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3rd EMMI Workshop on Plasma Physics

with Intense Laser and Heavy Ion Beams

K-alpha Spectra from Laser-Produced Solid-Density Plasmas

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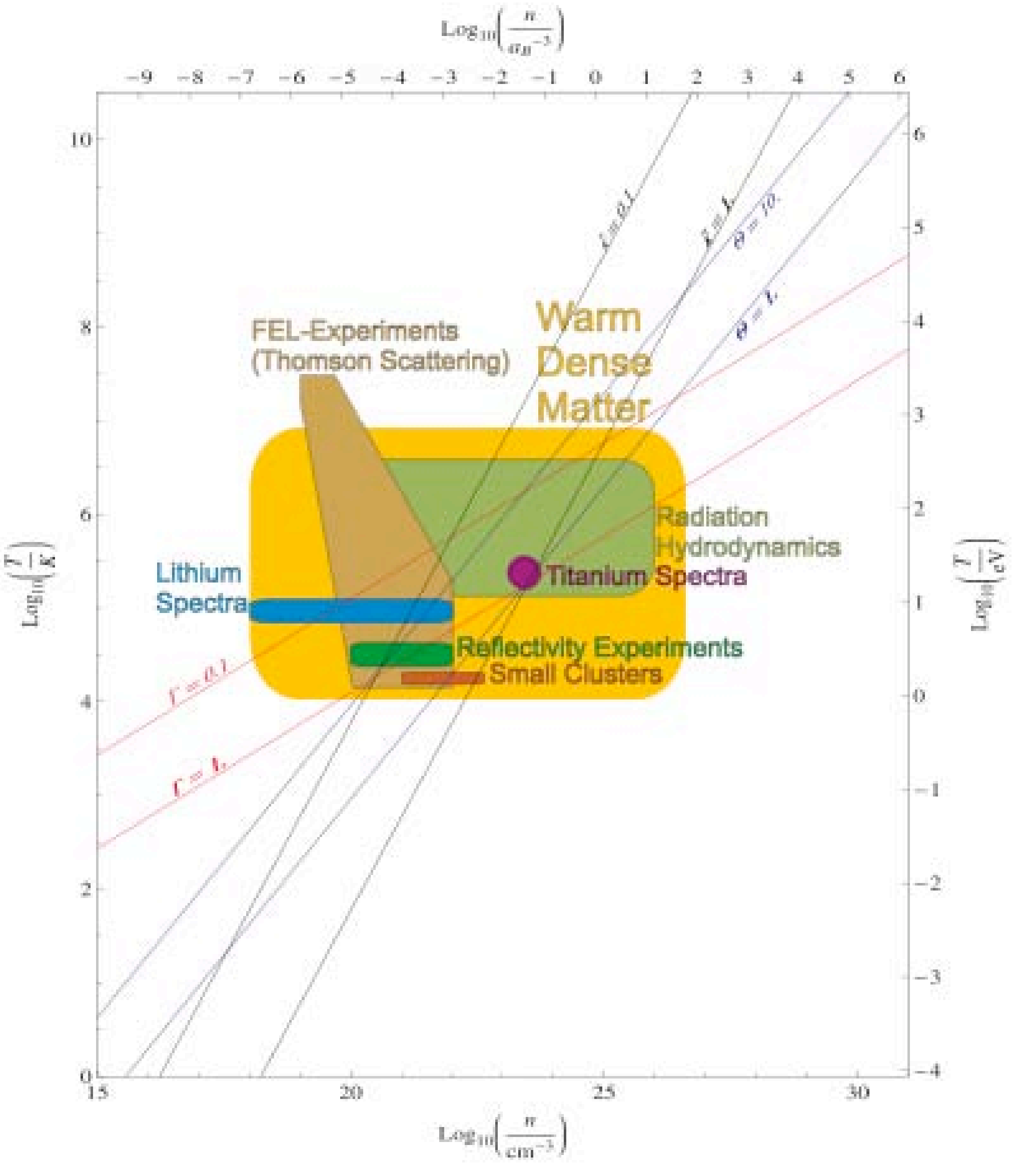
Rostock University

Outline

- Warm dense matter
- Line spectra, profiles
- X-ray spectroscopy and K-alpha lines
- The Titanium K-alpha experiment at LULI

The Plasma Phase Diagram



Research Activities in Our Rostock Central Research Unit

- experimental investigations of matter under extreme conditions using X-ray laser, intense short pulse laser, electric or magnetic fields
  ⇒ production/excitation, and diagnostics of warm dense matter
- Many–body theory
  ⇒ kinetic equations, linear response, molecular dynamics simulations
- Applications
  ⇒ transport properties: conductivity, Hall effect
  ⇒ optical properties:
  reflectivity, bremsstrahlung, Thomson scattering,
  spectral lines - optical spectrum, X-ray emission lines
  ⇒ cluster physics: size dependent properties

SFB 652

Quantum Statistical Approach to Nonequilibrium

- statistical operator for generalized grand canonical ensemble by introducing set of relevant observables $\{B_n\}$

$$\rho_{\rm rel} = \frac{1}{Z_{\rm rel}} \mathrm{e}^{-[\hat{\mathcal{H}}-\mu N+\sum_n \Phi_n B_n]} \qquad \hat{\mathcal{H}} = \hat{\mathcal{H}}_{\rm eq} - \sum_c e_c \vec{R}_c \vec{E}$$

- self-consistency condition for response parameter Φ_n

$\boxed{\mathrm{Tr}\,(B_n \rho_{rel}) = \mathrm{Tr}\,(B_n \rho)}$ with statistical operator $\rho = \rho_{rel} + \rho_{irrel}$

- solution in linear response:

response equation containing equilibrium correlation functions/ generalized BOLTZMANN equation

$$\begin{aligned} \langle B_m; \dot{\vec{R}}_c \rangle e_c \vec{E} &= \sum_n \langle B_m; \dot{B}_n \rangle \Phi_n \\ \mathrm{Tr}\,\{B_n \rho\} &= \sum_m (B_n; B_m) \Phi_n \end{aligned}$$

Zubarev, Morozov, Röpke, Stat. Mech. of Non-equilibrium Processes, Berlin 1996

Fluctuation - Dissipation Theorem for Absorption

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equilibrium correlation functions

$$\langle A;B\rangle_z = \int_0^\infty dt\, e^{izt}\,(A(t);B) = -\frac{i}{\beta}\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\,\frac{1}{z-\omega}\,\frac{1}{\omega}\,\mathrm{Im}\,G_{AB^+}(\omega-i0)$$

$$(A(t);B) = \frac{1}{\beta}\int_0^\infty d\tau\,\mathrm{Tr}\left[A(t-i\hbar\tau)\,B^+\,\rho_0\right]$$

- application to electrical current density using set $\{B_n\} = \vec{P} = m_e\dot{\vec{R}}$

$$\vec{J} = \left\langle\vec{j}\right\rangle = \mathrm{Tr}\left\{\rho\vec{j}\right\} = \frac{e}{\Omega}\mathrm{Tr}\left\{\rho\dot{\vec{R}}\right\} = \frac{e}{\Omega\, m_e}\mathrm{Tr}\left\{\rho_{\mathrm{rel}}\vec{P}\right\} = \sigma\vec{E}$$

- solution for electrical conductivity

$$\sigma = \beta\Omega\langle j;j\rangle = \frac{\beta e^2}{\Omega\, m_e}\,\frac{(P;P)^2}{\langle\dot{P};\dot{P}\rangle}$$

Kubo-Greenwood formula ⟺ force force correlation functions

$(\dot{P} = F_{ei} + F_{ee} + F_{ea})$

Röpke, Meister, Ann. Phys. ***36*** *(1979) 377; Röpke, PRA* ***38*** *(1988) 3001; Reinholz et al. , PRE 52 (1995) 6368*

Optical Properties

$$\boxed{\epsilon(\mathbf{k},\omega) = 1 + \frac{1}{\epsilon_0 k^2}\Pi(\mathbf{k},\omega) \qquad \Pi(\mathbf{k},\omega) = \Pi_1(\mathbf{k},\omega) + \Pi_2(\mathbf{k},\omega) + \ldots}$$

- polarization function $\Pi(\mathbf{k},\omega)$ from many-body theory using cluster decomposition
  - $\Pi_1(\mathbf{k},\omega)$ - single-particle contribution[1]
  - $\Pi_2(\mathbf{k},\omega)$ - two-particle contributions (bound states) [2]
- optical information: refraction index & absorption coefficient
  - $\Pi_1(\mathbf{k},\omega)$ - bremsstrahlung [1,3], $\Pi_2(\mathbf{k},\omega)$ - spectral line profiles [2]

$$\lim_{k\to 0} \epsilon(\mathbf{k},\omega) = \left(n(\omega) + \frac{ic}{2\omega}\alpha(\omega)\right)^2$$

- dynamical structure factor [1] → Thomson scattering

$$S(\mathbf{k},\omega) = \frac{1}{\pi V(k)} \frac{1}{\mathrm{e}^{-\beta\hbar\omega} - 1} \mathrm{Im}\epsilon_l^{-1}(\mathbf{k},\omega)$$

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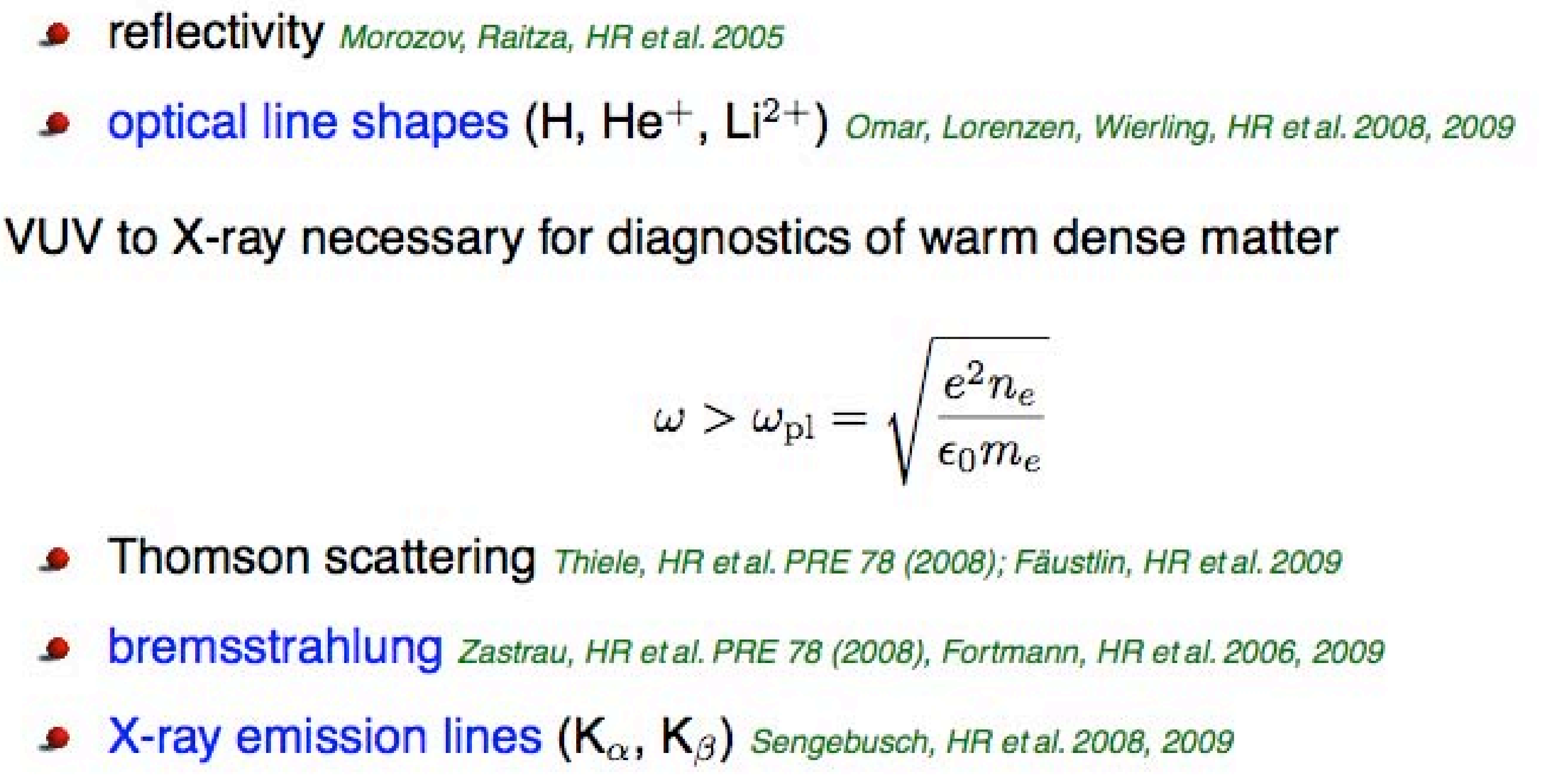
[1] Reinholz, Ann. de Phys. (2005); [2] Omar et al. PRE 2007; [3] Wierling et al. PoP (2001); Fortmann et al. HEDP

Some Applications



- reflectivity *Morozov, Raitza, HR et al. 2005*
- optical line shapes (H, He^{+}, Li^{2+}) *Omar, Lorenzen, Wierling, HR et al. 2008, 2009*

VUV to X-ray necessary for diagnostics of warm dense matter

$$\omega > \omega_{\mathrm{pl}} = \sqrt{\frac{e^2 n_e}{\epsilon_0 m_e}}$$

- Thomson scattering *Thiele, HR et al. PRE 78 (2008); Fäustlin, HR et al. 2009*
- bremsstrahlung *Zastrau, HR et al. PRE 78 (2008), Fortmann, HR et al. 2006, 2009*
- X-ray emission lines (K_α, K_β) *Sengebusch, HR et al. 2008, 2009*

X Ray Thomson Scattering

scattering cross section:

$$\frac{d^2\sigma}{d\Omega\, d\omega} = \sigma_{\mathrm{T}} \frac{k_1}{k_0} S(k,\omega)$$

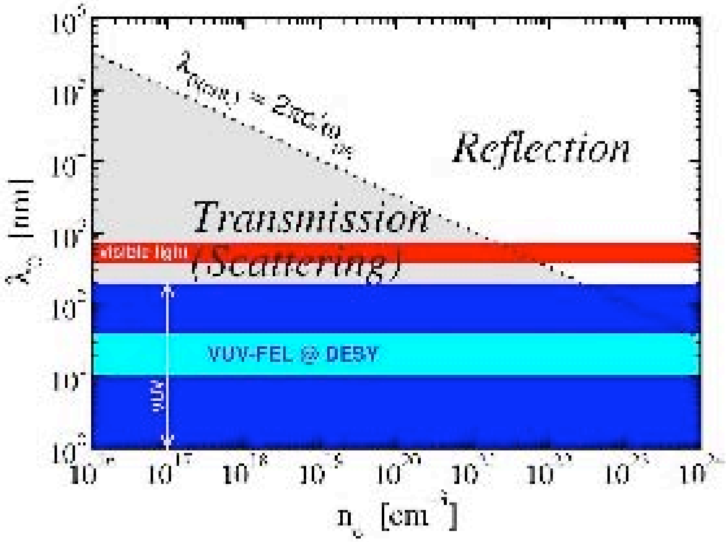
$$S_{ee}(\mathbf{k},\omega) = -\frac{\epsilon_0 \hbar k^2}{\pi e^2 n_{\mathrm{e}}} \frac{\mathrm{Im}\, \epsilon^{-1}(\mathbf{k},\omega)}{1-\exp\left(-\hbar\omega/k_{\mathrm{B}}T_{\mathrm{e}}\right)}$$

$\mathbf{k} = \mathbf{k}_0 - \mathbf{k}_1,\ \omega = \omega_0 - \omega_1$

$k_0 (k_1)$: incident (scattered) wavevector

$\sigma_{\mathrm{T}} = 8\pi\, r_{\mathrm{e}}^2/3$: Thomson cross section

$$S(k,\omega) = |f_{\mathrm{I}}(k) + q(k)|^2\, S_{\mathrm{ii}}(k,\omega) + Z_{\mathrm{f}} S_{\mathrm{ee}}(k,\omega) + Z_C \int d\omega'\, \widetilde{S}(k,\omega-\omega') S_{\mathrm{s}}(k,\omega')$$



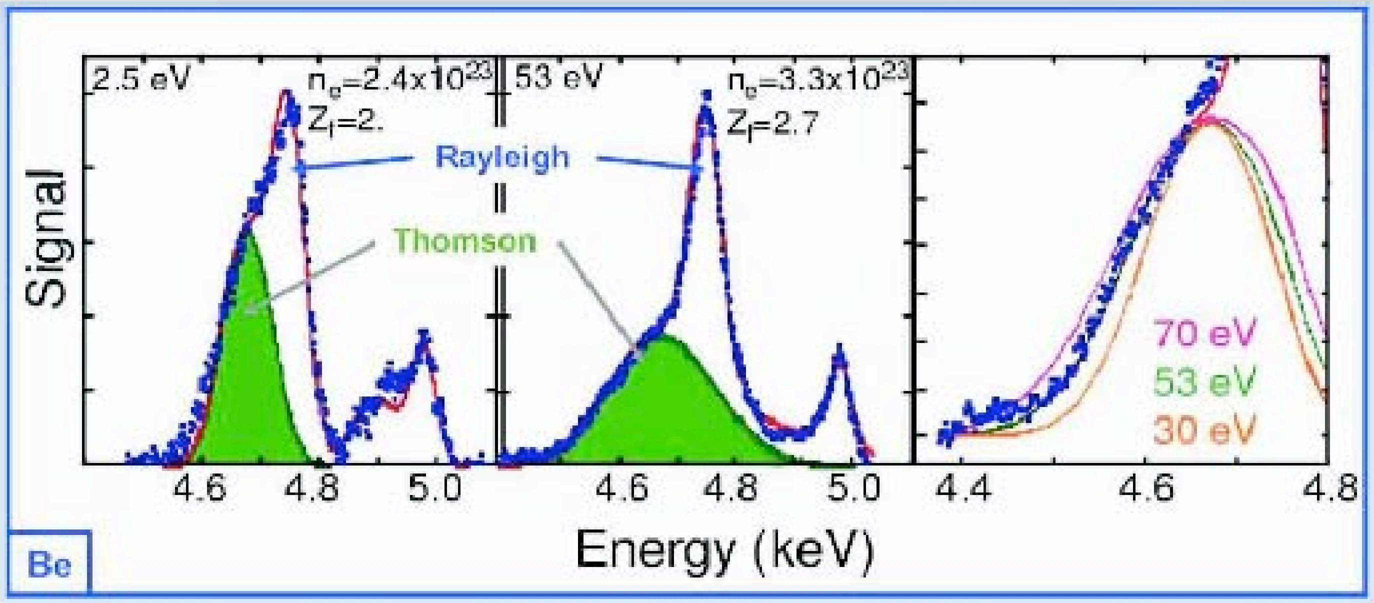
scattering parameter

$$\alpha = \frac{1}{k\lambda_D} \propto \frac{\lambda_0 \sqrt{n_{\mathrm{e}}}}{\sqrt{T}\sin\theta_S/2}$$

$\alpha > 1$ collective, $\alpha < 1$ non-collective

Fortmann, PhD thesis, Rostock 2008

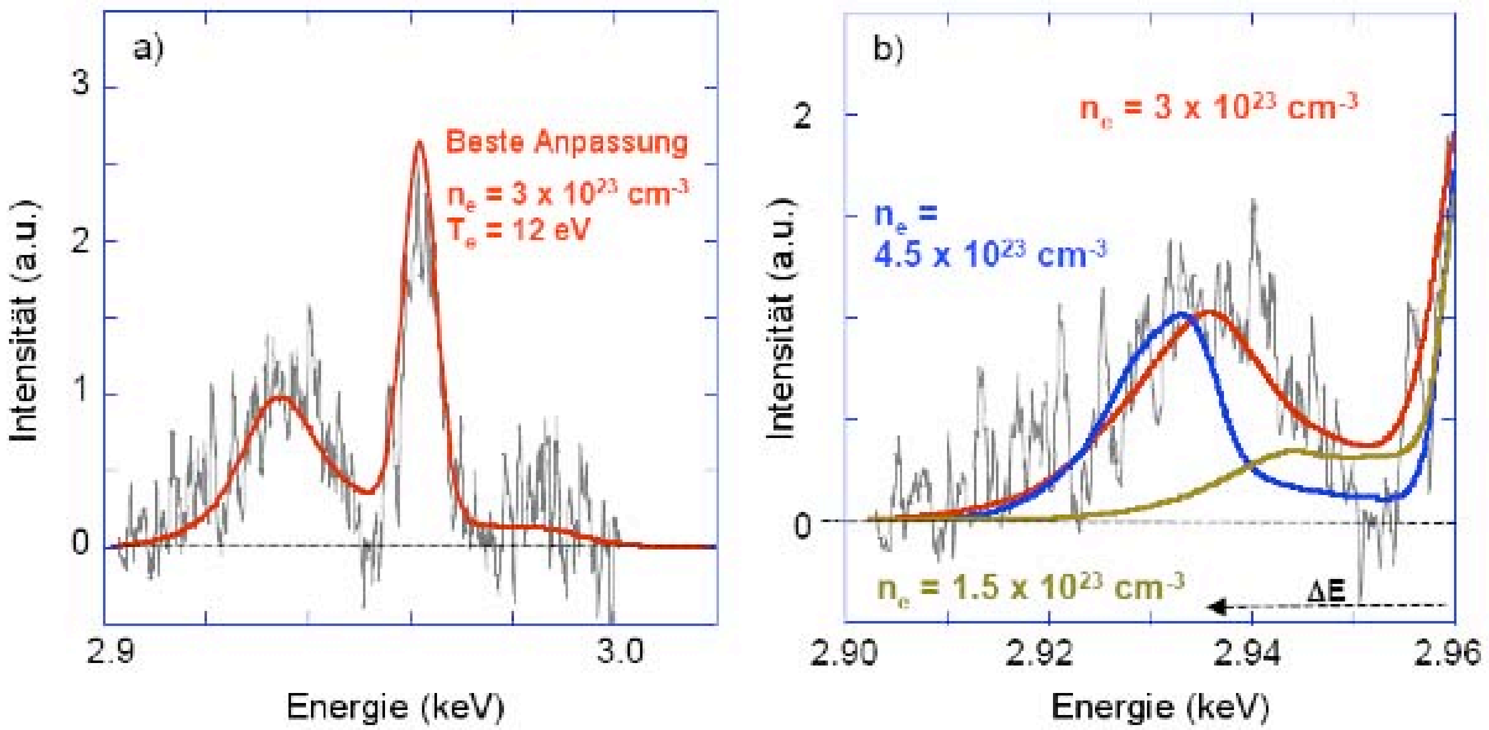
Plasmons in Beryllium Plasmas



Glenzer et al., PRL 90 (2003) 175002

- Experiment on Beryllium at 30 kJ Omega laser facility in Rochester
- heating: Rh X-ray (2.7 keV - 3.4 keV)
- scattering source: He-like Ti α-line (4.75 keV), scattering angle: $\Theta_S = 125°$

Plasma Parameters from Born - Mermin Fit



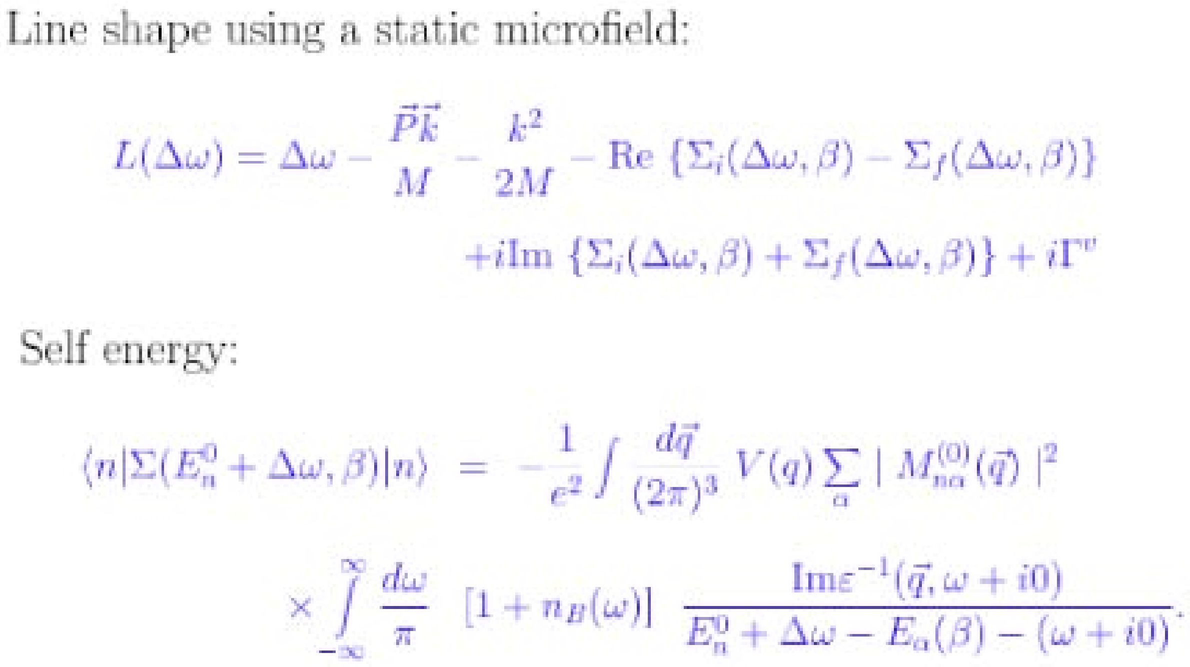
- Be with Cl Ly$_\alpha$ at E=2.96keV (λ_0 = 0.42 nm)
- scattering angle θ_s = 40°, $T_e = 12$ eV
- best fit of free electron density using Born-Mermin approximation

Glenzer et al. , PRL 98 (2007) 065002

Profiles of Spectral Lines

Absorption coefficient

from the quantum statistical evaluation of the polarization function



Line shape using a static microfield:

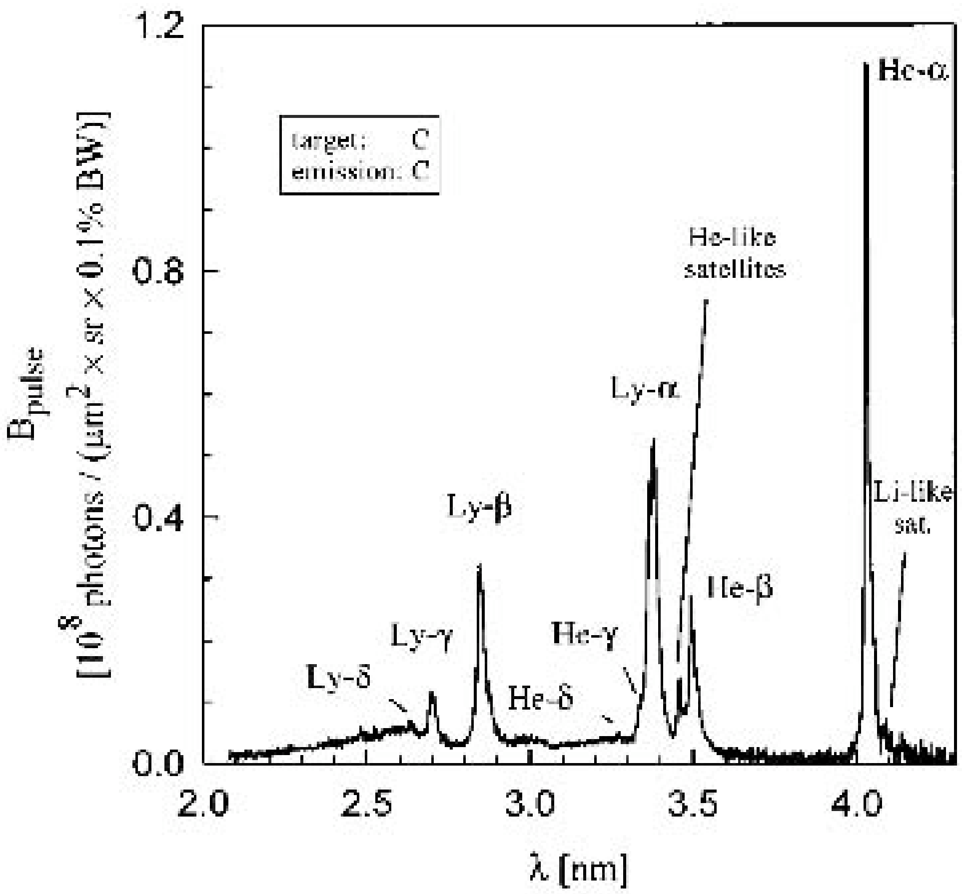
$$L(\Delta\omega) = \Delta\omega - \frac{\vec{P}\vec{k}}{M} - \frac{k^2}{2M} - \mathrm{Re}\,\{\Sigma_i(\Delta\omega,\beta) - \Sigma_f(\Delta\omega,\beta)\}$$
$$+i\mathrm{Im}\,\{\Sigma_i(\Delta\omega,\beta) + \Sigma_f(\Delta\omega,\beta)\} + i\Gamma^V$$

Self energy:

$$\langle n|\Sigma(E_n^0 + \Delta\omega,\beta)|n\rangle \;=\; -\frac{1}{e^2}\int\frac{d\vec{q}}{(2\pi)^3}\,V(q)\sum_\alpha |\,M_{n\alpha}^{(0)}(\vec{q})\,|^2$$
$$\times\int_{-\infty}^{\infty}\frac{d\omega}{\pi}\;[1+n_B(\omega)]\;\frac{\mathrm{Im}\varepsilon^{-1}(\vec{q},\omega+i0)}{E_n^0+\Delta\omega-E_\alpha(\beta)-(\omega+i0)}.$$

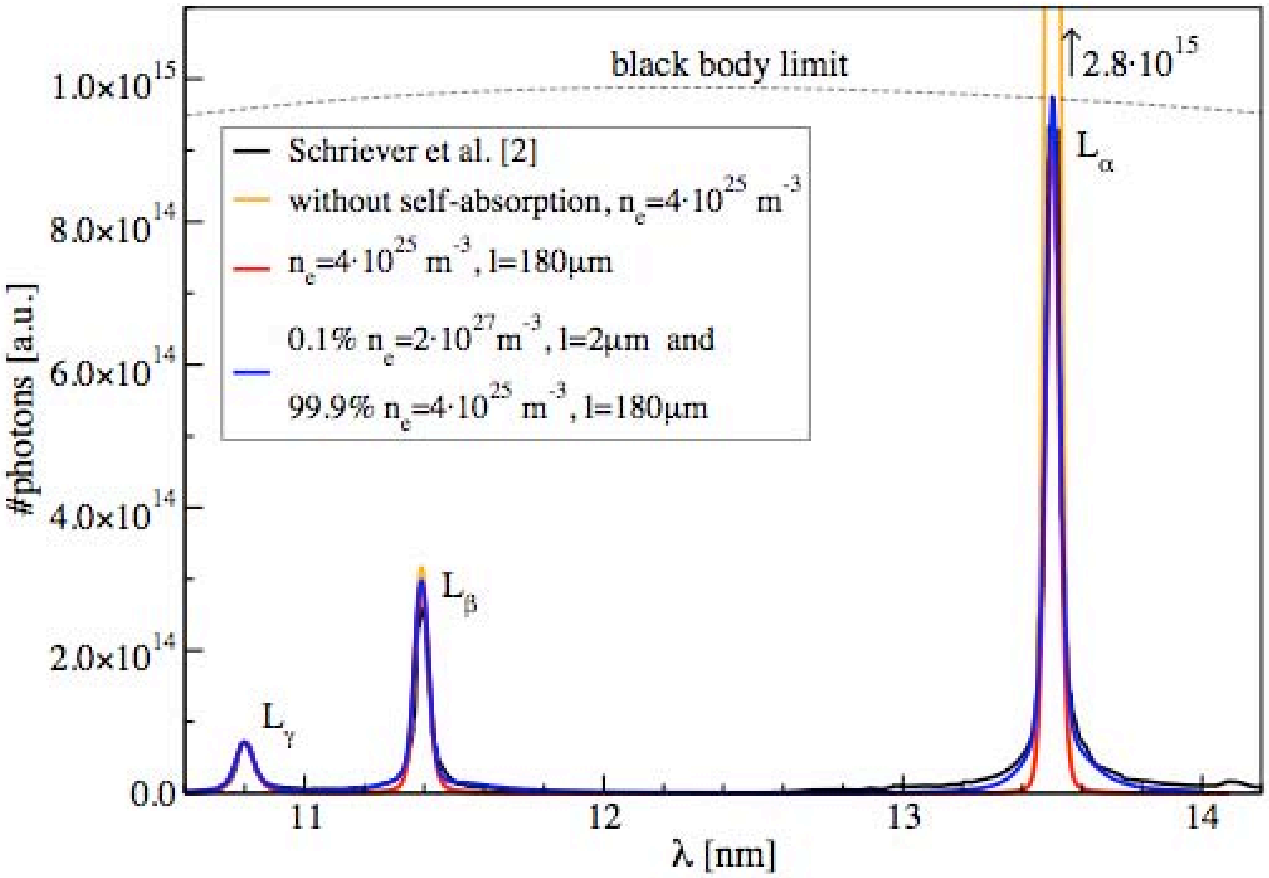
Hydrogen like Carbon spectrum

$$n_e = 4 \times 10^{22}\,\mathrm{cm}^{-3} \;,\; T = 90\,\mathrm{eV}$$



T. Wilhein, D. Altenbernd, U. Teubner, E. Förster, R. Häßner, W. Theobald, R. Sauerbrey, J. Opt. Soc. Am. B **15**, 1235 (1998)

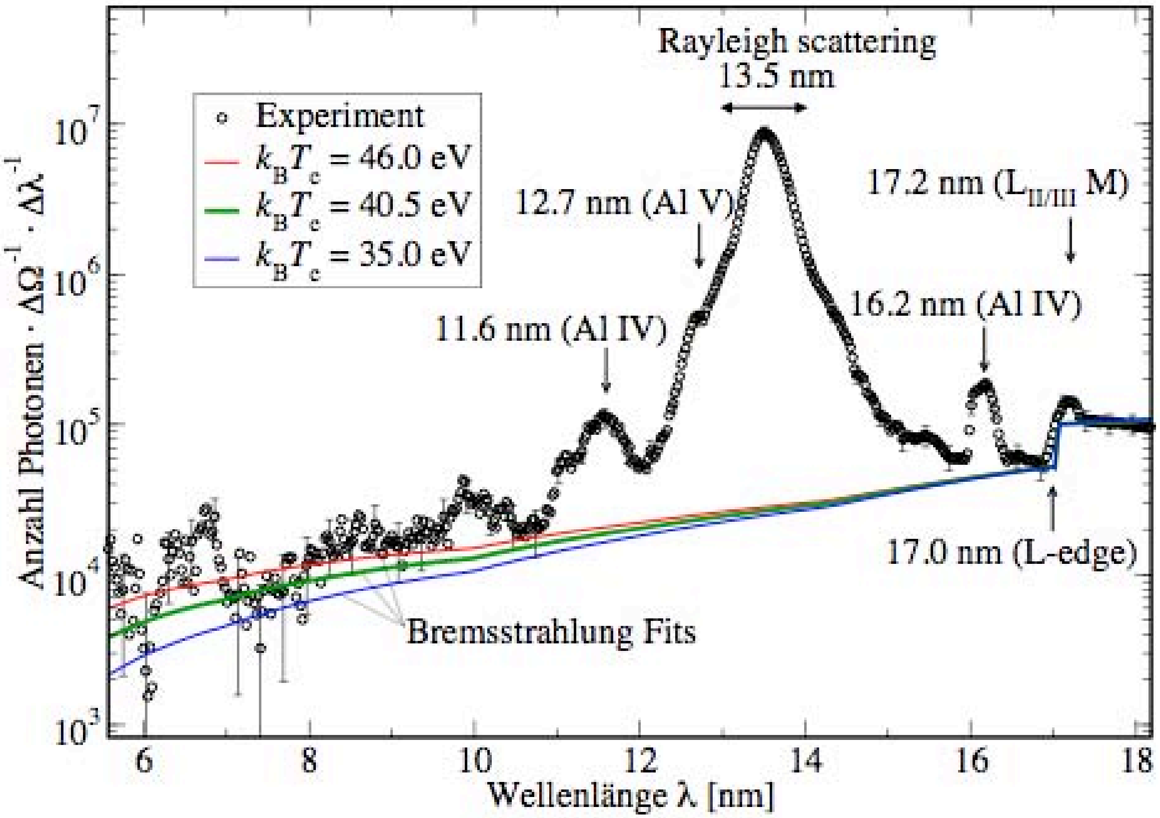
Line Spectrum of Li^{2+} Plasmas



- temperature $3 \cdot 10^5$ K determined via intensity ratio of L_β and L_γ lines
- consideration of self absorption for L_α line

S. Lorenzen et al., CPP **48** *(2008) 657, G. Schriever et al. , J. Appl. Phys.* **83** *(1998) 4566*

XUV - FEL Excited Al Plasmas



- emission spectrum of warm dense matter ($2 \cdot 10^{22}$ cm^{-3}) in XUV range
- temperature determined via intensity ratio of spectral lines as well as from bremsstrahlung ⇒ consistent results of $T = (40.5 \pm 5.5)$ eV

Zastrau et al., PRE **78** *(2008) 066406*

X-ray spectroscopy and K_{alpha} lines

- X-rays: diagnostic tool

- Experiment: Ti K_{alpha} emissions (LULI 100 TW)

- Theory: emitter + perturbing plasma
  - Ionization and polarization shifts
  - Synthetic spectra

- Analysis: Ti K_{alpha} emissions (LULI 100 TW)

Titanium K_{alpha} emission

Measured by Zastrau et al. at LULI (2008)

laser: up to 14 J at 1057 nm in 330 fs, d = 8 mu

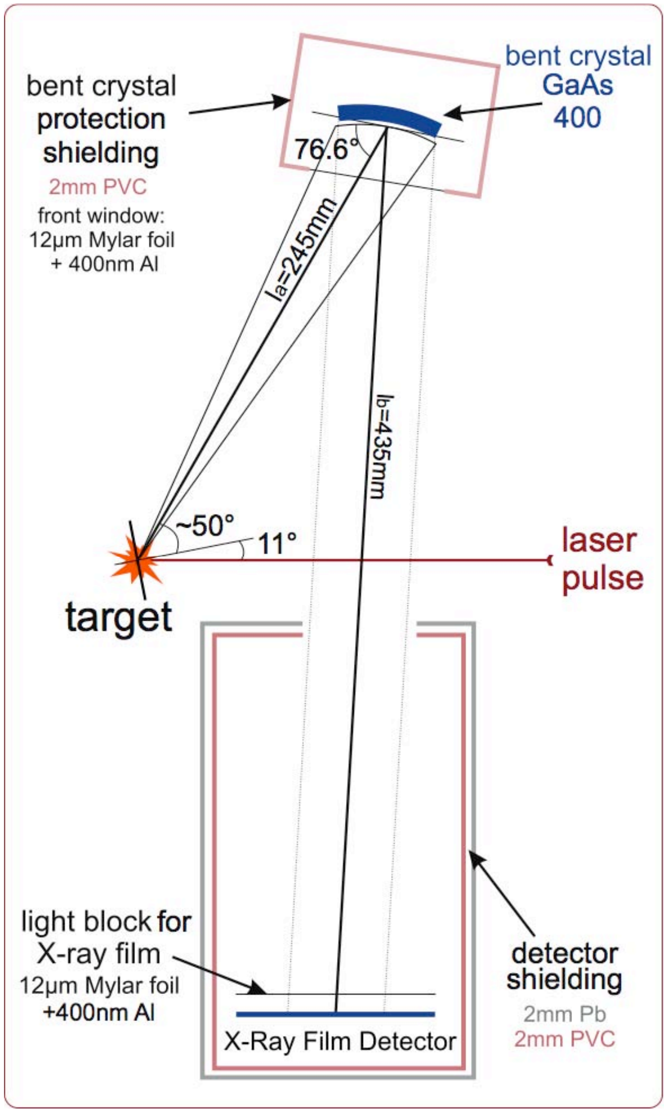
spectrometer: toroidal bent GaAs crystals,
resolution: E/Delta E = 15 000

targets: solid density titanium foils

spacial resolution: 13.5 mu

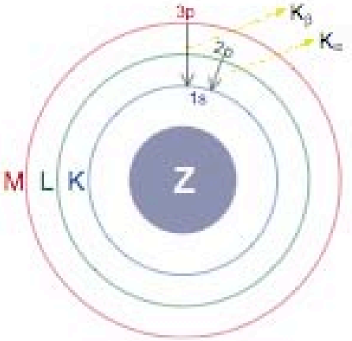
Abel deconvolution

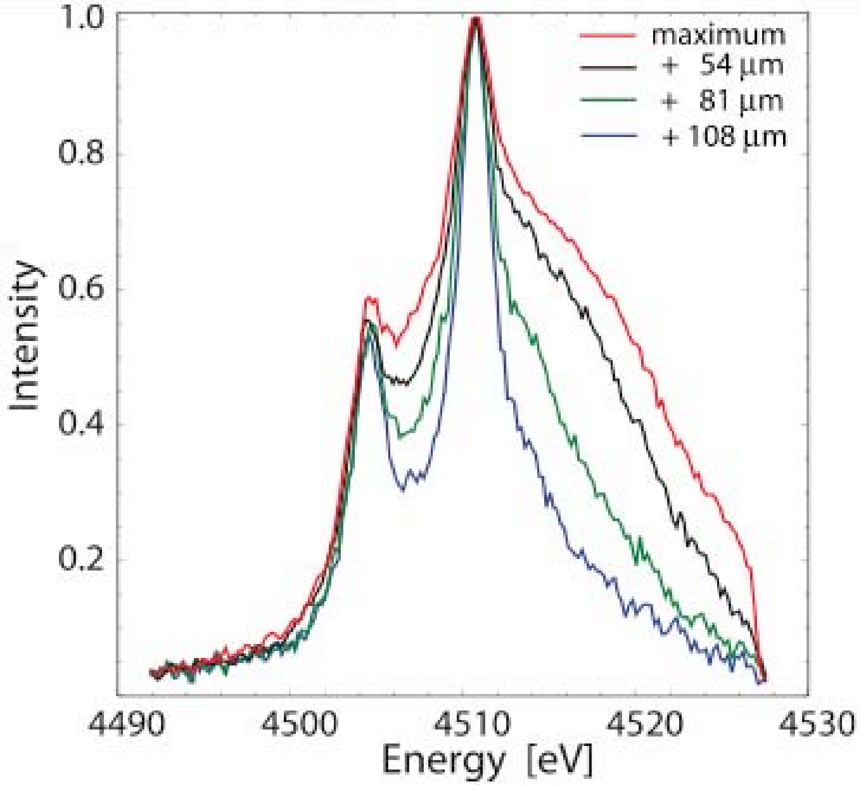
Phys. Rev. E 81, 026406 (2010)



X-Ray Plasma Diagnostics

- K_α lines of laser excited titanium plasma @ LULI
  $Z = 22, E_{K_\alpha} = 4.5$ keV





- line profile shifted and broadened with increasing temperature and free electron density as well as higher ionization stages
- considering radial distribution after deconvolution

Zastrau et al., FSU Jena (2008), Sengebusch et al., J. Phys. A accept. (2009)

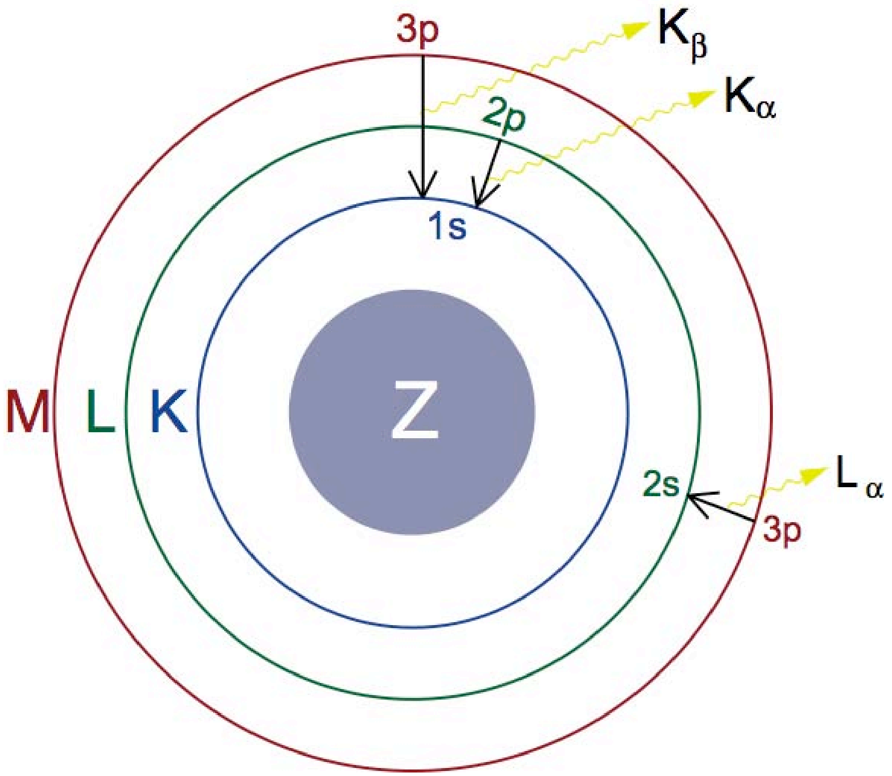
Characteristic X-Ray Emission

Mid-Z M-shell ions:
inner shell transitions

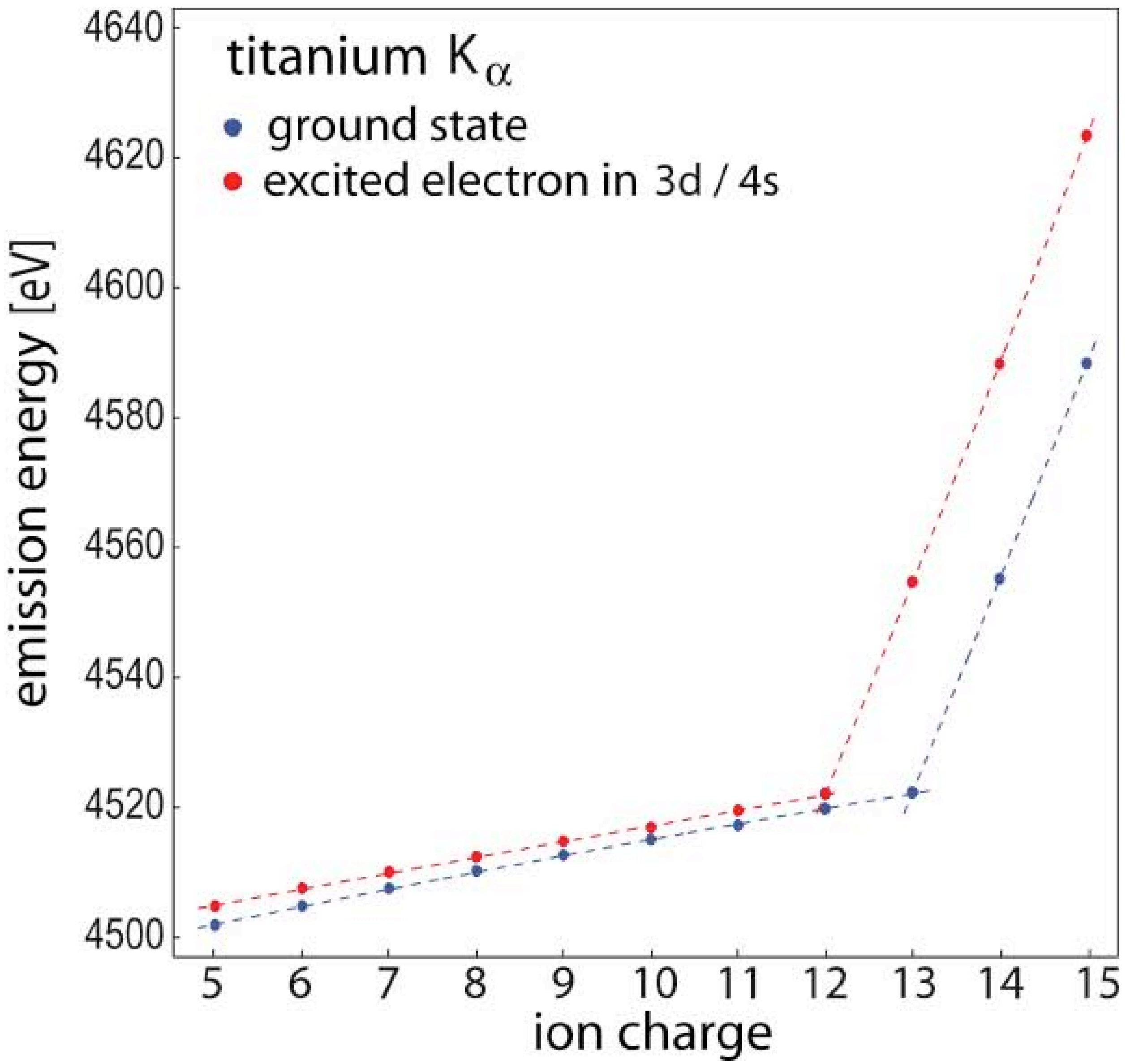
Roothan-Hartree Fock calculation,
depending on configuration

perturbing plasma potential,
self-consistent ion sphere model

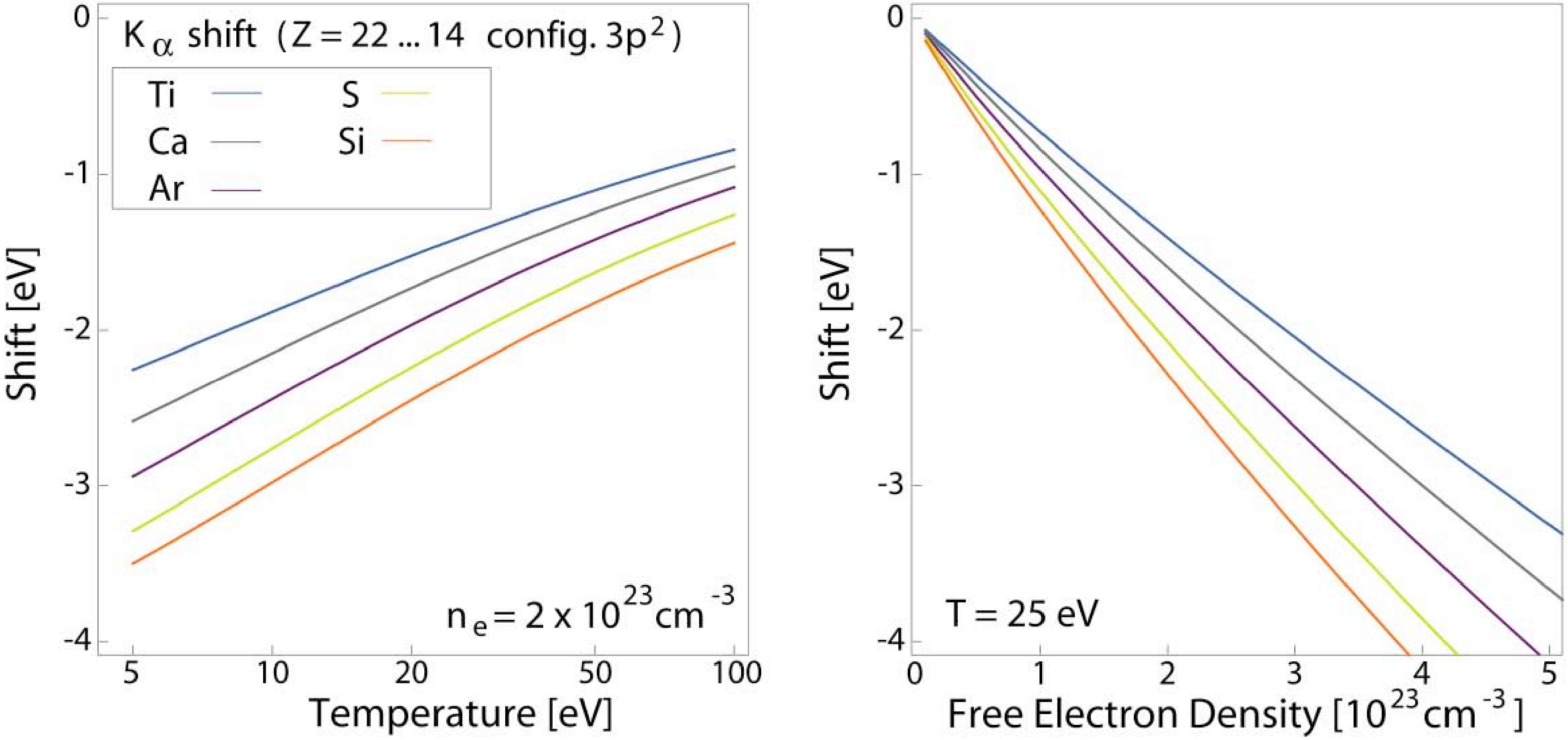
first order perturbation theory:
spectral line shift, continuum lowering



Ionization Blue Shift in Titanium



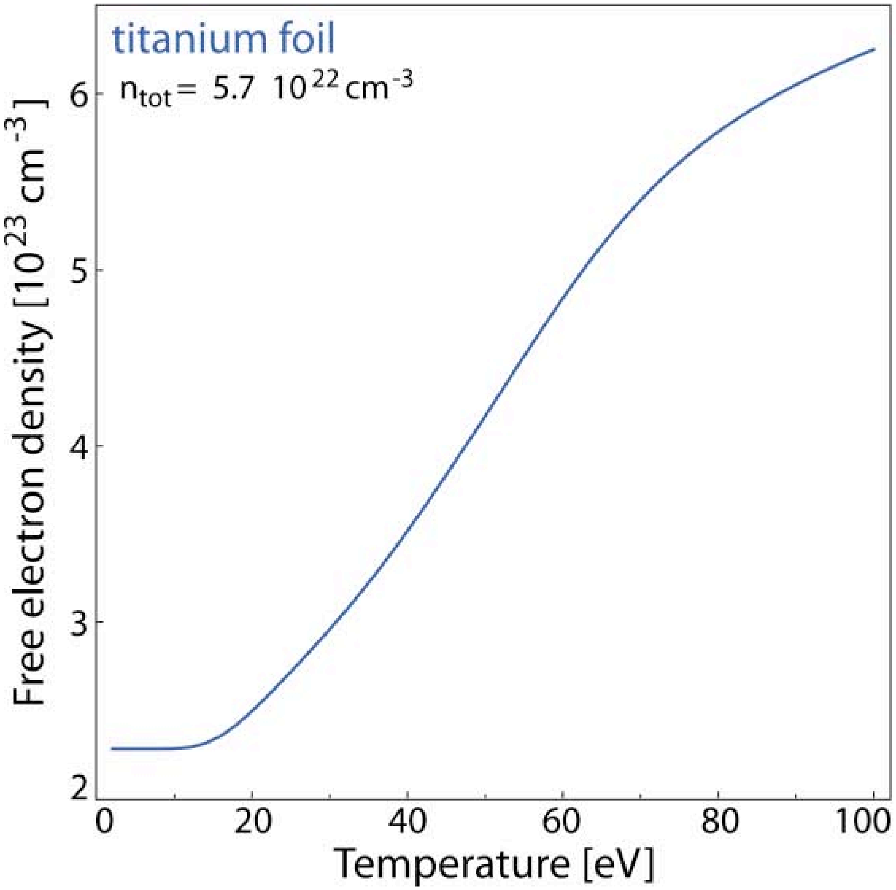
Polarization Shift of K_{alpha}

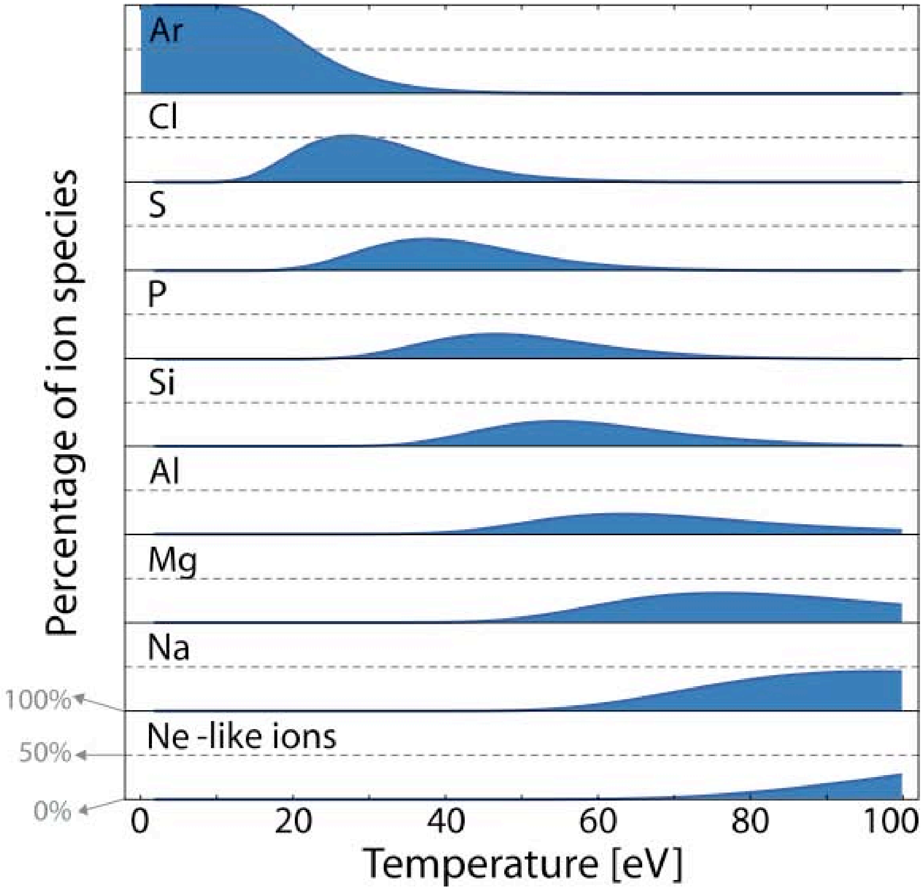


red shift due to screening

- decreases with increasing temperature or nuclear charge
- increases with increasing free electron density

Plasma Composition via Coupled Saha equations



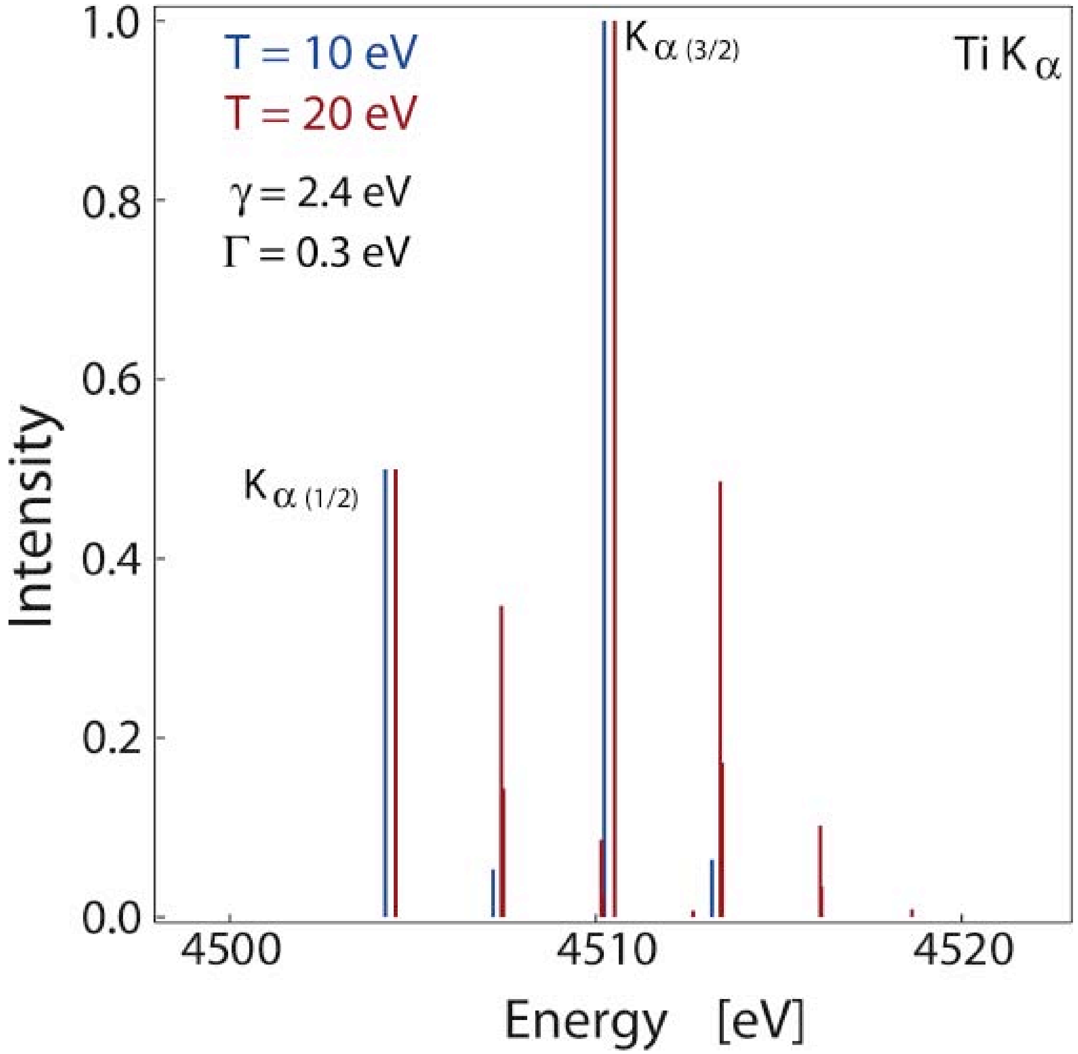


metallic titanium: conduction electrons + self-consistent ionization

Synthetic Spectra

-shifted spectral line positions

-relative intensities according to composition



Synthetic Spectra

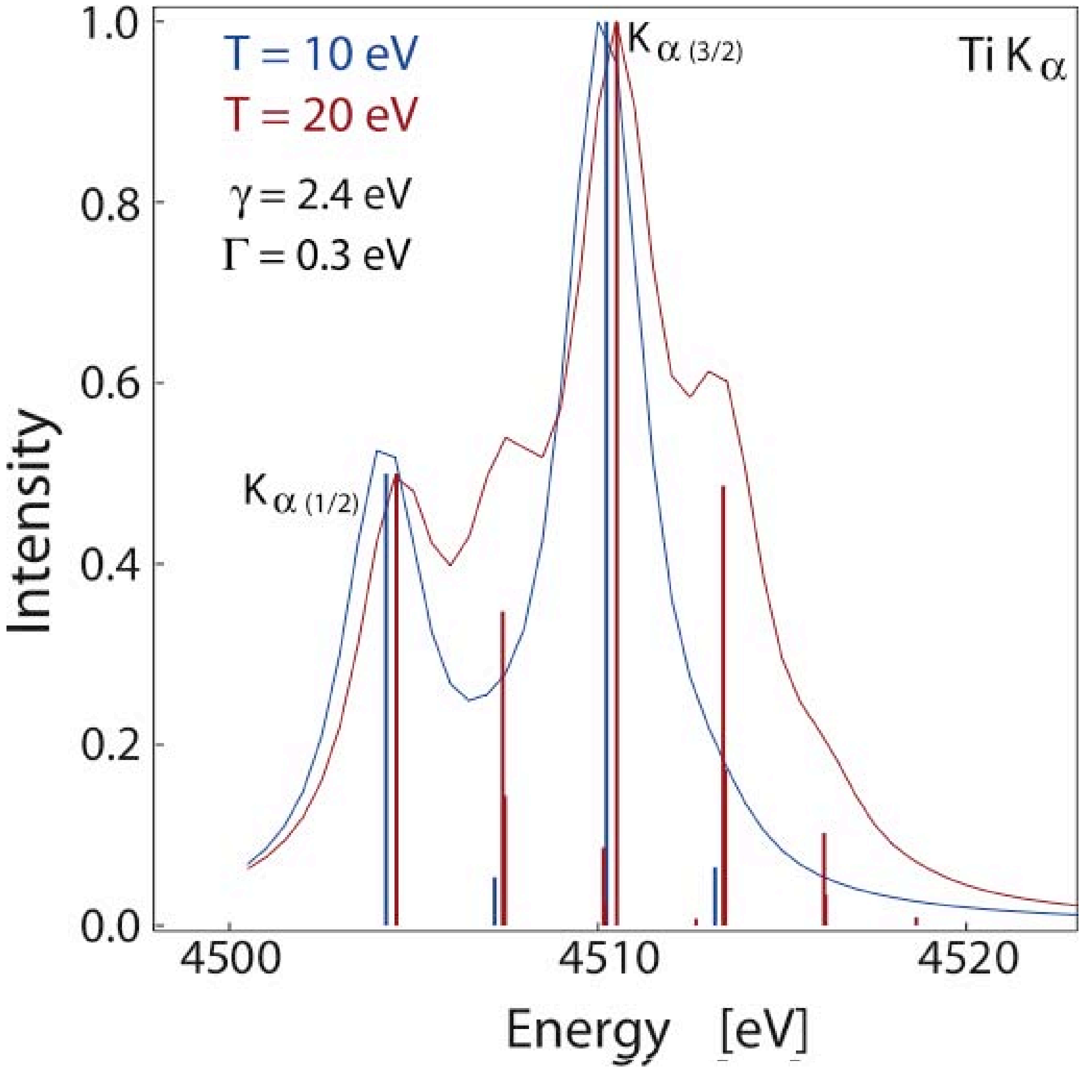
-shifted spectral line
positions

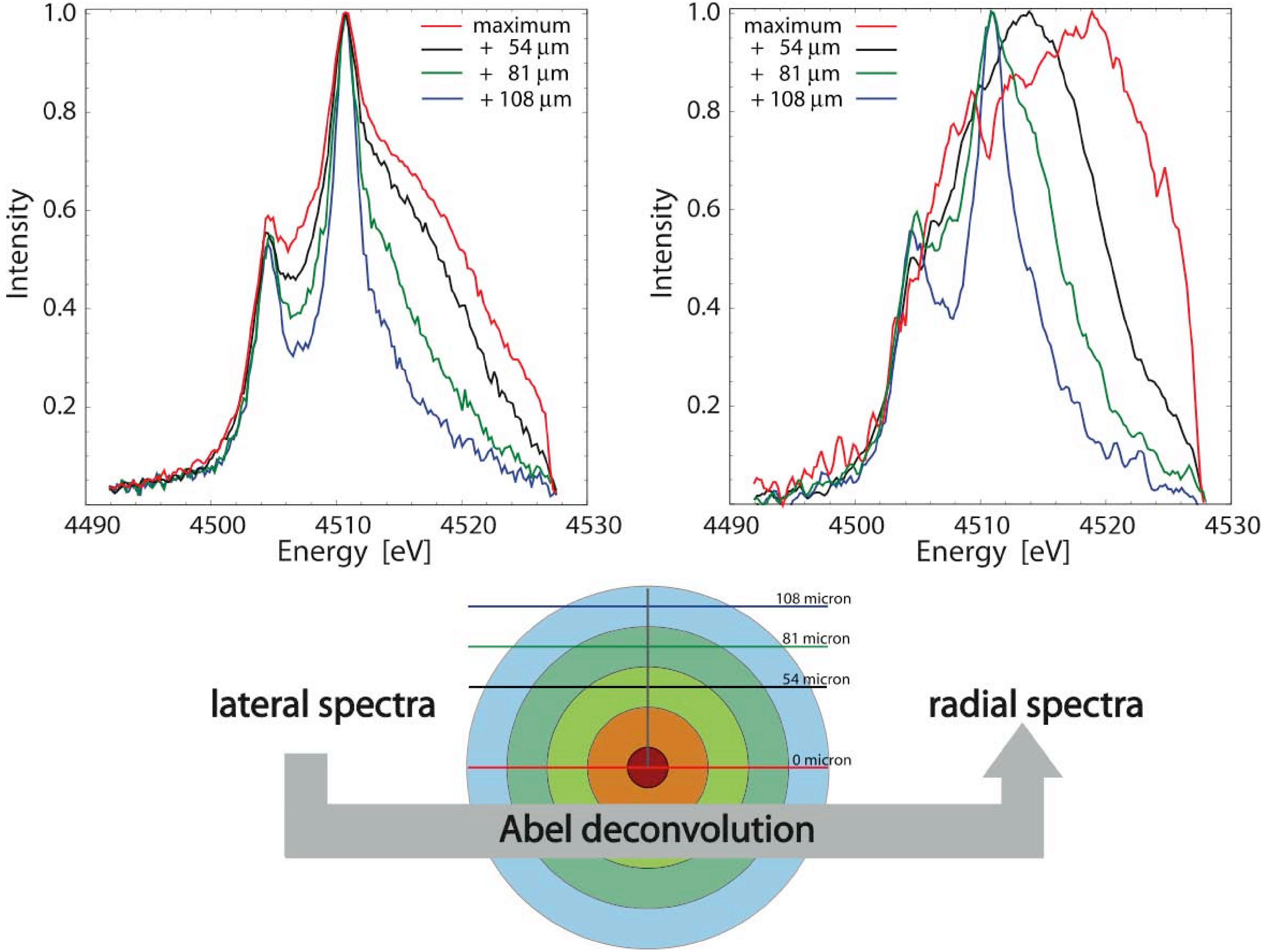
-relative intensities
according to composition

-Lorentzian line shape

empirical spectral line width

-Gaussian instrumental
broadening Gamma

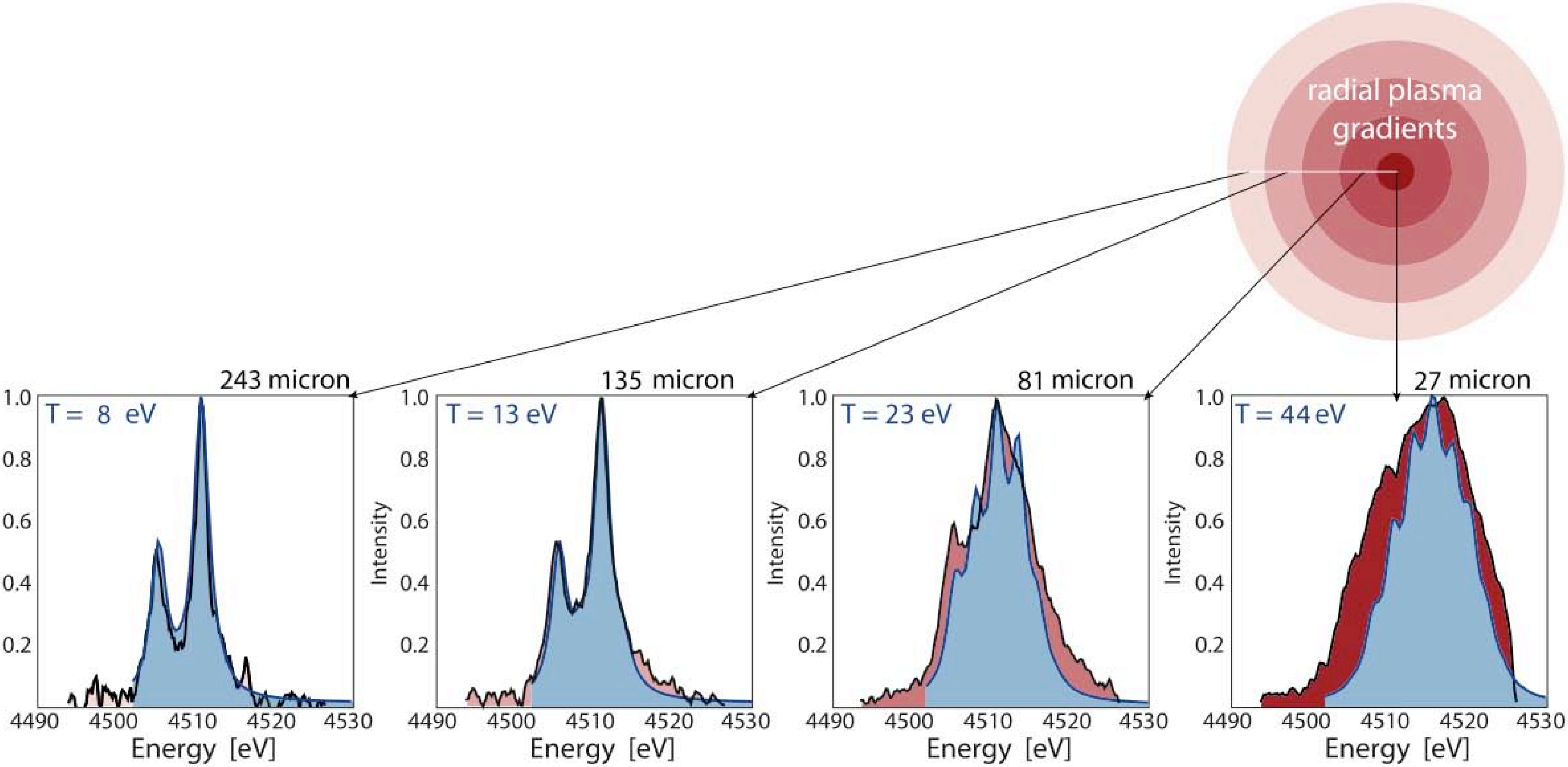



1.0
0.8
0.6
0.4
0.2
Intensity
4490
4500
4510
4520
4530
Energy [eV]
maximum
+ 54 µm
+ 81 µm
+ 108 µm
1.0
0.8
0.6
0.4
0.2
Intensity
4490
4500
4510
4520
4530
Energy [eV]
maximum
+ 54 µm
+ 81 µm
+ 108 µm
108 micron
81 micron
54 micron
0 micron
lateral spectra
radial spectra
Abel deconvolution

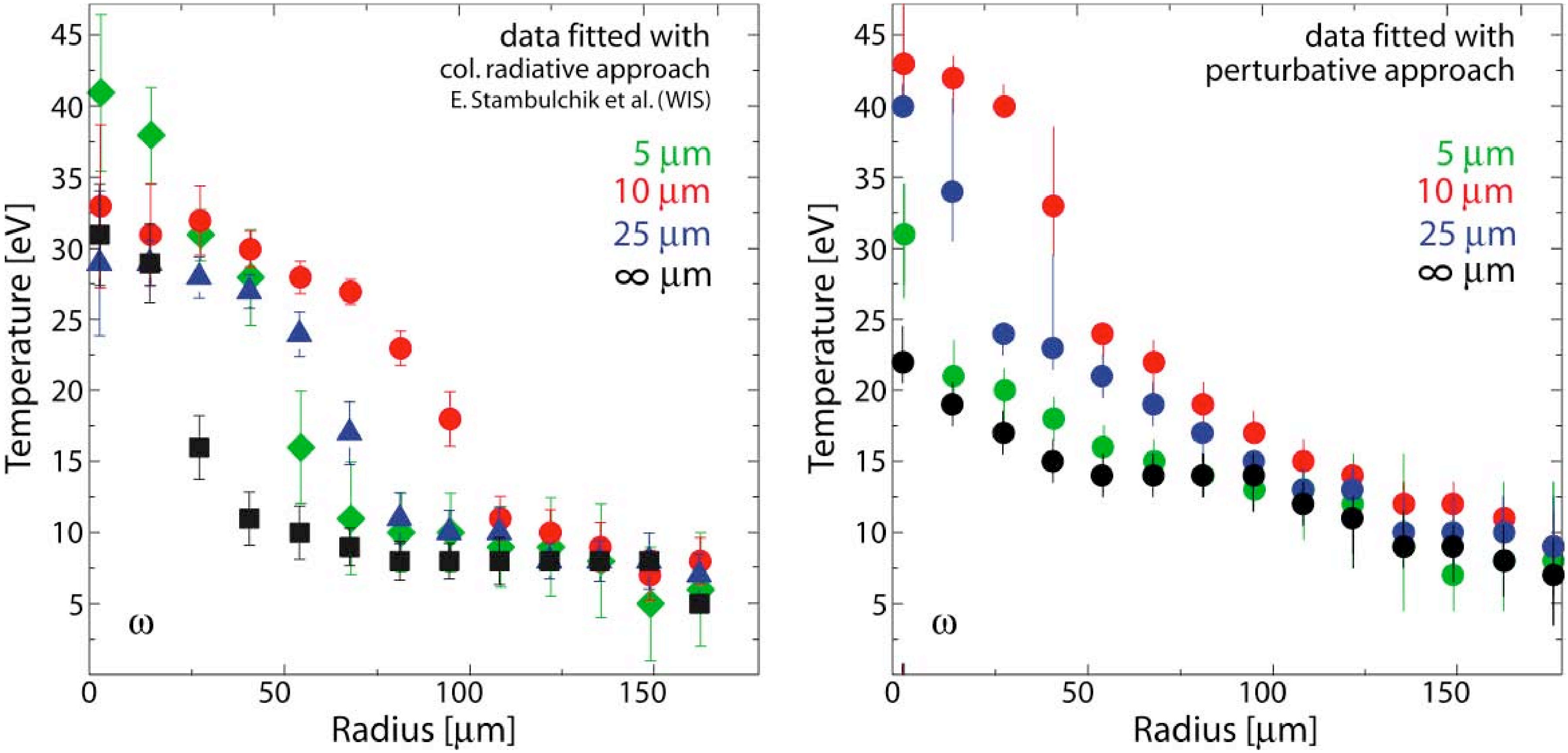
Interpretation of Deconvoluted Ti K_{alpha} Spectra

synthetic spectra fitted with respect to plasma temperature

radial temperature profile



Plasma Temperature Profile



U. Zastrau et al., Phys. Rev. E 81, 026406 (2010)

Chlorine K-shell emission

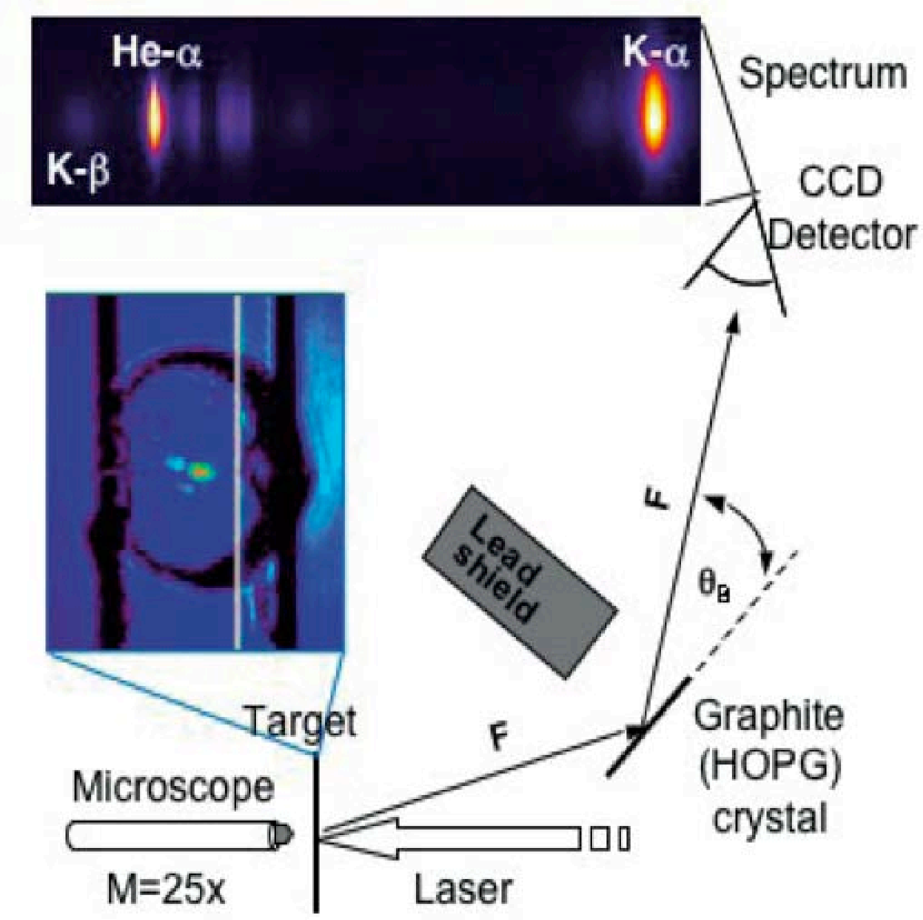
measured by Kritcher et al. (LLNL)

laser: 10 J at 800 nm in 150 fs, d=7 nm

spectrometer: HOPG crystals
resolution E/Delta E = 1500

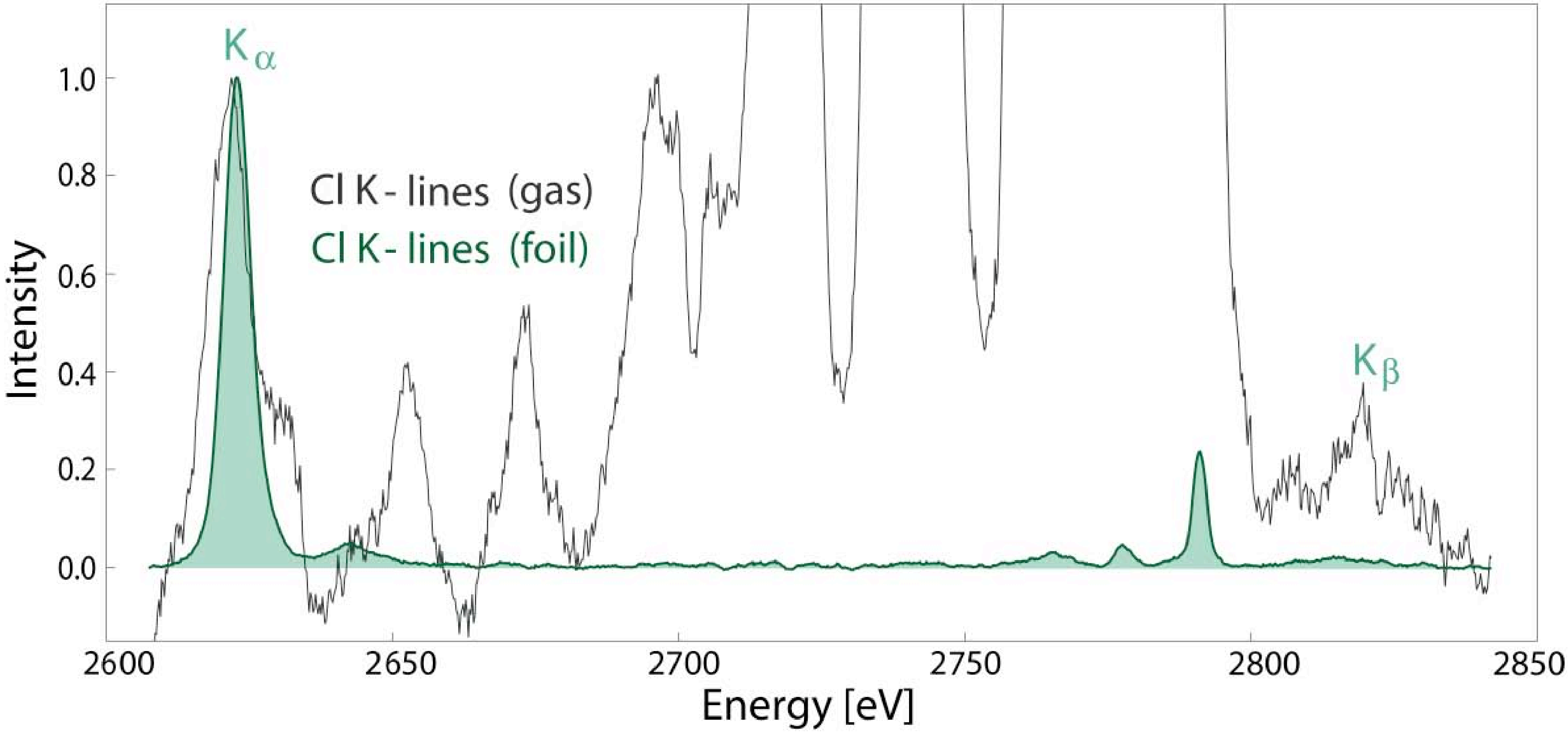
target: polymere foil n(C2H2Cl2)

gas jet with 6 % Cl

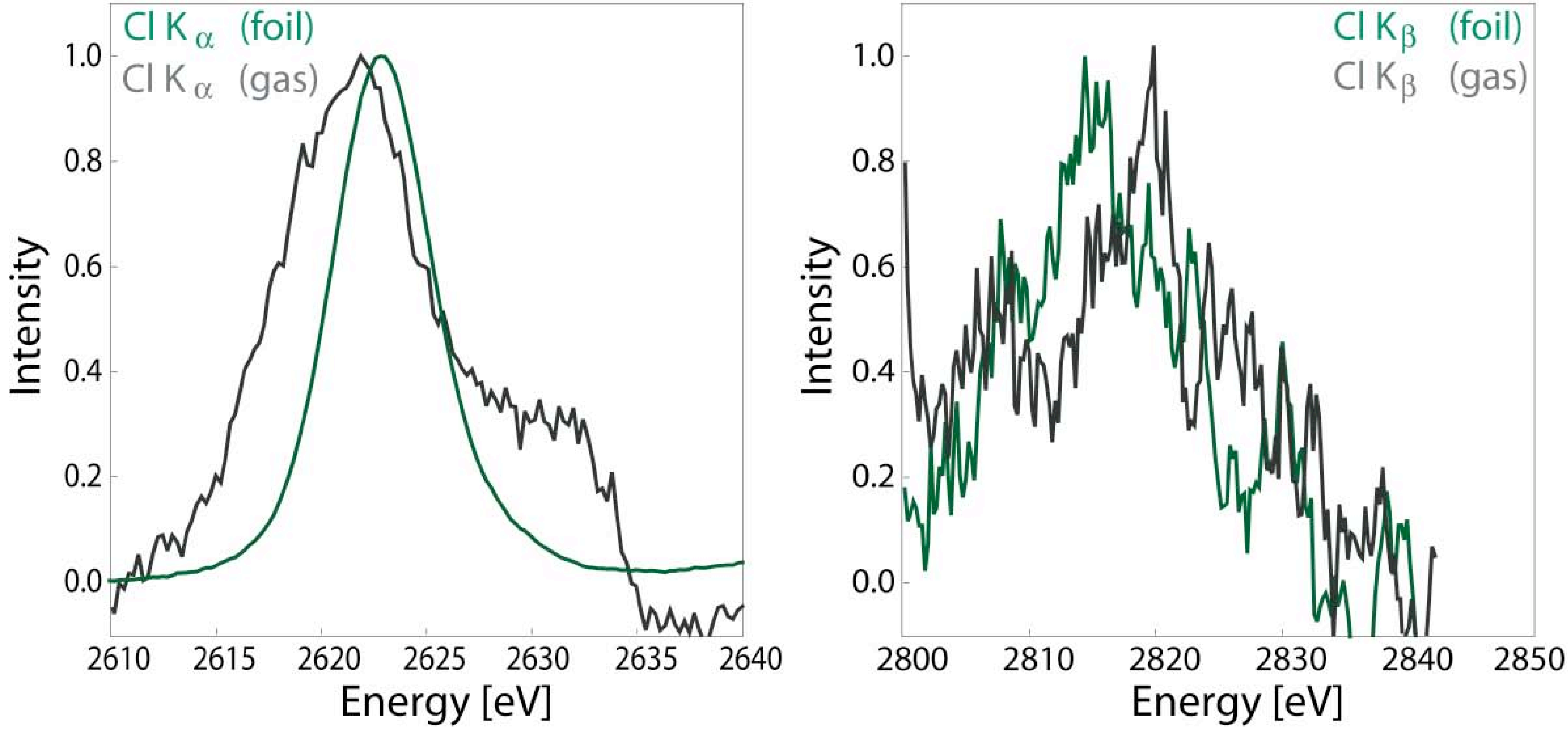


Chlorine K-shell Spectra

solid target (saran foil) $n_e=10^{22}$ cm^{-3}
gas target $n_e=10^{20}$ cm^{-3}

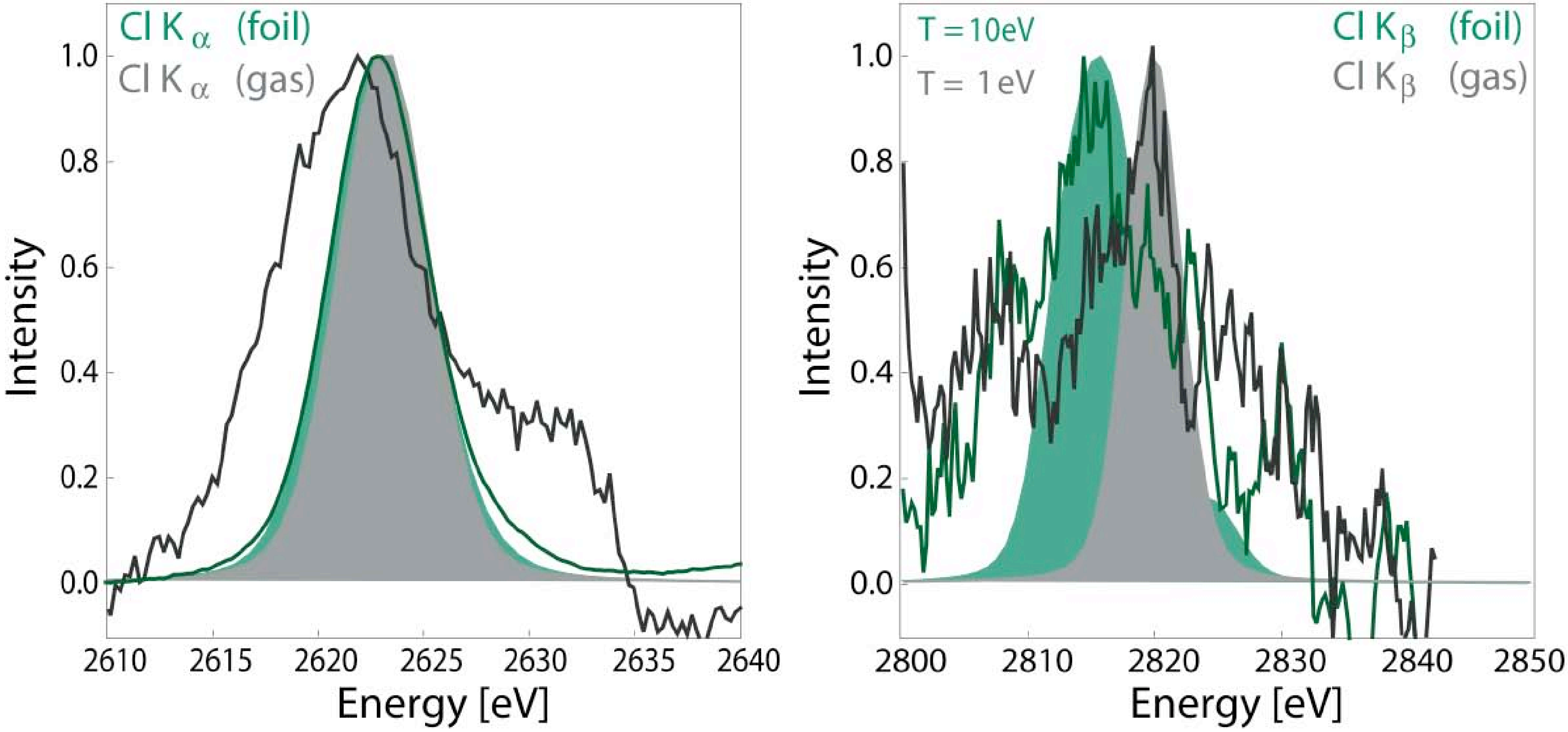


Comparison of Normalized K_{alpha} and K_{beta} Spectral Lines



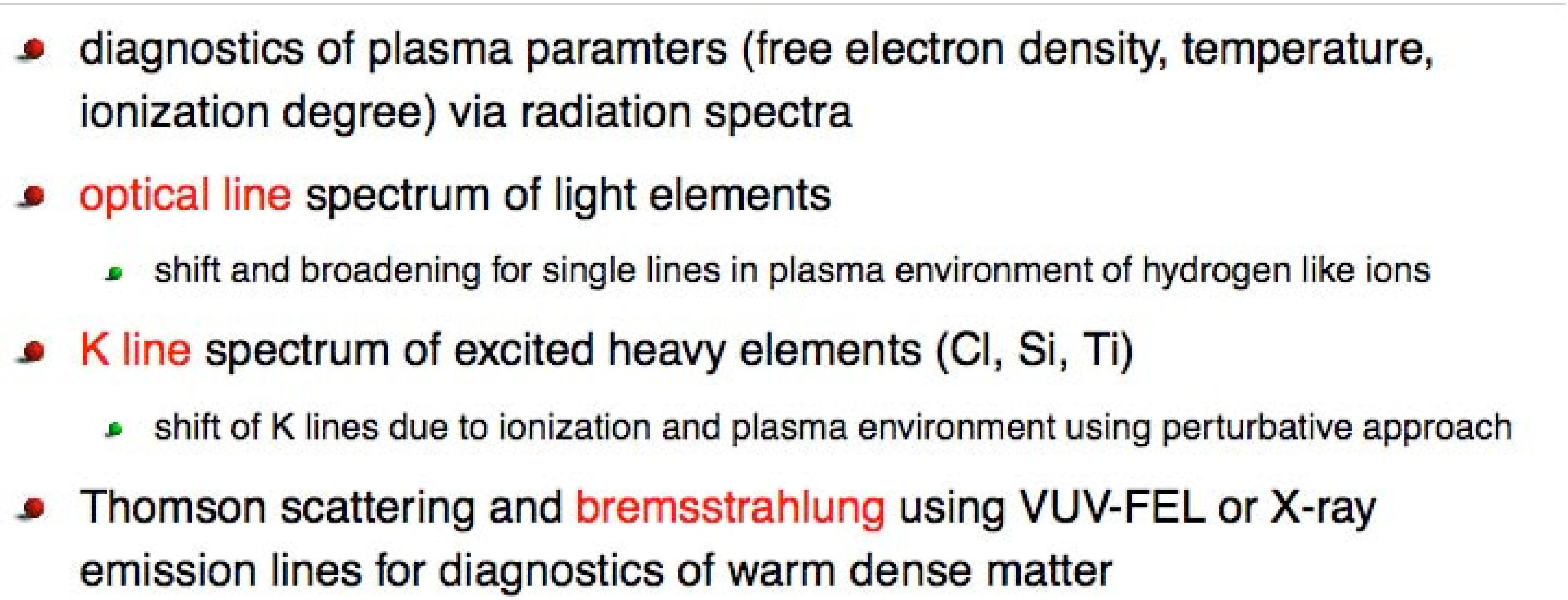
Spectral line shifts due to target density?

Comparison of Normalized K_{alpha} and K_{beta} Spectral Lines



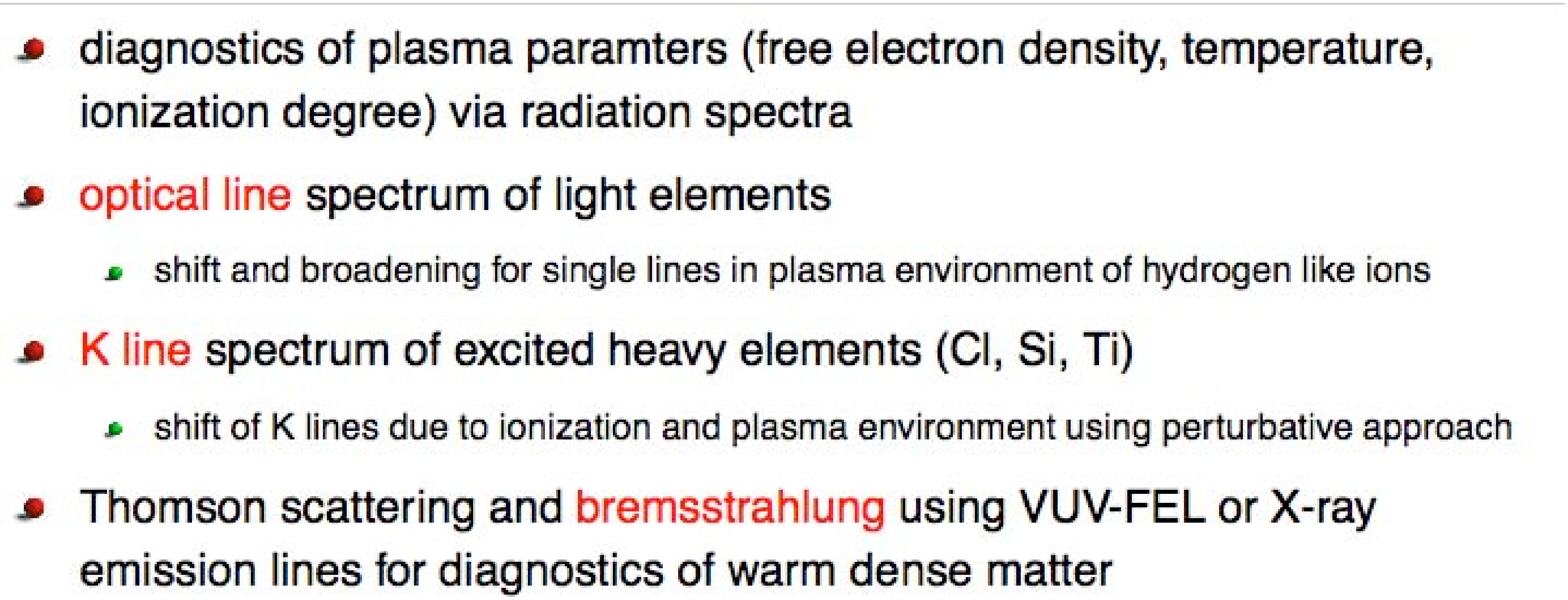
Spectral line shifts due to target density?

Summary



- diagnostics of plasma paramters (free electron density, temperature, ionization degree) via radiation spectra
- optical line spectrum of light elements
  - shift and broadening for single lines in plasma environment of hydrogen like ions
- K line spectrum of excited heavy elements (Cl, Si, Ti)
  - shift of K lines due to ionization and plasma environment using perturbative approach
- Thomson scattering and bremsstrahlung using VUV-FEL or X-ray emission lines for diagnostics of warm dense matter

Summary



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Thanks for attention