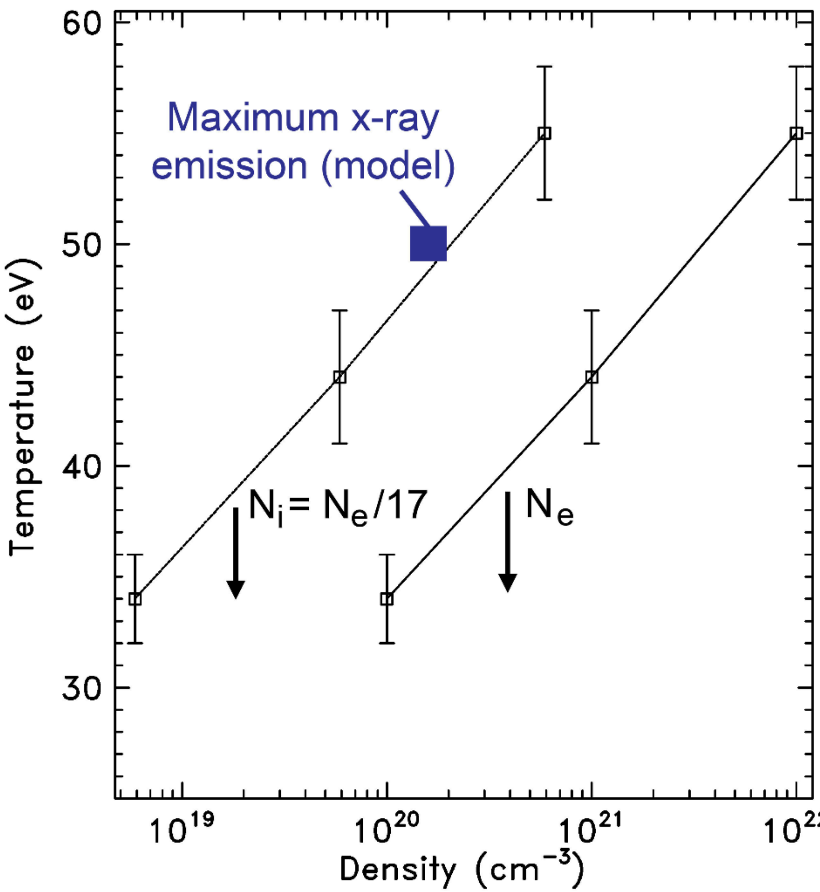
L-Shell Transition Energies are Accurately Calculated

Modified Grant MCDF code (Polasik, Słabkowska, *et al*.) calculates the W L-shell transition energies with few eV absolute accuracy, and transition energy differences have eV accuracy.

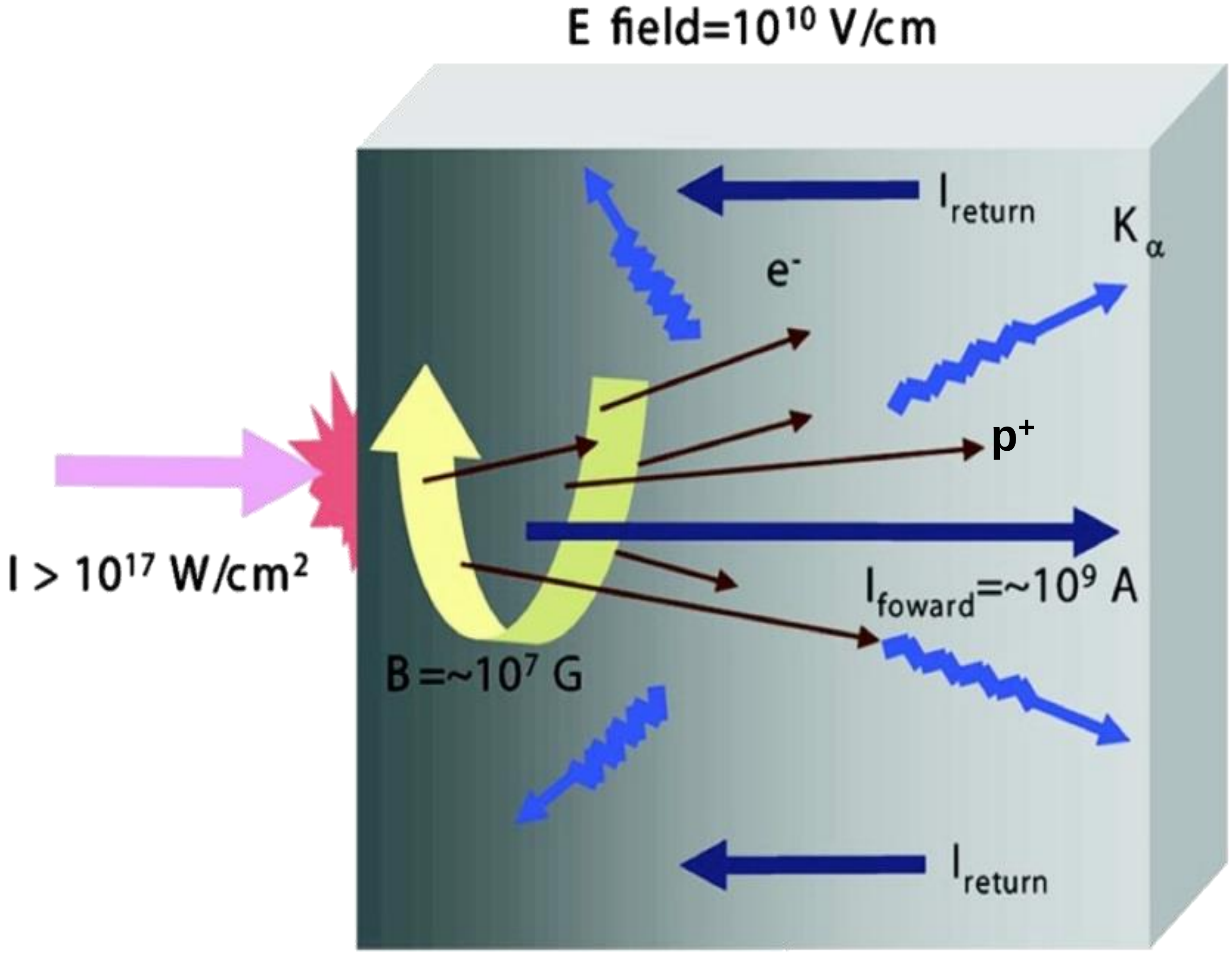


Measured Ionization is used to Determine Temperature and Density





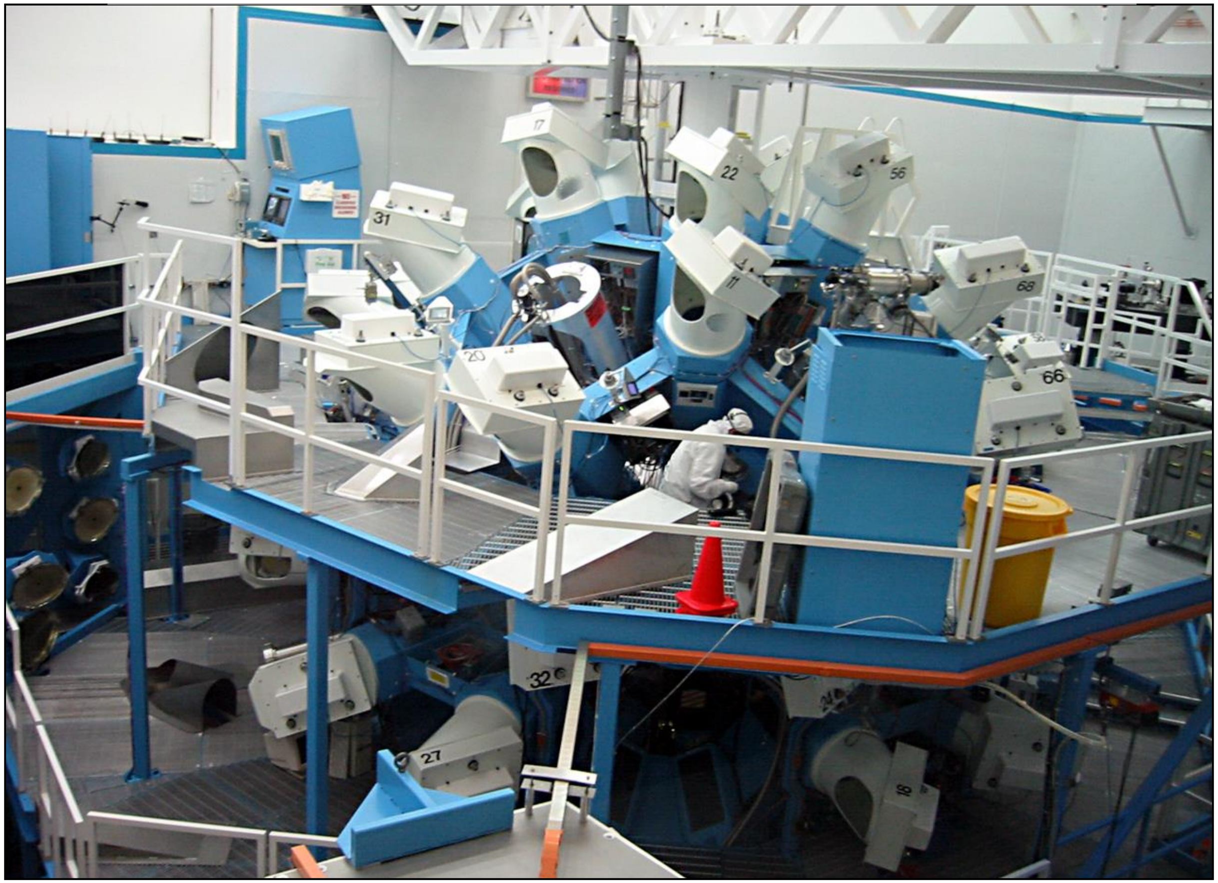
Intense Lasers Create Energetic Electrons, Positrons, Protons, X-Rays/Gammas, Strong Magnetic Fields, Etc.

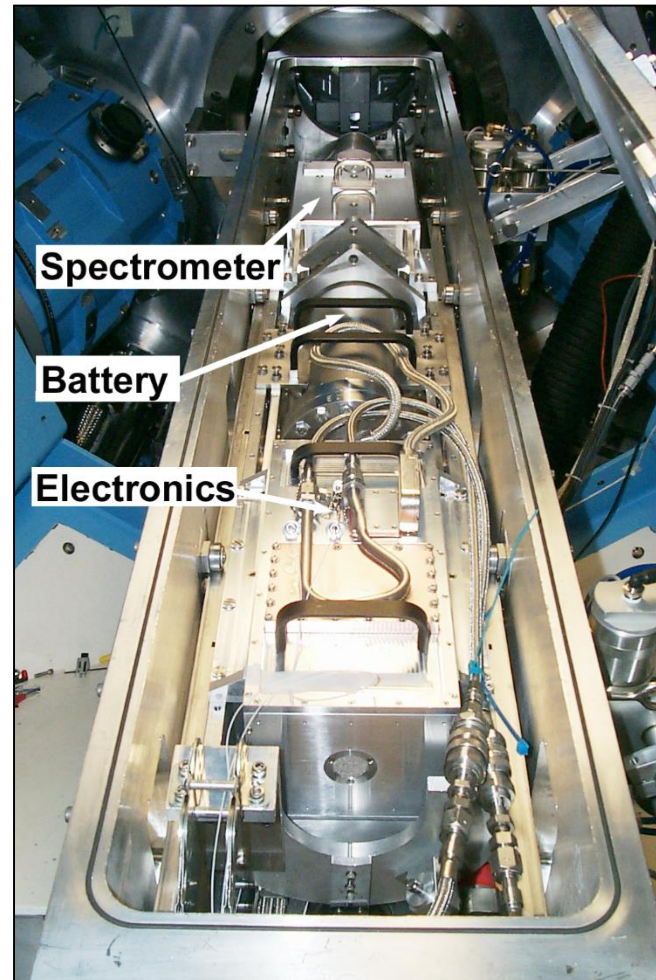


Park H.-S. et al. Phys. Plasmas **13** (2006) 056309

Omega Laser at the Laboratory for Laser Energetics (LLE) Rochester, NY, USA

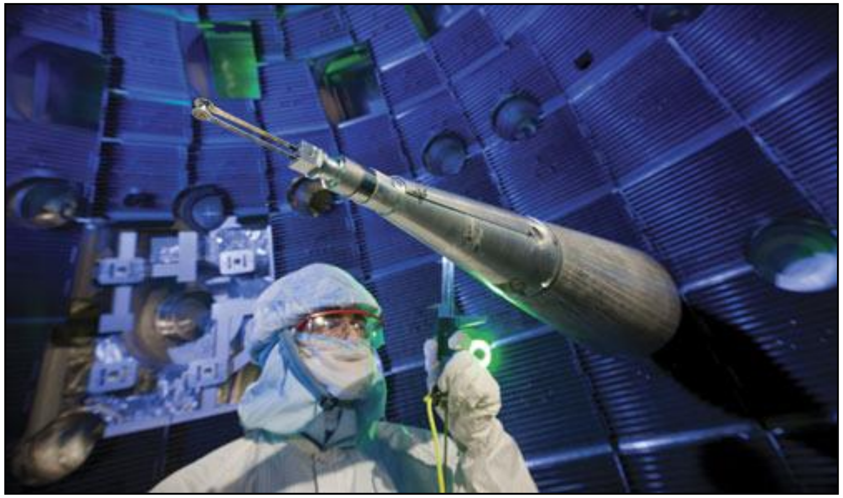
60 laser beams, 40 kJ, few ns



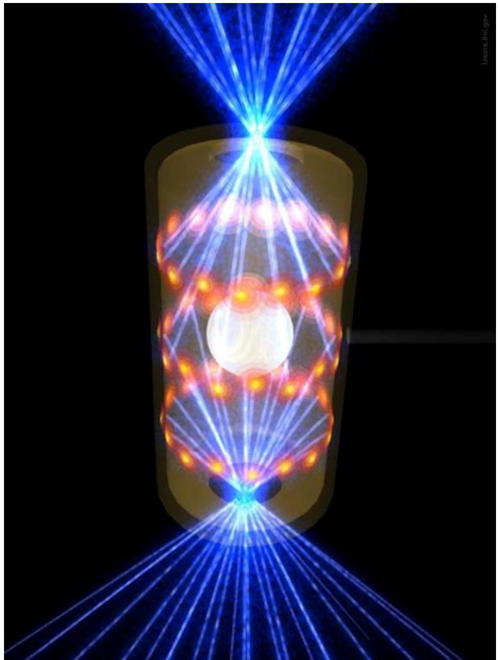


National Ignition Facility (NIF)
Lawrence Livermore National Laboratory (LLNL)

196 laser beams, 1.6 MJ, few ns

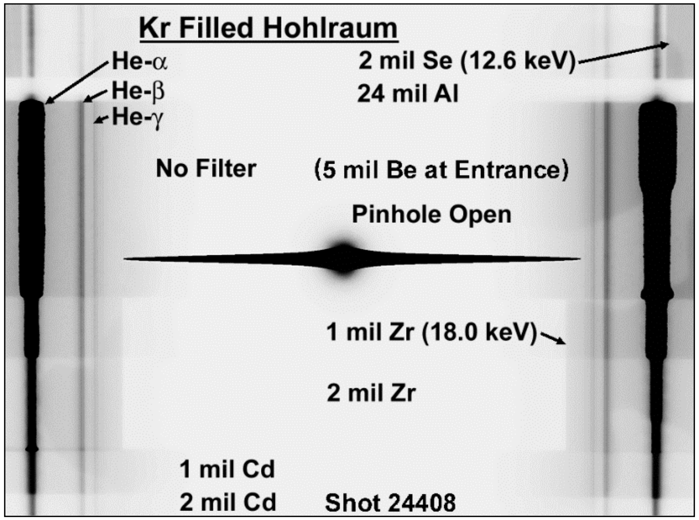


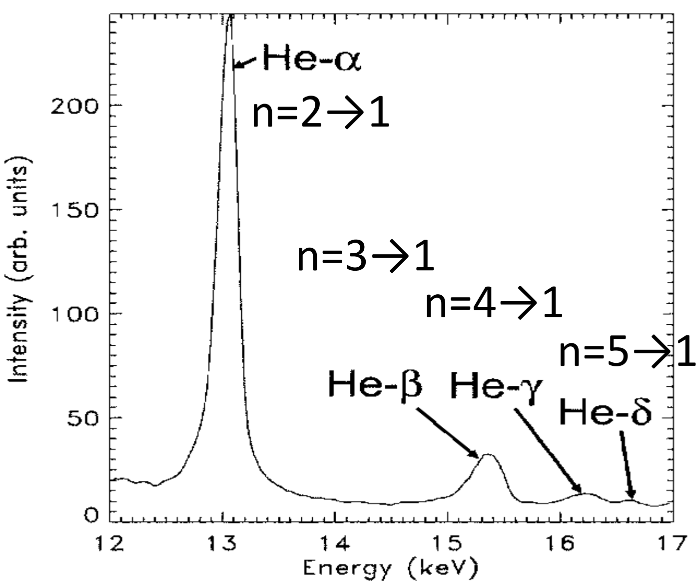
Capsule in hohlraum:



Kr K-Shell Spectra at Omega

Kr filled hohlraum





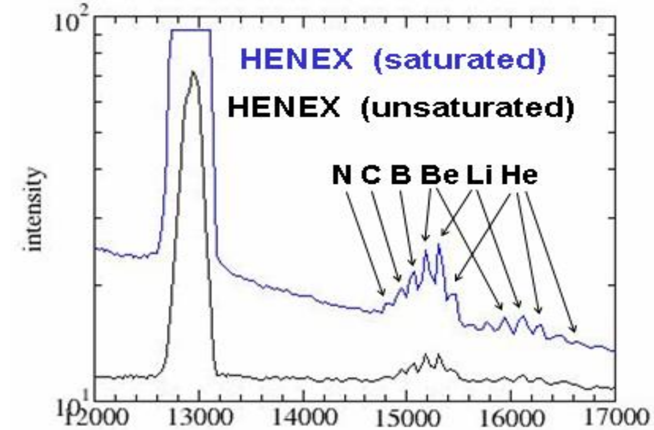
Kr filled gasbag (bulk heating, no super-thermal electrons)

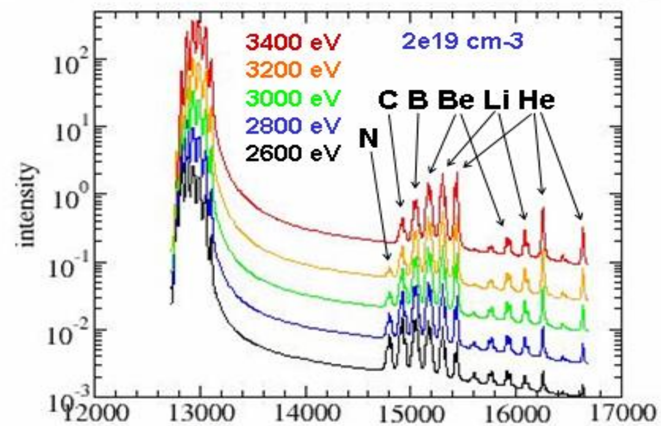
Experimental spectrum

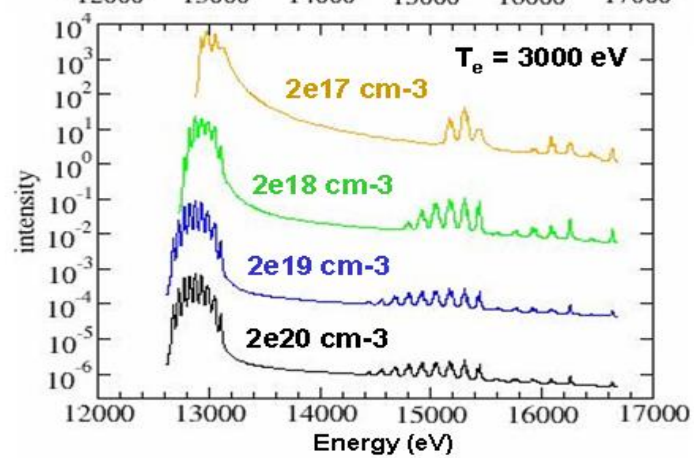
FLYCHK by H.-K. Chung:

T_e = 2.6 keV

$N_e = 2\times10^{18}$ cm^{-3}

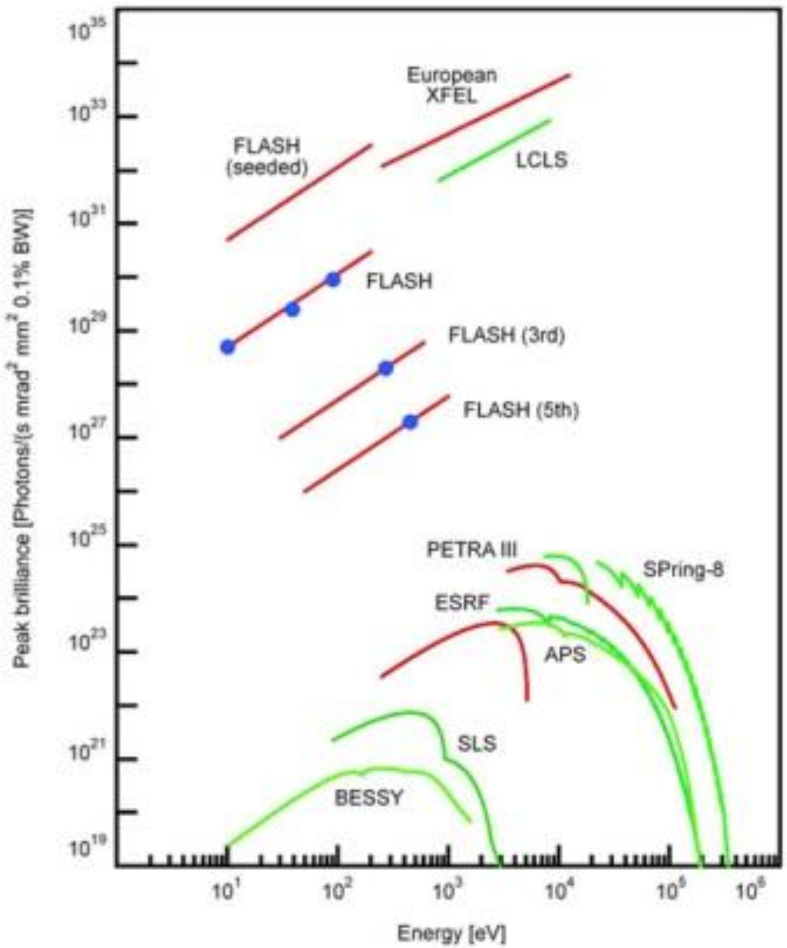




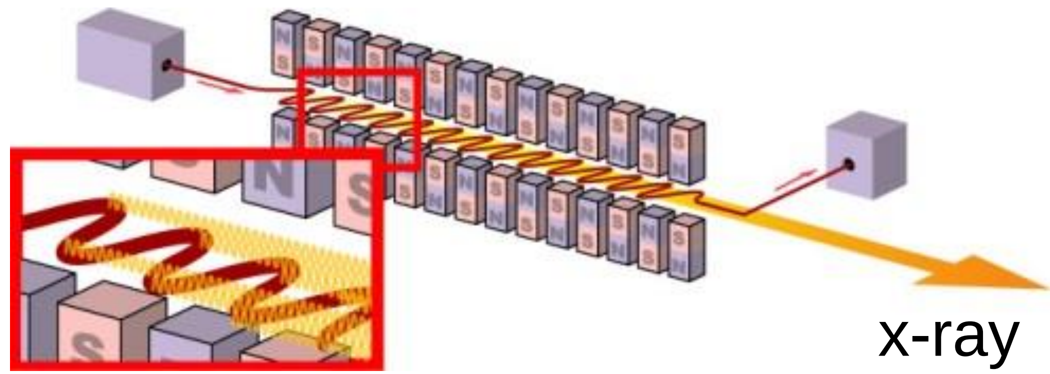


X-Ray Free Electron Laser (XFEL)

Bright, coherent, short duration, narrow bandpass, tunable energy.

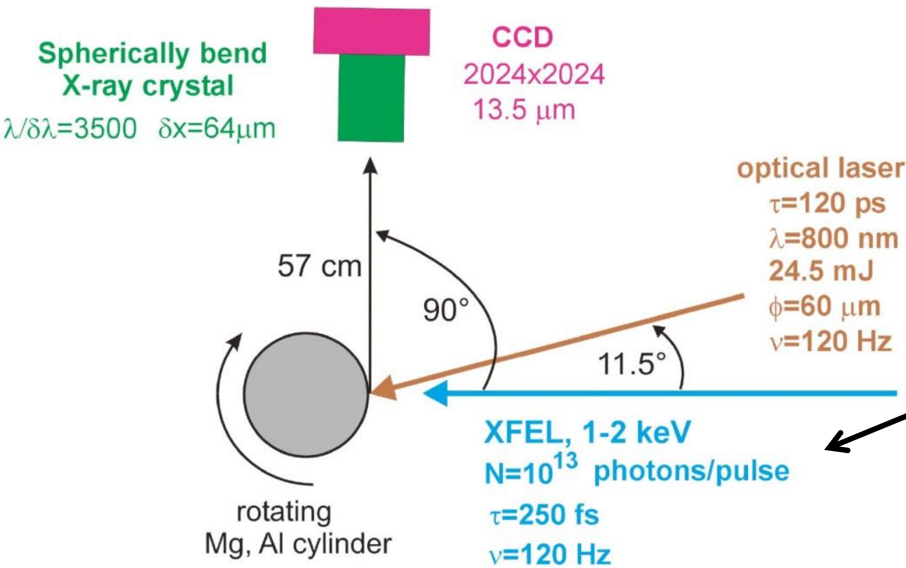


Electron bunches in undulator



x-ray beam

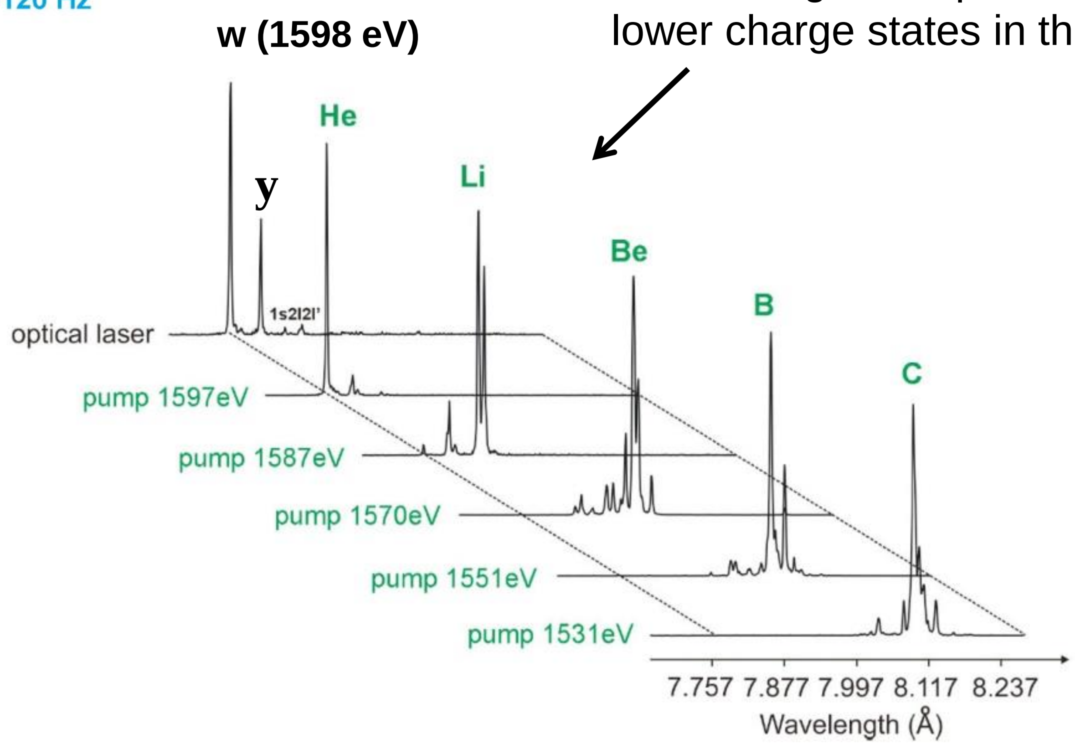
Photopumping Selected Transitions in an Aluminum Plasma



Optical laser pulse pre-forms the Al plasma (pump laser).

Time-synchronized XFEL pulse is tuned in energy to photopump transitions in selected charge state (probe laser).

Decreasing XFEL photon energy pumps lower charge states in the Al plasma.



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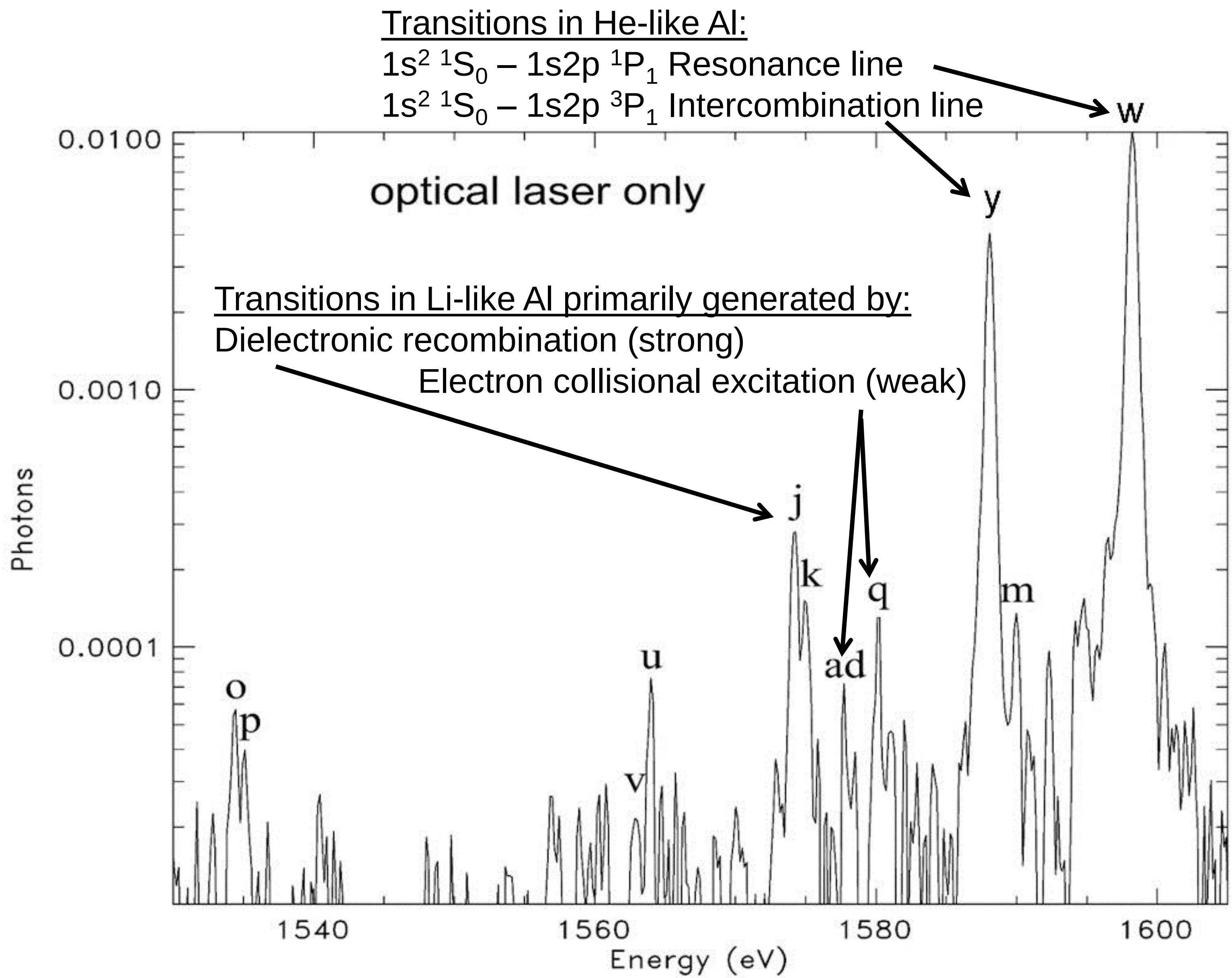
E. Galtier
O. Renner
LCLS Staff
Yuri Ralchenko

Emission Produced by Optical Laser Only

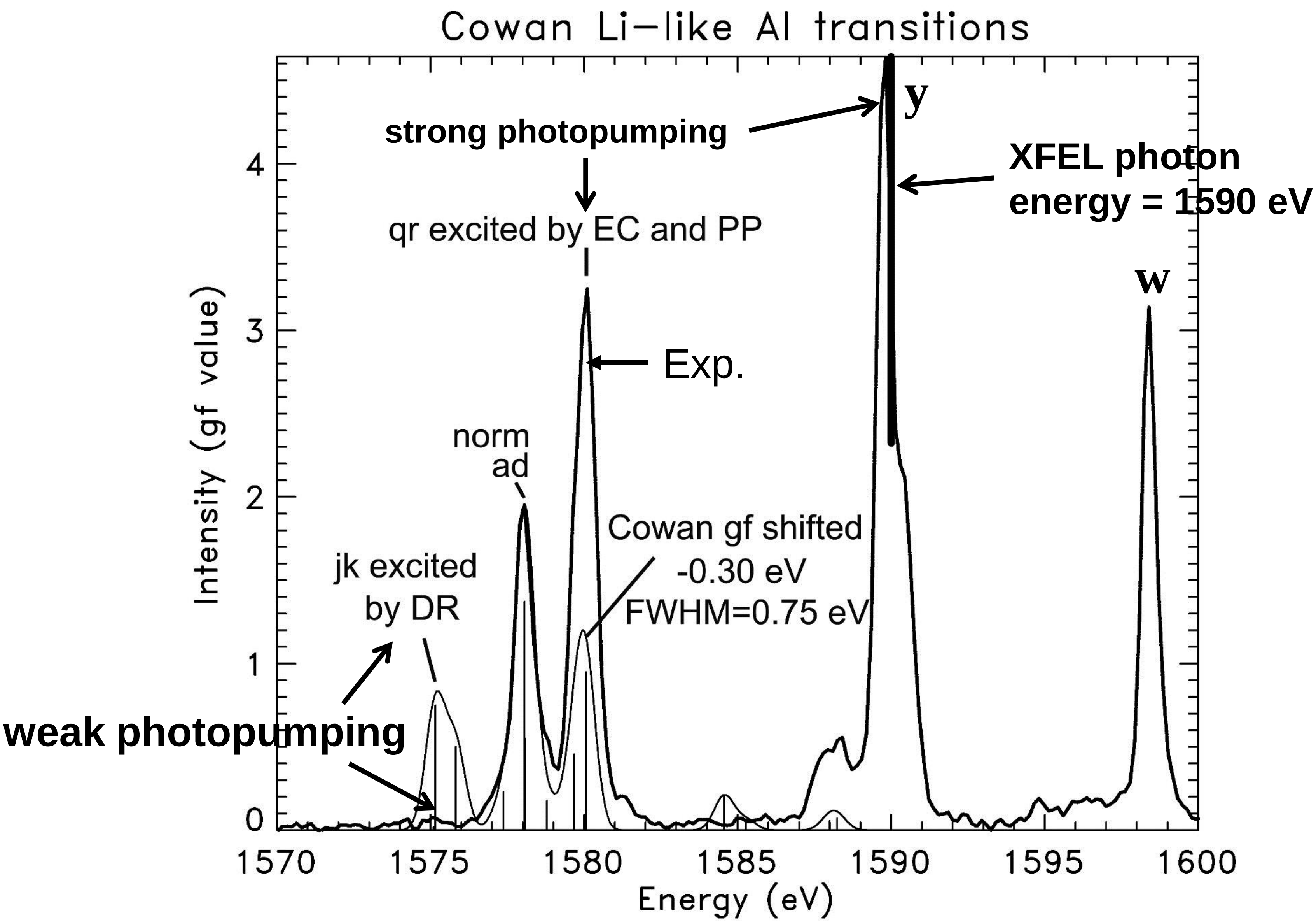


Satellites to the He-like Resonance Line

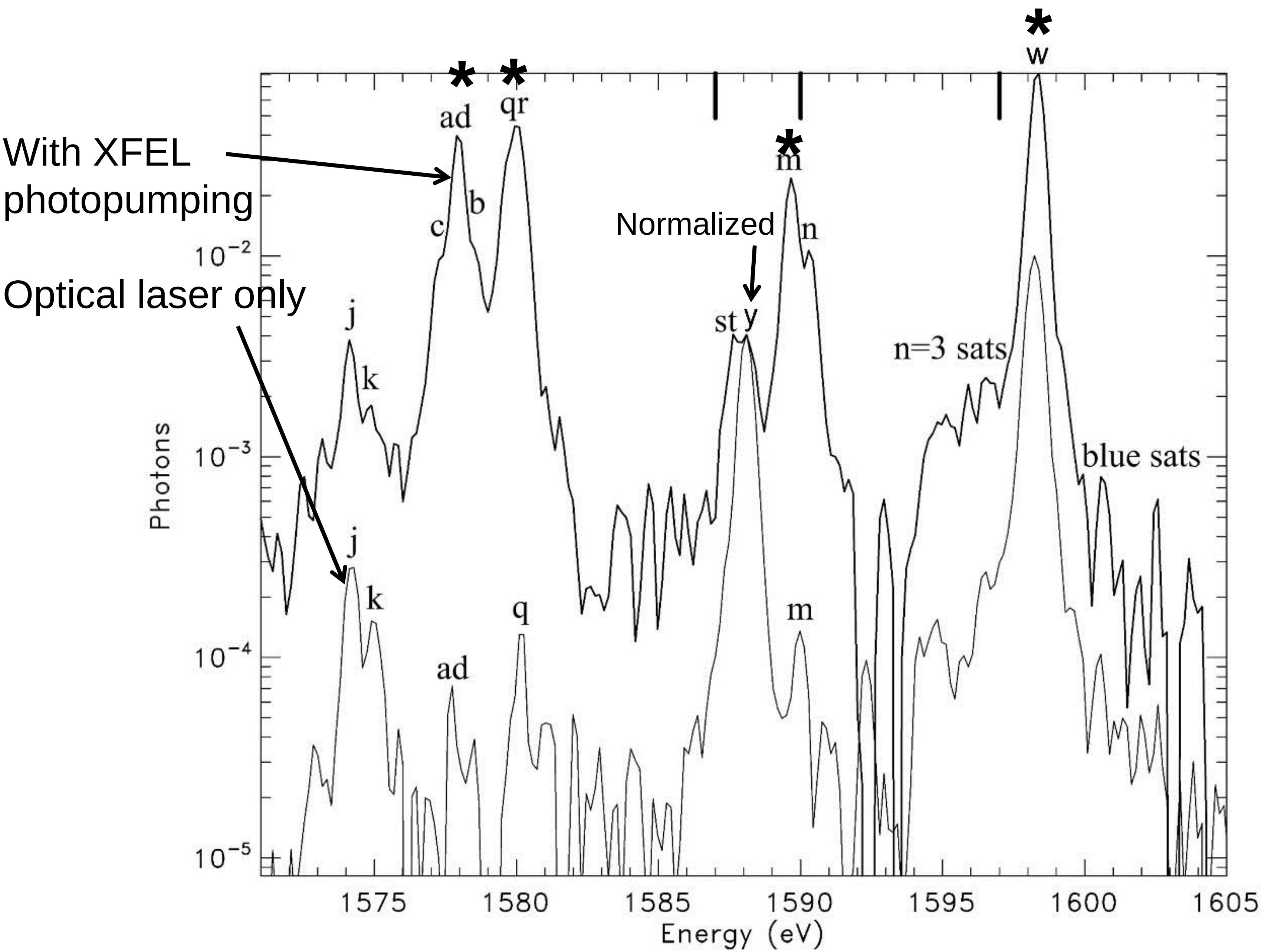
Li-like transitions from doubly-excited states.

Array	Multiplet	Line	Key letter	
$1s^2 2p$–$1s 2p^2$	$^2P^0$–^2P	1½–1½	a	Electron collisional excitation
		½–1½	b	
		1½–½	c	
		½–½	d	
	$^2P^0$–^4P	1½–2½	e	
		1½–1½	f	
		½–1½	g	
		1½–½	h	
		½–½	i	
	$^2P^0$–^2D	1½–2½	j	Dielectronic recombination
		½–1½	k	
		1½–1½	l	
	$^2P^0$–^2S	1½–½	m	
		½–½	n	
$1s^2 2p$–$1s 2s^2$	$^2P^0$–^2S	1½–½	o	
		½–½	p	
$1s^2 2s$–$1s 2p 2s$	^2S–$(^1P)\,^2P^0$	½–1½	q	
		½–½	r	Electron collisional excitation
	^2S–$(^3P)\,^2P^0$	½–1½	s	
		½–½	t	
	^2S–$^4P^0$	½–1½	u	
		½–½	v	
$1s^2$–$1s 2p$	^1S–$^1P^0$	0–1	w	He-like transitions
	^1S–$^3P^0$	0–2	x	
		0–1	y	
$1s^2$–$1s 2s$	^1S–^3S	0–1	z	

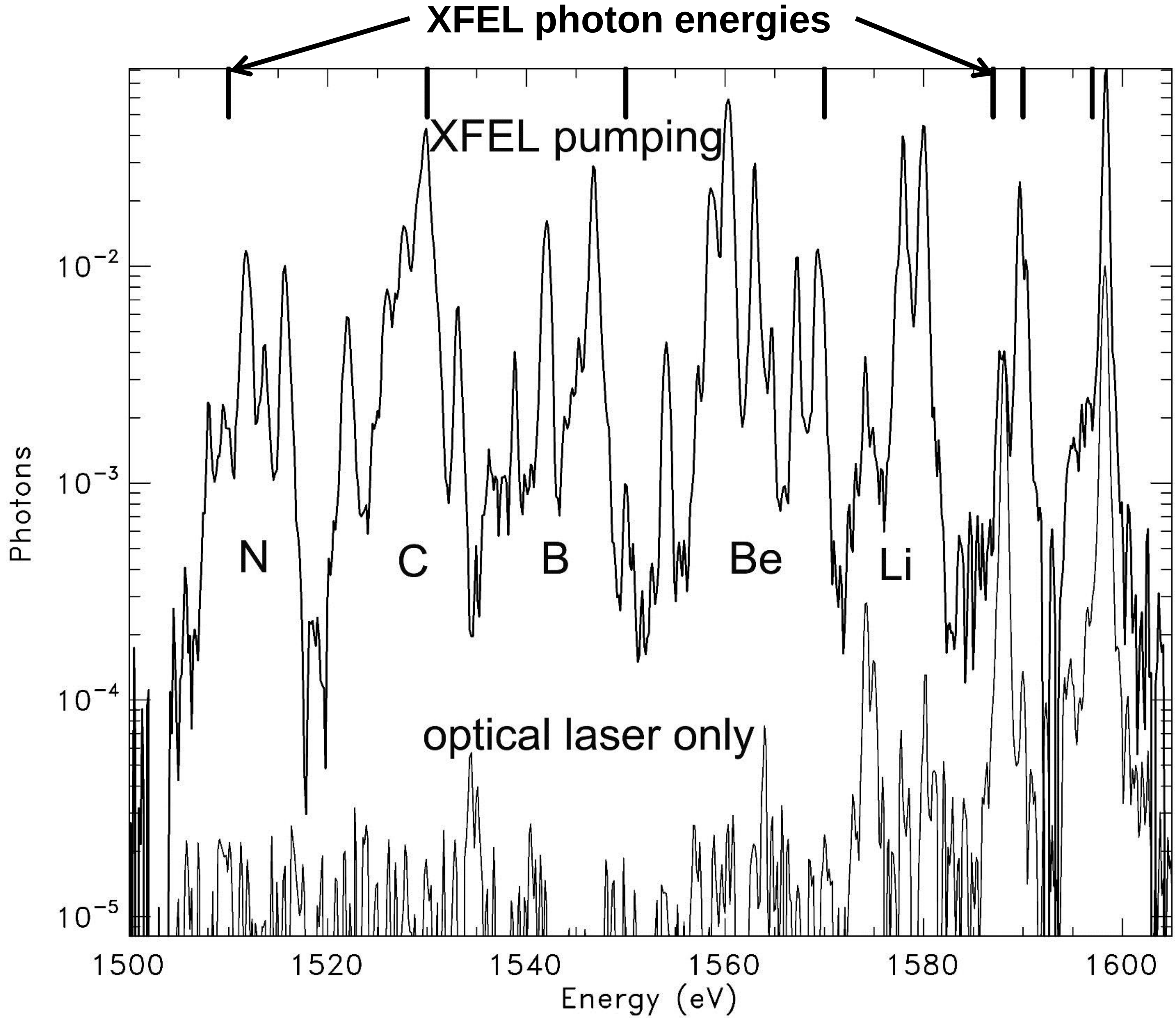
Transitions Photopumped by 1590 eV XFEL



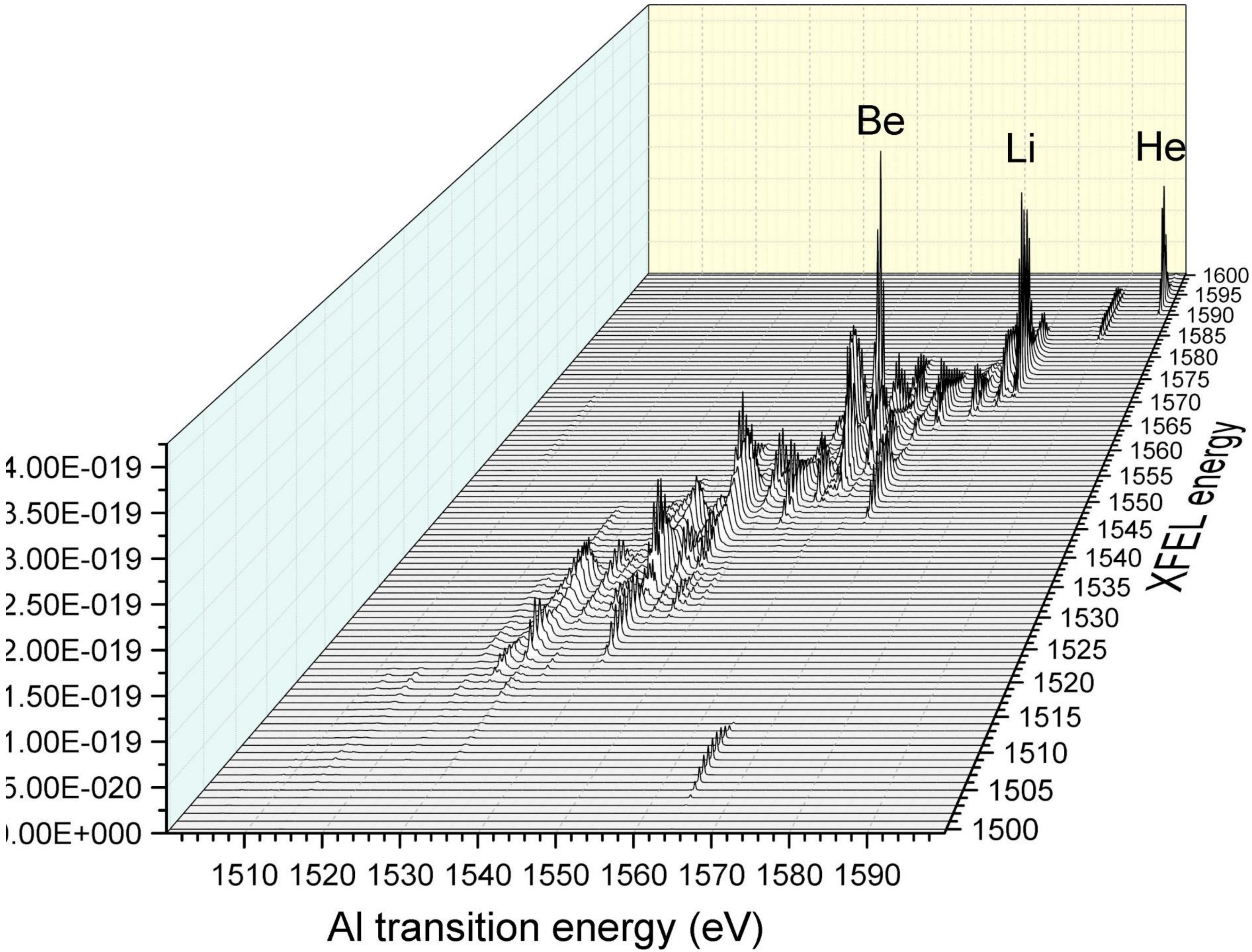
Transitions with Large Oscillator Strengths are Selectively Photopumped



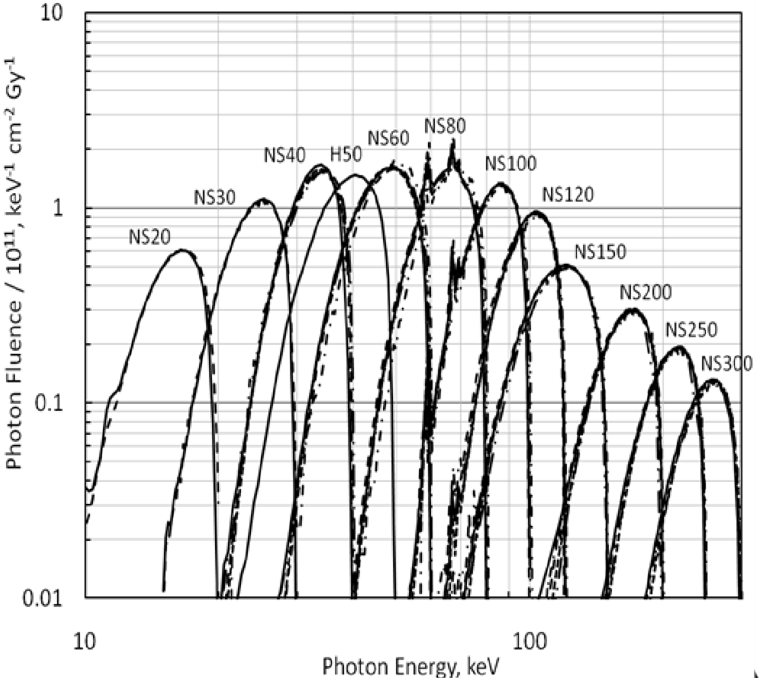
Composite Photopumped Transitions



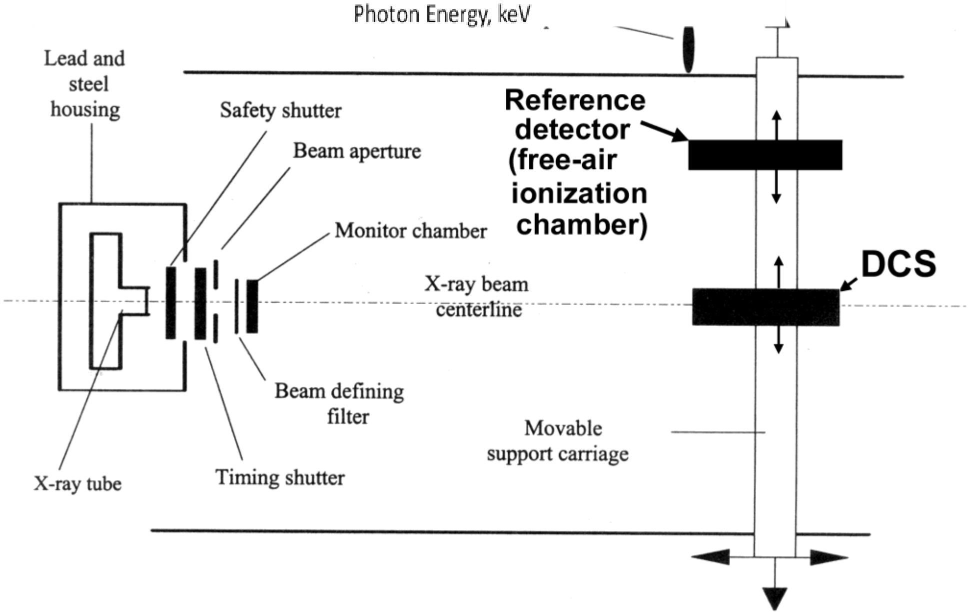
Ralchenko NOMAD Code

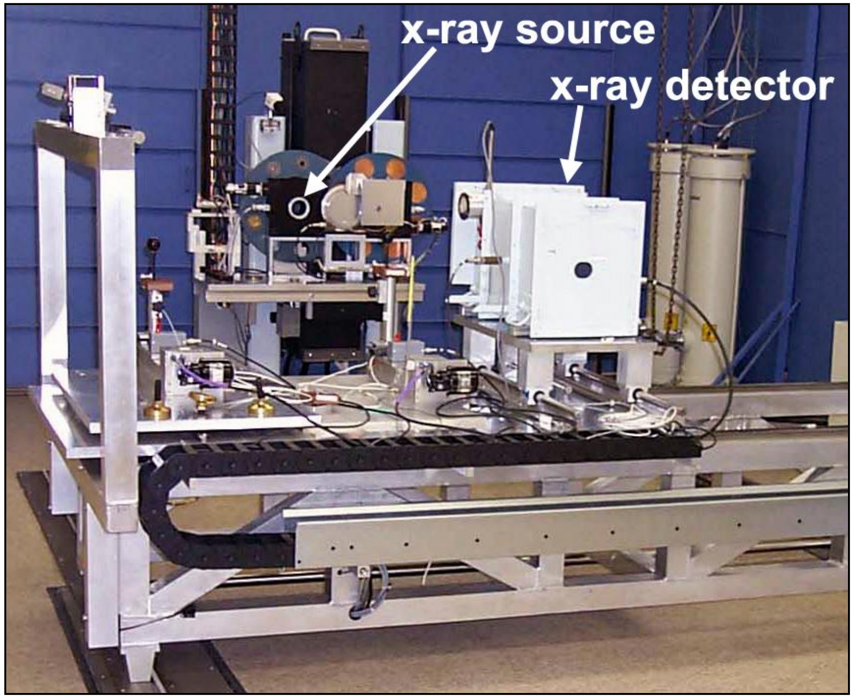


Spectrometer Calibrations (NIST)

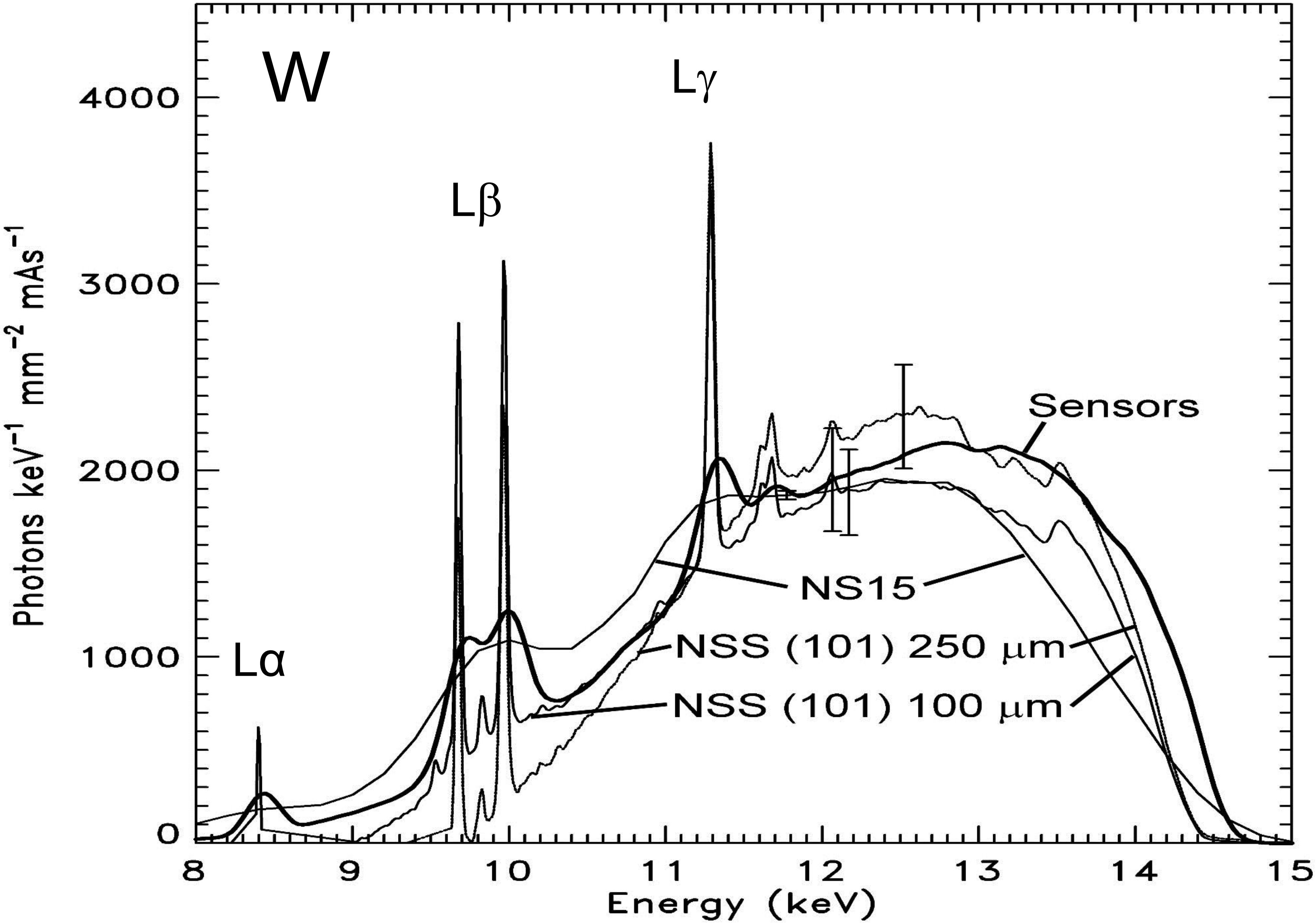


- Calibrated x-ray fluences in energy bandpasses.
- Spectrometer signal is related to the source fluence.
- Provides instrument sensitivity calibration.





Different Calibrated Instruments Measure the Same Source Fluence (within about 13% experimental uncertainty)



Experimental X-Ray Spectroscopy: Part 2

We will use the skills you have learned this week to analyze this spectrum: