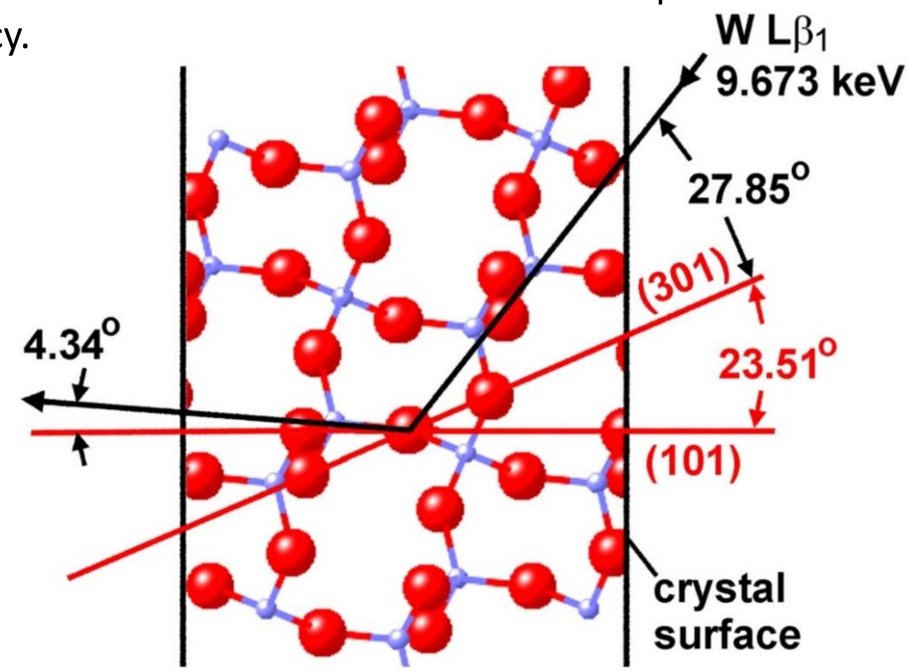
High-Resolution Hard X-Ray Spectroscopy at Titan (Work in Progress)

John Seely, 10/6/2015

- A new type of high-resolution transmission crystal spectrometer was developed and tested at the NIST W laboratory source and deployed at Titan in August:
  - Diffraction from quartz (301) planes at an angle of 23.51^o to the (101) planes that are perpendicular to the crystal surface.
  - Spectral lines in the 10-20 keV range are diffracted nearly perpendicular to the back surface of the crystal resulting in practically zero aberrations associated with the cylindrical crystal bending and the crystal thickness, and this produces excellent focusing on the image plate (hi-res Fuji TR) detector and high spectral resolution (35 eV/mm).
- The spectrometer was set up in the Titan chamber with Jeff Fein and Mario Manuel (University of Michigan) and using Titan 3 ns pulses and large focal spot (100 µm) to produce a quasi-steady state thermal plasma.
- Recorded spectra from highly-charged ions of GaAs (He-like through Ne-like K shell transitions) and Au and Ta (L shell transitions).
- The time-integrated plasma electron energy distribution and density were determined from the line ratios: T_e=1100 eV, 3% 30 keV hot electrons, and $N_e=1x10^{19}$ cm^{-3}. The line widths indicate the ion temperature was much less than the electron temperature.
- **The spectral lines were fitted to Voigt profiles, and the Gaussian and Lorentzian components have few eV FWHM values which enables line shape measurements with sub-eV accuracy.**
- ***The spectrometer is compact (0.5 m crystal to detector length) and can be deployed in instrument insertion modules.***

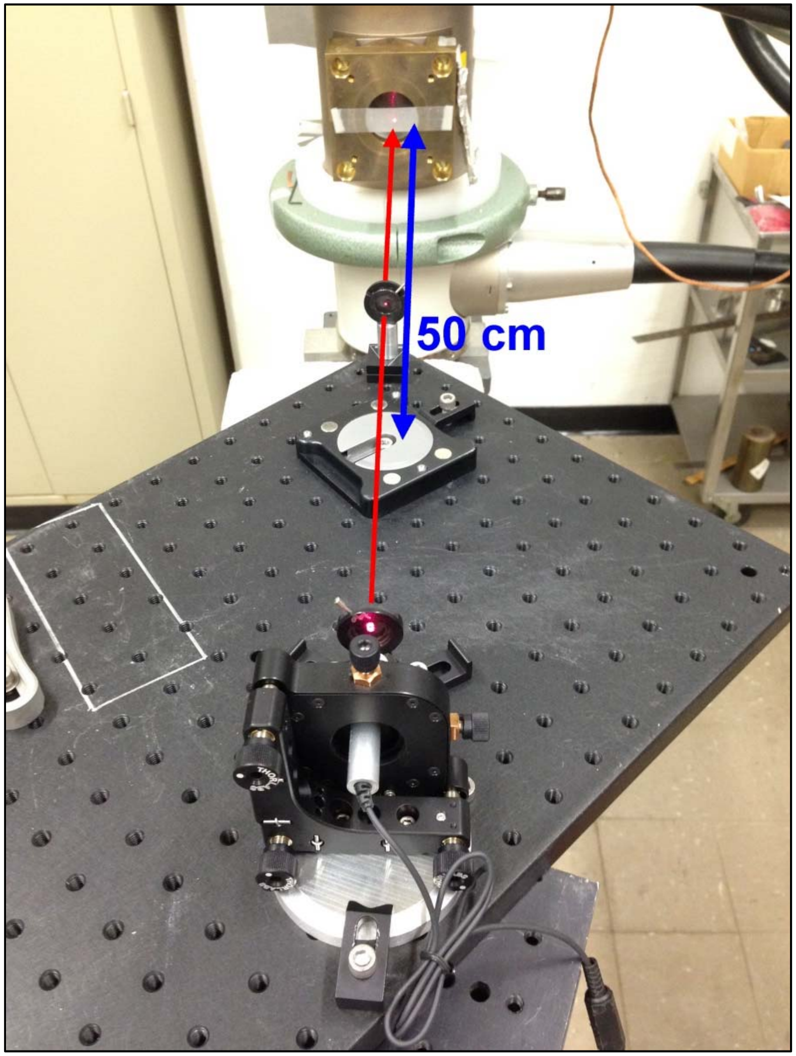
High-Dispersion Diffraction from the Quartz (301) Planes

- The quartz crystal is cut with the (101) planes perpendicular to the surface and is bent to 0.5 m radius of curvature.
- The (301) planes are at an angle of 23.51° to the (101) planes and have lattice spacing 2d=0.2744 nm.
- The W Lβ_1 9.673 keV line has Bragg angle 27.85° on the (301) planes, and the crystal is rotated by 51.36° from the spectrometer axis to diffract the Lβ_1 line from the (301) planes at the center of the illuminated length of the crystal.
- The diffracted Lβ_1 x-rays emerge from the back of the bent crystal nearly perpendicular to the crystal surface (at 4.34° to the local surface normal), and this results in nearly zero aberrations associated with the cylindrical bending of the crystal and the crystal thickness and produces excellent focusing on the detector and high spectral resolution.
- The dispersion on the IP detector (placed 25 mm behind the Rowland circle) is 35 eV/mm or 0.88 eV per 25 µm Fuji scanner step used at Titan.
- The observed spectral lines have few eV widths which enables the measurement of spectral line shapes and energy shifts with sub-eV absolute accuracy.

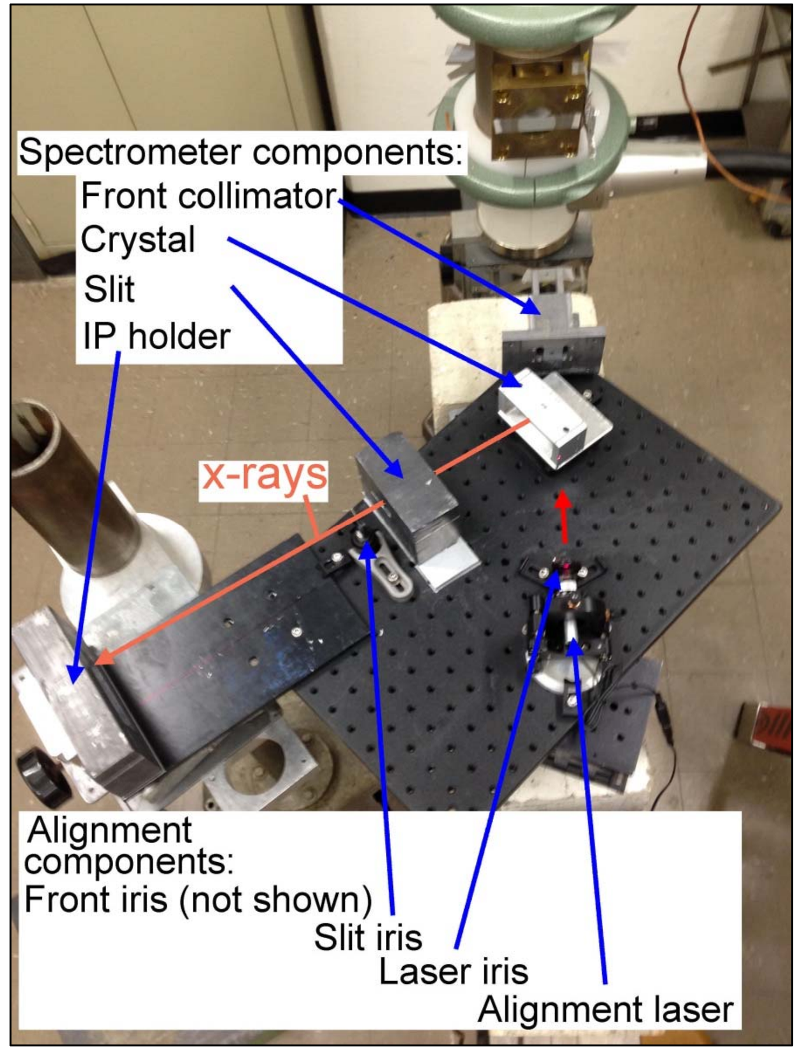


Spectrometer Alignment and Testing at the NIST W Source

<u>Baseplate alignment:</u> The red alignment beam points to the center of the x-ray source and propagates through the front and rear irises, and this defines the spectrometer axis:

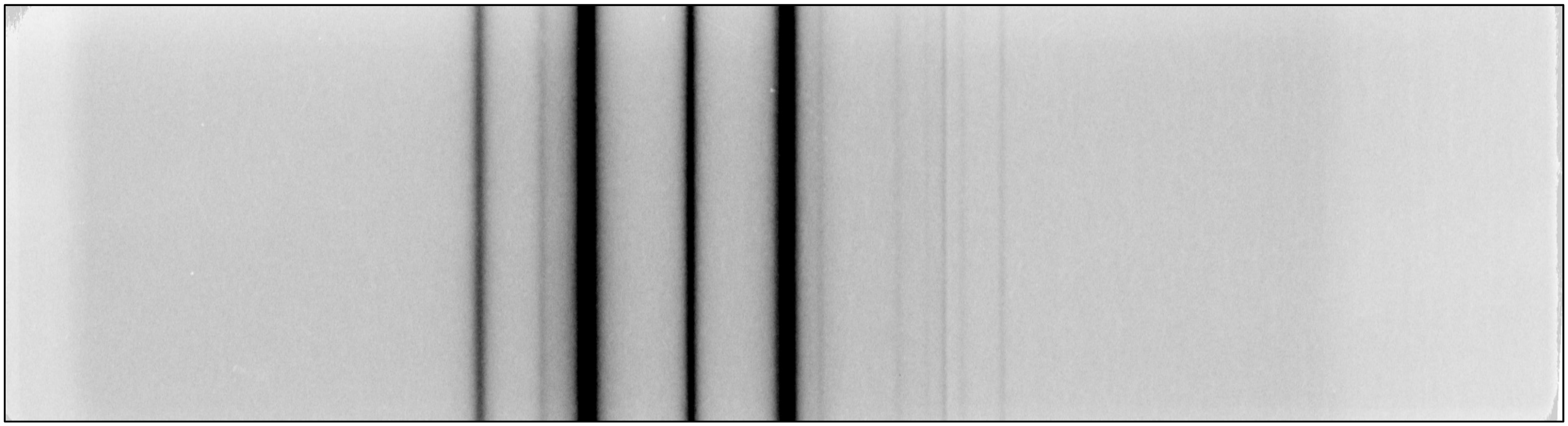


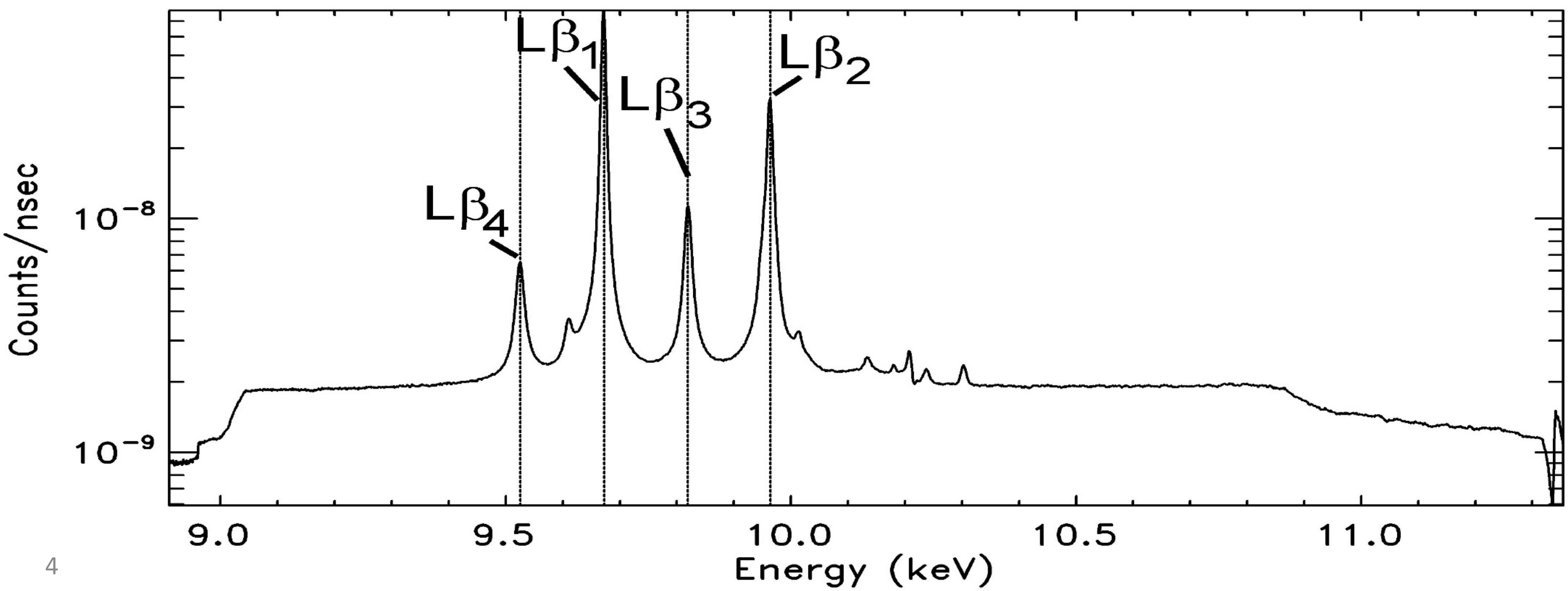
<u>Crystal alignment:</u> The crystal is mounted on a precision rotation stage and is rotated to the Bragg angle + (301) asymmetric angle $\Theta_B+\Theta_A$. The slit and IP holder are aligned to the red beam reflected from the back of the crystal when rotated by the Bragg angle Θ_B:



W Lβ Spectrum from the NIST Source

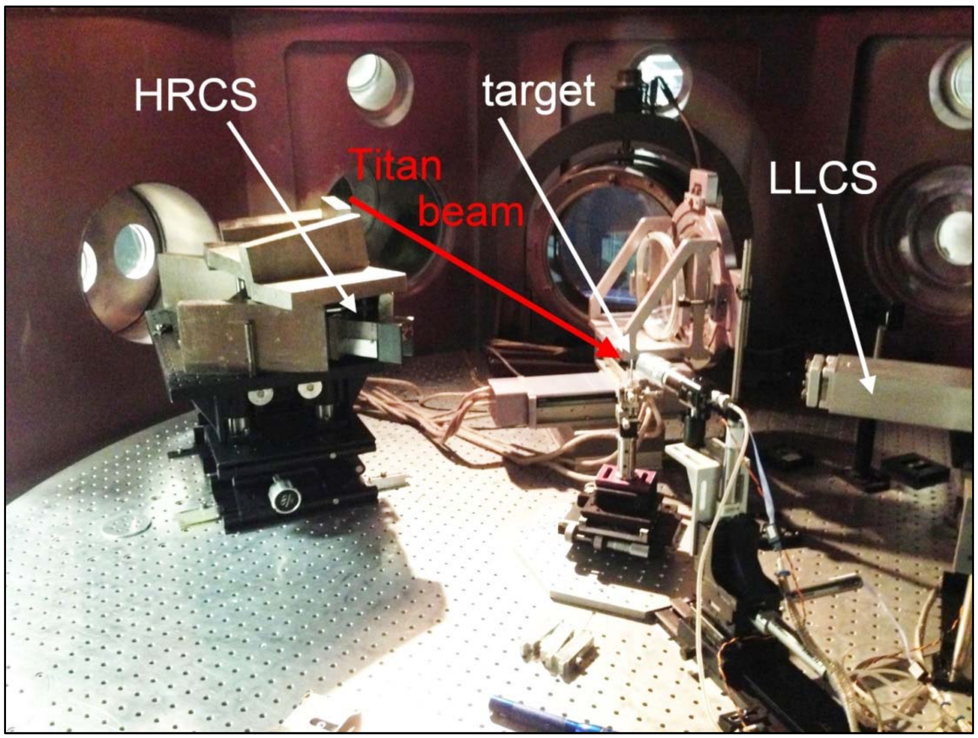
- Crystal rotation angle 51.36°, source to crystal distance 50 cm.
- 100 kVp, 10 mA, 3 min. exposure on TR IP.

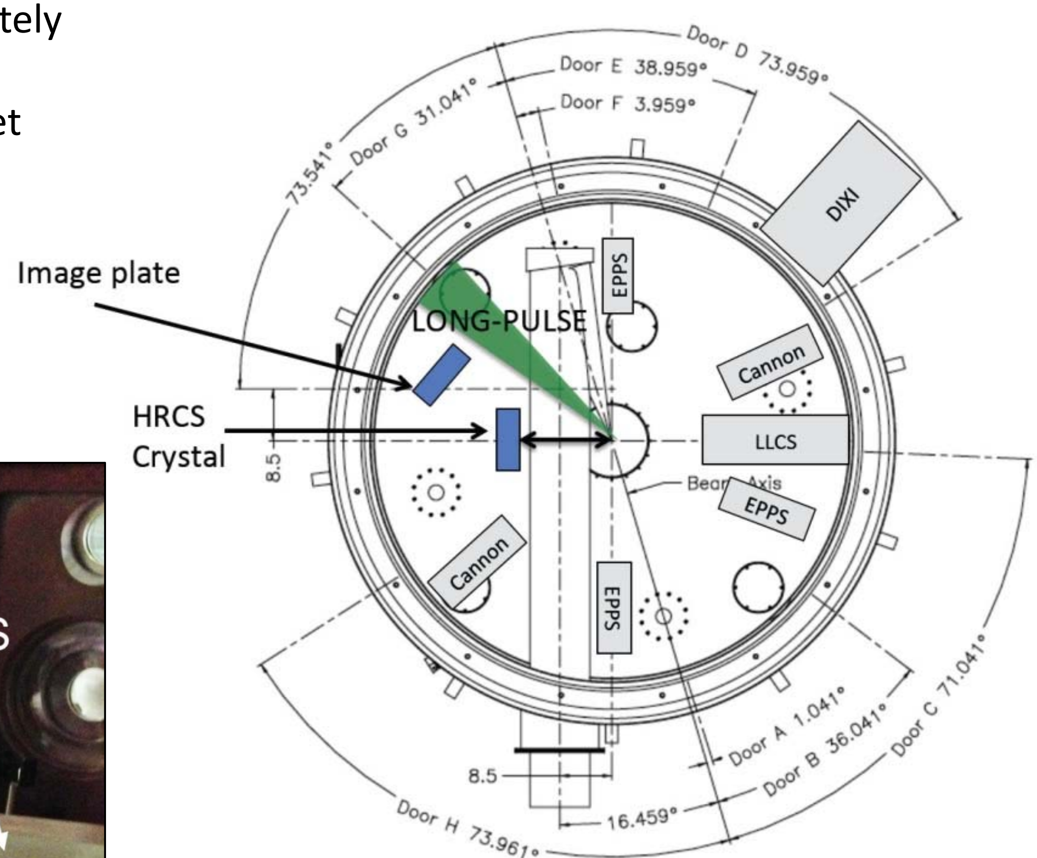




Spectrometer Alignment in the Titan Chamber

- The spectrometer was positioned in the Titan chamber with the spectrometer axis approximately 45° to the incident Titan long-pulse beam.
- For all but one Titan shot, the plane of the target was rotated so the spectrometer viewed at an angle of approximately 20° to the edge of the target.
- The target to crystal distance was 25 cm.
- Numerous 1” thick Pb bricks surrounded the spectrometer:





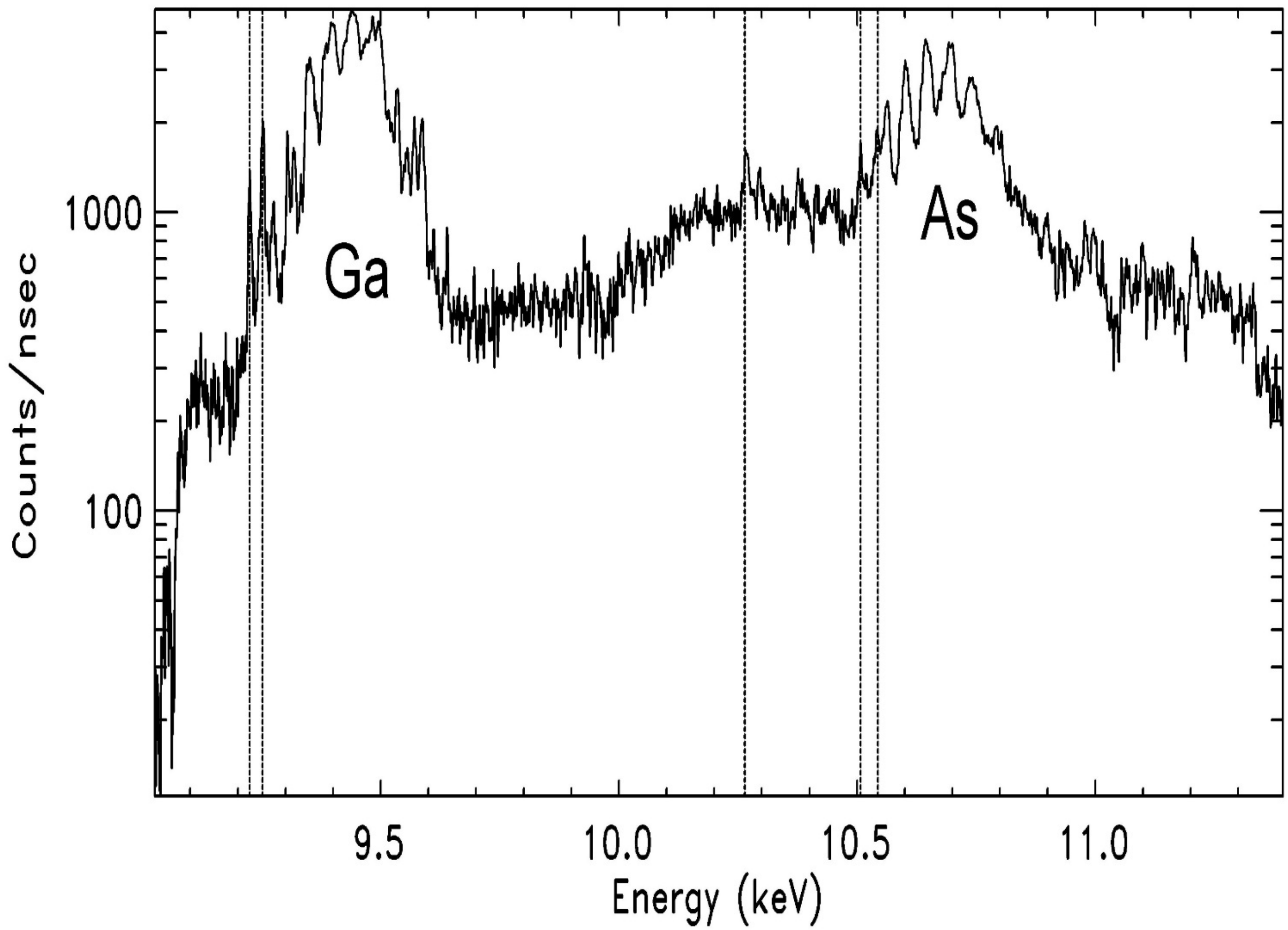
Titan Long-Pulse Shots Produced Thermal Plasmas

- The Titan laser pulse was designed to produce a relatively large thermal plasma with high ionization:
  - Long pulse duration (3 ns square pulse) reduces time-dependent effects.
  - Large focal spot (≈100 μm) reduces edge effects and differential hydrodynamic motions.
  - λ = 1 μm (1ω) and no phase-plate beam smoothing produce high pulse energy: average 770 J and ≈ 3×10^{15} W/cm^2 focused intensity.
- Absence of beam smoothing results in hot spots that produce non-thermal energetic electrons (approximately 30 keV), inner-shell vacancies in neutral atoms outside the focal spot, and characteristic K and L shell radiation from the neutral atoms.
- Targets were selected that have K-shell lines (Ga and As) or L-shell lines (Au and Ta) in the 9.0–11.5 keV energy range covered by the spectrometer.
- The targets were 250 μm GaAs wafer pieces and 25 μm thick Au or Ta foils.
- Spectra were recorded on a MS image plate or on horizontally split MS/TR image plate pieces.
- Spectra were recorded from 5 high-energy Titan shots and a half-energy shot that was designed to produce a null result:

Shot Number	Scan File	Target	Edge View Angle (deg)	Laser Energy (J)	Image Plate	Spectrum Comments
1	820151147	GaAs	20	779	MS	Intense Ga and As lines
2	820151311	Au	20	780	MS	Intense Au L lines
3	820151503	Ta	20	786	MS/TR	Intense Ta lines
4	820151621	GaAs	90	725	MS/TR	Out of focus: weak Ga and As lines
5	820151722	GaAs	20	776	MS/TR	Intense Ga and As lines
6	820151810	GaAs	20	331	MS/TR	Very weak Ga lines, no As lines

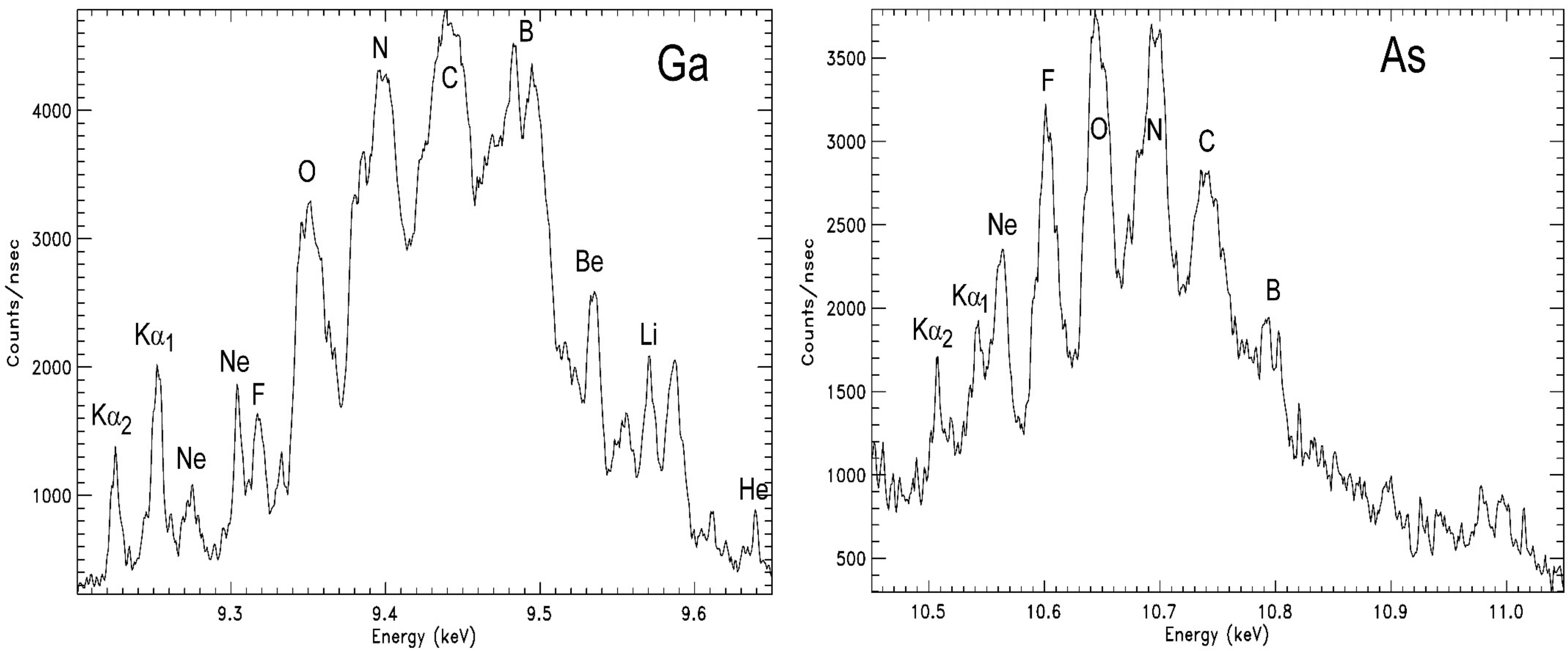
Spectrum from a GaAs Target

- Intense Ga and As K-shell lines were recorded:
- Ga $K\alpha_1$, $K\alpha_2$, $K\beta_1$ and As $K\alpha_1$, $K\alpha_2$ lines from neutral atoms outside the focal spot were used to establish an energy scale with 1 eV absolute accuracy as indicated by the 5 vertical lines on the spectra.
- K-shell lines from highly charged Ga and As ions at energies higher than the Ga and As $K\alpha$ lines.



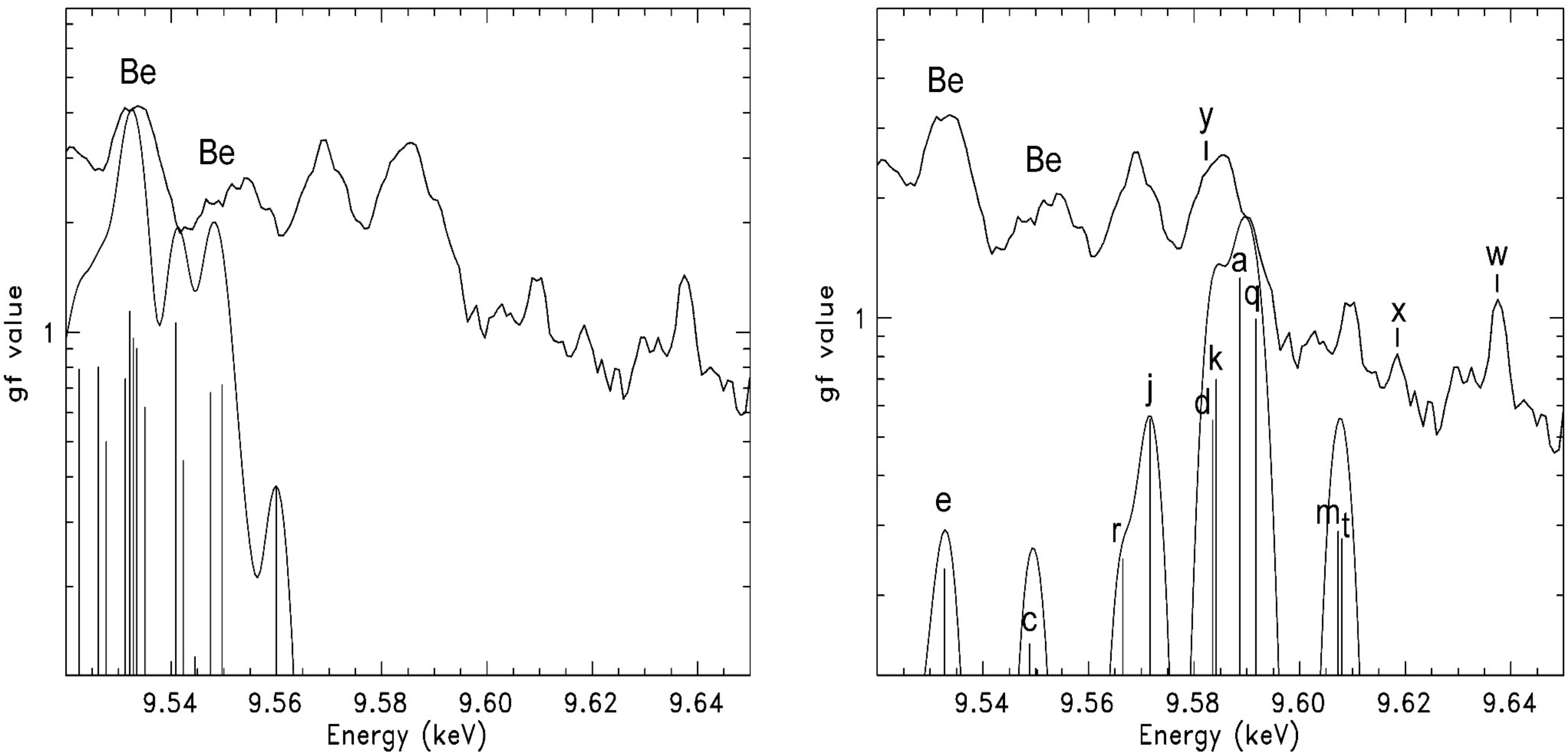
Identification of the Ga and As K-Shell Transitions

- Cowan code calculations for the transition energies and gf values for K-shell transitions in the Ga and As ionization stages He-like through Ne-like.
- FLYCHK calculations for the ionization balance vs. T_e and N_e.
- Detailed FAC and NOMAD calculations by Yuri Ralchenko simulated the spectra.
- The Ga spectrum extends to the He-like ionization stage and the As spectrum to B-like:



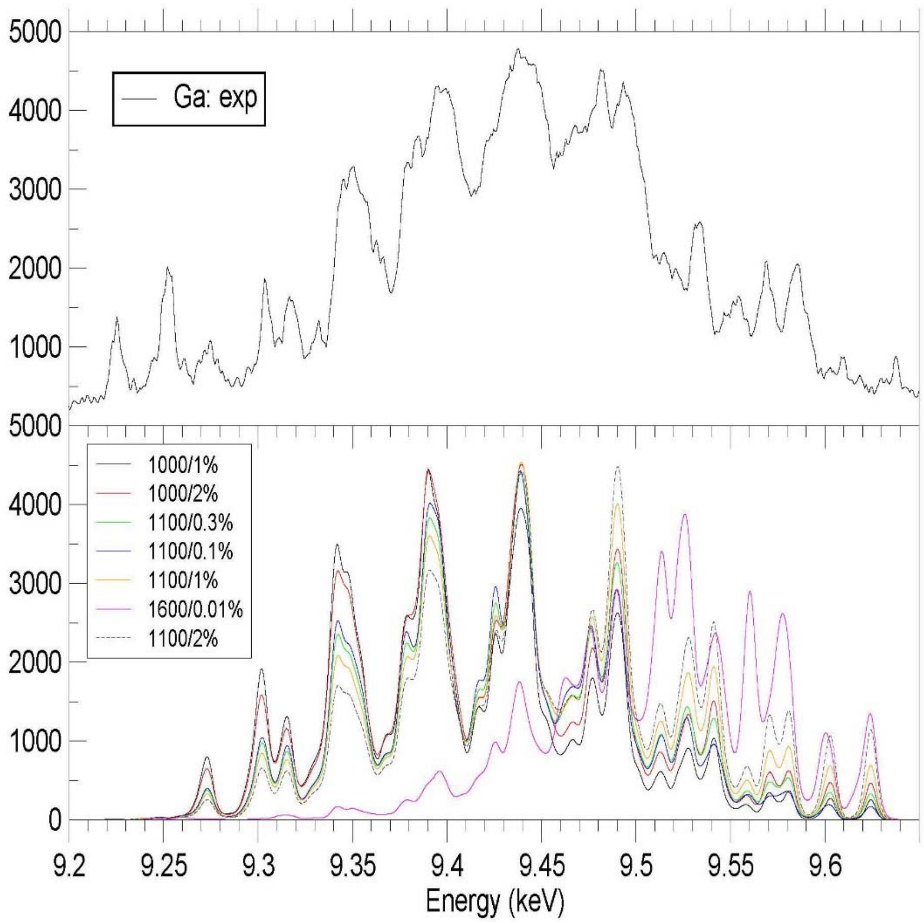
Cowan Code Calculations

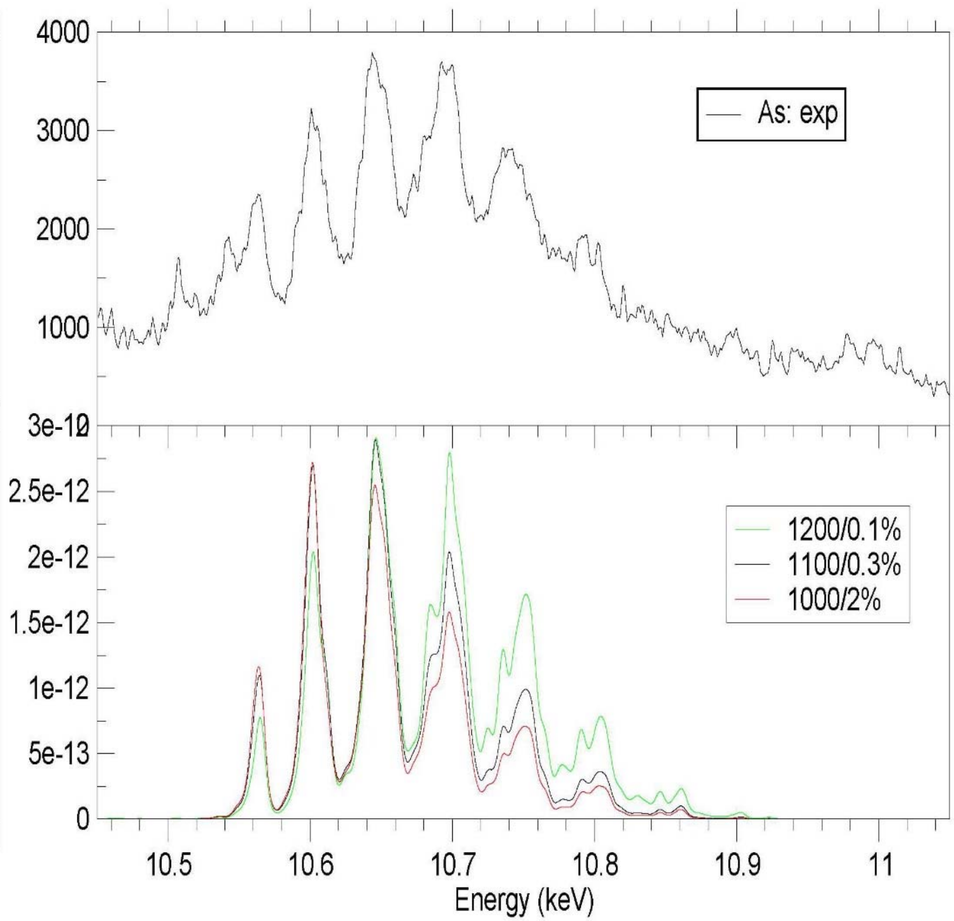
- Transition energies are accurate to a few eV.
- The gf values give an indication of the blending of lines for a given charge state.
- Examples for the Ga Be-like and Li-like transitions:



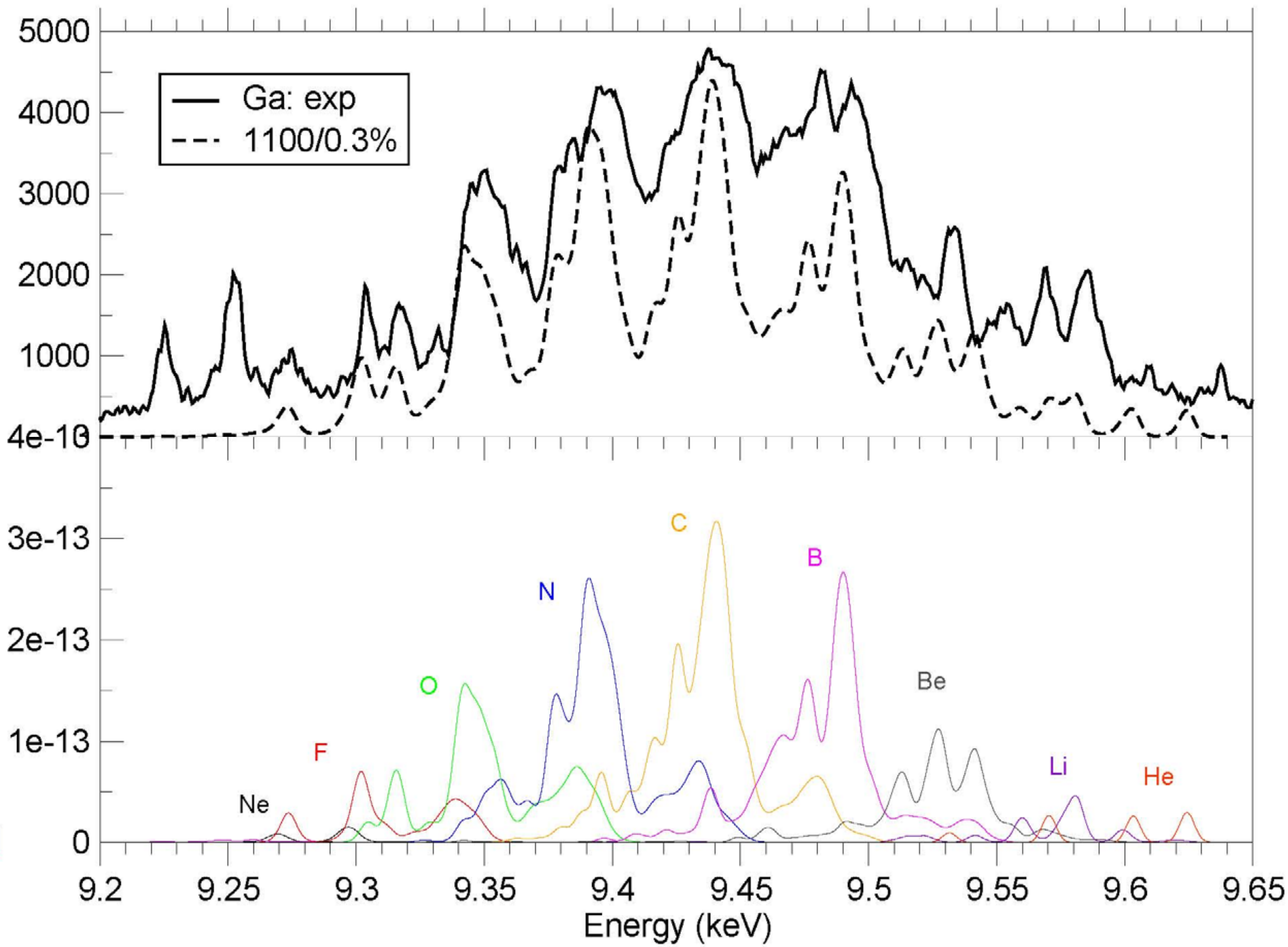
Yuri Ralchenko (NIST) Spectrum Simulations

- Ionization balance is sensitive to electron temperature and relatively insensitive to electron density.
- Li-like and He-like line ratios, in particular the q/y ratio, are sensitive to the electron density and indicate N_e= $1x10^{19}$ cm^{-3}.
- Ga and As spectrum simulations at N_e= $1x10^{19}$ cm^{-3} and variable thermal and hot electron distributions indicate T_e=1100 eV and 3% 30 keV electrons.:



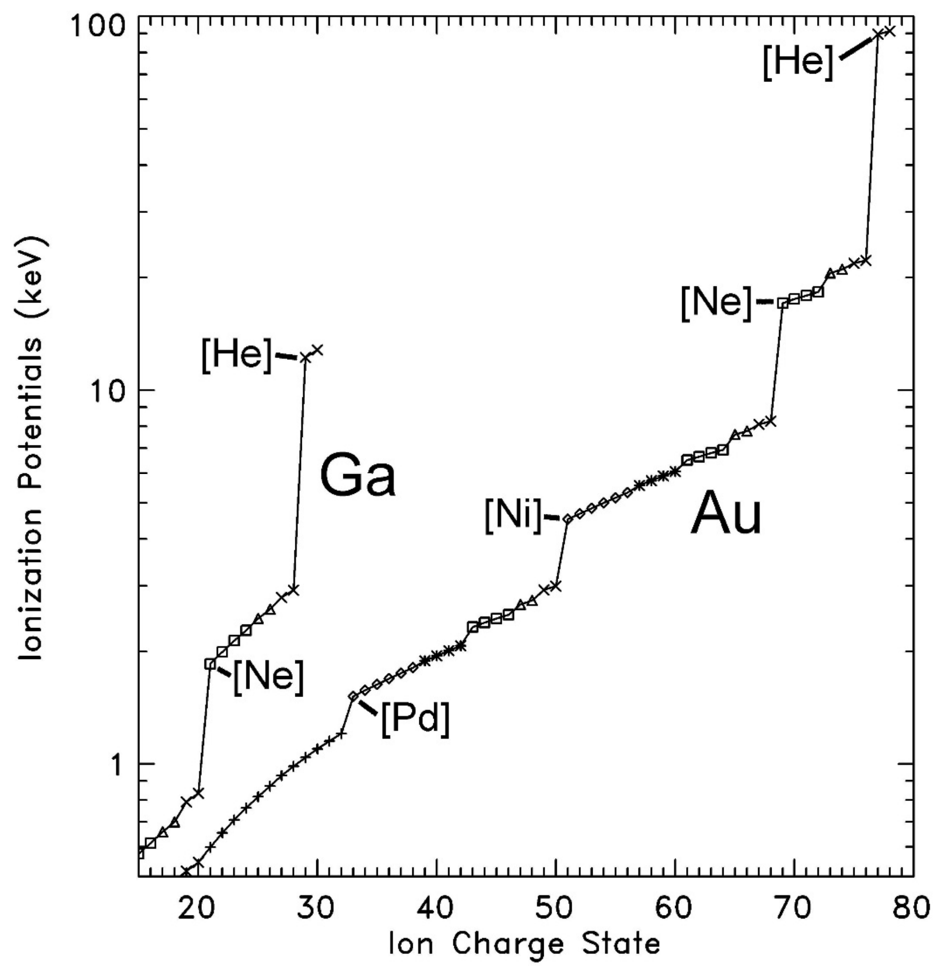


Ga Charge State Contributions to the Spectrum



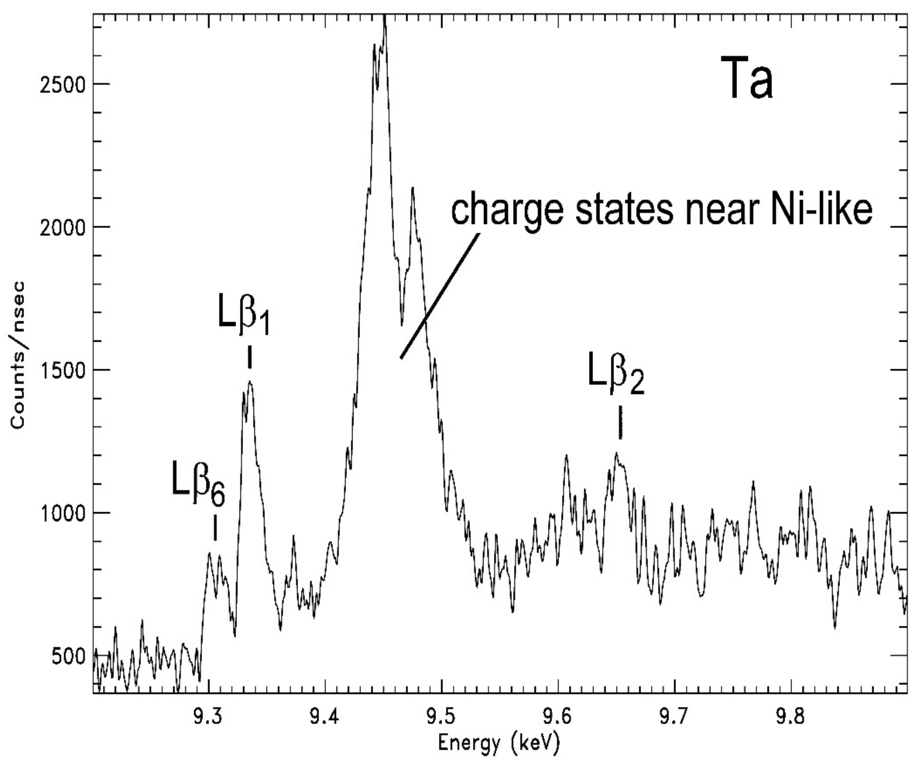
Au and Ta Ionization Stages

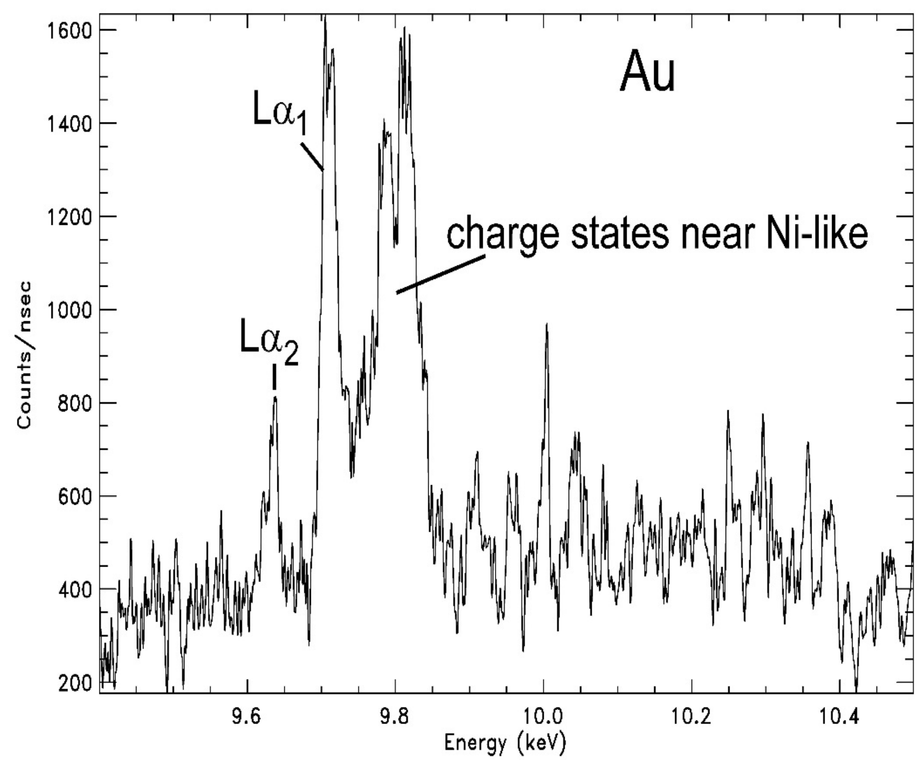
Based on the ionization potentials of the Ga and Au ions and the observed He-like through Ne-like Ga transitions, we expect the Au and Ta spectra to contain transitions from charge states near the Ni-like closed shell.



Transitions in Au and Ta

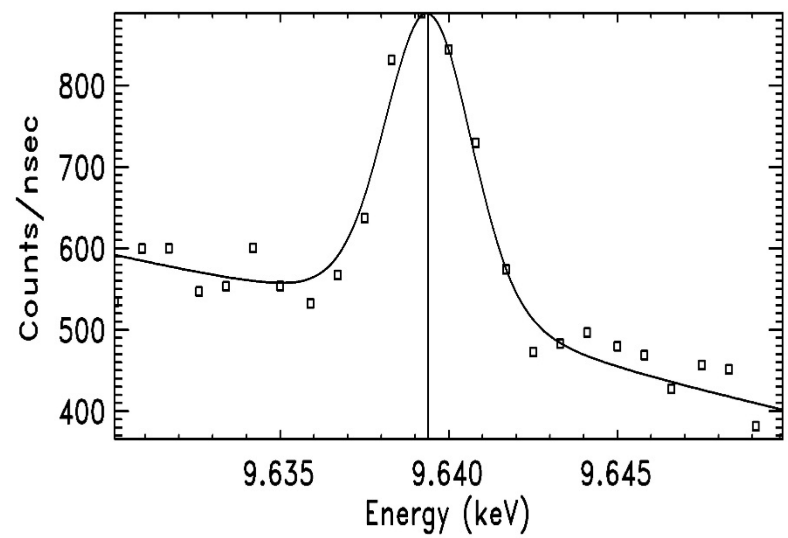
- The L transitions in the neutral atoms enable an energy scale with eV accuracy.
- The comparison of a relativistic code such as FAC with the experimental spectra should result in identification of the transitions in highly-charged Au and Ta and should provide validation of the accuracy of the calculated transition energies and line intensities.

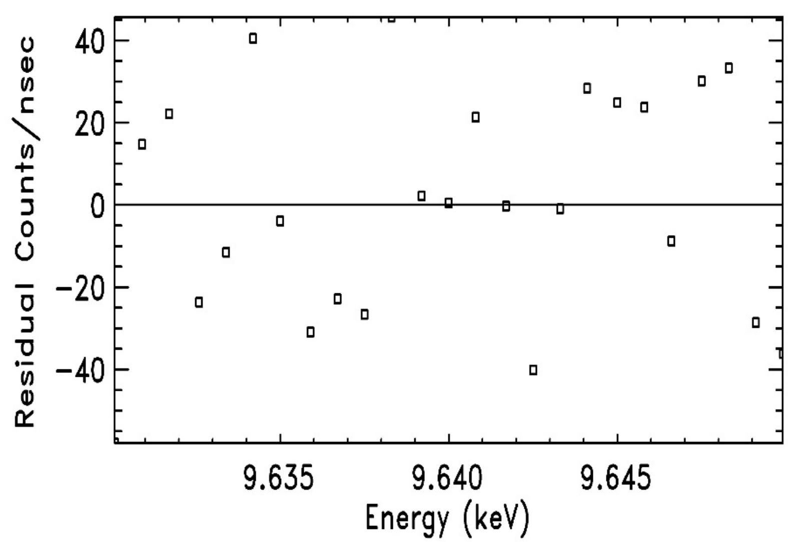




Voigt Fit to the Ga He-like Resonance Transition (w)

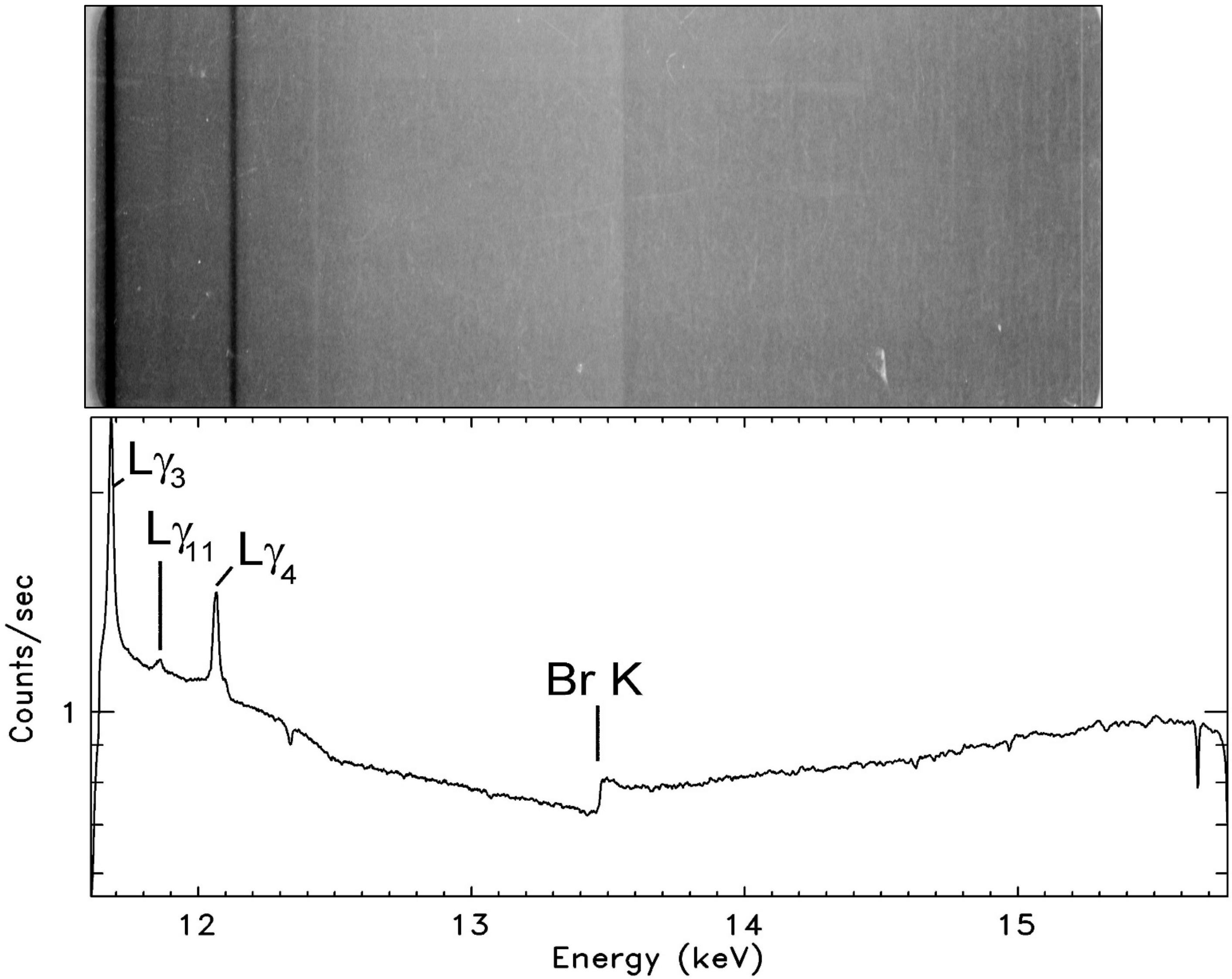
- The Gaussian component has 2.56 ± 0.03 eV FWHM and the Lorentzian component has 1.00 ± 0.03 eV FWHM.
- Using the opaque edge technique, the IP edge spread function and the line spread function were measured, and the IP spatial resolution contributes 2.6 ± 0.2 eV Gaussian FWHM to the observed line profile (the Lorentzian component of the IP line spread function is zero within the accuracy of the measurement); thus the observed Gaussian broadening can be attributed entirely to IP detector broadening.
- Assuming the ion temperature is equal to the 1.1 keV electron temperature, the ion thermal Doppler (Gaussian) broadening would be 3 eV which exceeds the observed Gaussian 2.56 eV width (before removal of the IP broadening); this implies the ***Ga ion temperature is much less than the electron temperature***.
- Calculations indicate the Stark broadening is negligible even for electron densities up to 10^{21} cm^{-3}.
- The natural lifetime (Lorentzian) broadening resulting from the Ga w radiative transition rate (9×10^{14} s^{-1}) is 0.6 eV.
- ***The intrinsic Lorentzian broadening of the (301) planes is 1.0 eV – 0.6 eV = 0.4 eV FWHM.***





TR Image Plate Br K Absorption Edge at 13.5 keV

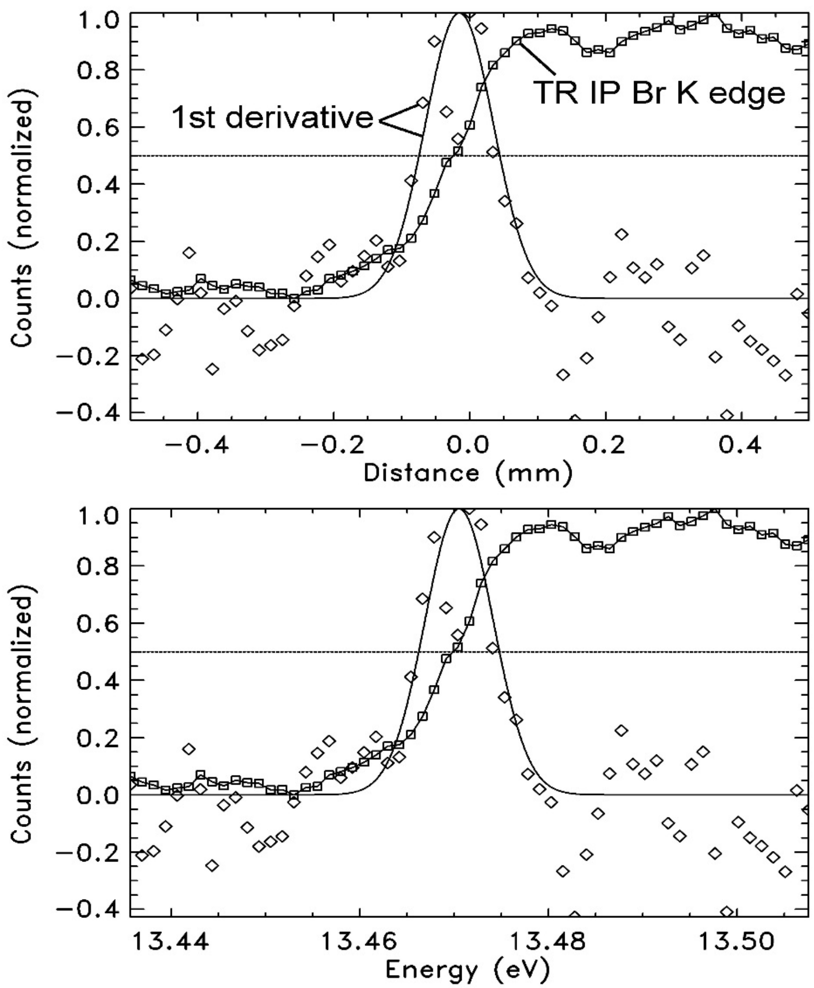
- According to Fuji the TR image plate composition is $BaFBr_{0.85}I_{0.15}$:Eu.
- The enhanced absorption at the 13.4705 keV Br K edge was recorded using the Bremsstrahlung continuum radiation from the NIST W source.

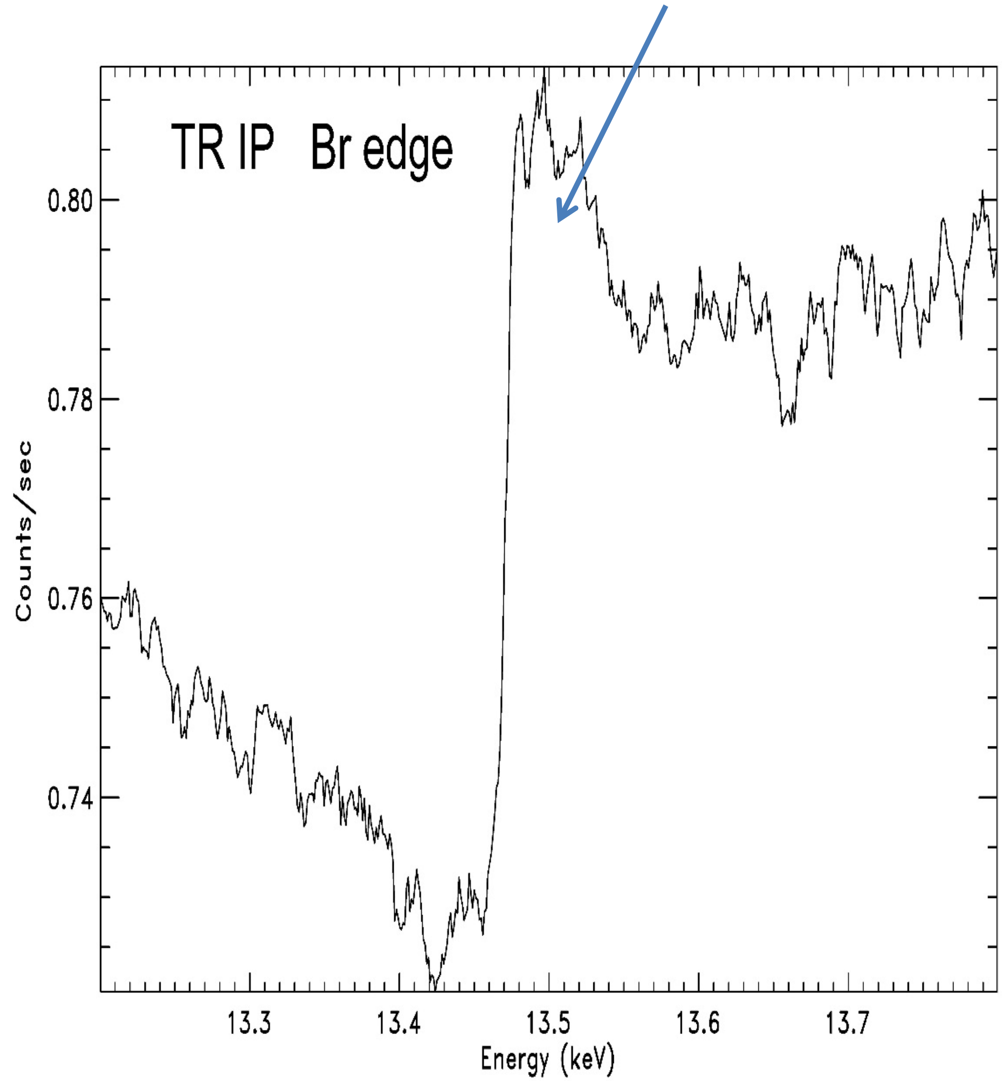


High-Resolution TR IP Br K Edge

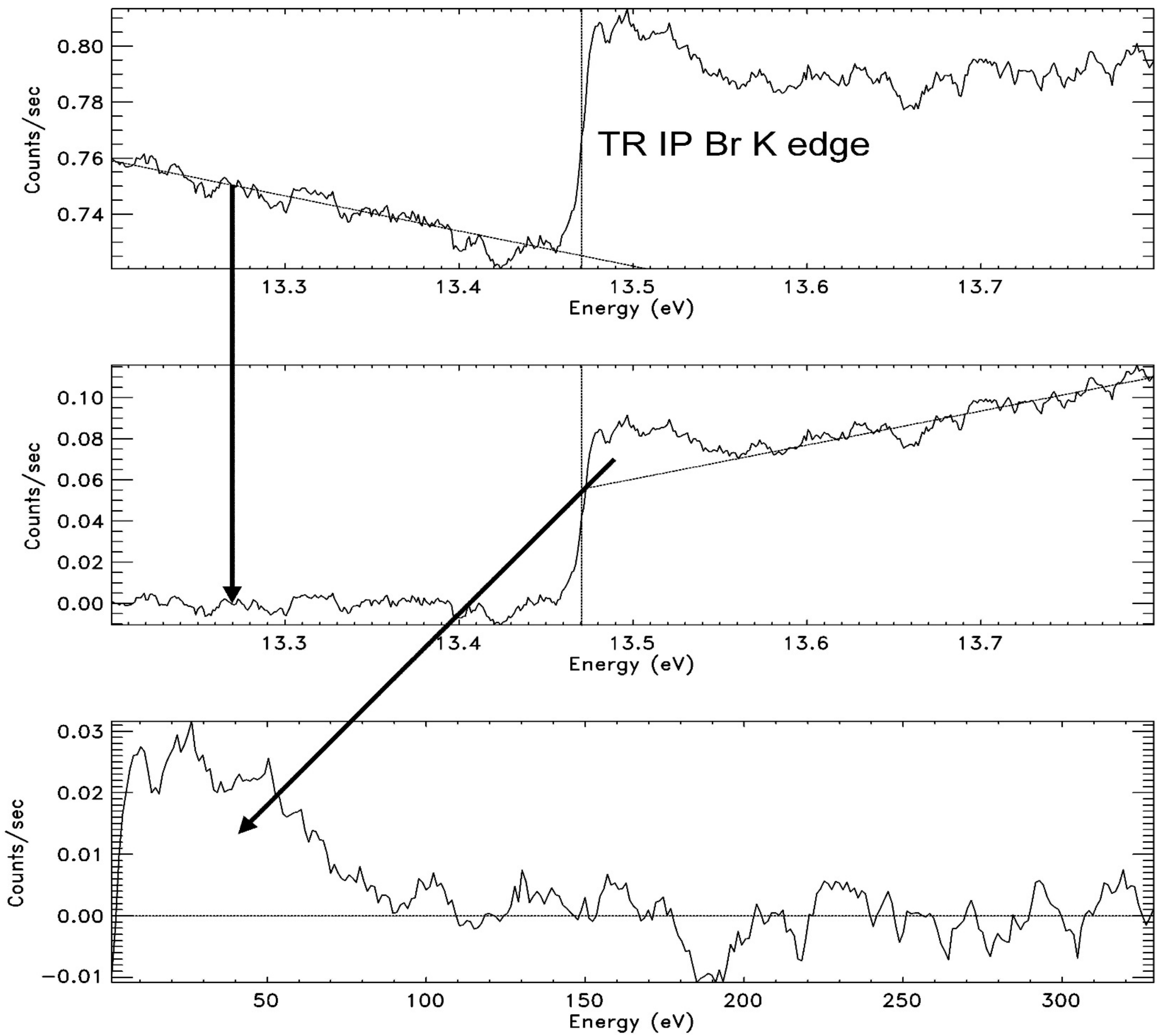
The FWHM width of the Br K edge derived from the 1st derivative is 8.6 eV which includes the 2.7 eV natural (lifetime) width of the Br K level and 3 eV TR IP spatial broadening.

The Br K absorption edge has fine structure on the high-energy side with typical 20 eV period, much larger than the crystal's intrinsic resolution.

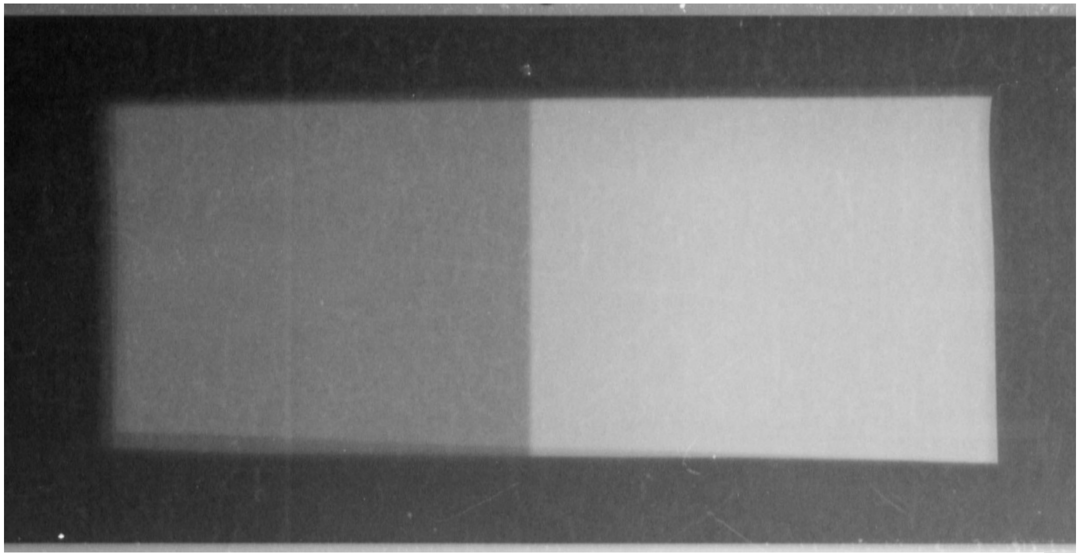


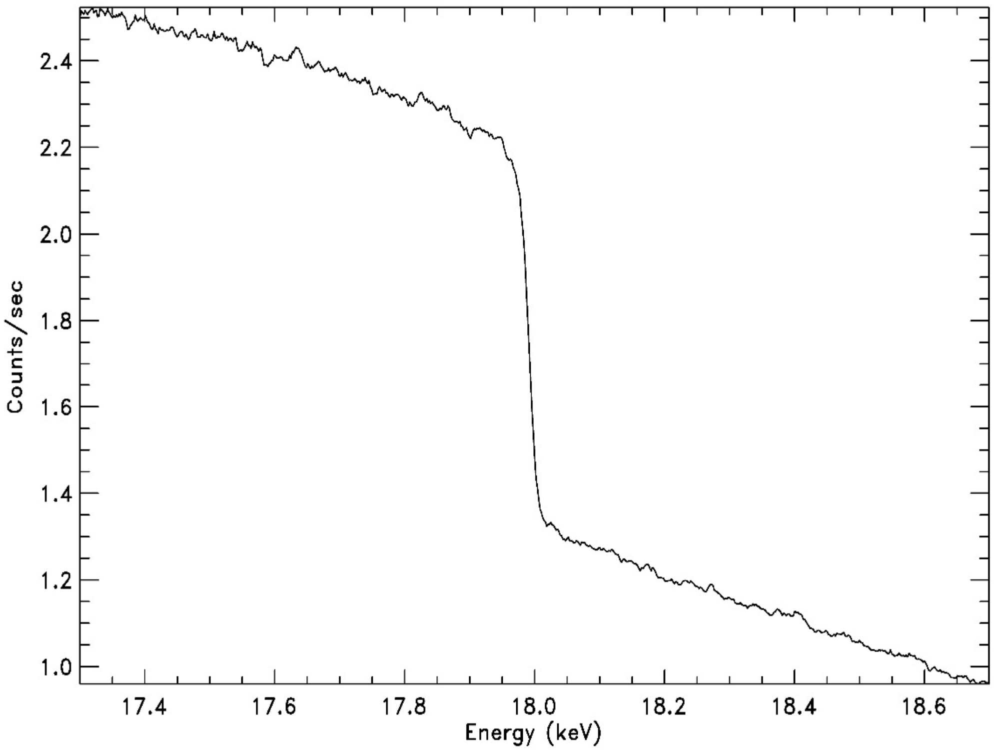


Analysis of the Fine Structure Above the Br K Edge



Zr K Edge at 18 keV





Conclusions (Work in Progress)

- A new type of high-resolution quartz crystal transmission spectrometer using the (301) planes at an asymmetric angle of 23.51^o to the crystal surface was developed and tested using the NIST W source.

- X-rays in the 10-20 keV region that are diffracted by the (301) planes emerge nearly perpendicular to the crystal surface and have practically zero aberration broadening associated with the cylindrical crystal bending and crystal thickness.

- The spectrometer was fielded at the Titan laser and recorded high-resolution spectra from GaAs (K shell transitions) and from Au and Ta (L shell transitions).

- Based on FAC and NOMAD spectrum simulations, the Titan 3 ns laser pulse without beam smoothing generated a quasi-steady state thermal plasma with 1100 eV electron temperature and $1x10^{19}$ cm^{-3} electron density and hot spots that generated 3% 30 keV non-thermal electrons that caused inner-shell vacancies in the neutral atoms outside the focal spot, and the ion temperature was much smaller than the electron temperature.