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# X-ray Diagnostics for High Energy Density Plasma

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*Sandia National Laboratories*

High Energy Density Science Summer School

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# Outline

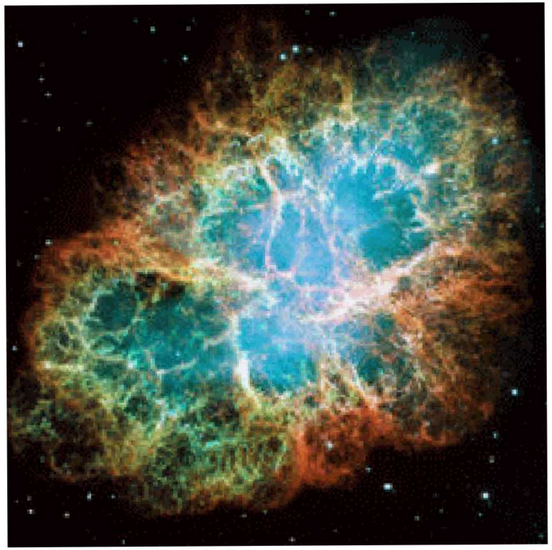
- General thoughts on HEDP diagnostics

- X-ray methods: basic ideas & handy estimates
  - emission & absorption spectroscopy
  - scattering & diffraction

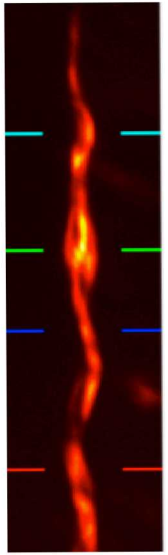
- Introduction to projects

# At the object scale, we have two basic techniques to learn about HED plasmas:

## 1. Look at them

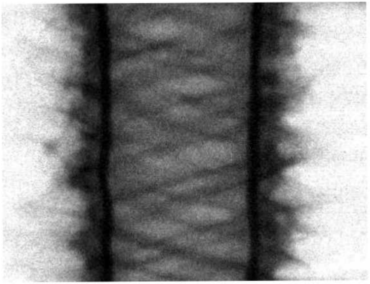


Optical image of the Crab nebula (HST)

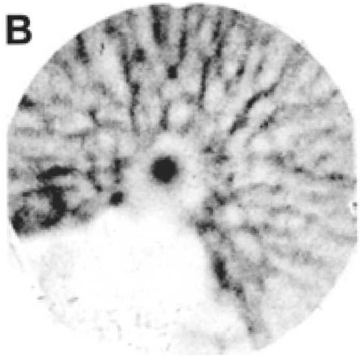


X-ray image of MagLIF (SNL)

## 2. Hit them with something



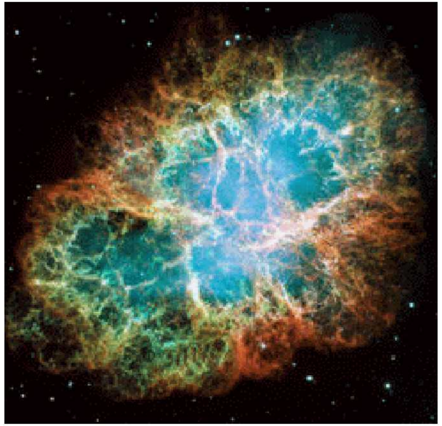
**X-rays**
(T. Awe, SNL)



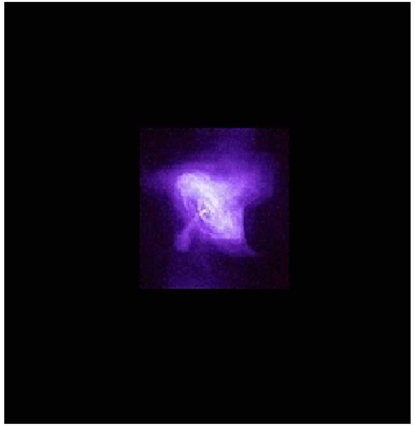

**Protons**
(R. Rygg, LLNL)

# What we see depends on how we image or probe the object

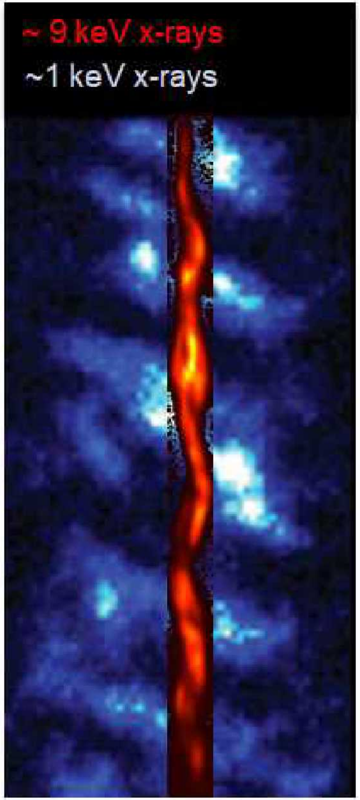
Gradients & energy-dependent atomic-scale processes determine what we can measure



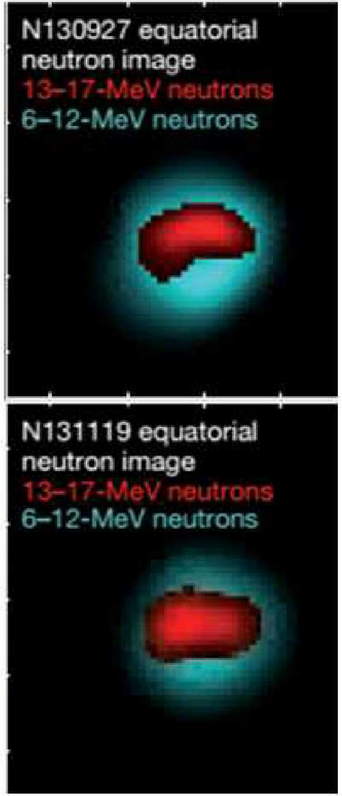
**Optical**



**X-ray**




Gomez *et al* PRL 2014




Hurricane *et al* Nature 2014

# Beyond imaging, there is a rich dimension of energy that can reveal details of object composition, conditions, and motion

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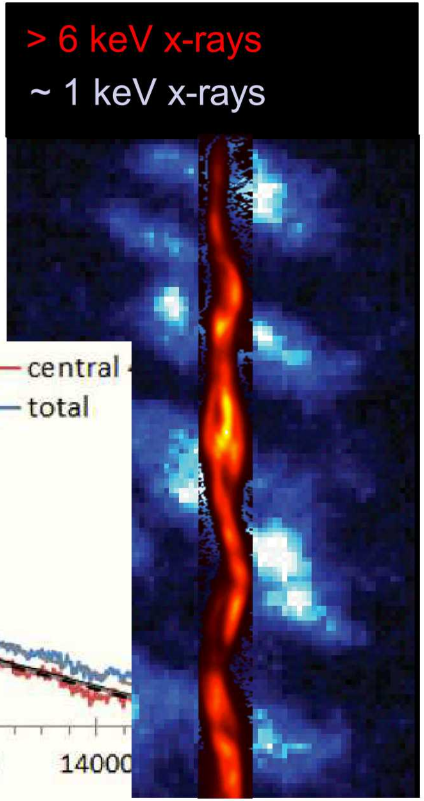
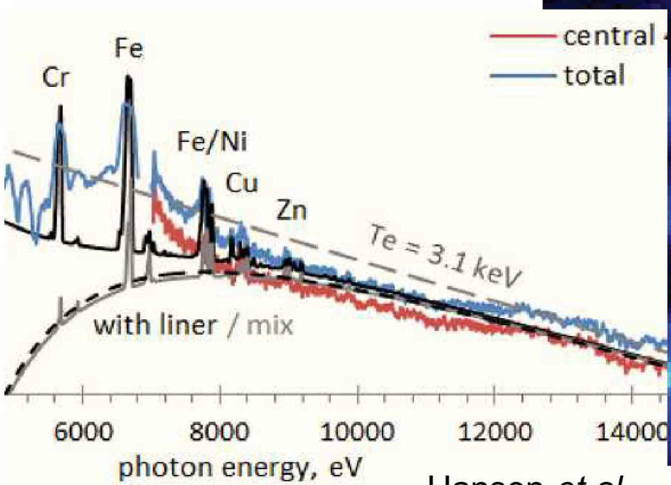
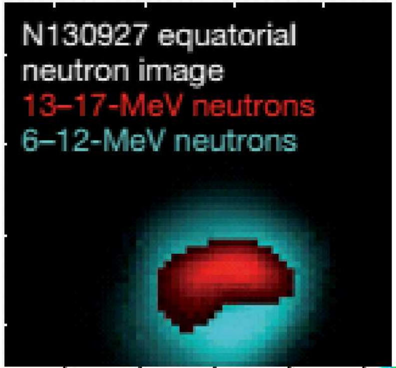
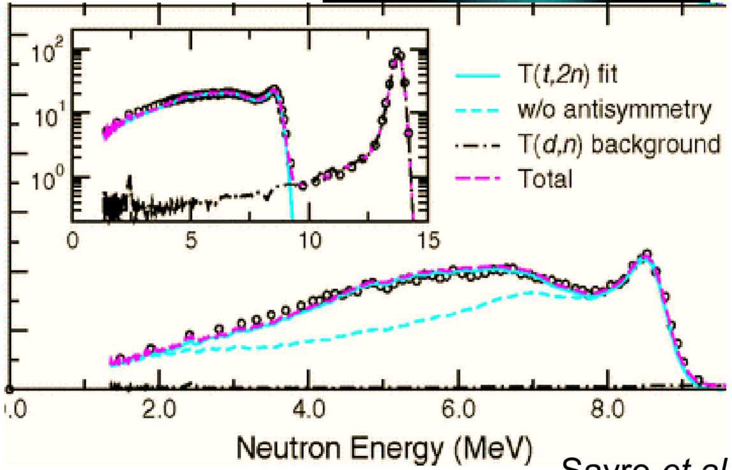
Interpreting energy-dependent data requires understanding atomic-scale structure and response




Hansen *et al*




Sayre *et al*

# At the atomic scale, we have two basic techniques to measure the properties of electrons and ions in HEDP:

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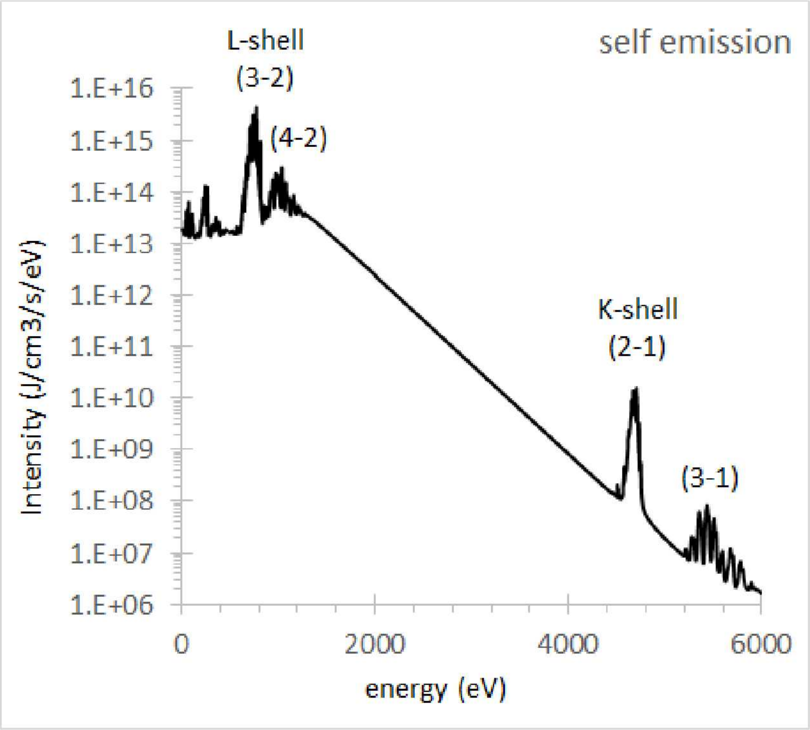
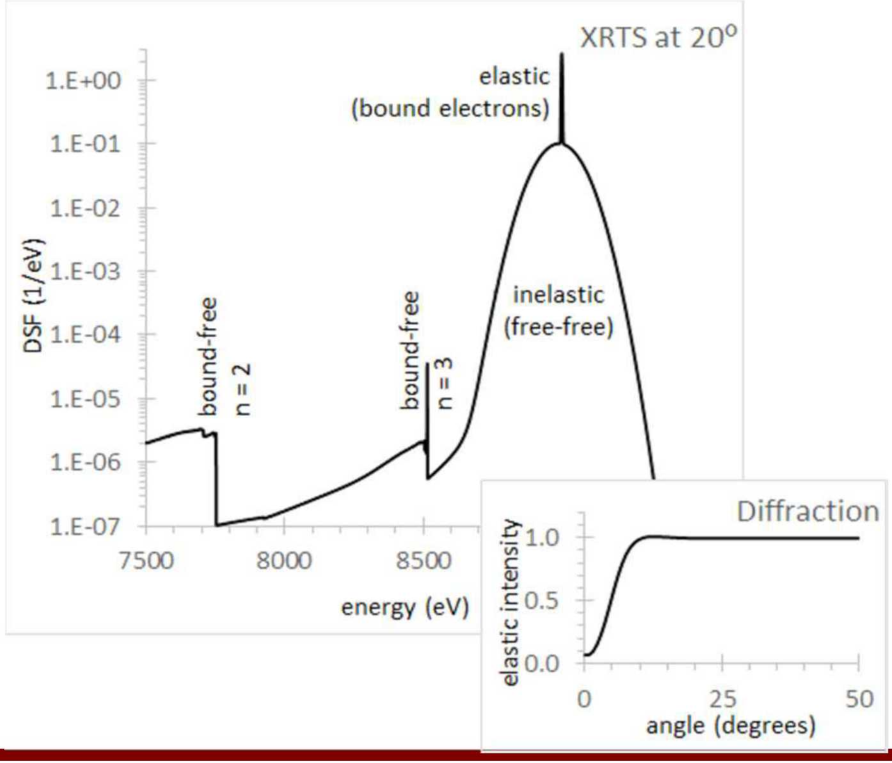
## 1. Look at their thermal self-emission

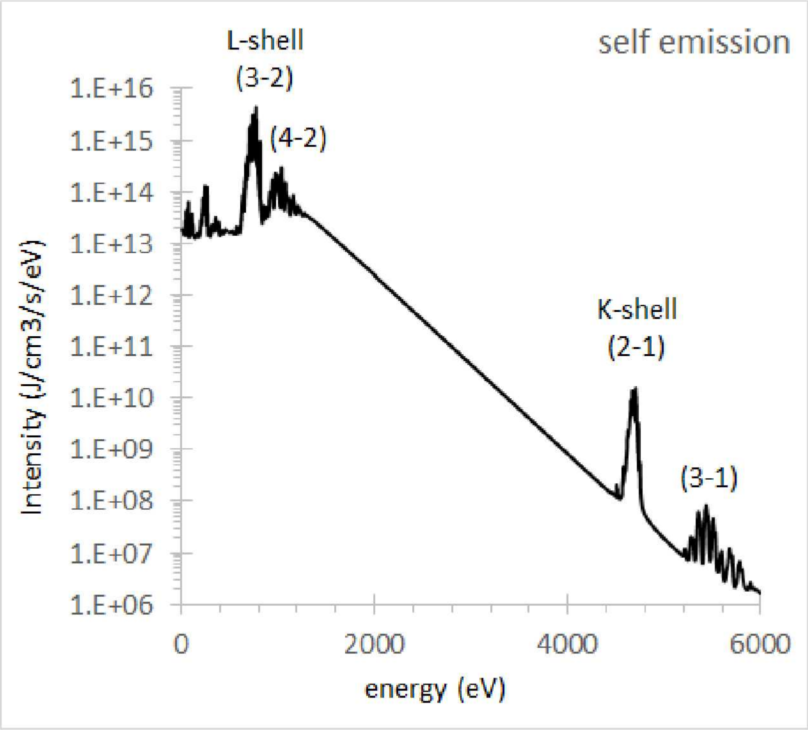



## 2. Hit them with something (here, a 9 keV narrow-band XFEL)

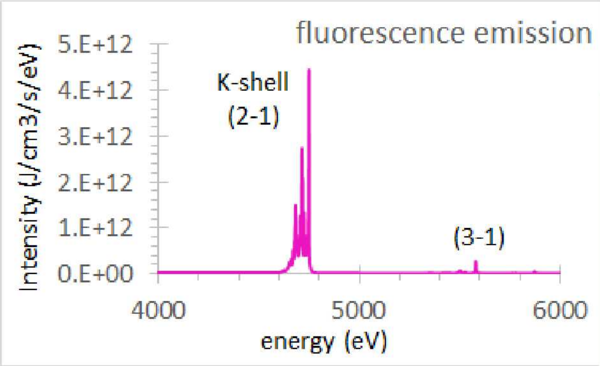


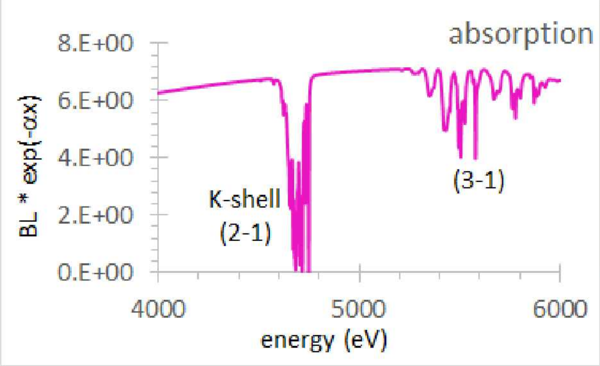
# At the atomic scale, we have two basic techniques to measure the properties of electrons and ions in HEDP:

## 1. Look at their thermal self-emission




## 2. Hit them with something (here, a broadband backlighter)



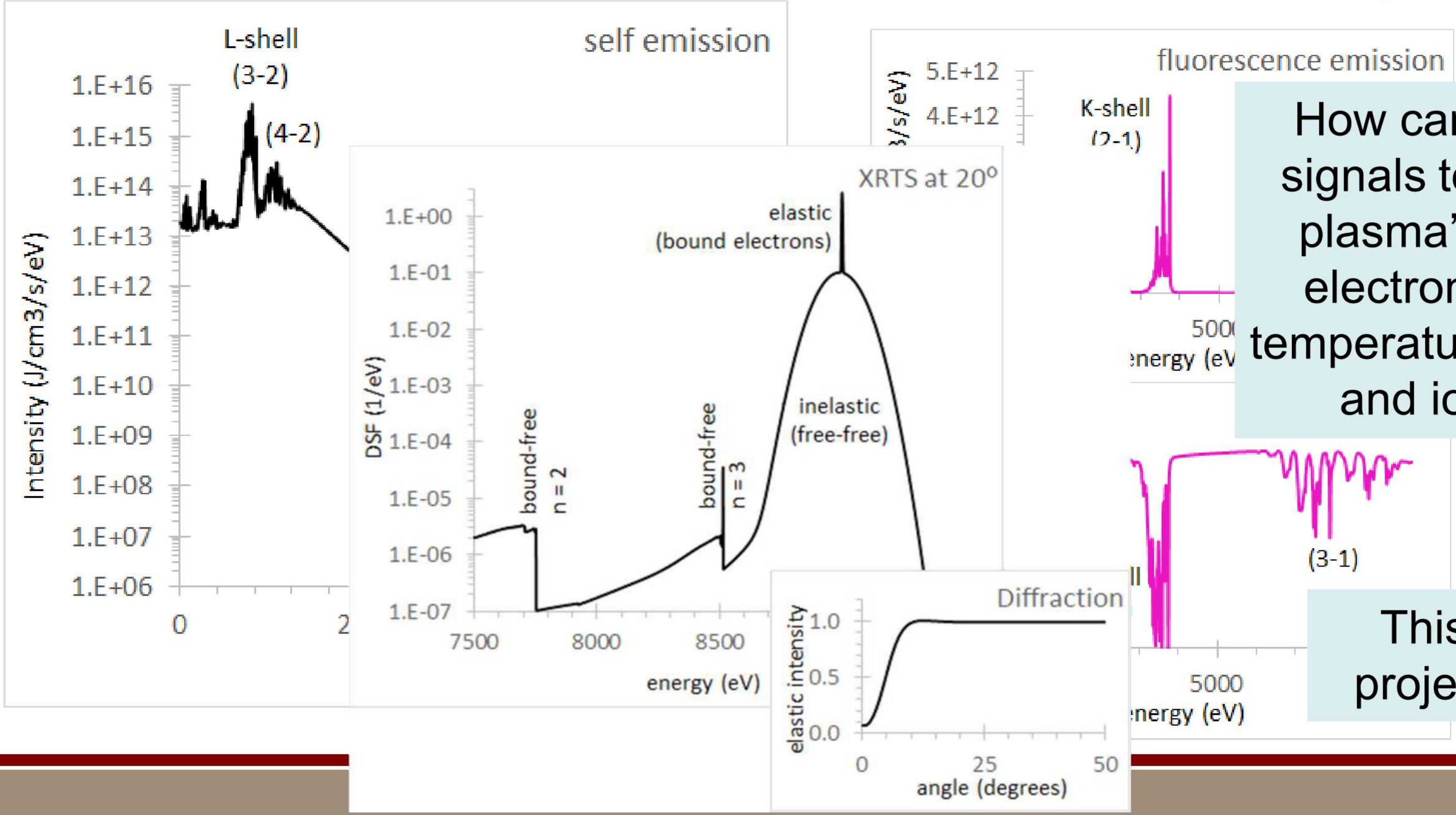




Plasma diagnostics relate image-scale observables to atomic-scale properties of the plasma’s constituent elements

# At the atomic scale, we have two basic techniques to measure the properties of electrons and ions in HEDP:

## 1. Look at their thermal self-emission

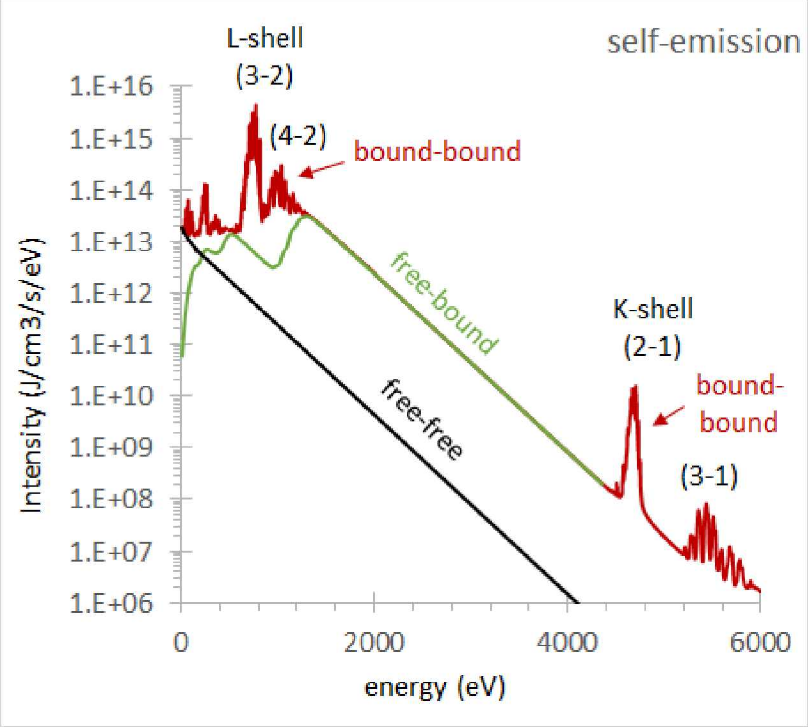
## 2. Hit them with something




How can we use these signals to determine the plasma's composition, electron and radiation temperatures, and electron and ion densities?

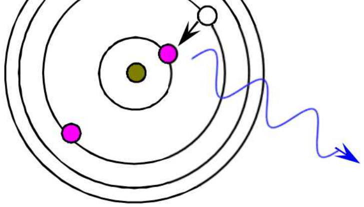
This is our course project – take notes!

# X-ray emission is a rich source of information



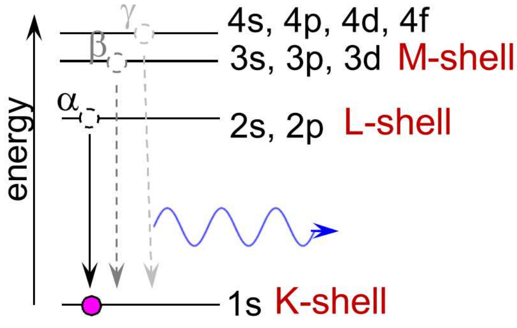

X-ray spectra are typically interpreted using collisional-radiative (CR) models, which track populations $X$ of many electronic configurations

$$\text{Intensity } I = I_{\text{f-f}} + I_{\text{b-f}} + I_{\text{b-b}}$$
$$I_{\text{b-b}} \sim X\, \mathrm{A}^{\text{rad}}\, \varphi(\varepsilon)$$



Bohr shell model:

$\varepsilon_n \sim 13.6 \text{ eV } (Z_{eff}/n)^2$

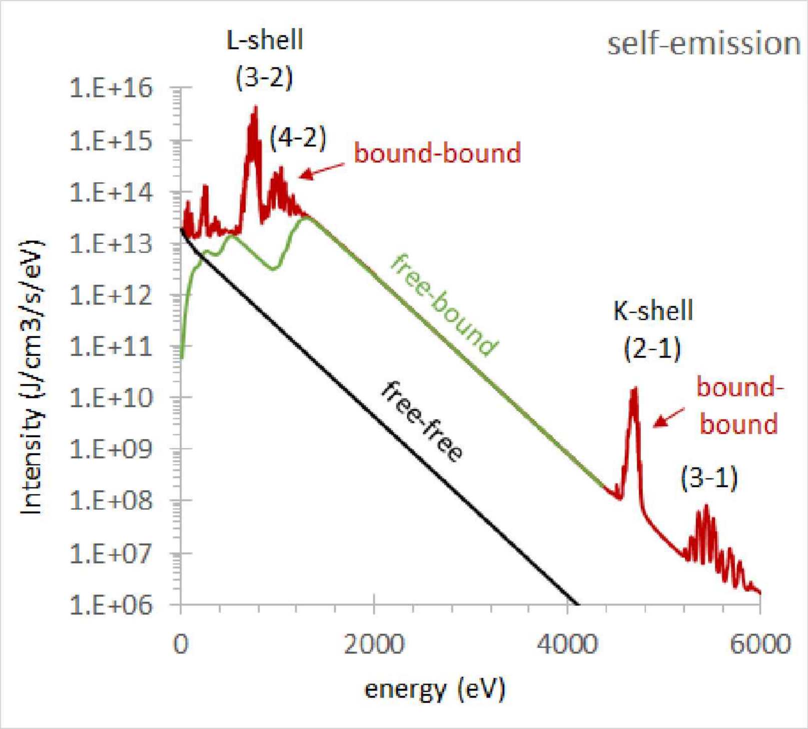



Schrödinger: $\Psi_{n1}$, $\varepsilon_{n1}$, and $A^{\text{rad}}$

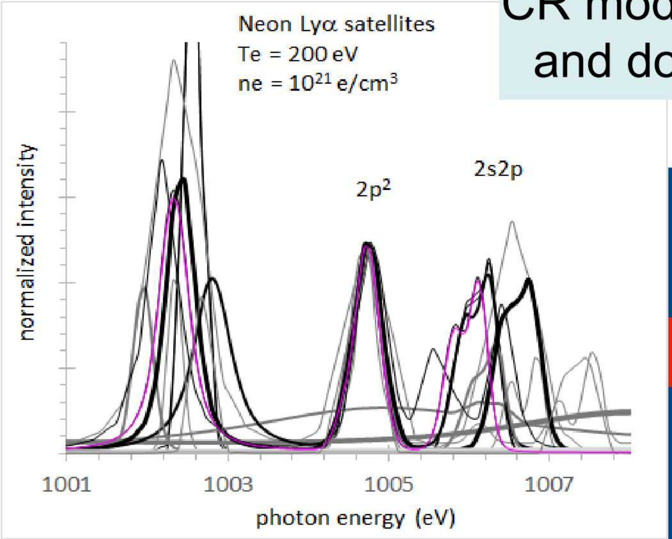
$A^{\text{rad}} \sim \langle \Psi_{n1} \,|\, r \,|\, \Psi_{n2} \rangle$

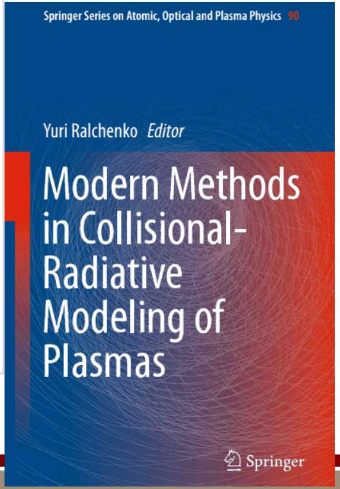
# X-ray emission, composed of free-free, free-bound, and bound-bound (line) features, is a rich source of information

X-ray spectra are typically interpreted using collisional-radiative (CR) models, which track populations $X$ of many electronic configurations

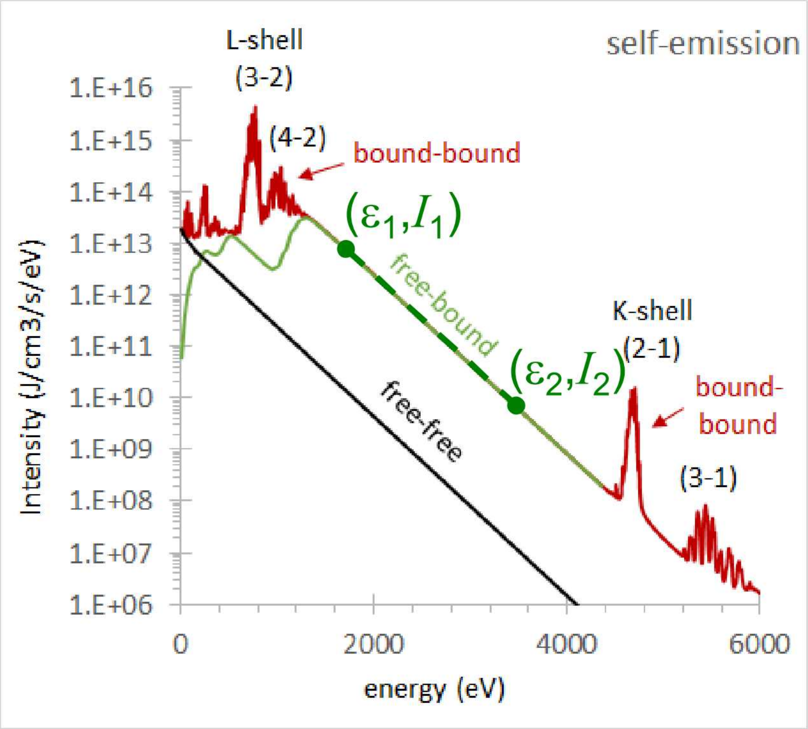



CR models can and do vary!



# The continuum slope is a useful thermometer, independent of CR model and plasma composition



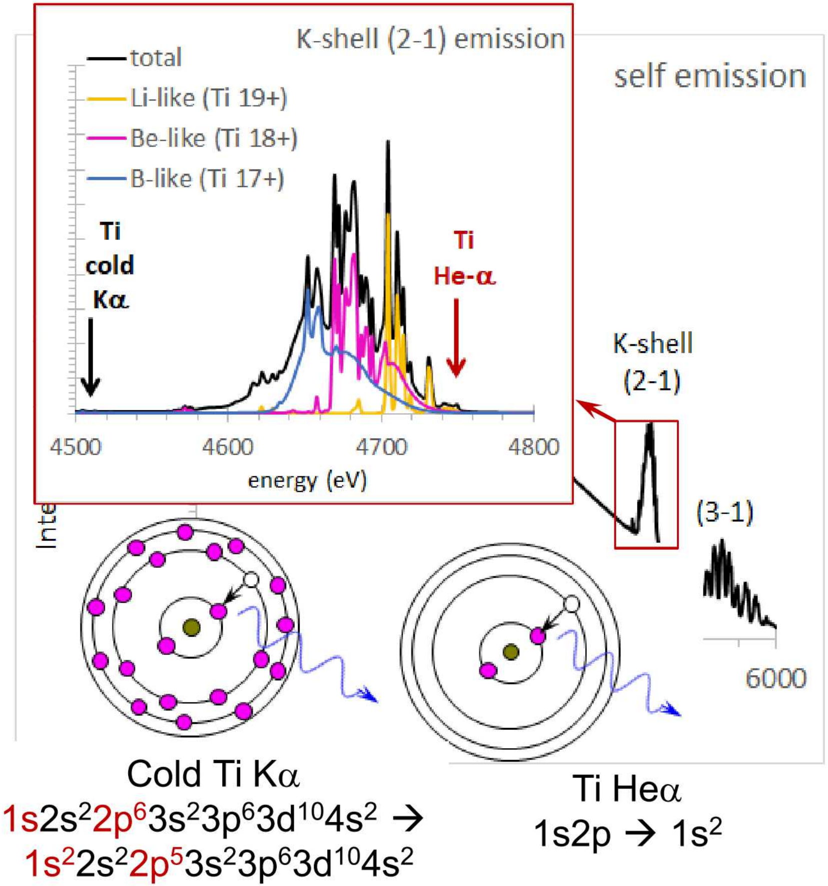

Free-bound emission $I \sim g(\varepsilon)\ \exp(-\varepsilon/T_e)$

$\rightarrow T_e(\text{eV}) \sim (\varepsilon_1 - \varepsilon_2)/\ln(I_2/I_1)$

Here, continuum slope indicates $T_e$ = 250 eV (same as actual)

Note that gradients can complicate this straightforward interpretation (and all that follow), but we exclude them for the projects

# Lines are unique to particular elements and charge states




Bound-bound line energies definitively identify elements in a plasma:

$\varepsilon_{line} \sim 13.6\text{ eV }(Z_{nuc}-1)^2\ [1/n_1^2 - 1/n_2^2]$

Here, K-shell ($n_2 = 2 \rightarrow n_1 = 1$) lines at ~4.6 keV indicate $Z_{nuc} = 22$ ($\varepsilon_{K\text{-}line}$ ~4.5 keV ~ cold Ti Kα) (Ti is the actual element!)

Line energies increase under ionization, enabling estimates of the average ion charge Z*

Here, Z* ~ 18 for Be-like Ti (actual Z* = 17.7)

Knowing Z* and $Z_{nuc}$, we can roughly estimate temperature: $T_e$ (eV) ~ $Z^{*3}/Z_{nuc}$

Here, $T_e$ ~ 265 eV (actual $T_e$ = 250 eV)

# Lines can also be sensitive to plasma density effects

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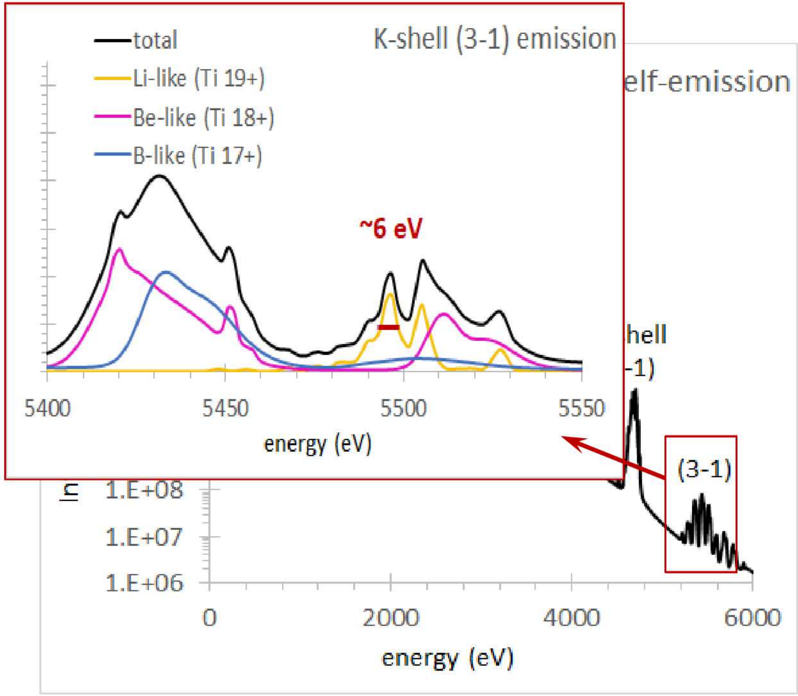


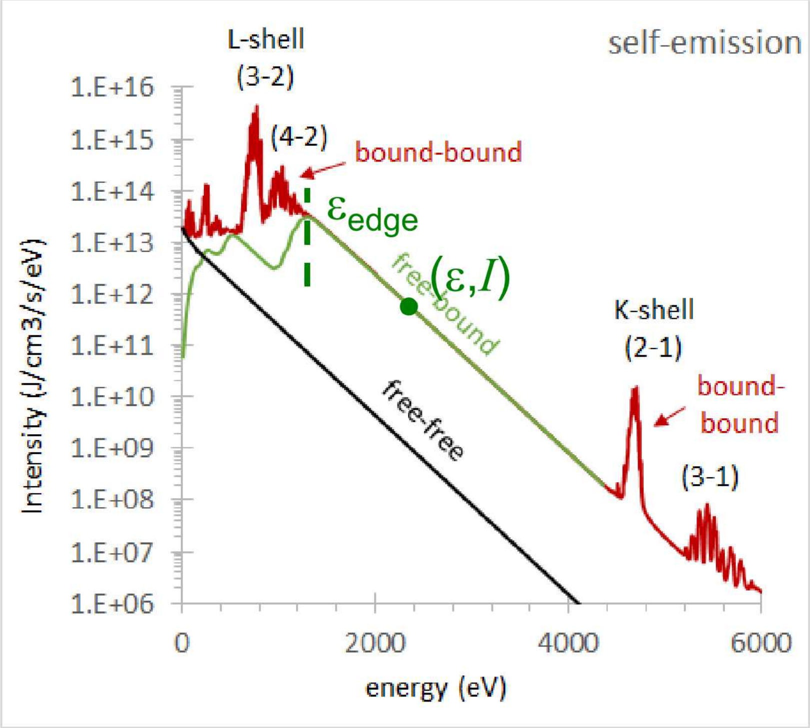

Lines are broadened by density-dependent collisions and Stark splitting.
3p -1s (K$\beta$) lines have widths that roughly follow:
$fwhm_{K\beta}$ (eV) ~ 40 / $Z_{nuc}$ $(n_e/10^{22})^{0.6}$

Here, $n_e$ ~ $7.5\times10^{22}$ e/cm$^3$
(actual $2.5\times10^{22}$ e/cm$^3$)

<u>Caution</u>: ion motion, opacity, and line blends (*not* excluded here) also broaden features!

<u>Advanced</u>: collisions also redistribute populations, leading to changes in relative line intensities (e.g. satellites & $He_{IC}/He\alpha$)

# Absolute emission intensities, when available, are good density diagnostics




Free-bound intensity increases with density:

$$I_{f\text{-}b}(\varepsilon) \sim 4e\text{-}31\ T_e^{-3/2}\ Z^{*4}\ n_i^2\ \exp[(\varepsilon_{edge} - \varepsilon)/T_e]$$

($I$ in J/cm$^3$/s/eV, $T_e$ in eV, $n_i$ in ions/cm$^3$)

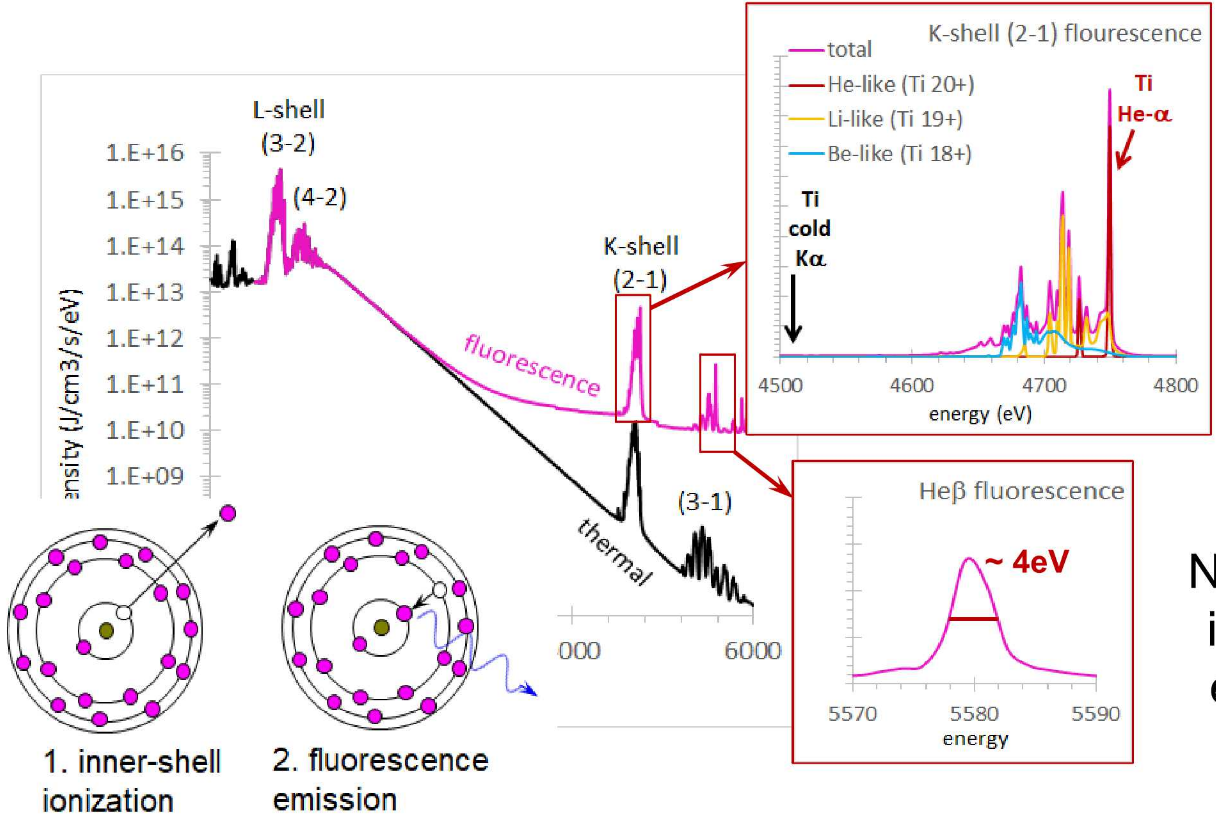
$$E_{n\text{-}edge} \sim 13.6\ \text{eV}\ (Z_{eff}/n)^2$$

$$Z_{eff} \sim \max[Z^*, Z_{nuc} - \Sigma_1^{(n-1)}(2n^2)]$$

Here, $Z_{eff} = 20 \rightarrow \varepsilon_{L\text{-}edge} = 1360$ eV.
With $Z^* = 18$, the continuum intensity indicates
$n_i = 1.7 \times 10^{21}$ e/cm$^3$
(actual $n_i = 1.4 \times 10^{21}$ e/cm$^3$)

Neutrality: $n_e = Z^* n_i$

# Cool plasmas + bright external radiation emit useful fluorescence lines

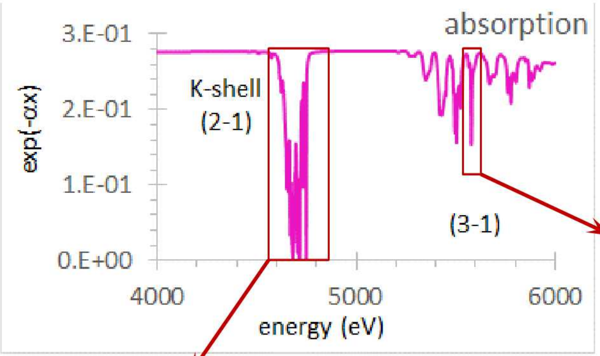


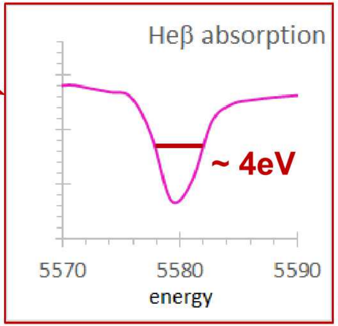

We can use these lines as before to identify the plasma composition and estimate $Z^*$, $T_e$, and $n_e$:

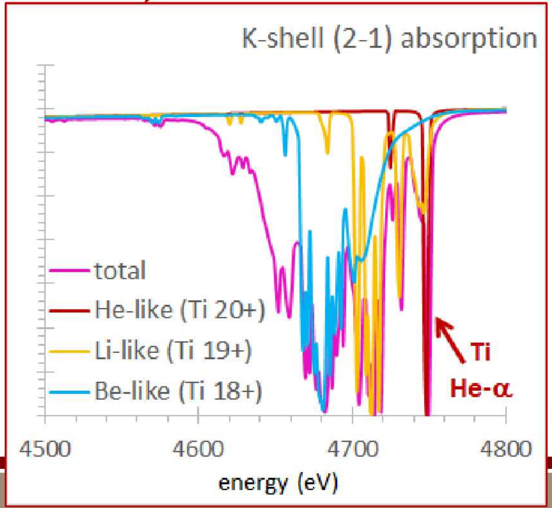
Here, $Z^*$ ~19 (17.7),
Te ~ 312 eV (250),
$n_e$ ~ $4\times10^{22}$ e/cm$^3$ ($2.5\times10^{22}$)

Note that *absolute* fluorescence intensities say more about the external radiation source than the plasma

# If the bright external source is a continuum, we can use absorption lines as diagnostics




Here,
for $x$ = 20 μm,
$n_i \sim 1.4\times10^{21}/cm^3$
($n_e \sim 2.6\times10^{21}/cm^3$)

We can *still* use lines to identify the plasma composition and estimate $Z^*$, $T_e$, and $n_e$:

Here, $Z^*$ ~18.5? (17.7),
Te ~ 290 eV (250),
$n_e \sim 4\times10^{22}$ e/cm$^3$ ($2.5\times10^{22}$)

When the plasma depth $x$ is known, absorption spectra can indicate densities:

Transmission = $\exp(-\kappa x)$

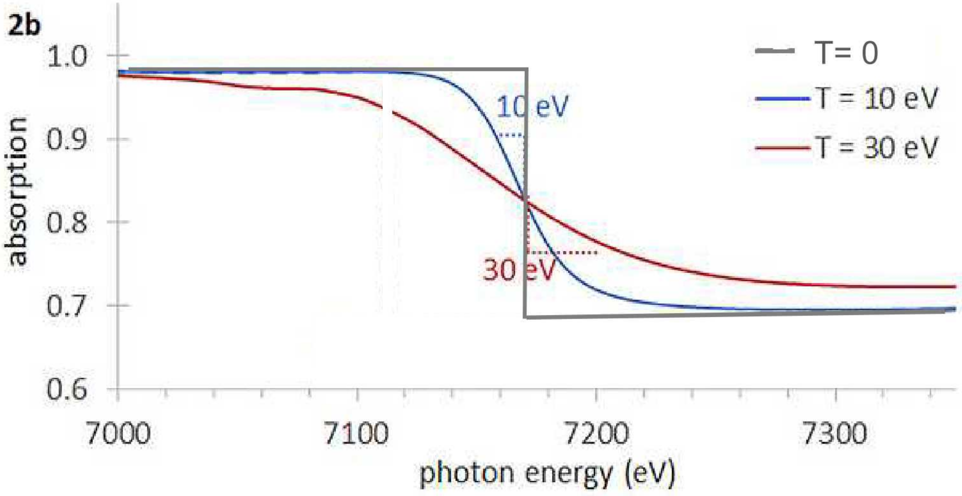
($\kappa = n_i\,\sigma$)

Note that fluorescence and self-emission (both excluded here) can complicate interpretation of real data

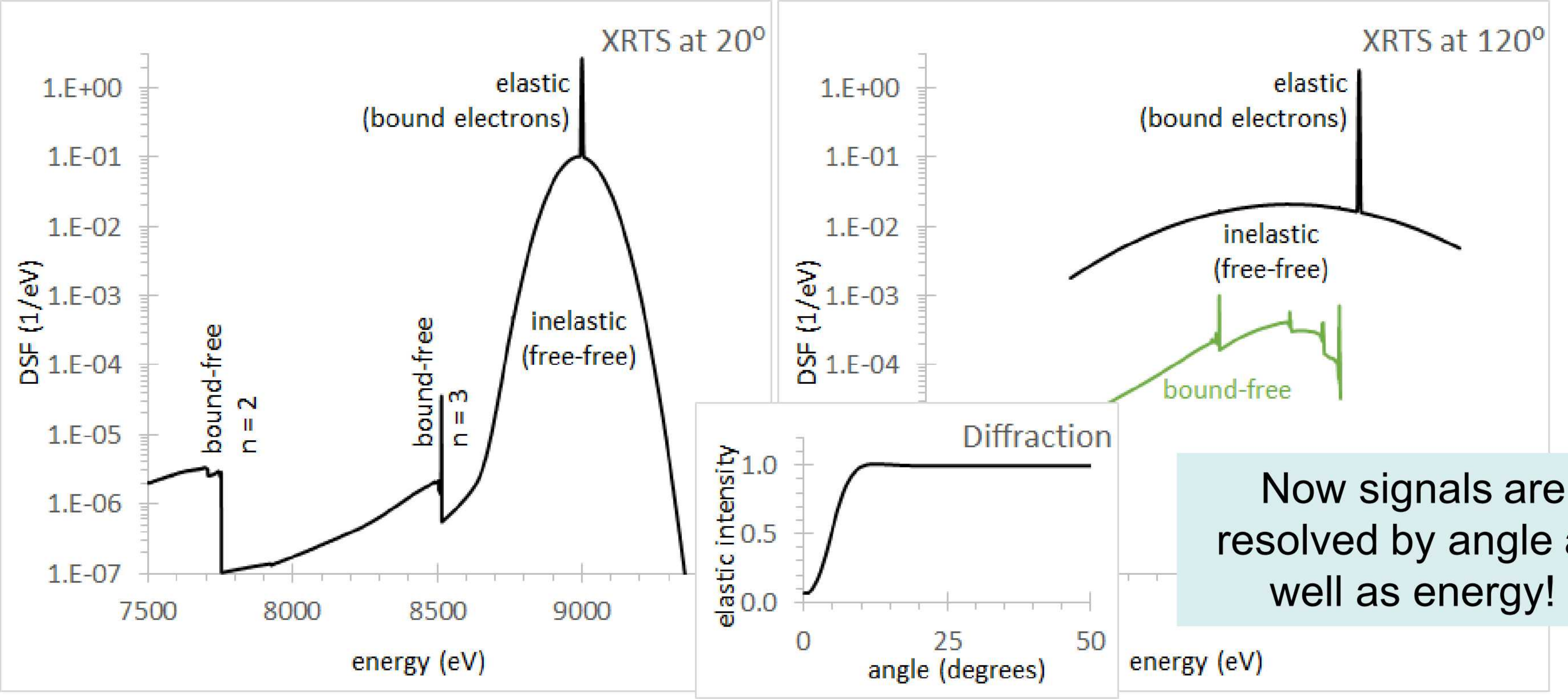
# If the plasma is very dense and/or cool, bound-free absorption edges are good thermometers

When electrons are degenerate ($T_e$ <~ $\varepsilon_{Fermi}$ ~ $1.7(n_e/10^{22})^{2/3}$ eV), thermal broadening of sharp absorption edges can indicate $T_e$

$hwhm_{edge}$ ~ $T_e$



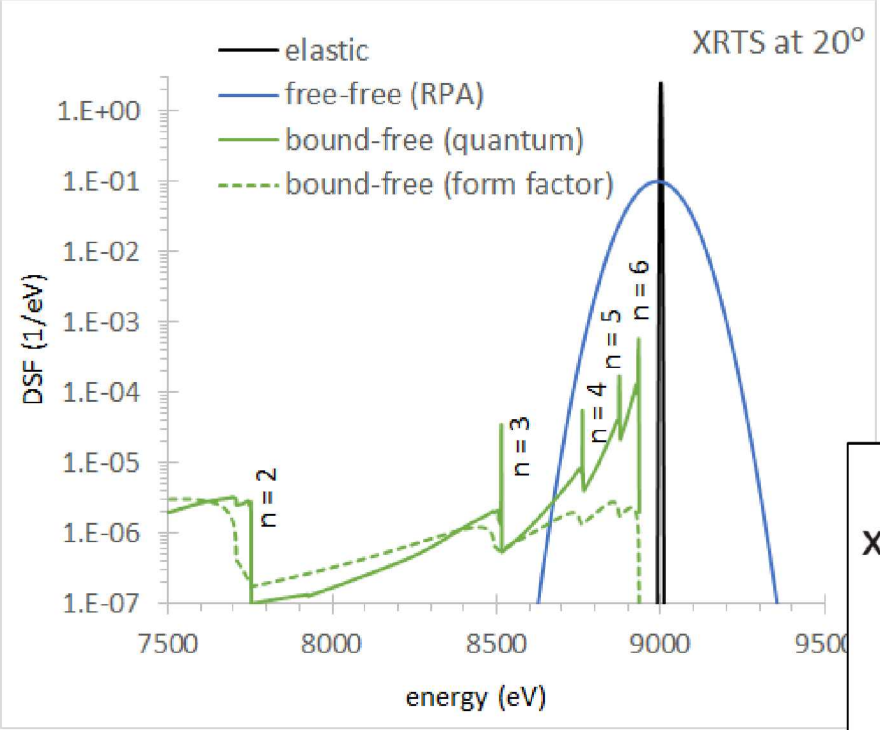
# If the bright external source is narrow-band (e.g. XFEL) x-ray scattering offers a rich source of diagnostic information




Now signals are resolved by angle as well as energy!

# XRTS data is most often interpreted using models based on the Chihara decomposition






$$S(k,\omega) = \underbrace{|f_I(k) + q(k)|^2 S_{ii}(k,\omega)}_{\text{elastic}}$$

$$+ \underbrace{\bar{Z} S_{ee}(k,\omega)}_{\text{free-free}} + \underbrace{S_{bf}(k,\omega)}_{\text{bound-free}}$$

This is similar to the decomposition of x-ray emission spectra ($I = I_{\text{f-f}} + I_{\text{b-f}} + I_{\text{b-b}}$), and each component can be treated with different levels of approximation.

REVIEWS OF MODERN PHYSICS, VOLUME 81, OCTOBER–DECEMBER 2009

X-ray Thomson scattering in high energy density plasmas

Siegfried H. Glenzer

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Ronald Redmer

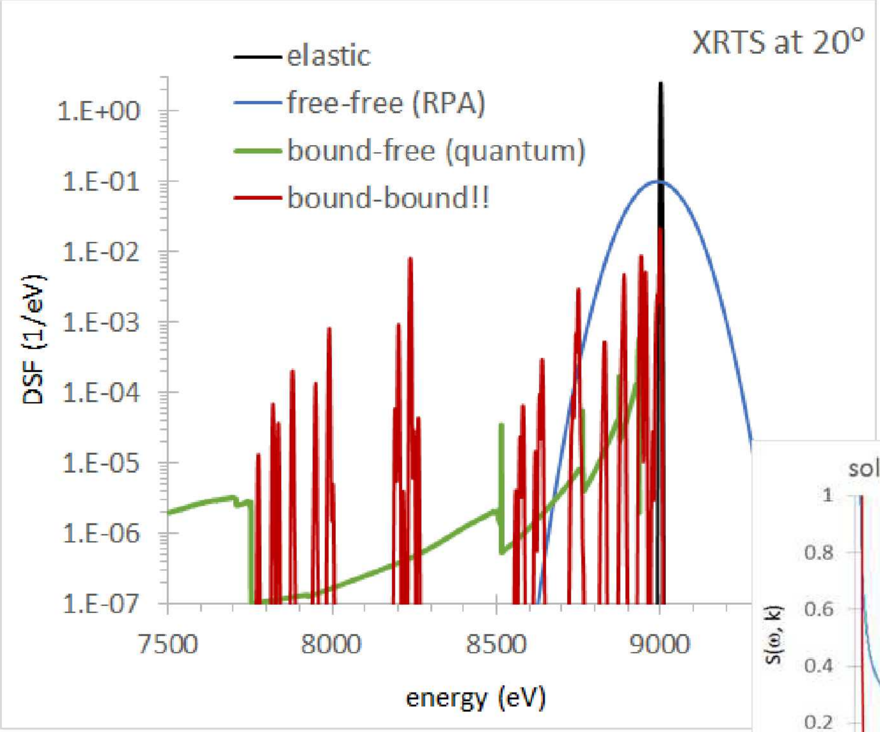
*Institut für Physik, Universität Rostock, Universitätsplatz 3, D-18051 Rostock, Germany*

Chihara, J. Phys. F **17**, 295 (1987); *c.f.* Baczewski *et al* PRL 116, 115004 (2016)

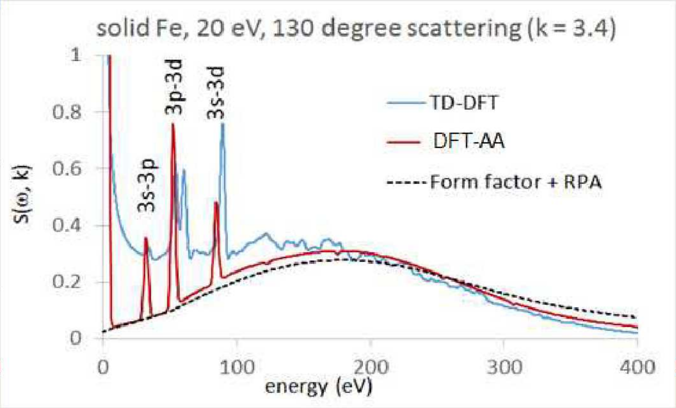
# The Chihara decomposition is not adequate for all HEDP (but we'll exclude b-b in the projects)

$$S(k,\omega) = \underbrace{|f_I(k) + q(k)|^2 S_{ii}(k,\omega)}_{\text{elastic}}$$

$$+ \underbrace{\bar{Z} S_{ee}(k,\omega)}_{\text{free-free}} + \underbrace{S_{bf}(k,\omega)}_{\text{bound-free}} + \underbrace{S_{bb}(k,\omega)}_{\text{bound-bound}}$$

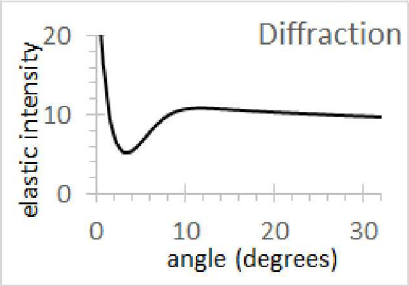


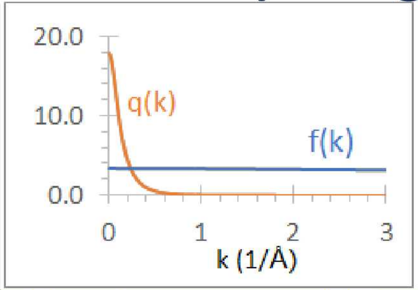

Hot plasmas are likely to have significant bound-bound contributions

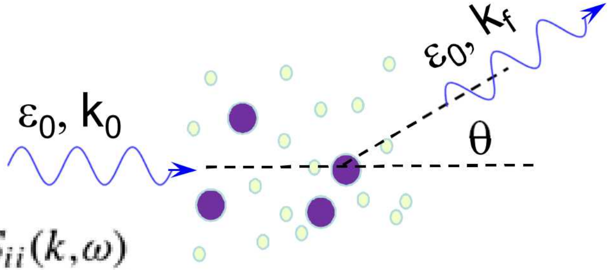



Baczewski *et al* PRL 116, 115004 (2016)

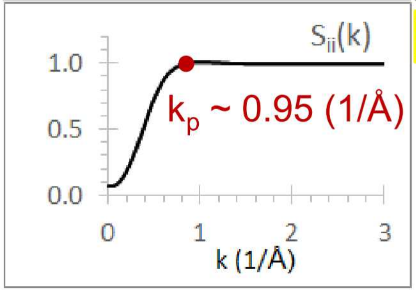
# The elastic scattering intensity depends on the angle/k and number (distribution) of tightly bound electrons



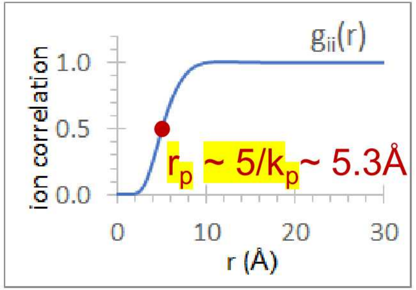

$$\underbrace{|f_I(k)+q(k)|^2 S_{ii}(k,\omega)}_{\text{elastic}}$$




$k_C(1/Å) \sim 0.51\sqrt{\varepsilon_C}(eV)$

Ion density can be estimated from the ion correlation function $g_{ii}(r)$, which is the transform of the ion structure factor $S_{ii}(k)$:

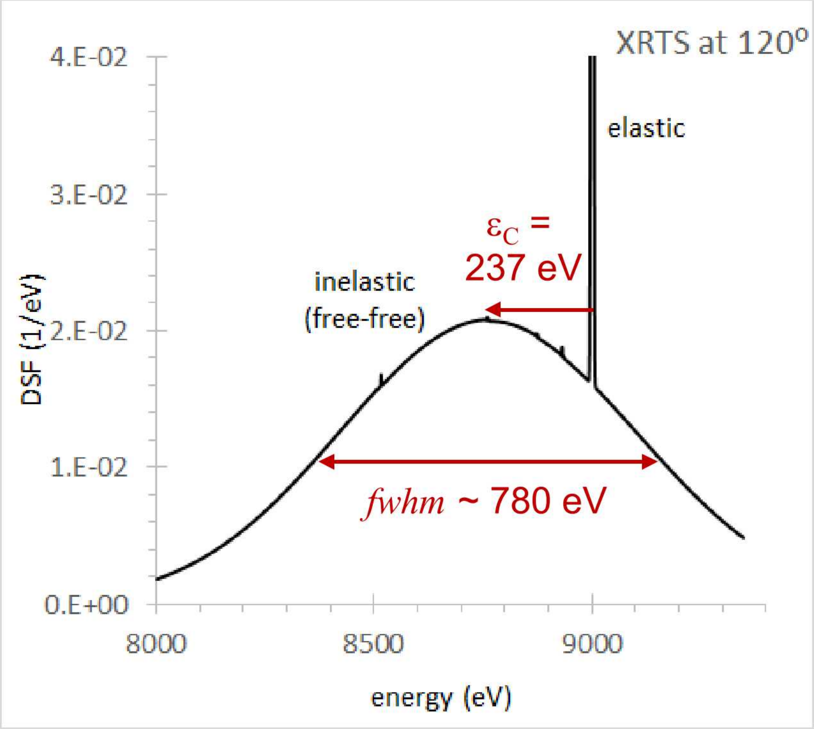
$3/(4\pi R^{*3}) = n_i \sim 2.4\text{x}10^{23} / r_p(Å)^3$ ion/cm$^3$

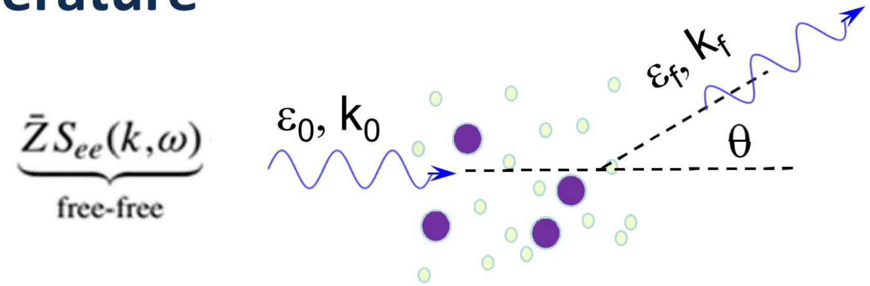



Here, $n_i \sim 1.6\text{x}10^{21}$ e/cm$^3$ (actual is $1.4\text{x}10^{21}$)

<u>Caution</u>: it's not always easy to locate the first diffraction peak, and small errors in $r_p$ are amplified

# Inelastic scattering from free electrons samples their velocity distribution, indicating temperature




Scattered photons are Compton shifted and Doppler broadened by plasma electrons:

$$\varepsilon_f \sim \varepsilon_0 - \varepsilon_C +/- \varepsilon_p$$

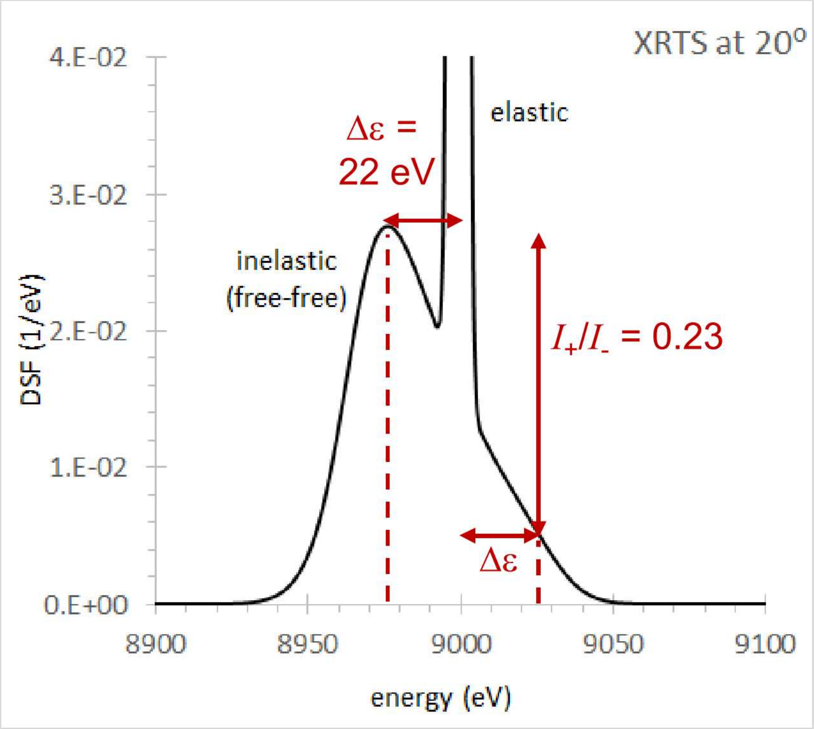
$$\varepsilon_C \text{ (eV)} \sim 1.96\, \varepsilon_0^2 (1 - \cos\theta);\ \varepsilon_0 \text{ in } \underline{\text{keV}}$$

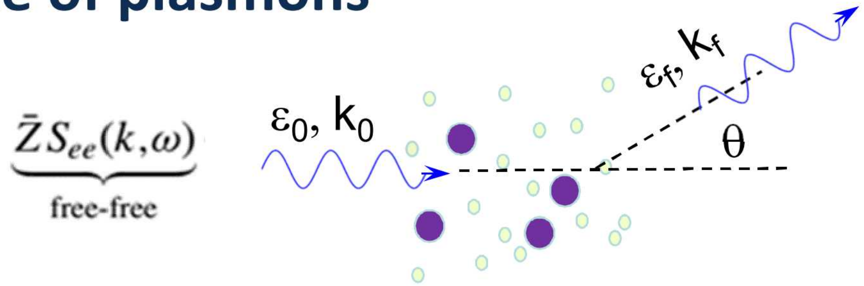
$$\varepsilon_p = \max(T_e, \varepsilon_{Fermi})$$

$$fwhm_{f\text{-}f} \sim \pi(\varepsilon_C \varepsilon_p)^{1/2}$$

Here, $T_e$ ~ 260 eV (actual is 250)

# Collective scattering from free electrons can indicate temperature through detailed balance of plasmons



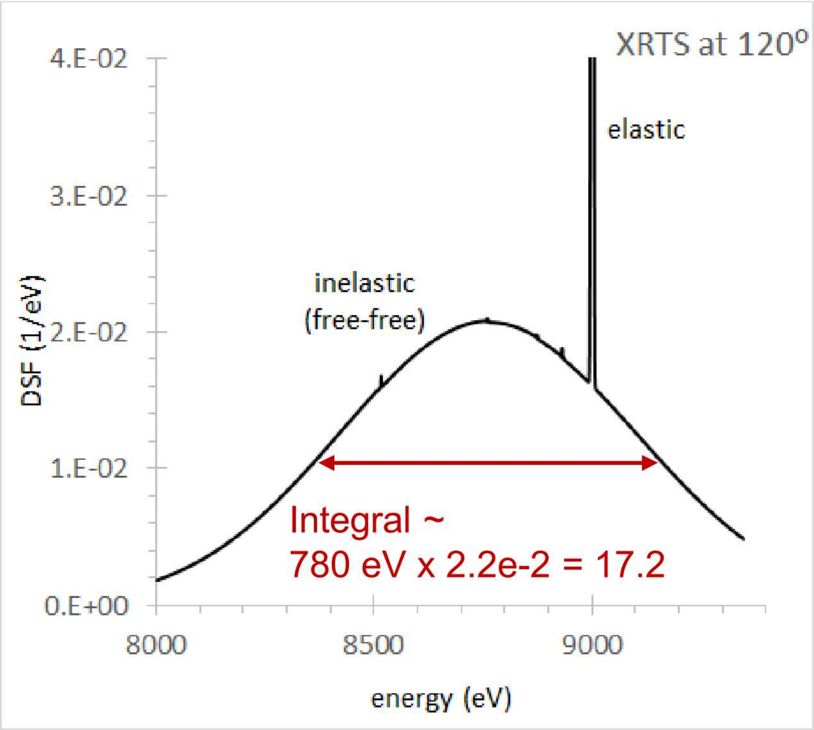




Collective plasma waves (plasmons) exchange energy with the photon beam following $| \{1 - \exp(\Delta\varepsilon/T_e)\}^{-1} |$

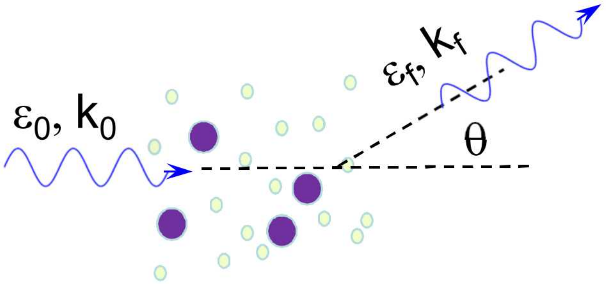
$T_e \sim \frac{1}{2}\,\Delta\varepsilon\,\ln(I_+/I_-)$

Here, $T_e \sim 16$ eV (actual is 15)

# The integral of the free-free feature can determine Z*




$$\underbrace{\bar{Z} S_{ee}(k,\omega)}_{\text{free-free}}$$



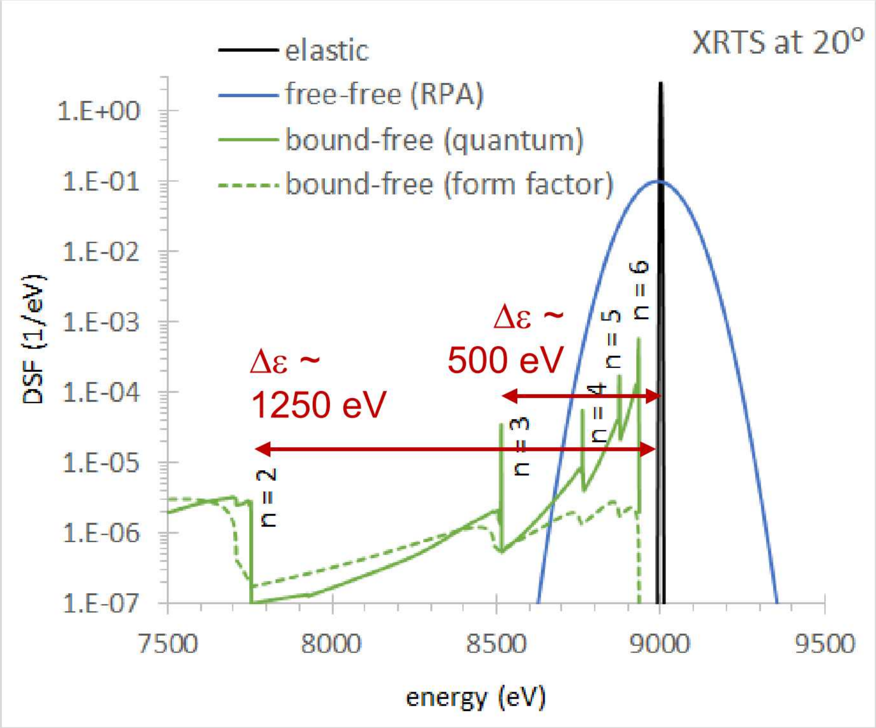

In absolutely calibrated data, sum rules ensure that $\int DSF_{ff}(\varepsilon)\, d\varepsilon = Z^*$

Here, Z* ~ 17.2 (actual is 17.7)

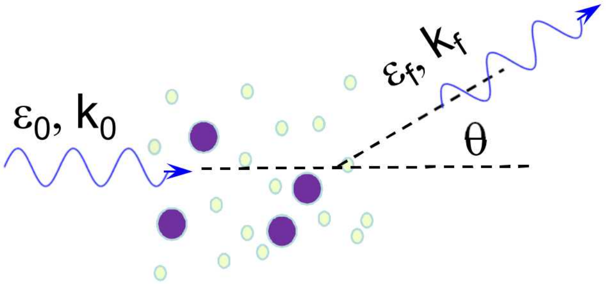
A trusted elastic feature can also be used to normalize the Z* integral

$$\underbrace{|f_I(k) + q(k)|^2 S_{ii}(k,\omega)}_{\text{elastic}}$$

# Bound-free edges can help identify constituent elements but do not discriminate as well as lines (would)




$$\underbrace{S_{bf}(k,\omega)}_{\text{bound-free}}$$




Only $\Delta\varepsilon > \varepsilon_n$ can give rise to bound-free (ionization) scattering

$$\varepsilon_n \sim 13.6 \text{ eV } (Z_{eff}/n)^2$$

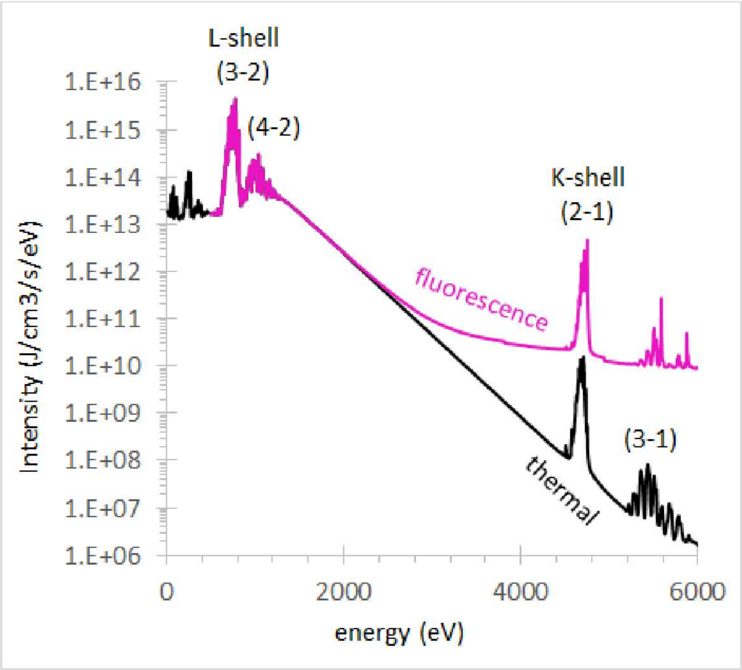
$$Z_{eff} \sim \max[Z^*, Z_{nuc} - \Sigma_1^{(n-1)}(2n^2)]$$

For $Z_{nuc}$ = 21, 22, 23, $\varepsilon_2$ = 1230, 1360, 1500 eV and for all three elements $\varepsilon_3$ = 450 eV → Sc? Ti?

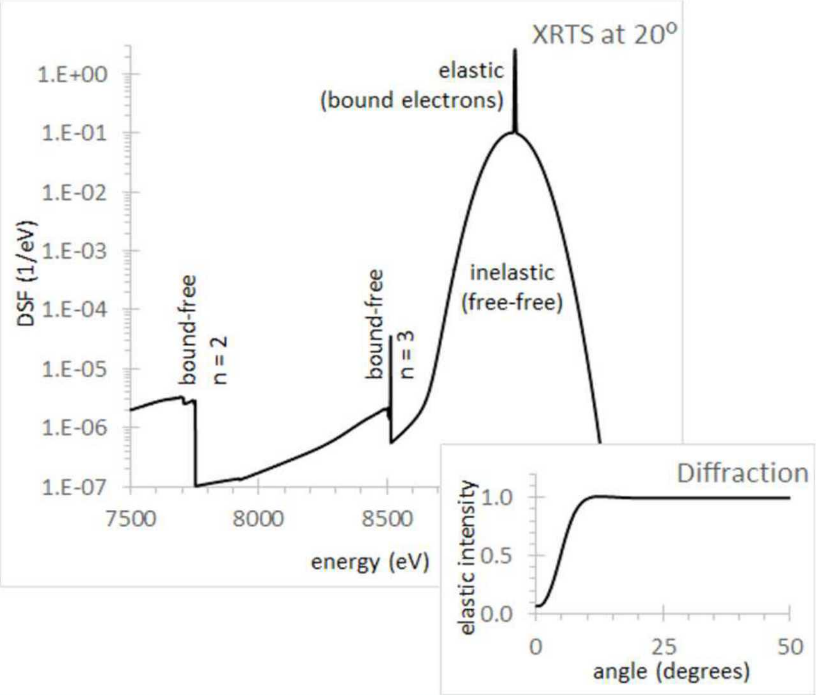
Caution: *n* may not be self-evident

# Projects: Diagnose $Z_{nuc}$, $Z^*$, $n_i$, $T_e$ from a "mystery" plasma using one of two synthetic data sets:

**1. X-ray spectroscopy:**
**Thermal or fluorescence emission; transmission spectra**




**2. X-ray scattering:**
**20 and 120 scattering signals; diffraction data**




*Fluorescence from 9 keV XFEL at $10^{16}$ W/cm$^2$

# First synthetic data sets have restricted dynamic range, degraded resolution, and missing information

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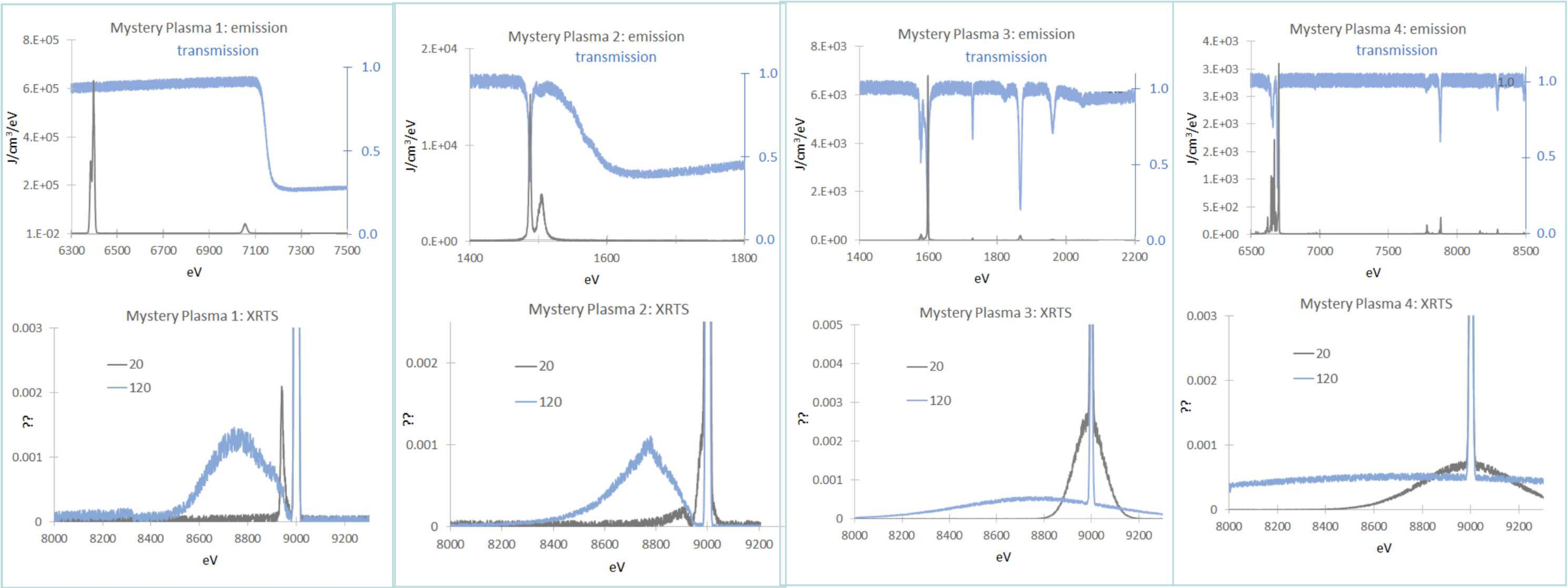


Next week we'll provide emission duration, absorption depth, XRTS units, and diffraction data plus infinite resolution and dynamic range

# Summary!

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## X-ray spectroscopy

free-bound: $T_e \sim (\varepsilon_1 - \varepsilon_2)/\ln(I_2/I_1)$

$I_{f\text{-}b}(\varepsilon) \sim 4e\text{-}31\ T_e^{-3/2}\ Z^{*4}\ n_i^2 \exp[(\varepsilon_{edge} - \varepsilon)/T_e]$

*(absolute units Monday!)*

$hwhm_{edge} \sim T_e$ (degenerate)

bound-bound:

$\varepsilon_{K\text{-}line} \sim \tfrac{3}{4}\ 13.6\ \mathrm{eV}\ (Z_{nuc}-1)^2$

$T_e \sim Z^{*3}/Z_{nuc}$

$fwhm_{K\beta} \sim 40\mathrm{eV} / Z_{nuc}\ (n_e/10^{22})^{0.58}$

$n_e = n_i/Z^*$

Transmission = $\exp(-n_i \sigma x)$

*($x$ Monday!)*

## X-ray scattering

$k_C(1/\text{Å}) \sim 0.51\sqrt{\varepsilon_C(\mathrm{eV})}$

elastic: $n_i \sim 2.4\mathrm{x}10^{23} / r_p(\text{Å})^3\ /\mathrm{cm}^3$

*(diffraction Monday!)* $r_p \sim 5/k_p$

free-free: $Z^* = \int DSF_{ff}(\varepsilon)\, d\varepsilon$

*(absolute units Monday!)*

$T_e \sim \tfrac{1}{2}\, \Delta\varepsilon\, \ln(I_+ / I_-)$ (collective)

$fwhm_{f\text{-}f} \sim \pi(\varepsilon_C T_e)^{1/2}$

for $\varepsilon_C \sim 1.96\ \varepsilon_0^2(1 - \cos\theta)$

free-bound: $\varepsilon_n \sim 13.6\ \mathrm{eV}\ (Z_{eff}/n)^2$

$Z_{eff} \sim \max[Z^*, Z_{nuc} - \Sigma_1^{(n-1)}(2n^2)]$

bound-bound neglected in synthetic data