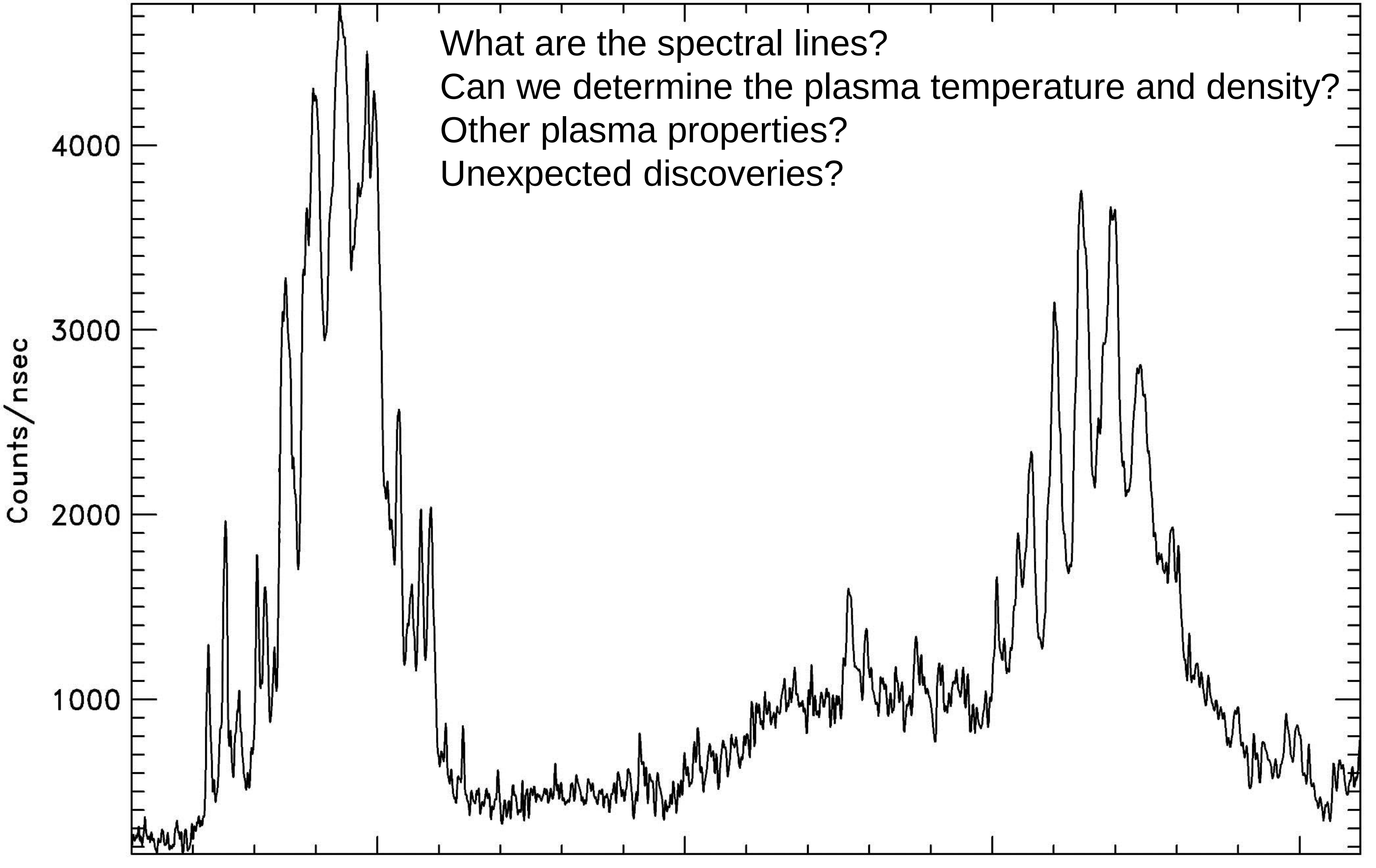
Experimental X-Ray Spectroscopy: Part 2

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



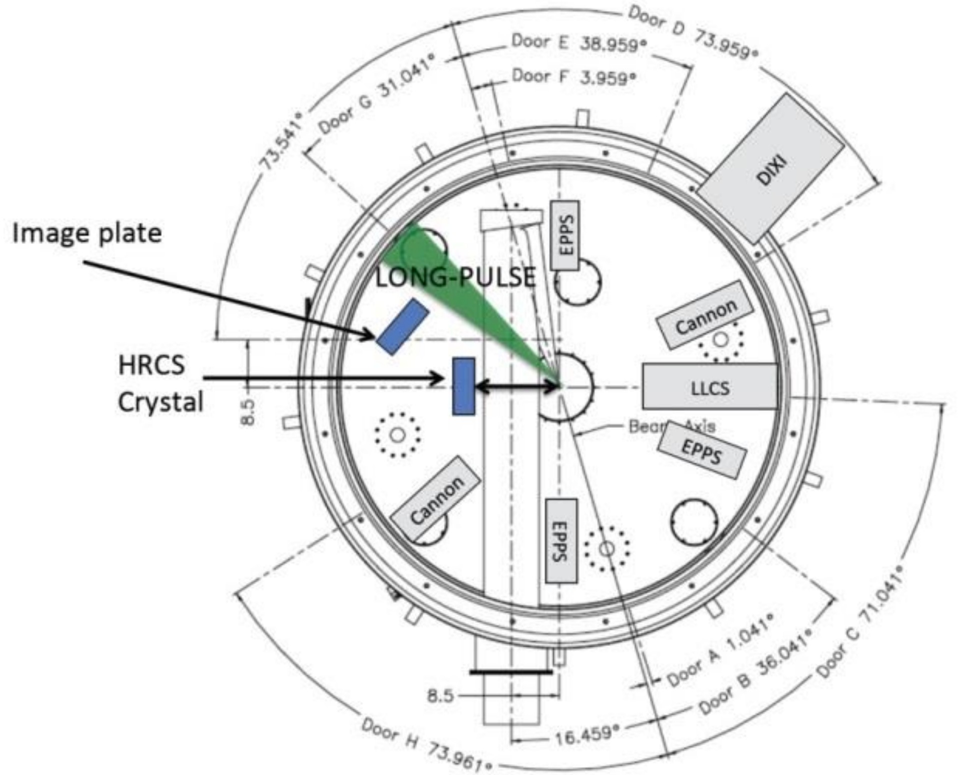
We need some information to start the analysis

What was the x-ray source?

What spectrometer recorded the spectrum?

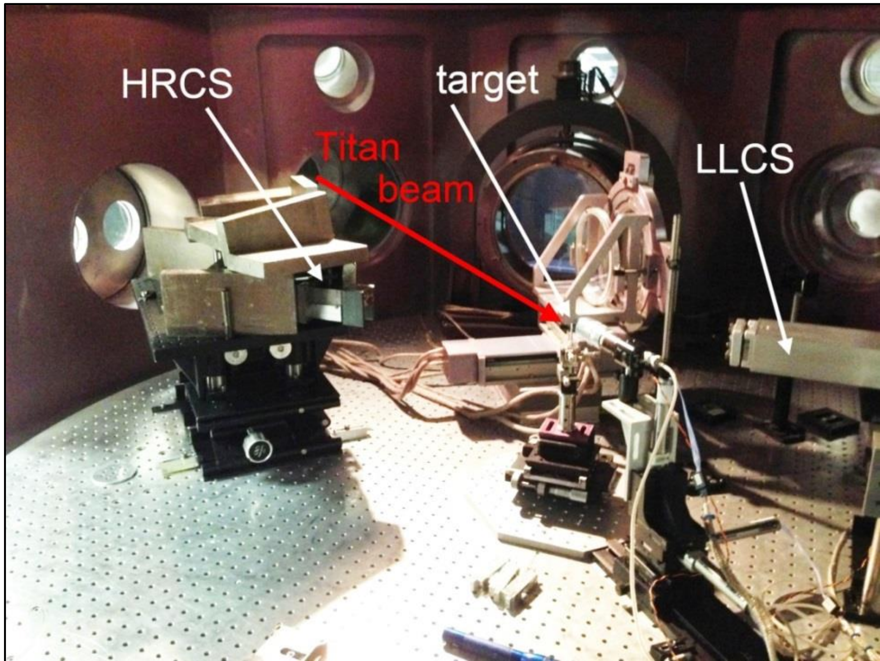
The X-Ray Source

- The x-ray source was a GaAs wafer that was irradiated by a pulse from the Titan laser at Livermore National Laboratory (LLNL).
- The focused laser intensity was 3×10^{15} W/cm^2, and this level of intensity is known from other studies to produce a hot, dense plasma.



The Spectrometer

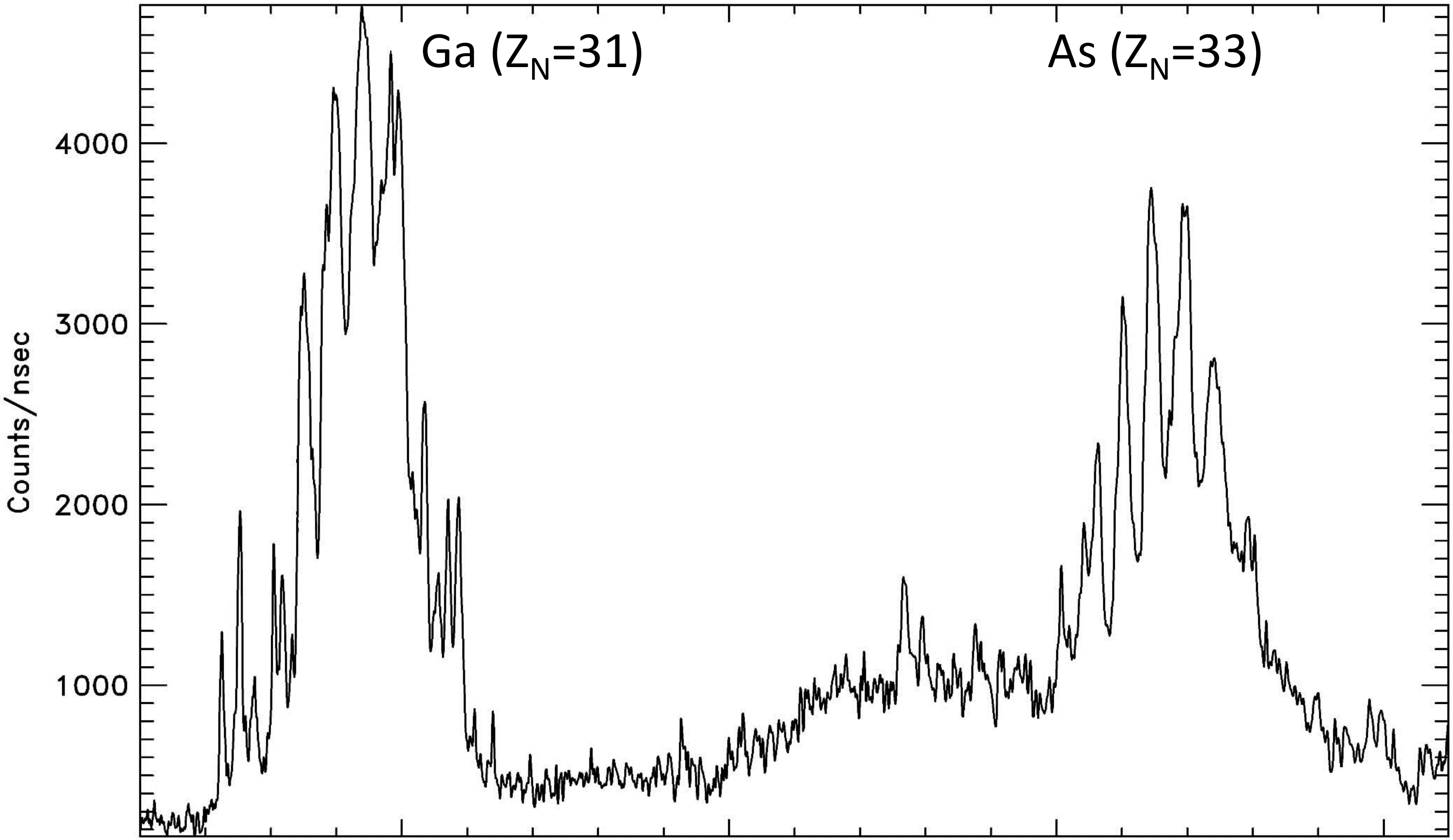
- The spectrometer used a transmission crystal to record spectra in the 9 - 11 keV x-ray energy range.
- The spectrometer had high spectral resolution and was named HRCS (High Resolution Crystal Spectrometer).



What We Know

- The spectral lines are from Ga and As.
- The energy range is 9 – 11 keV.

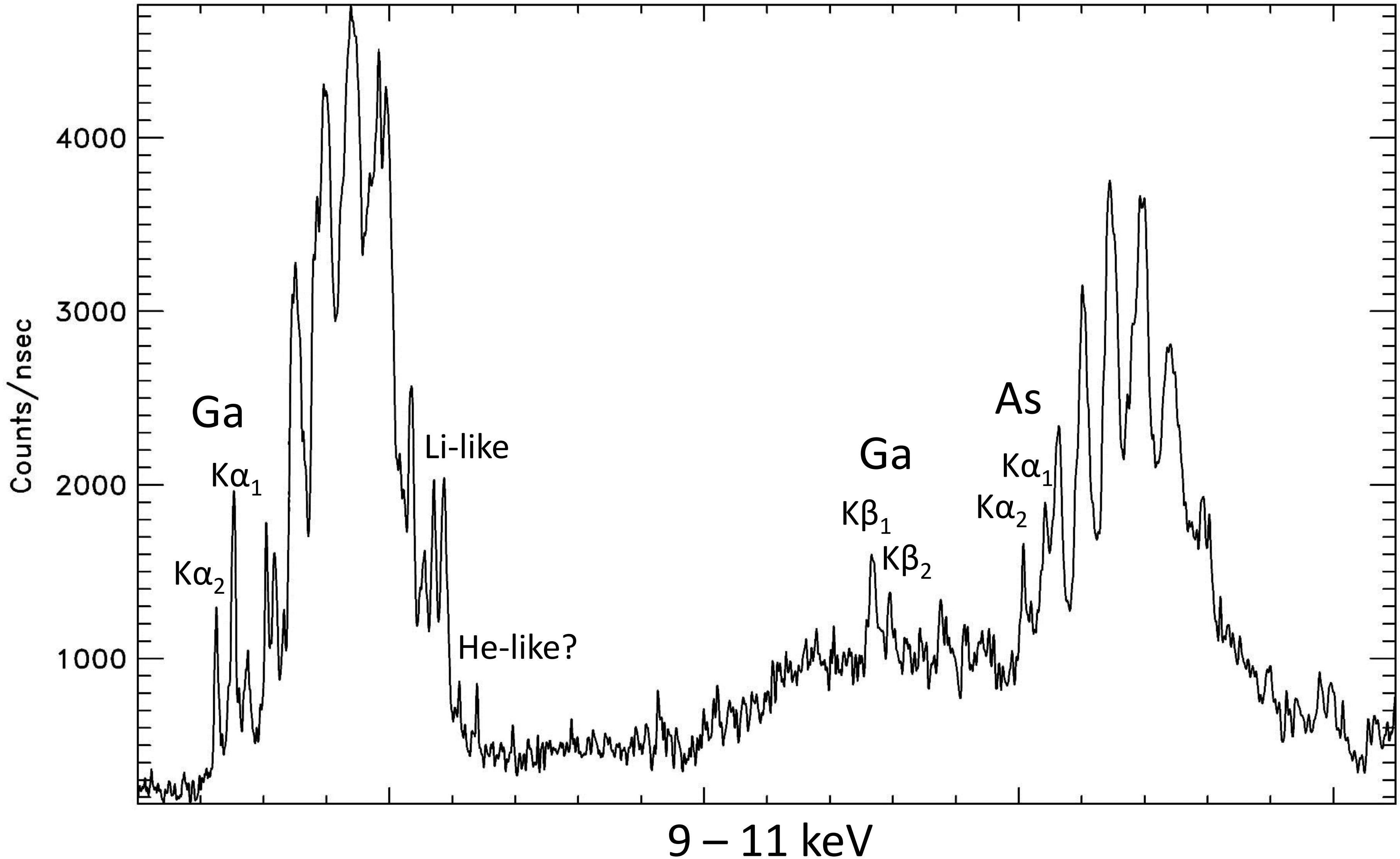
We know the spectral lines are from Ga and As and are in the energy range 9-11 keV.
How to establish an accurate energy scale?
Try to identify some strong lines: The Ga and As characteristic transitions at the lower energies and the He-like transitions and Li-like satellites at the higher energies.



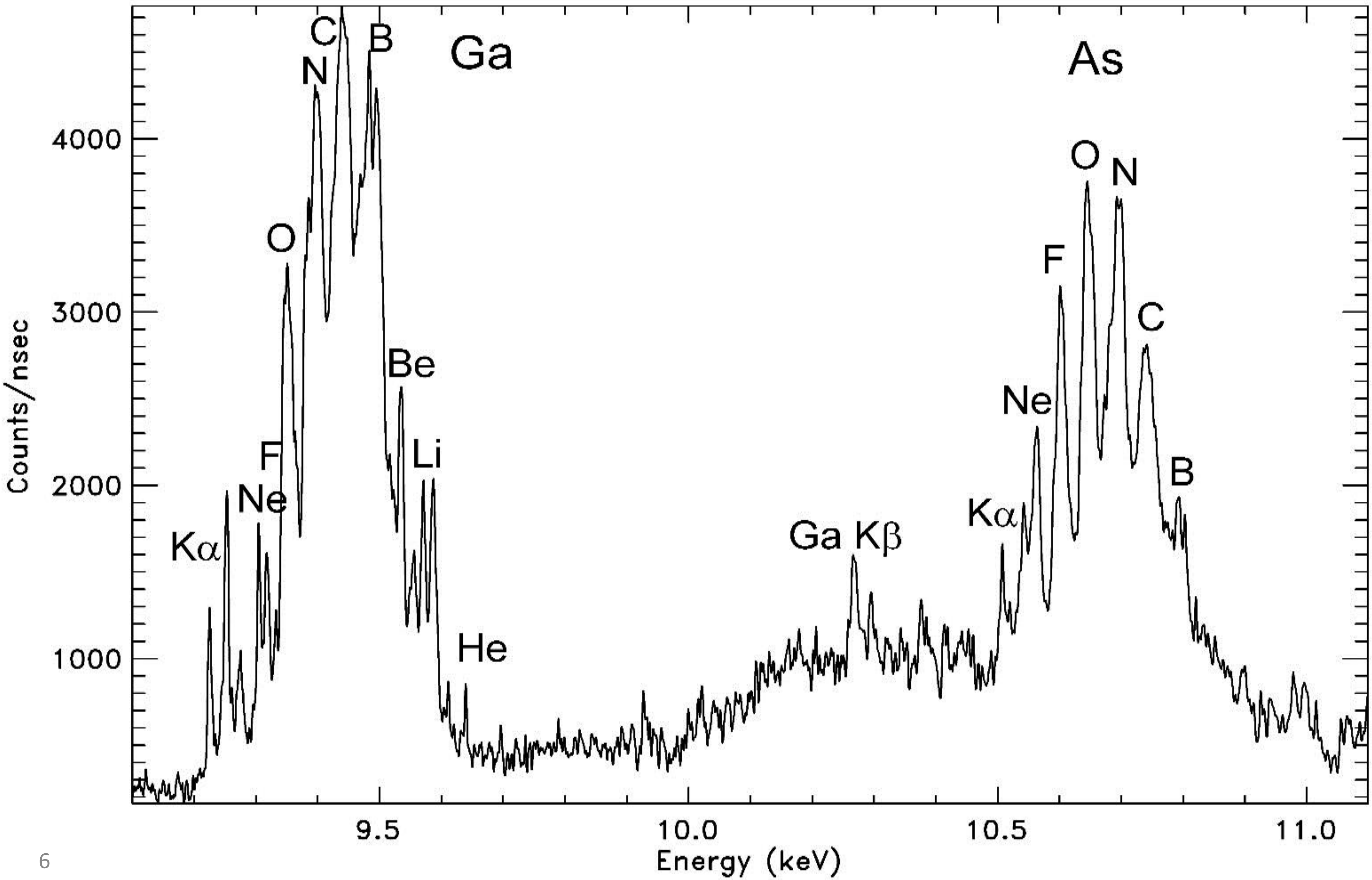
9 – 11 keV

Found the Ga and As characteristic transitions and maybe the Ga He-like and Li-like transitions.

Use the characteristic transitions to establish the energy scale and identify the other spectral features.

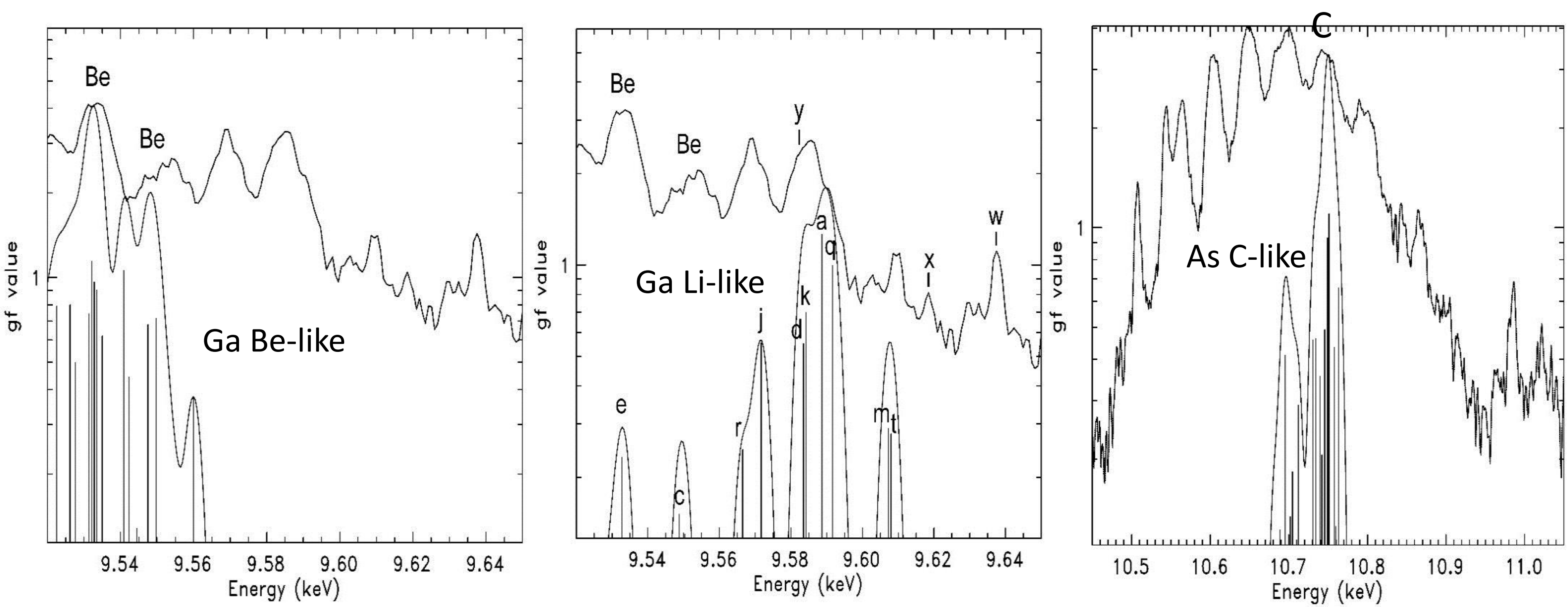


Now that we have an accurate energy scale, we guess that the other spectral features between the characteristic lines (neutrals) and the Li-like lines are from the Be-Ne charge states. Compare to calculated transition energies in Li-Ne ions and see if the identifications are correct.

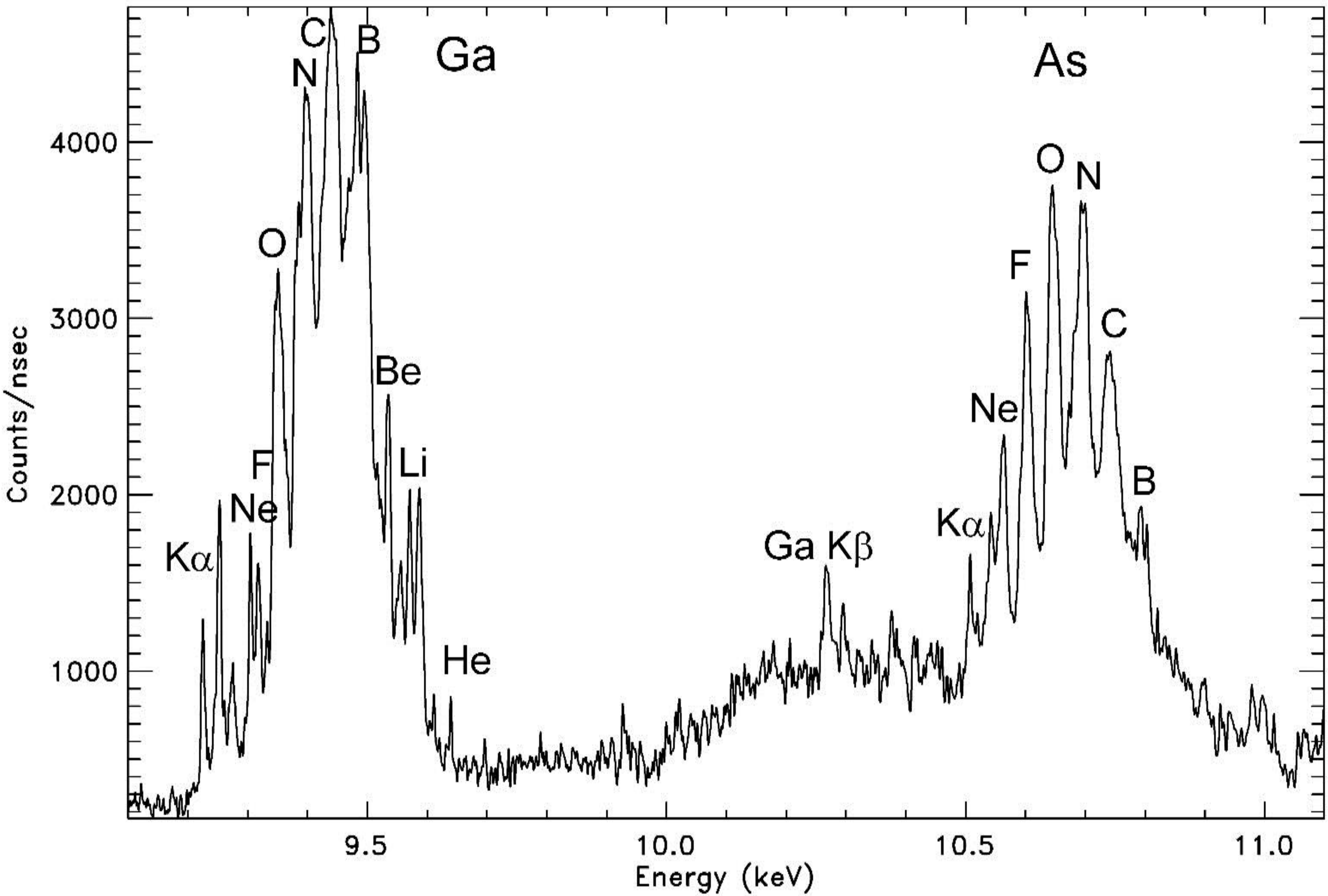


Comparisons to Cowan Code Transition Energies and gf Values

- Examples of Cowan Ga and As gf values convolved with 10 eV Gaussians to simulate the experimental line widths.
- The transition energies are shifted to lower energies by ≈ 10 eV.
- The gf values indicate the blending of numerous lines from a given charge state.
- The agreement confirms the experimental lines identifications.



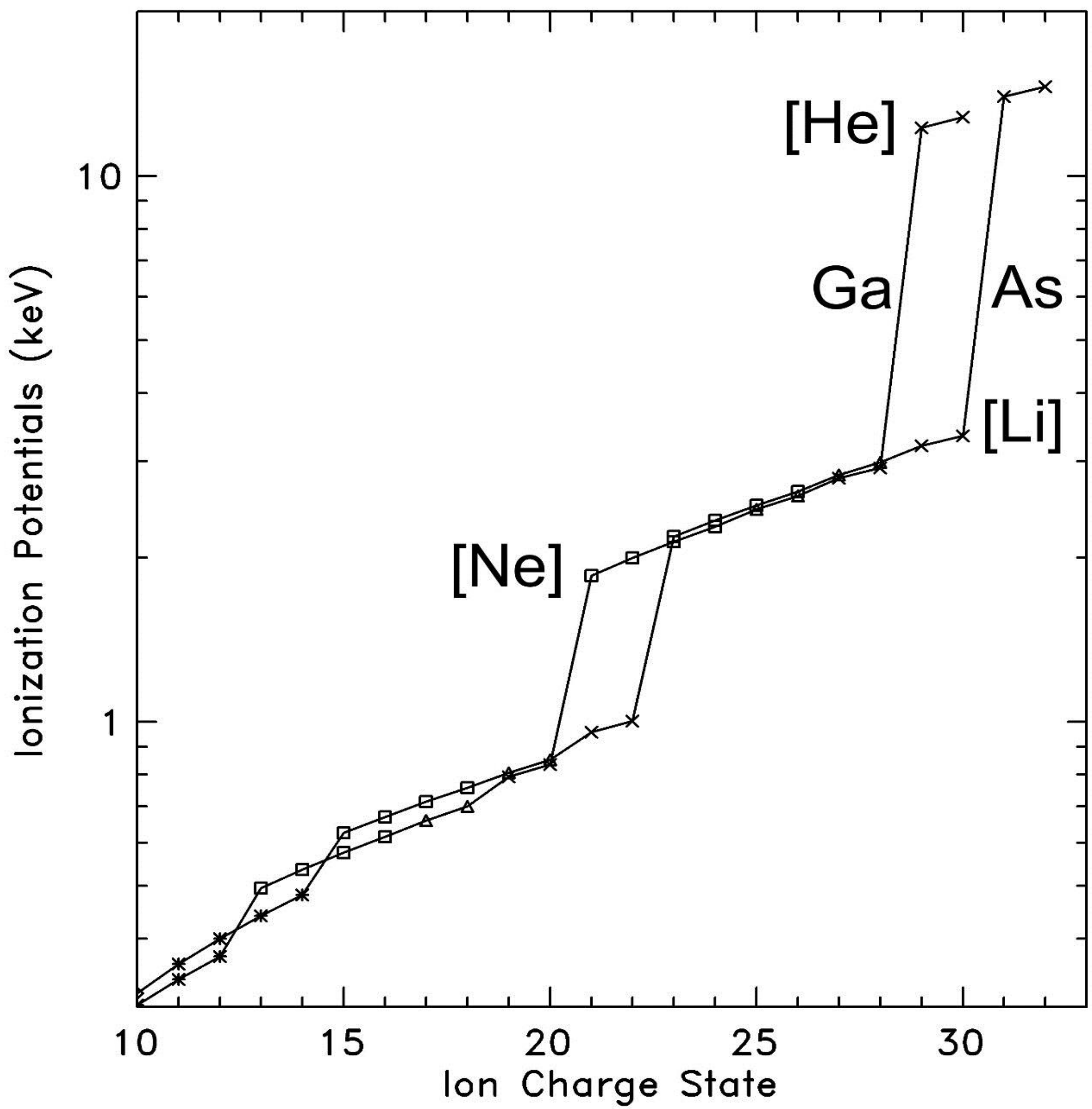
Now that we are confident of the line identifications, let's simulate the line intensities using a kinetics code and determine the temperature and density of the plasma emission region.



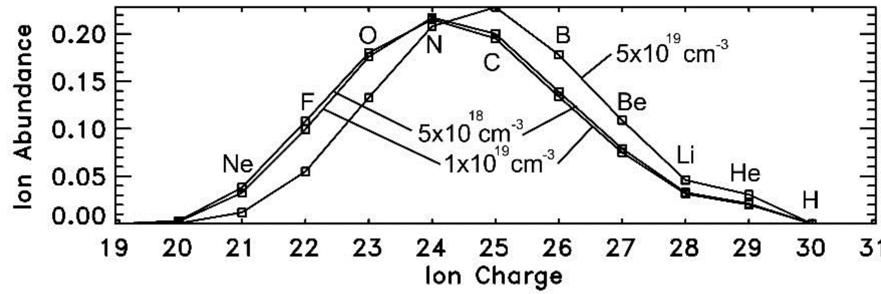
Where to begin?

What T_e and N_e to choose for the spectrum simulations?

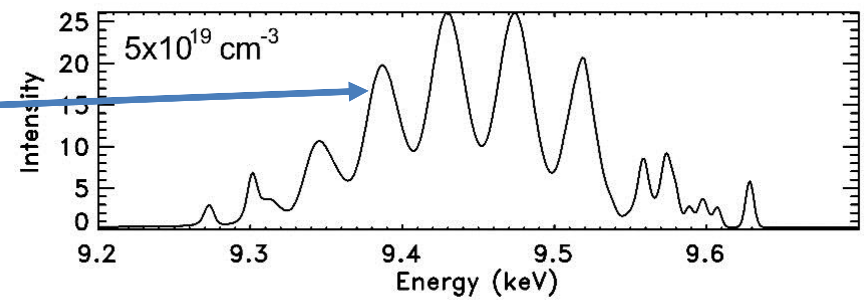
We know that the most abundant charge states in a thermal plasma have ionization potential ≈ $3T_e$, so choose $T_e \approx 2$ keV.



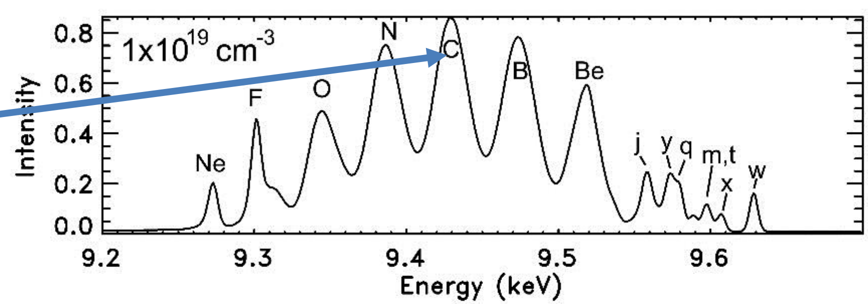
FLYCHK Simulations of the Ga Spectrum with T_e = 2 keV and Variable N_e



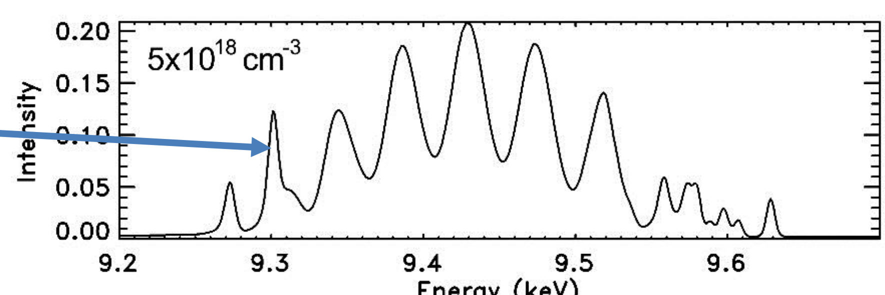
Low charge states too low



C is highest. Good

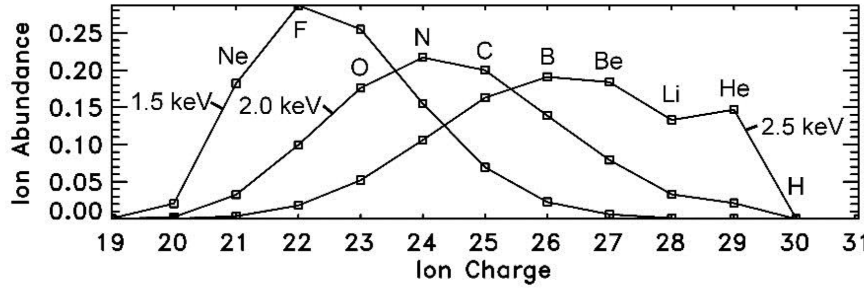


Lower charge states too high

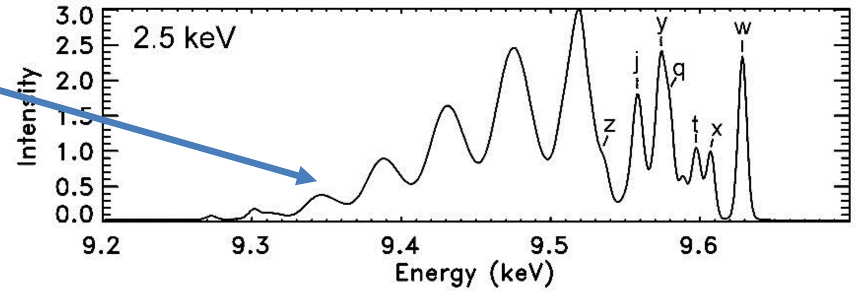


FLYCHK Simulations of the Ga Spectrum with Variable T_e and Fixed N_e

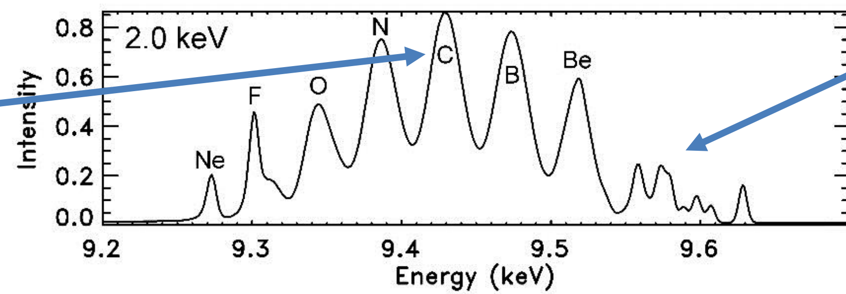
$N_e = 1 \times 10^{19}\ cm^{-3}$



Low charge states too low

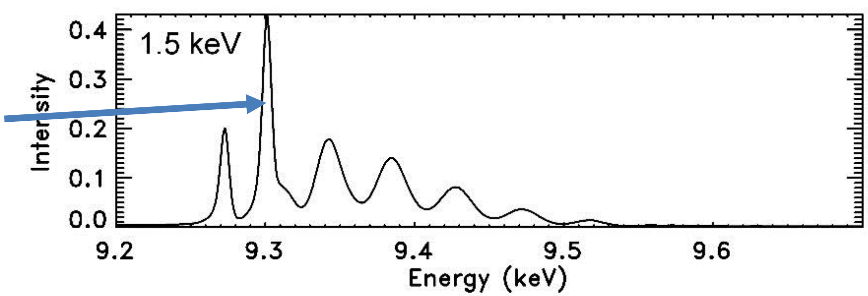


C is highest. Good

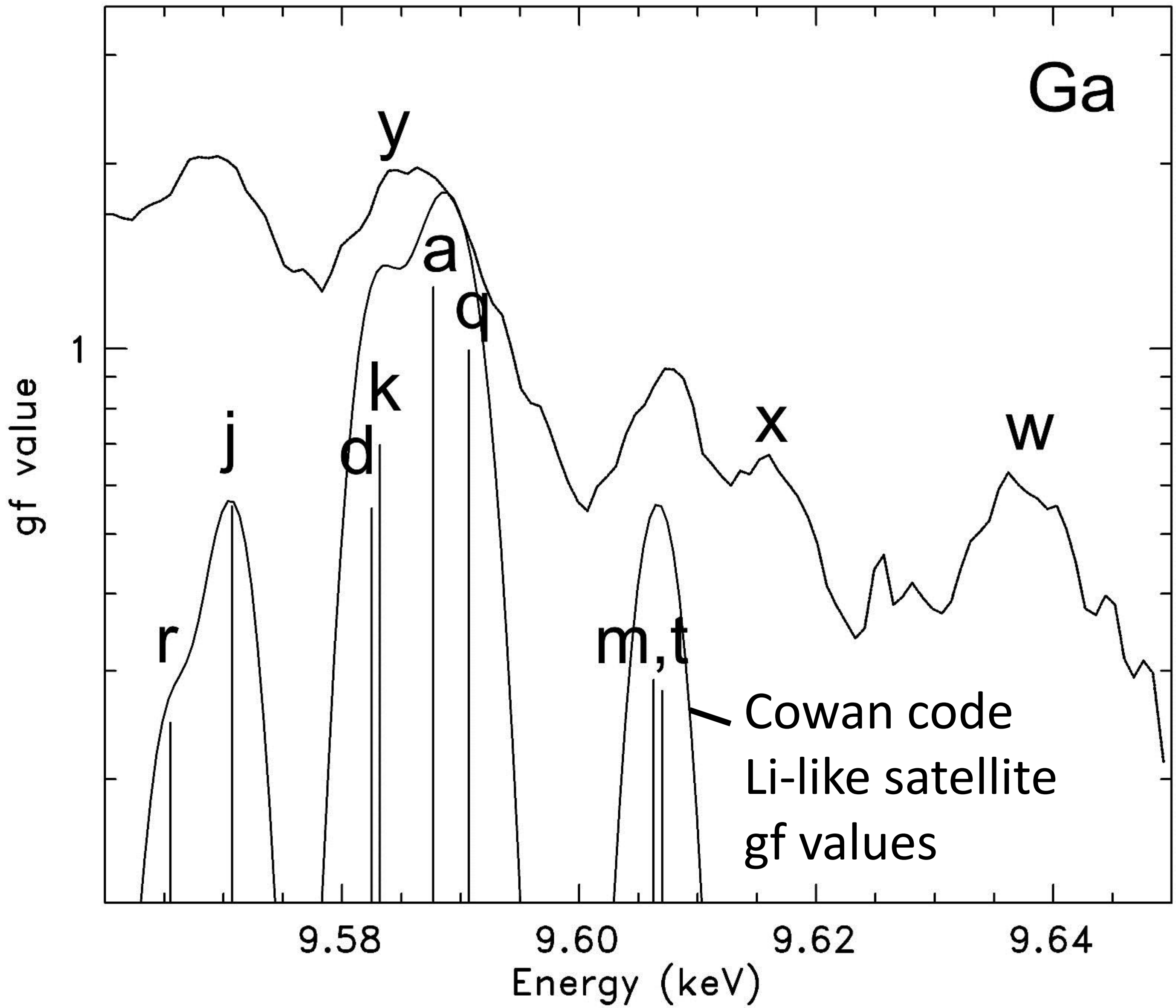


He-like transitions and Li-like satellites have good intensities.

Lower charge states too high



The He-like and Li-like transition intensities are sensitive to T_e, N_e , and other plasma conditions. We need improved simulations of these transitions.



How can the intense Ga and As characteristic x-rays, resulting from 1s vacancies with up to 11.87 keV ionization energy, be generated by the 2 keV thermal electrons?

They can't.

Moreover, the abundance of neutrals in the 2 keV plasma is low, so the Ga and As characteristic transitions must originate elsewhere.

The answer: The Ga and As characteristic x-rays are generated by super-thermal electrons that are accelerated by the intense laser irradiation and propagate outside the focal spot into the surrounding cold GaAs material where they create 1s vacancies in the neutrals and characteristic x-rays.

From previous studies, the standard formula for the super-thermal electron energy is E_{hot} = (100 keV)$(I\,\lambda^2/10^{17})^{1/3}$ where $I=3\text{x}10^{1/3}$ W/cm^2 , λ=1 μm, and **E_{hot}=30 keV**.

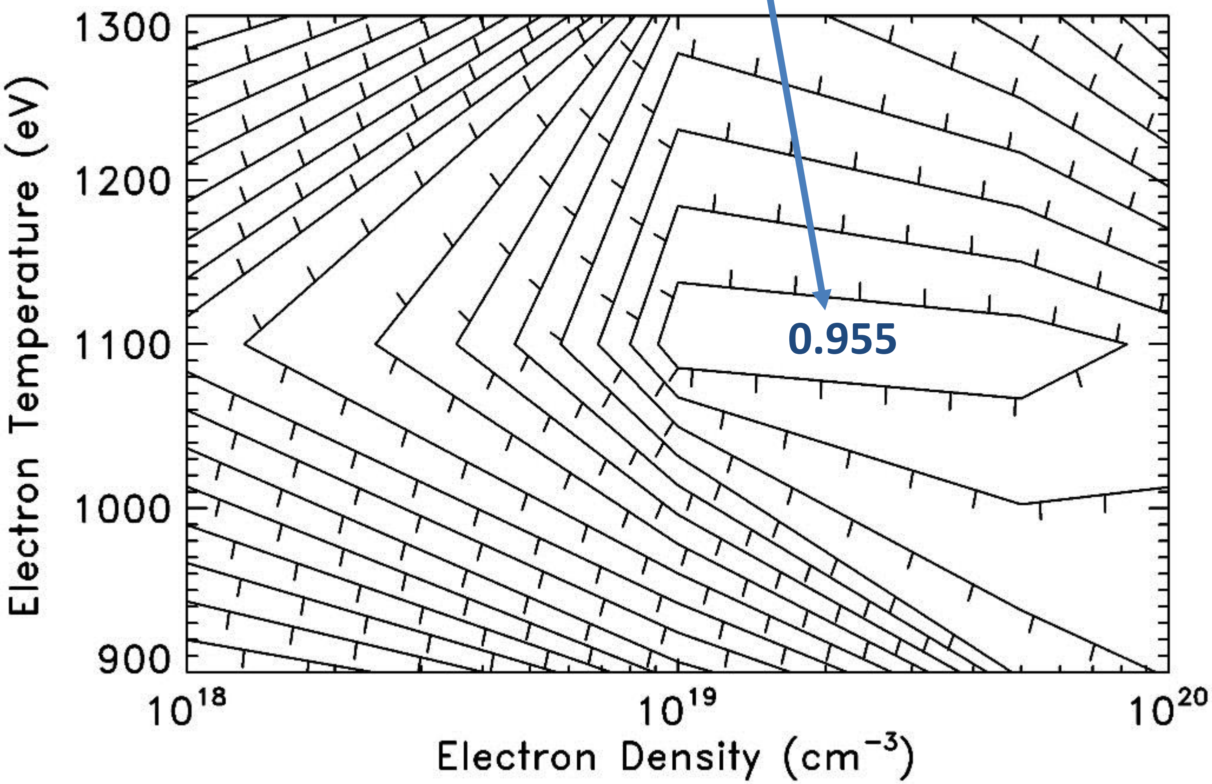
The 30 keV electrons also exist in the plasma, so we must include a 30 keV hot electron component in the spectrum simulations, and the fraction of hot electrons is unknown and is a variable.

FLYCHK simulations of the Ga spectrum were performed with variable T_e, N_e, and hot electron fraction. The correlations between the calculated and experimental spectra were calculated. The highest correlation occurred for:

$T_e = 1100$ eV ± 5%

$N_e = 3\mathrm{x}10^{19}$ cm^{-3} ± 50%

Fraction of hot electrons = 0.025 ± 0.005

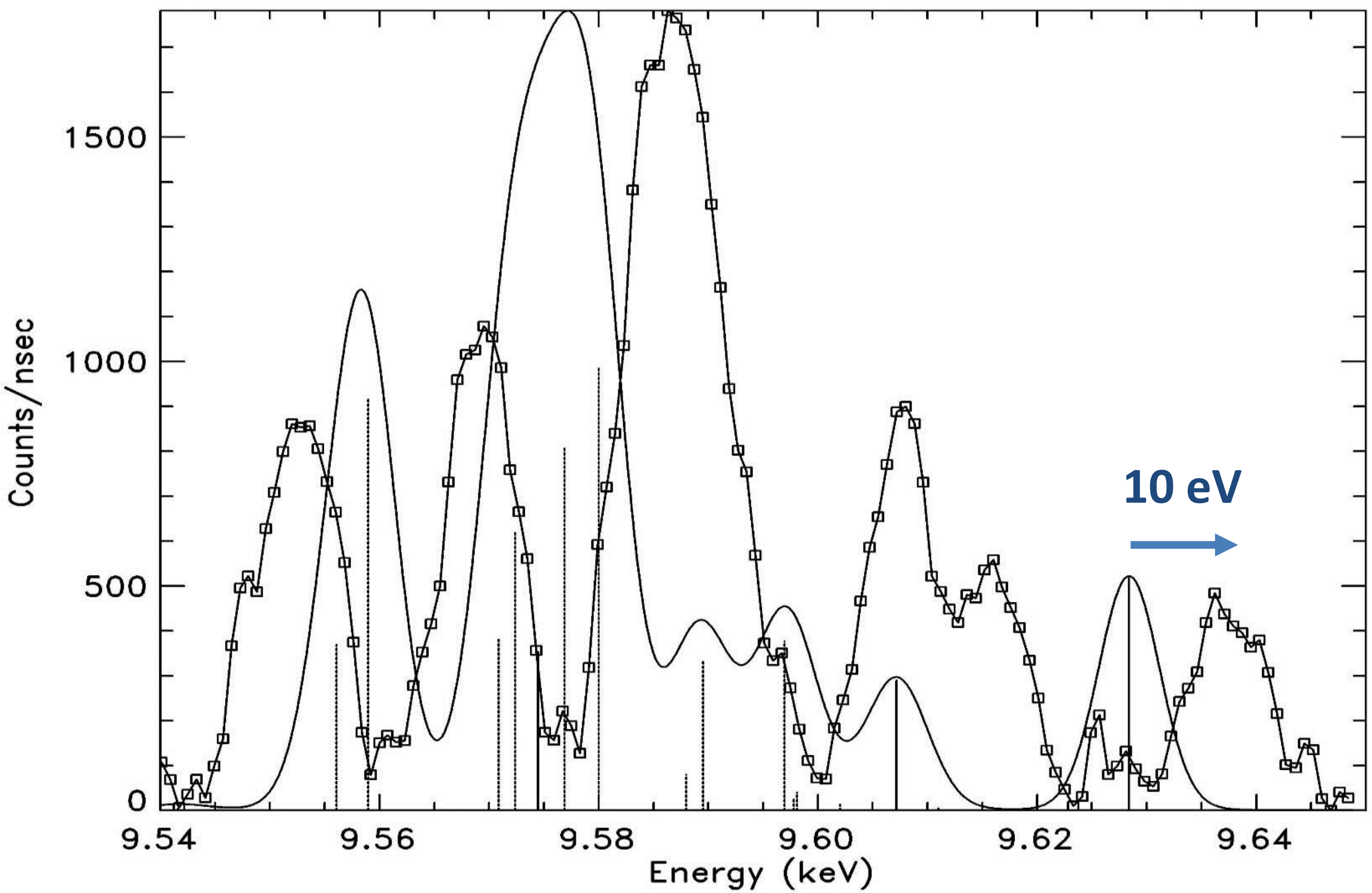


The FLYCHK line intensities were convolved with Voigt profiles having widths corresponding to:

- Gaussian – thermal Doppler broadening, detector broadening, crystal broadening
- Lorentzain – natural lifetime, detector broadening

Compared to the FLYCHK spectrum, the experimental spectrum appears to be blue-shifted by 10 eV when using the experimental energy scale established by the K lines from the cold Ga and As atoms.

But are the FLYCHK transition energies accurate?



The best calculated and measured transition energy in highly-charged Ga is the He-like resonance transition w.

Calculated:

Grant code (1980) 9628 eV

Artemyer (2005) 9628.2 eV

Measured:

Aglitsky (1984) Low inductance vacuum spark 9631 ± 7.5 eV

Aglitsky (1988) LIVS corrected for plasma motion 9627.5 ± 0.7 eV

FLYCHK: 9628.4 eV

The FLYCHK transition energies are accurate!

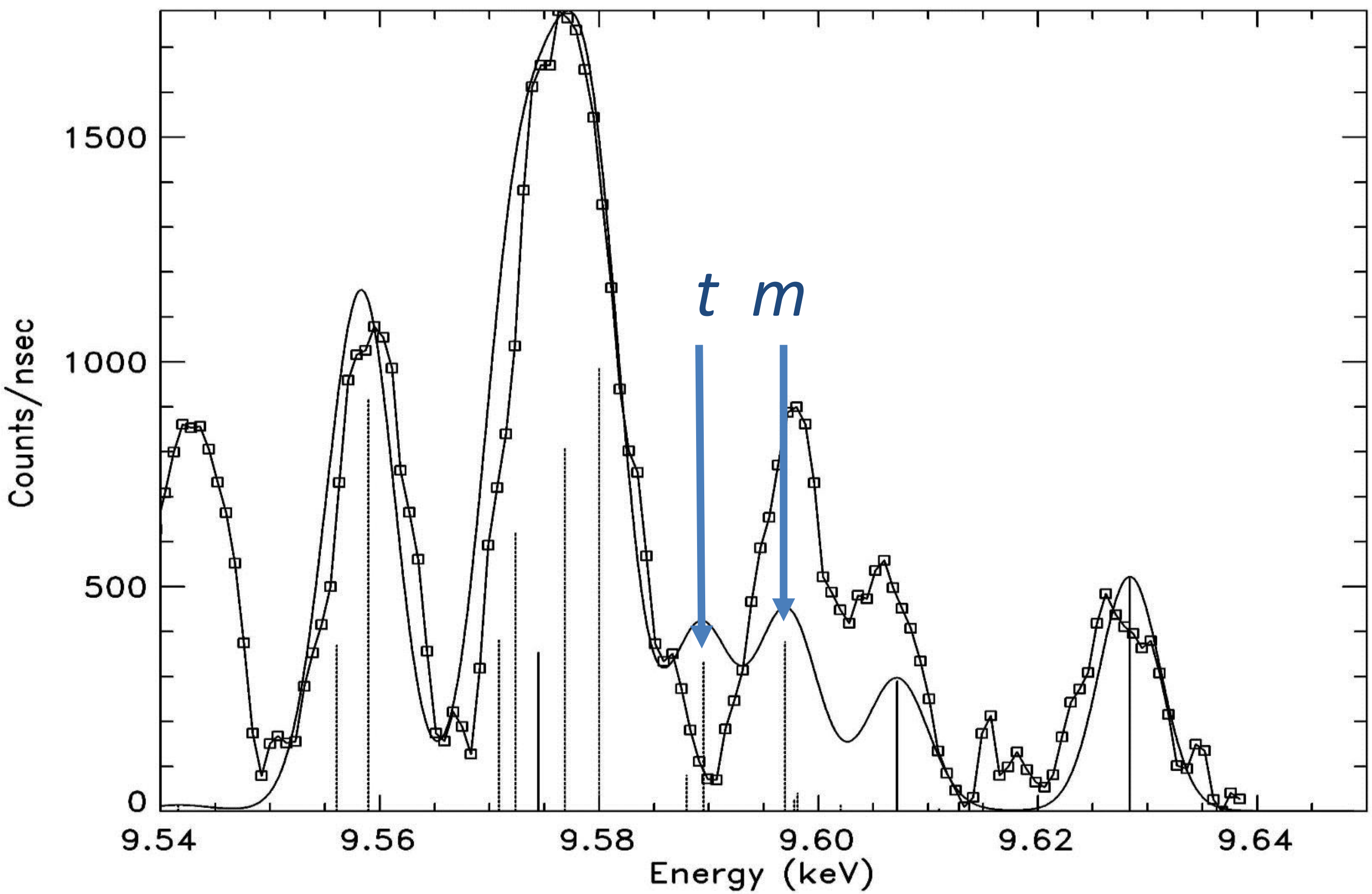
This indicates the 10 ev blue shift of the transitions from the highly-charged Ga plasma, measured with respect to the transitions from cold Ga atoms outside the focal spot, is real.

This blue shift results from bulk plasma streaming motion toward the spectrometer with velocity (10 eV / 9.6 keV) (3×10^{10} cm/s) = **3×10^{7} cm/s** which is reasonable for a laser-produced plasma blow-off velocity (hydrodynamic expansion).

Shift the experimental spectrum by -10 eV to account for bulk plasma motion.

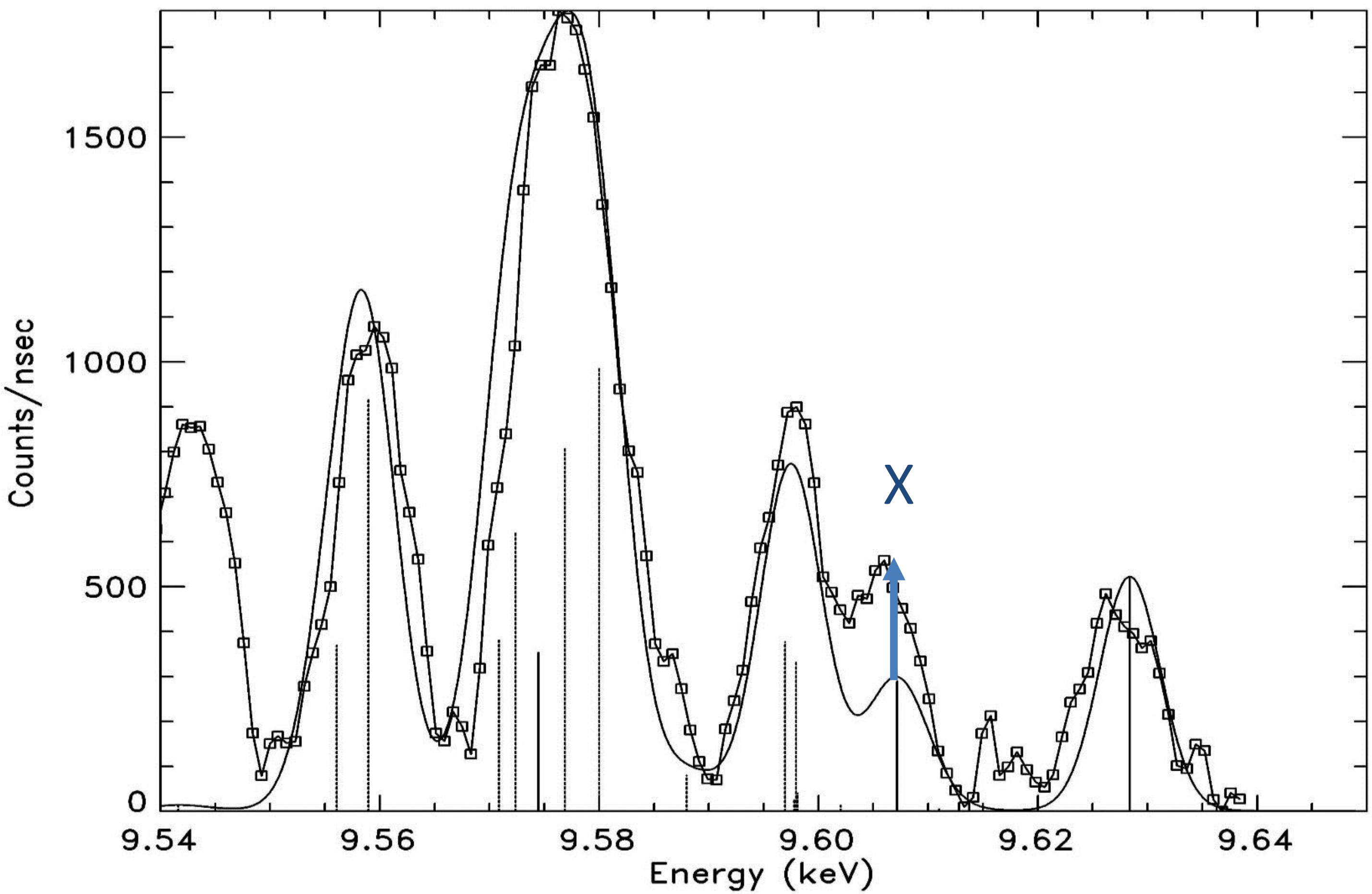
The *t* satellite transition has incorrect energy. According to the Cowan code it should be 0.7 eV on the high energy side of the *m* transition.

Move the *t* satellite to this position.

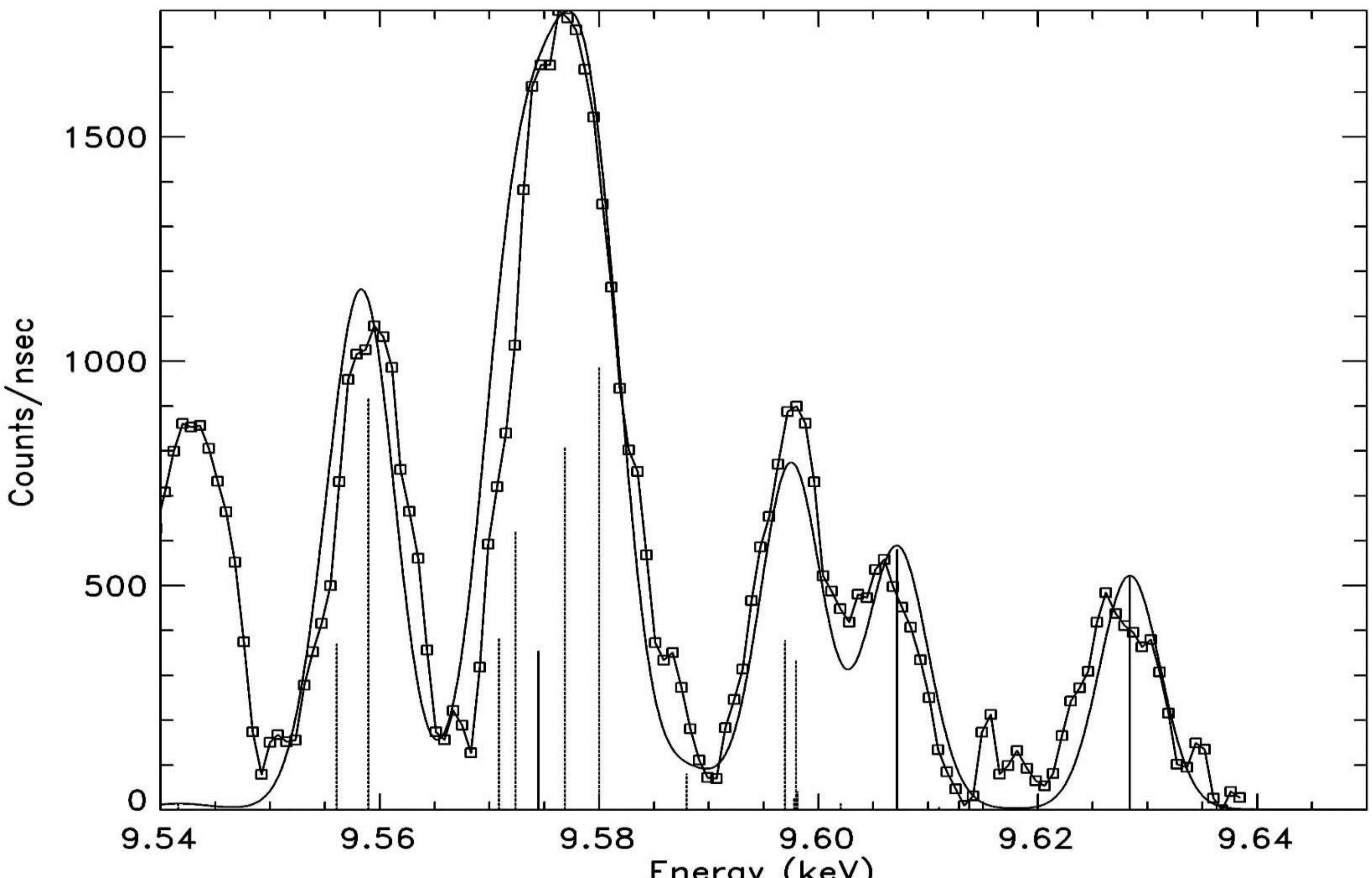


The intensity of the He-like $1s^2\ ^1S_o$–$1s2p\ ^3P_2$ M2 transition designated x is too low by a factor of 2.

Increase the x intensity by a factor of 2.

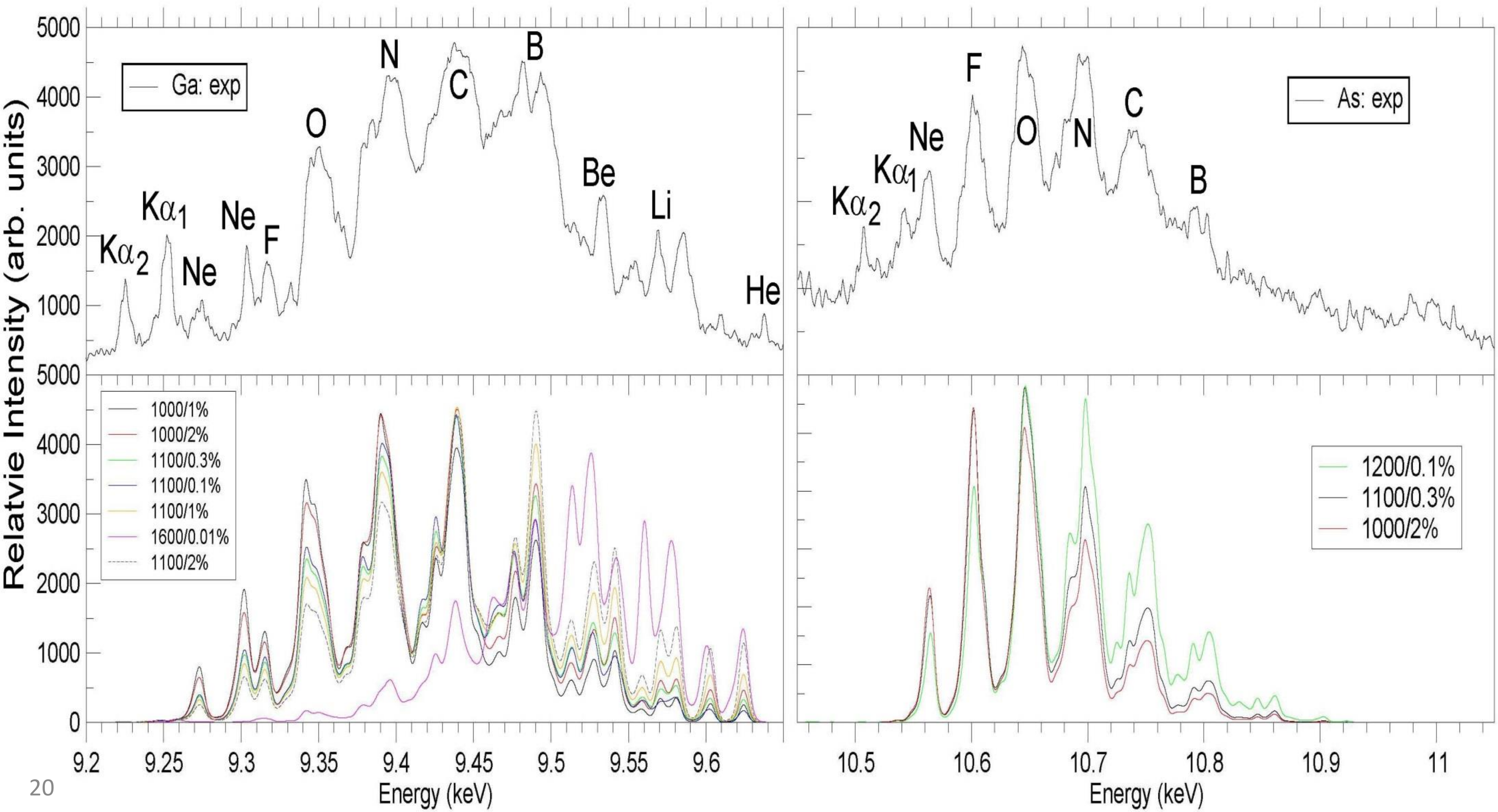


Good agreement, after a few adjustments!



NOMAD/FAC Spectrum Simulations (Y. Ralchenko)

Ga and As spectrum simulations for $N_e = 1x10^{19}\ cm^{-3}$ and variable thermal and hot electron distributions.

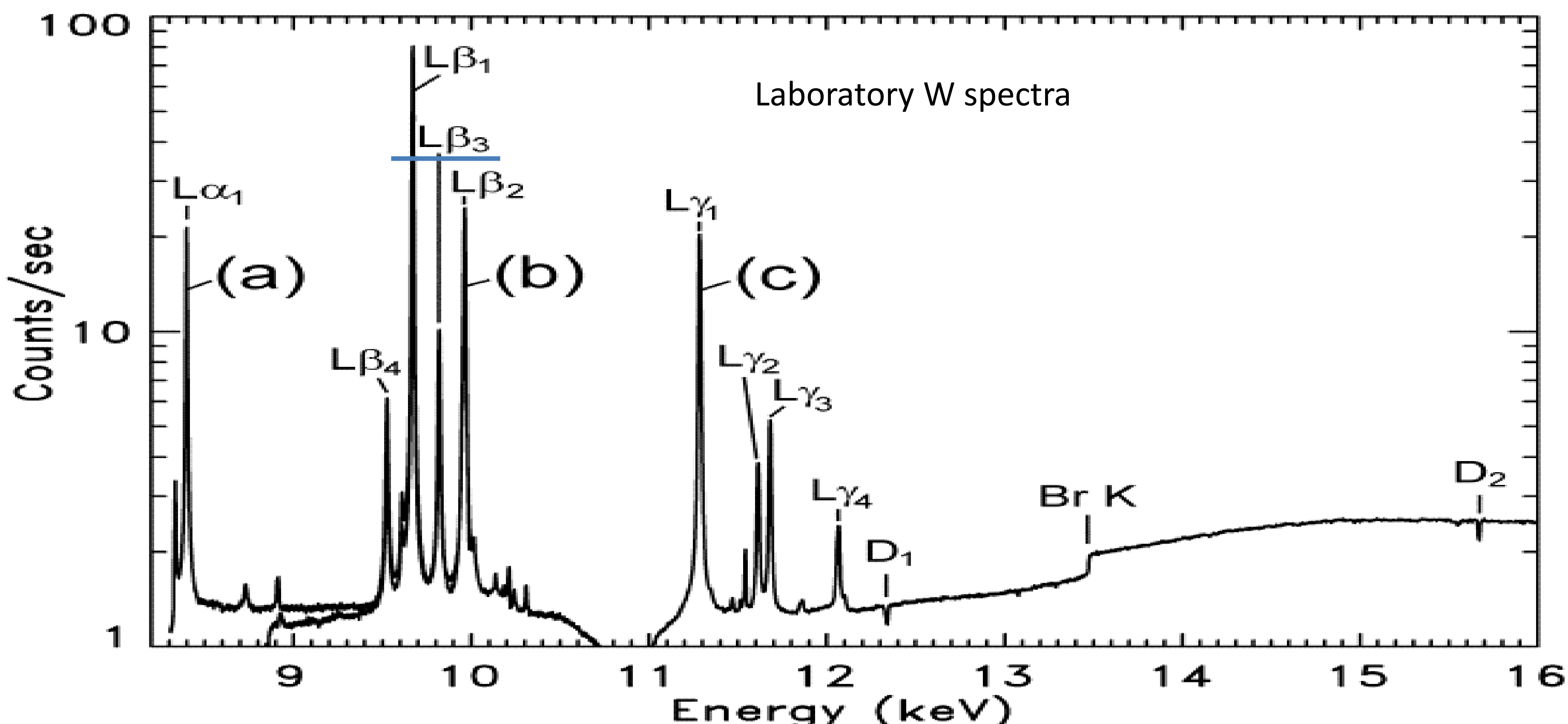


Now that we understand the spectrum and the plasma conditions, we can analyze the spectral line shapes.

In order to do this, we must know the spectrometer's instrumental broadening.

The instrumental broadening was determined using the characteristic lines from a laboratory W source.

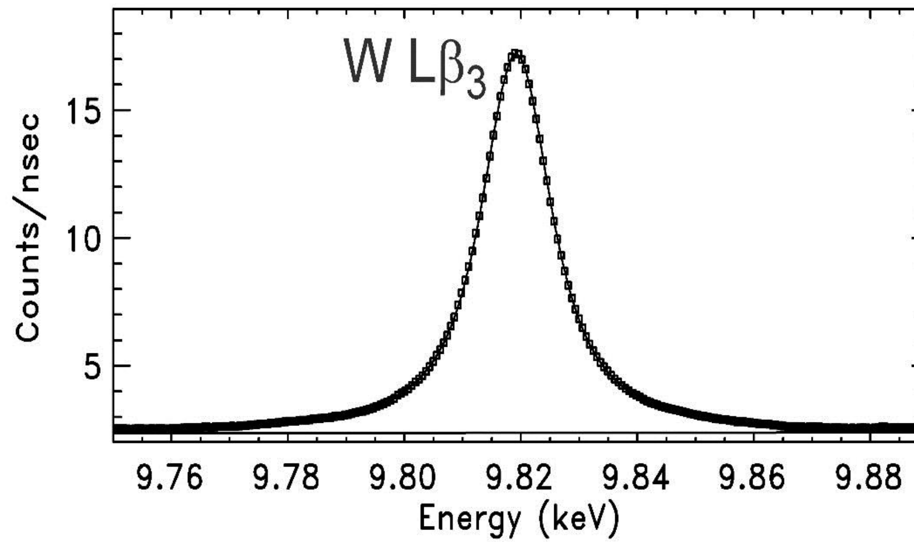
The spectrometer's instrumental broadening was measured by fitting a Voigt profile to the $L\beta_3$ line which is isolated from other spectral lines and is unblended by weaker W L lines.

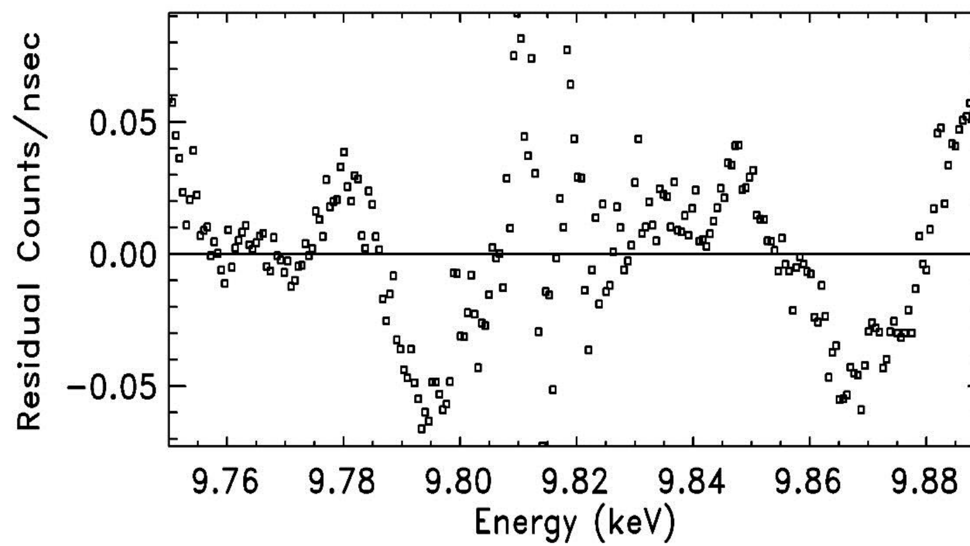


- The measured Lorentzian FWHM is 12.80 ± 0.01 eV and the Gaussian FWHM is 4.82 ± 0.01 eV.

- After subtracting the natural (lifetime) Lorentzian width* 12.8 ± 1.4 eV and the detector Lorenztian FWHM 0.78 ± 0.01 eV, the resultant Lorentzian width is -0.8 ± 1.4 eV which is effectively zero within the measurement uncertainty.

- After subtracting in quadrature the detector Gaussian FWHM 0.84 ± 0.01 eV, the resultant Gaussian width is 4.75 ± 0.02 eV and represents the intrinsic crystal broadening.





*Natural widths of the characteristic x-ray lines are from Campbell and Papp, ADNDT **77**,1 (2001)

A Voight Profile is Fitted to the Cold Ga Kα_2 from Outside the Focal Spot

Lorentzian component:

Fitted FWHM = 2.71 ± 0.04 eV.

Subtract the natural (lifetime) width 2.53 ± 0.33 eV

and the detector Lorentzian FWHM 0.11 ± 0.09 eV.

The resultant is 0.07 ± 0.46 eV (zero within the uncertainties).

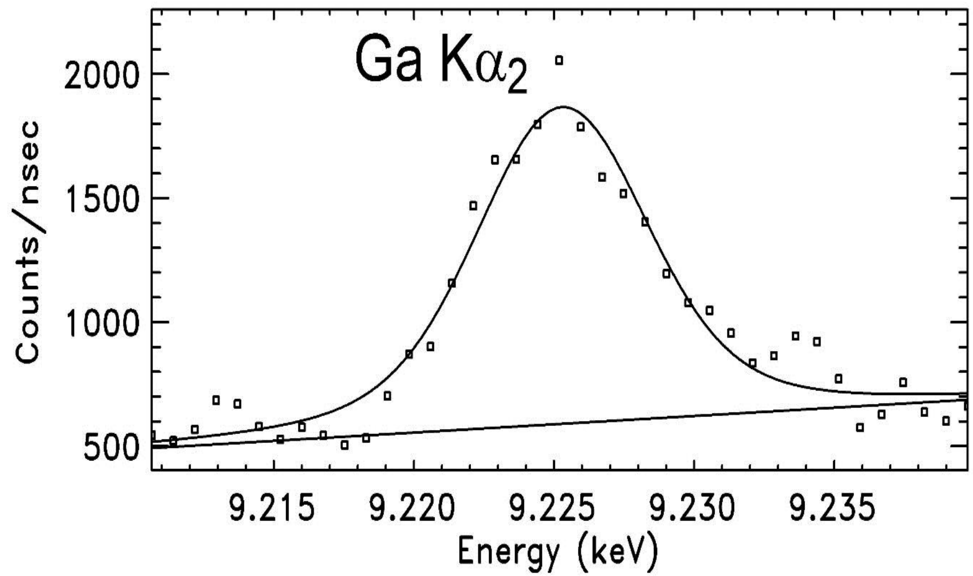
Gaussian component:

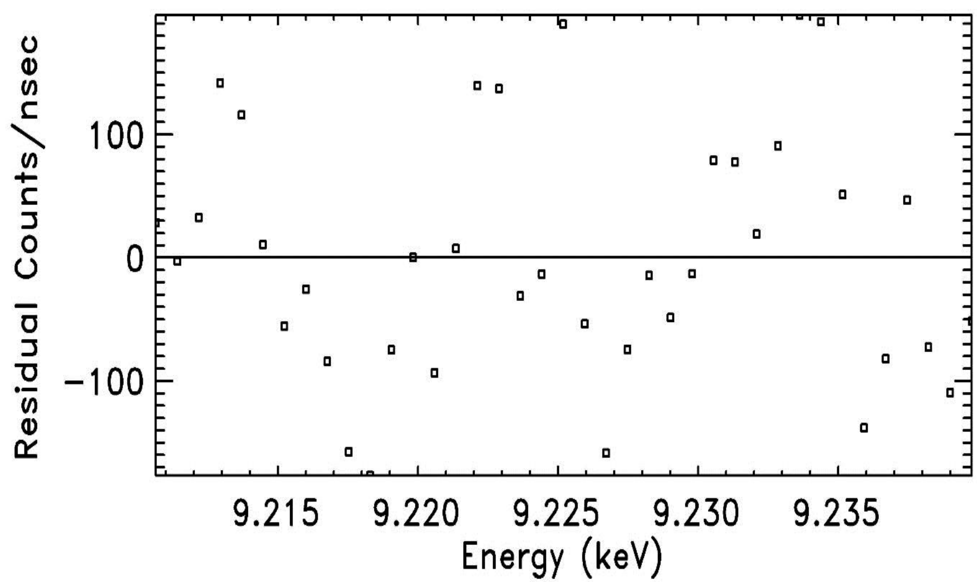
Fitted FWHM = 5.78 ± 0.03 eV.

Subtract in quadrature the detector Gaussian FWHM 2.24 ± 0.06 eV

and the resultant is 5.33 ± 0.07 eV.

This is slightly larger than the 4.75 ± 0.02 eV crystal broadening measured in the laboratory.



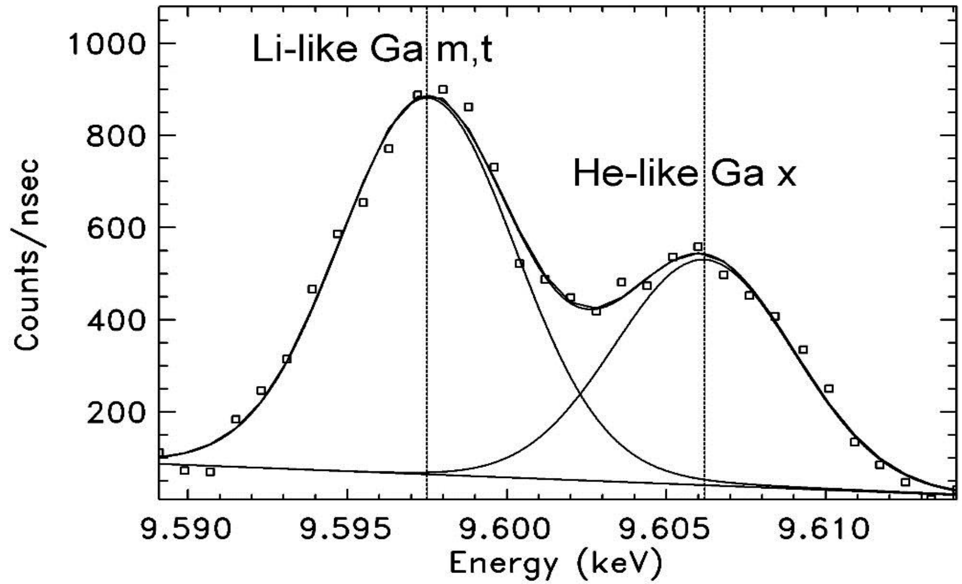


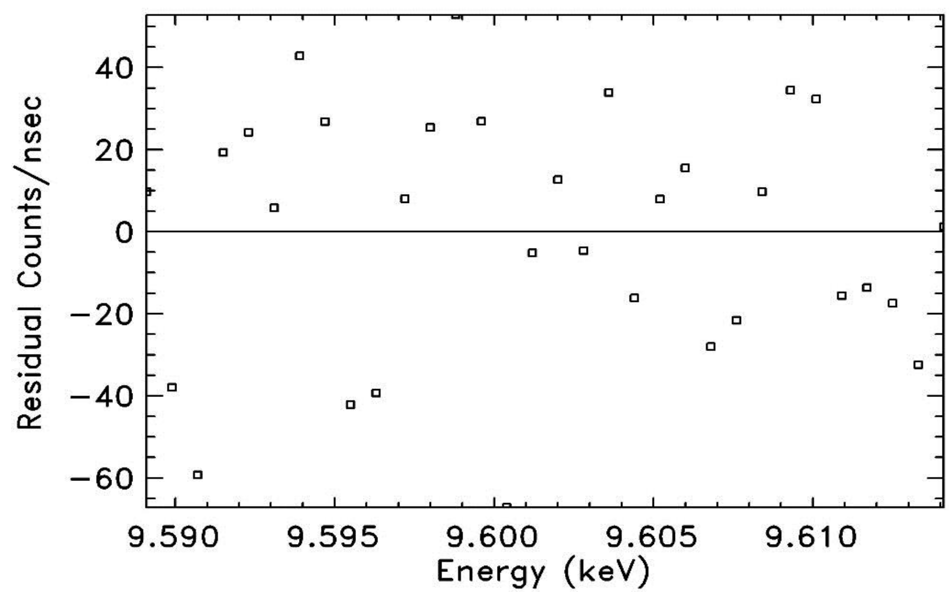
Two Voigts are Fitted to Partially Blended Li-Like and He-like Lines

	m,t	x
Lorentzian	FWHM (eV)	FWHM (eV)
Measured	0.41 ± 0.10	0.01 ± 0.10
Natural	0.31	0.001
Detector	0.12 ± 0.10	0.12 ± 0.10
Resultant	**-0.02 ± 0.20**	**-0.11 ± 0.20**
Gaussian	FWHM (eV)	FWHM (eV)
Measured	6.30 ± 0.10	6.61 ± 0.10
Crystal	4.75 ± 0.02	4.75 ± 0.02
Detector	2.45 ± 0.07	2.45 ± 0.07
Thermal *	2.94 ± 0.13	2.94 ± 0.13
Resultant	**1.58 ± 0.30**	**2.55 ± 0.30**
	5×10^6 cm/s	8×10^6 cm/s

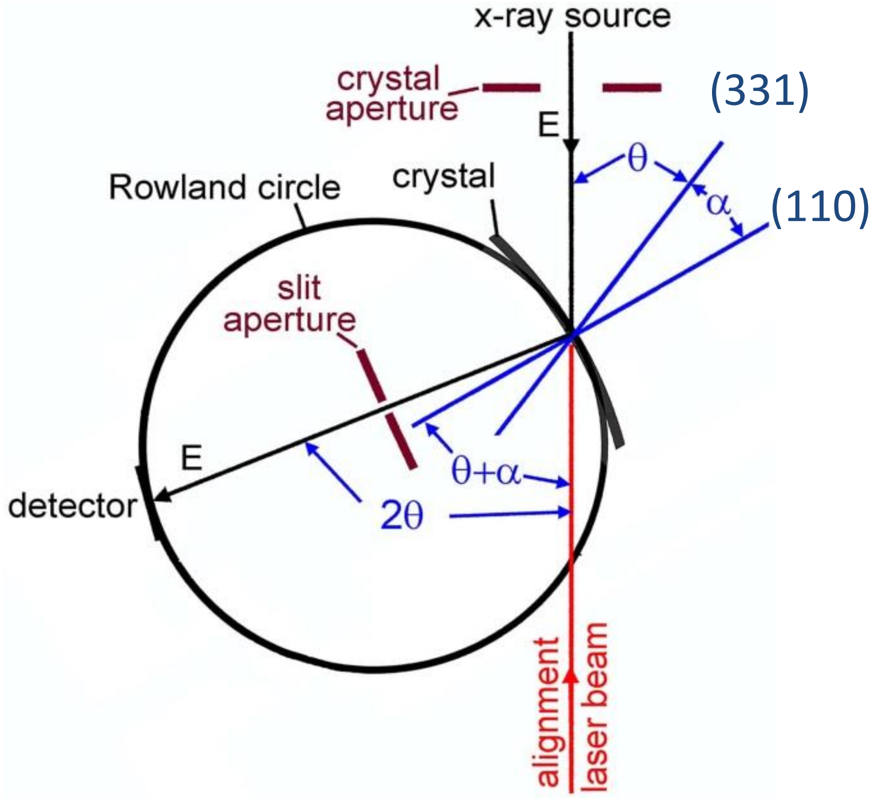
Doppler spread (turbulence) in the 3×10^7 cm/s plasma streaming motion.

*Thermal Doppler FWHM assuming the ion temperature is the same as the electron temperature, 1100 eV. This is valid because the ion-electron equilibration time is 0.9 ps.



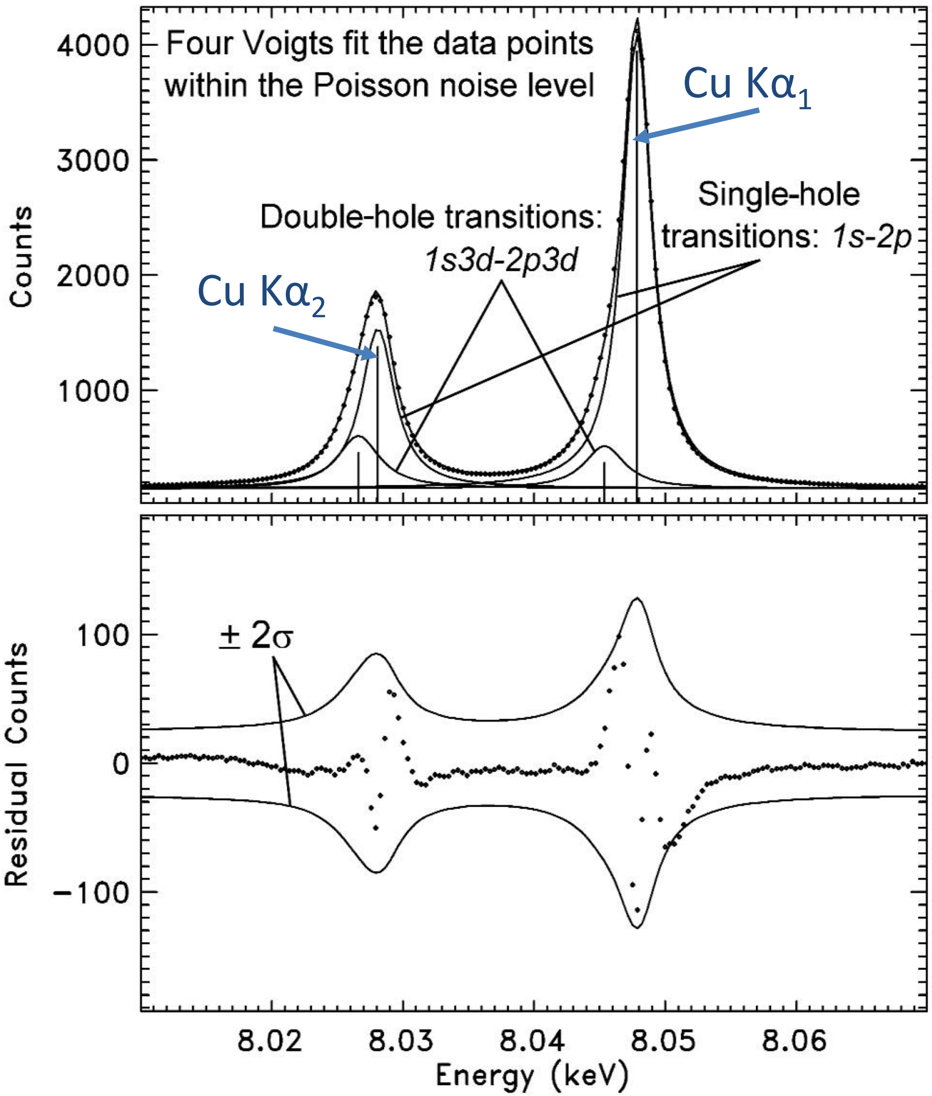


Transmission-crystal spectrometer having > 20,000 resolving power has been developed

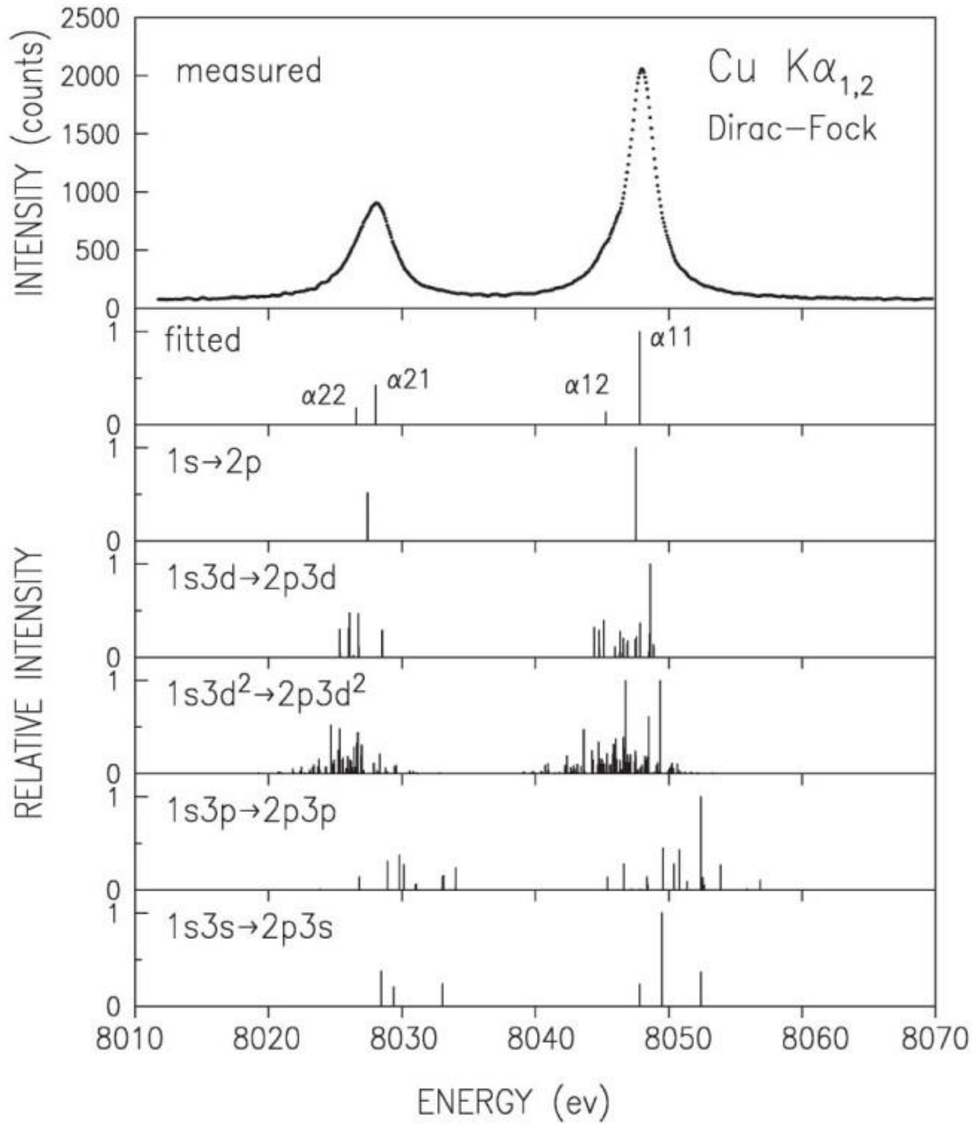


Observed Double-Hole 1s3d–2p3d Transition in Cu

1s–2p type transition with a 3d vacancy

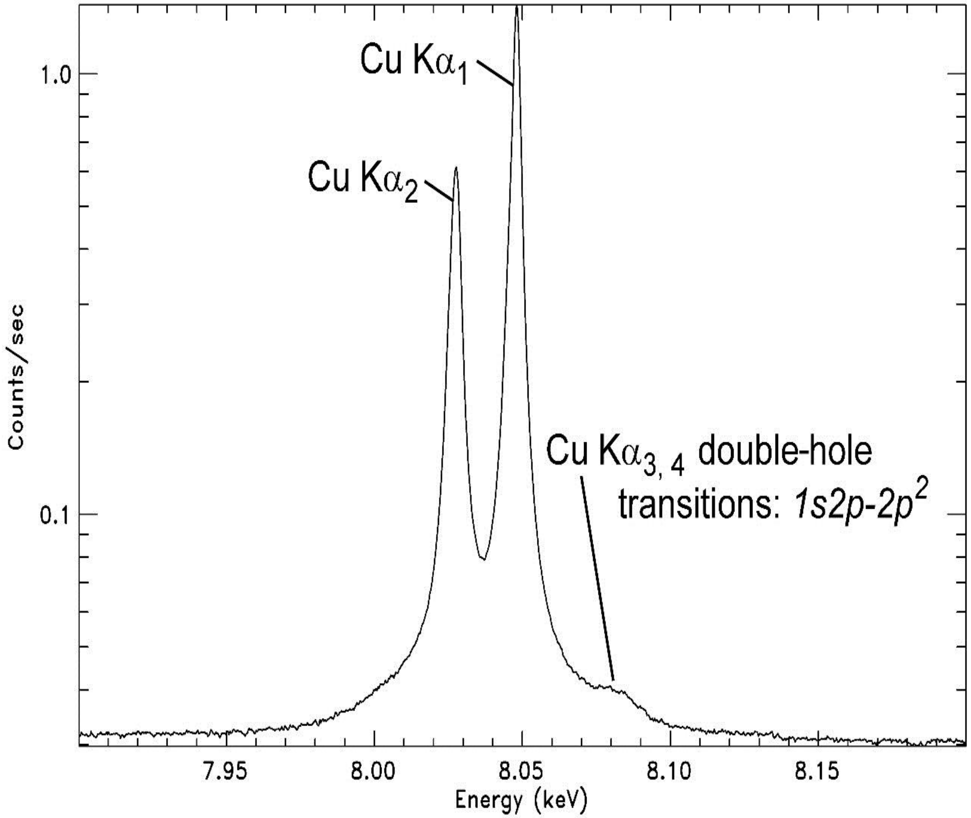


Previous synchrotron measurement:



Double-Hole 1s2p–2p^2 Transitions

1s-2p type transition with a 2p vacancy



Previous synchrotron measurement: