The K-shell fluorescence yields and electron impact ionization cross sections for all bromine ions relevant to the plasma temperature diagnostics in laser-solid experiments

Maxime Brasseur, Loïck Morcrette and Patrick Palmeri

Atomic Physics and Astrophysics Unit, University of Mons
(7000), Belgium

The 15th International Colloquium on Atomic Spectra and Oscillator Strengths
for Astrophysical and Laboratory Plasmas (ASOS 15)

July 1 2026

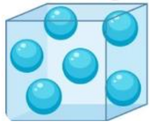
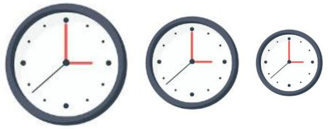
1. Introduction
   - Inertial confinement fusion (ICF) (proton-boron fusion)
   - High Z dopants in laser-solid experiments (the case of bromine)
   - K-line emission and Auger effects

2. The K-shell electron impact ionization (EII) cross section
   - FAC atomic code (relativistic distorted-wave approximation)
   - The MRBEB + density effects model for higher incident electron kinetic energies ($\epsilon >$100 keV)
   - The total K-shell EII cross sections

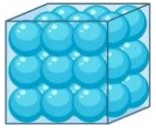
3. The K-shell fluorescence yields
   - The pseudo-relativistic Hartree-Fock (HFR) method
   - K_α and K_β fluorescence yields
   - The K_α/K_β ratio for temperature diagnostics in laser-plasma experiments

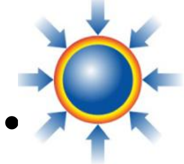
Introduction

Inertial confinement fusion

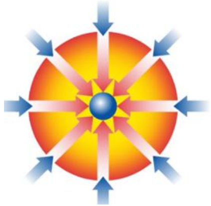
- Magnetic confinement fusion (MCF) :  and 

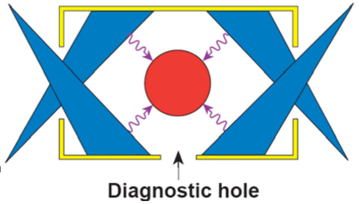
  ≠

  Inertial confinement fusion (ICF):  and  (nsec)



- Direct laser-drive: laser beams directly focused on the capsule surface, the hot plasma at the surface is rapidly created and expand outwards pushing inward the non-evaporated material by conservation of momentum creating the implosion. The surface between the two regions is the ablation surface





- Indirect laser-drive: laser beams are focused on the inner walls of a centimeter size cavity of high-Z material (gold, uranium, etc.). A hot plasma is created on the surface and emits soft X-ray radiation which produced the ablation of the target and its implosion.

- Both scheme have advantages and weaknesses on the efficiency and the irradiation uniformity

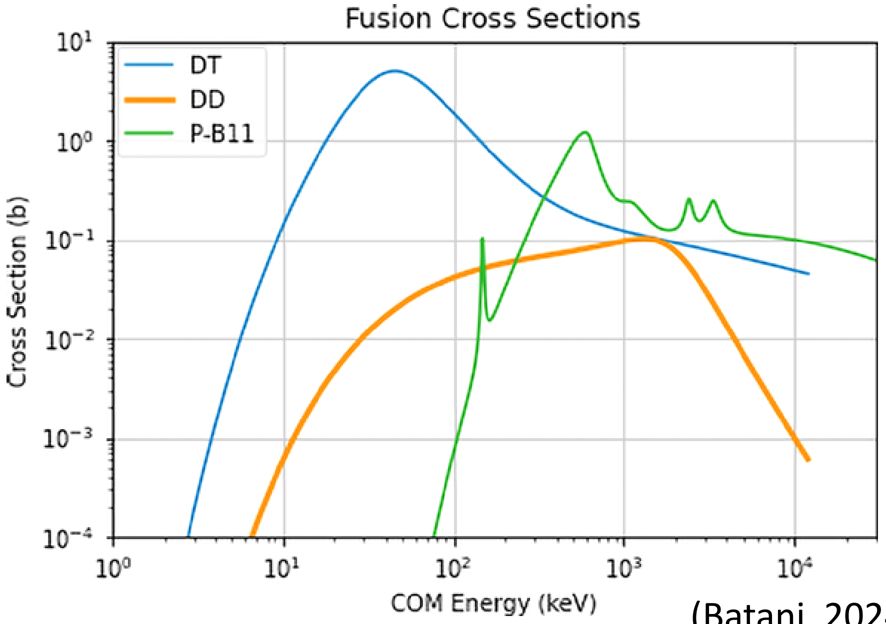
Proton-boron ICF

- This work is part of the PROBONO (proton boron nuclear fusion) COST Action but could also prove useful for any other inertial fusion reaction.

- The advantage of PB or HB nuclear fusion is that it produces neither neutrons nor radioactive wastes :

$$p + B^{11} \rightarrow 3\ He^{4} + 8.7\ \mathrm{MeV}$$

- Higher cross section than other reactions but requires higher energy conditions accessible thanks to the ICF



(Batani, 2024)

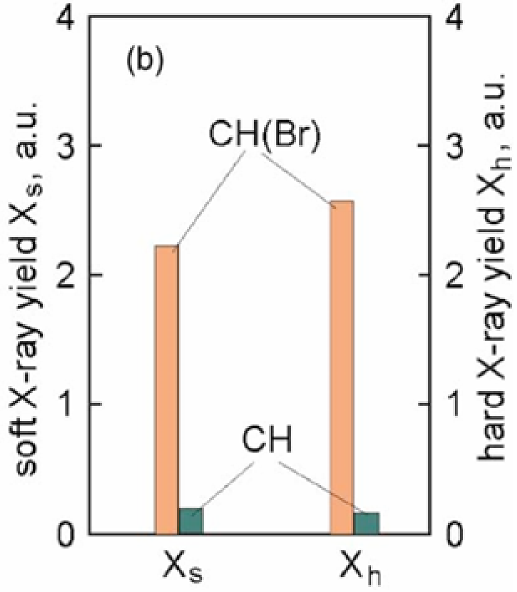
High-Z dopants in laser-solid experiments (the case of bromine)

- In the conventional direct-drive approach to ICF, some instabilities are produced in the ablation surface like the Rayleigh-Taylor (RT) instability → reduction of energy gain

- The idea is to create a double plasma ablation (DA): one ablation surface is formed due to the electron heat conduction induced by laser light and a new ablation surface is created by the X-rays emitted by high-Z atoms doped into the low-Z material (often plastic) (Badziak,2008):
  - ➢ Deletion of the RT instability
  - ➢ High-gain fusion targets
  - ➢ Higher kinetic energy and density

- This idea was proved using a brominated plastic [CH(Br)]
  and a OCT (cellulose acetate)-Cu

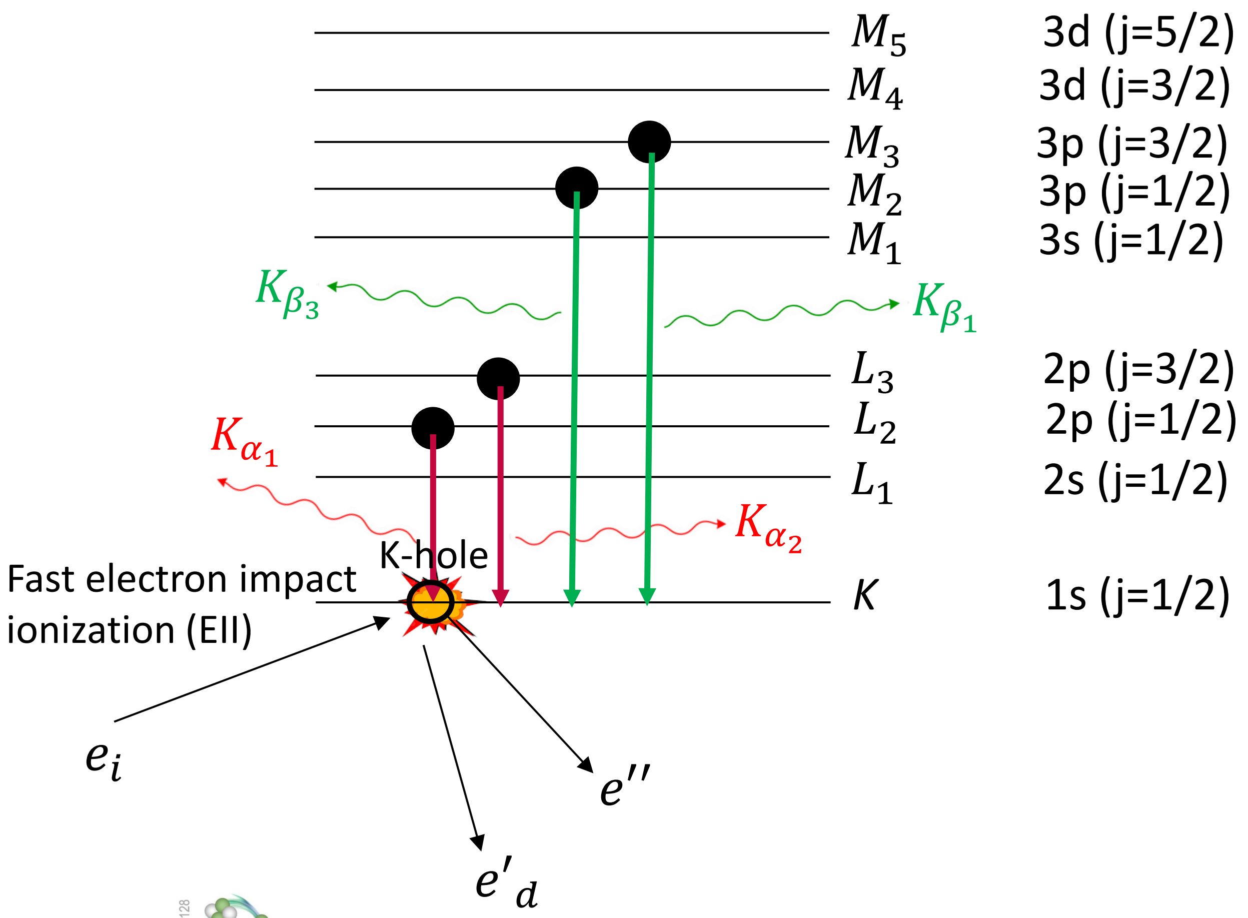
- Cu in all charge states have already been studied by Palmeri *et al.* (2015a,2015b)



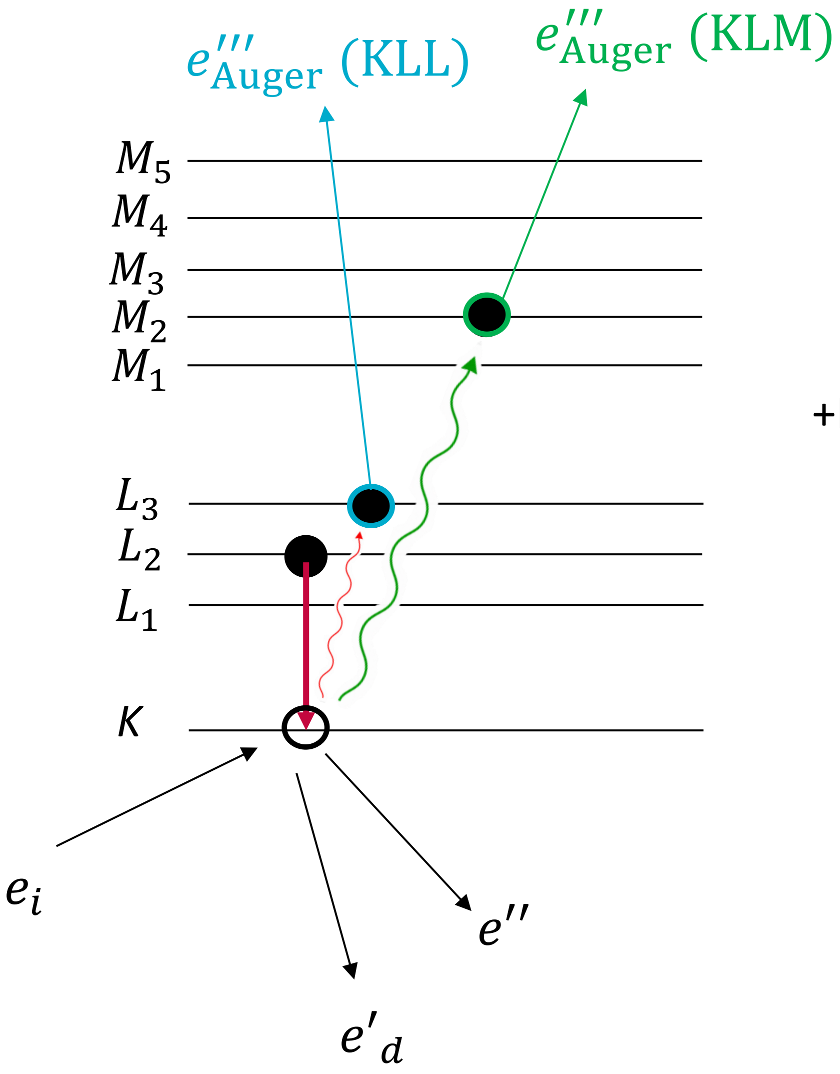
(Badziak,2008)

The K-line emission

In this work, we focused on
$K_\alpha(K_{\alpha_1} + K_{\alpha_2})$ and
$K_\beta\ (K_{\beta_1} + K_{\beta_3})$



Auger effect



+KLN,KMM,KMN, KNN, etc

The K-shell EII cross section

FAC atomic code (relativistic distorted-wave approximation) [Gu, 2002a, 2002b]

- To model the process of K-shell emission, the knowledge of the K-shell EII cross section is required

→ FAC atomic code based on the Dirac Hamiltonian and the central field approximation (eigenvalue problem)

- The Atomic State Functions (ASF) are written as a linear combination of well chosen basis wave functions referred to as Configuration State Functions (CSF), Φ_{r}, in jj coupling:

$$\Psi(\gamma, P, J, M_J) = \sum_{r=1}^{n_c} c_r \, \Phi_r(\gamma_r, P, J, M_J) \text{ where } c_r \text{ are the mixing coefficients.}$$

- The CSF's, Φ_r, are built after optimizing the large, $P_{n,k}(r)$, and small, $Q_{n,k}(r)$, radial parts in the one-electron Dirac spinors, $\varphi_{nkm} = \frac{1}{r}\begin{pmatrix} P_{n,k}(r)\chi_{k,m}(\theta,\phi) \\ i\, Q_{n,k}(r)\chi_{k,m}(\theta,\phi) \end{pmatrix}$.

- $P_{n,k}(r)$ and $Q_{n,k}(r)$ are obtained for a known local central field, $V(r) = V^N(r) + V^{ee}(r)$, by solving the coupled Dirac equation iteratively.

- The potential is optimized for a fictitious mean configuration with fractional occupation numbers and it is used to determine both bound and continuum orbitals

FAC atomic code (relativistic distorted-wave approximation) [Gu, 2002a, 2002b]

- The calculation of the EII cross sections from the initial state ψ_0 to the final state ψ_1 is obtained in terms of the collision strength, Ω_{01}, in the relativistic distorted-wave approximation:

$$\sigma(\varepsilon_0, \varepsilon) = \frac{1}{k_0^2(2J_0+1)}\,\Omega_{01},$$

where ε_0 and k_0 are the energy and the kinetic momentum of the incident electron, ε is the energy of the ejected electron and

$$\Omega_{01} = 2\sum_{k_o,k_1,k}\sum_{J,J_T}(2J_T+1)\left|\left\langle \psi_0 k_0, J_T M_T \left|\sum_{i<j}\frac{1}{r_{ij}}\right| (\psi_1 k)J k_1, J_T M_T\right\rangle\right|^2,$$

with k_1 and k the relativistic angular quantum number of the scattered and ejected electrons

- The total ionization cross section : $\sigma(\varepsilon_0) = \int_0^{\frac{\varepsilon_0 - I_{01}}{2}} \sigma(\varepsilon_0, \varepsilon)\ d\varepsilon$, where I_{01} is the ionization energy for the fine structure transition $\psi_0 \rightarrow \psi_1$.

The MRBEB + density effects (DEF) model

- The modified relativistic binary encounter Bethe (MRBEB) model (Guerra *et al.*,2012) with the density effect correction is used to extrapolate the EII cross sections to higher relativistic energies of the incident electrons ($\varepsilon > 100\ keV$) as suggested by Davies *et al.* (2013):

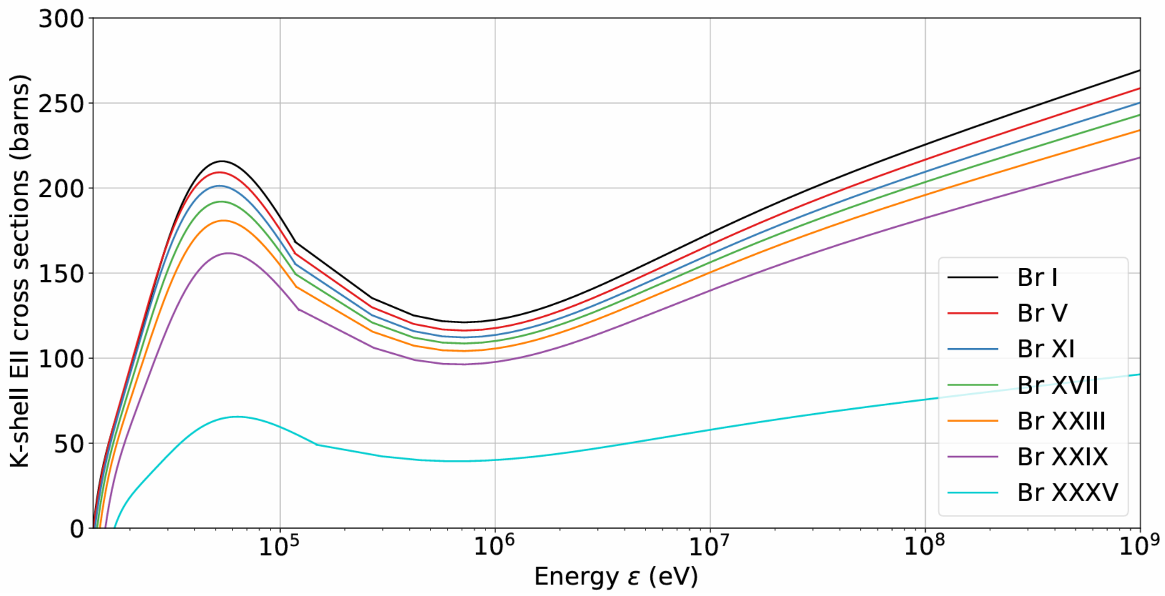
$$\sigma_{ij}(u) = K_{ij}\,\frac{5.1*10^5}{I_{ij}}\left\{\frac{1}{2}\left[\ln\left(\frac{\gamma+1}{2}u\right)-\beta^2-\frac{\delta}{2}\right]*\left(1-\frac{1}{u^2}\right)+1-\frac{1}{u}+\left(\frac{2}{\gamma+1}\right)^2*\left[\frac{u-1}{2J^2}-(2\gamma-1)\,\frac{\ln(u)}{1+u}\right]\right\}*$$

$$\left\{\beta^2+(0.126-0.213*Z+0.195*Z^2)\,\frac{2\,Ry}{I_{ij}}\,\beta_I^2\right\}^{-1}$$

with $u = \frac{\varepsilon}{I_{ij}}, J = \frac{m_e c^2}{I_{ij}}, \gamma = 1+\frac{u}{J}, \beta^2 = 1-\frac{1}{\gamma^2}, \frac{\delta}{2} = \ln\left[1+(\gamma+1)\frac{h\nu_p}{I_{ex}}\exp(-0.5)\right], \beta_I^2 = 1-\frac{1}{\left(1+\frac{1}{J}\right)^2}$

- For bromine, I_{ex} (mean excitation potential)=343 eV and $h\nu_p$ (plasmon energy)=$28.816*\left(\frac{\rho_0 Z}{A_0}\right)^2 =$ 55.06 eV

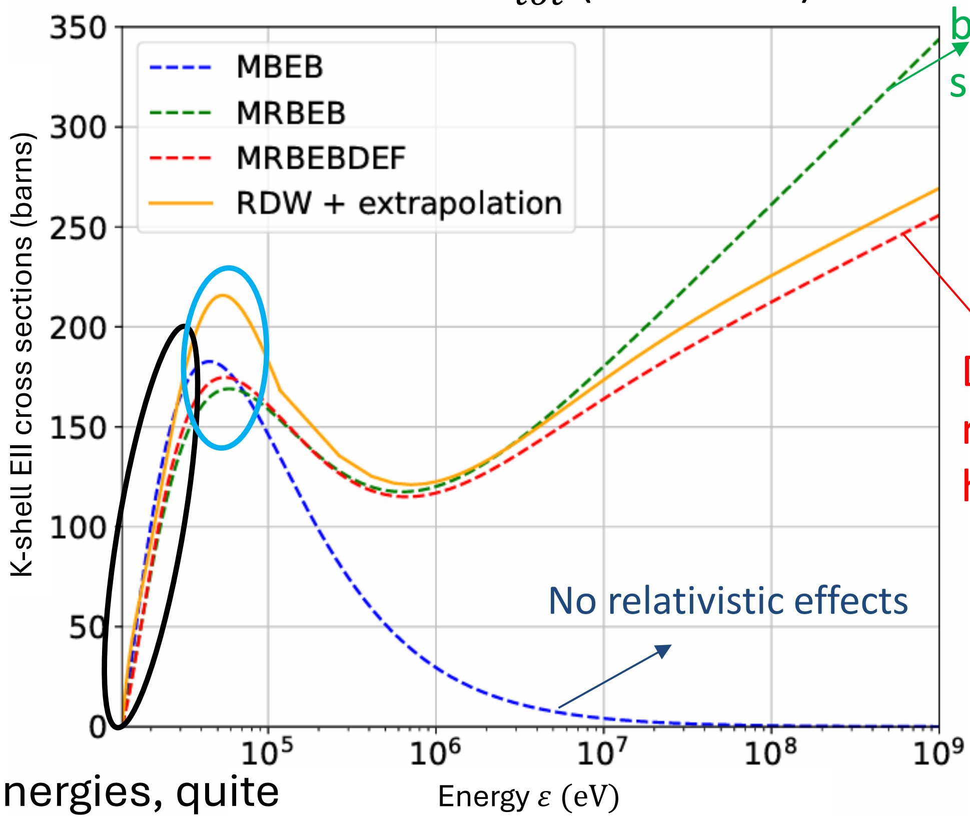
The total K-shell EII cross sections



σ_{tot} is obtained summing all partial KEII cross sections from the parent ion (Z^*) ground level to all final daughter ion (Z^*+1)

σ_{tot} decreases and the K-shell ionization threshold increases with Z* as expected due to the decreasing nbre of bound electrons as Z* increases

Different calculation models of σ_{tot} (Br I → Br II)



Relativistic rise (Breit interaction becomes significant)

Density effects reduce the high-energy rise

At low energies, quite good agreement between all models
→ all σ_{tot} peak around 54 keV with an uncertainty of less than 7%

The peak of our σ_{tot} is higher of nearly 20% than the other models as already observed for Cu (Palmeri *et al.*, 2015a) and V (Palmeri *et al.*, 2015b)

The K-shell fluorescence yields

The pseudo-relativistic Hartree-Fock (HFR) method [Cowan, 1981]

- Solve $H\Psi = E\Psi$ where $H = \sum_{i=1}^{N}\left(-\frac{1}{2}\Delta_i + V(r_i)\right)$ (central field approximation)

- $H_i\varphi_i = E_i\varphi_i \;\rightarrow\; \varphi_i(r_i,\theta_i,\phi_i,s_i) = \frac{1}{r_i}P_{n_il_i}(r_i)Y_{l_i}^{m_i}(\theta_i,\phi_i)\sigma_{m_{s_i}}(s_i)$

- $P_{n_il_i}(r_i)$? → solve Hartree-Fock equations (Self-Consistent Field method)

- HF equations obtained by variational principle on the average energy of each electronic configuration

- Atomic State Functions (ASFs) : $\Psi(\alpha, P, J, M_J) = \sum_{r=1}^{n_c} c_r\, \Phi_r(\alpha_r, P, L_r, S_r, J, M_J)$

  → Configuration State Functions (CSFs) are built thanks to Slater determinants

- The relativistic corrections are introduced perturbatively (spin-orbit + mass-velocity + Darwin corrections)

K_α and K_β fluorescence yields

- The upper K-vacancy fine structure level (i) formed after fast-electron impact ionization can decay through either a radiative (K_α or K_β transition) or a non-radiative channel (Auger transition)

- For a particular fine structure radiative transition i → j, the fluorescence yields is defined as a branching ratio :

$$Y(i,j,Z^*) = \frac{A_r(i,j,Z^*)}{\sum_{k<i} A_r(i,j,Z^*) + A_a(i,Z^*)},$$

where the sum runs over all radiative transitions i → k

- The average K-shell fluorescence yields for a K-vacancy configuration of a charge state Z^*:

$$Y^{K_\alpha \ or \ K_\beta}(Z^*) = \frac{\sum_{i,j} Y(i,j,Z^*)}{n(Z^*)},$$

where the sum runs over all K_α or K_β fine-structure i → j transitions and $n(Z^*)$ is the total number of level of the K-vacancy configuration

Atomic model (Br XVIII, 17+)

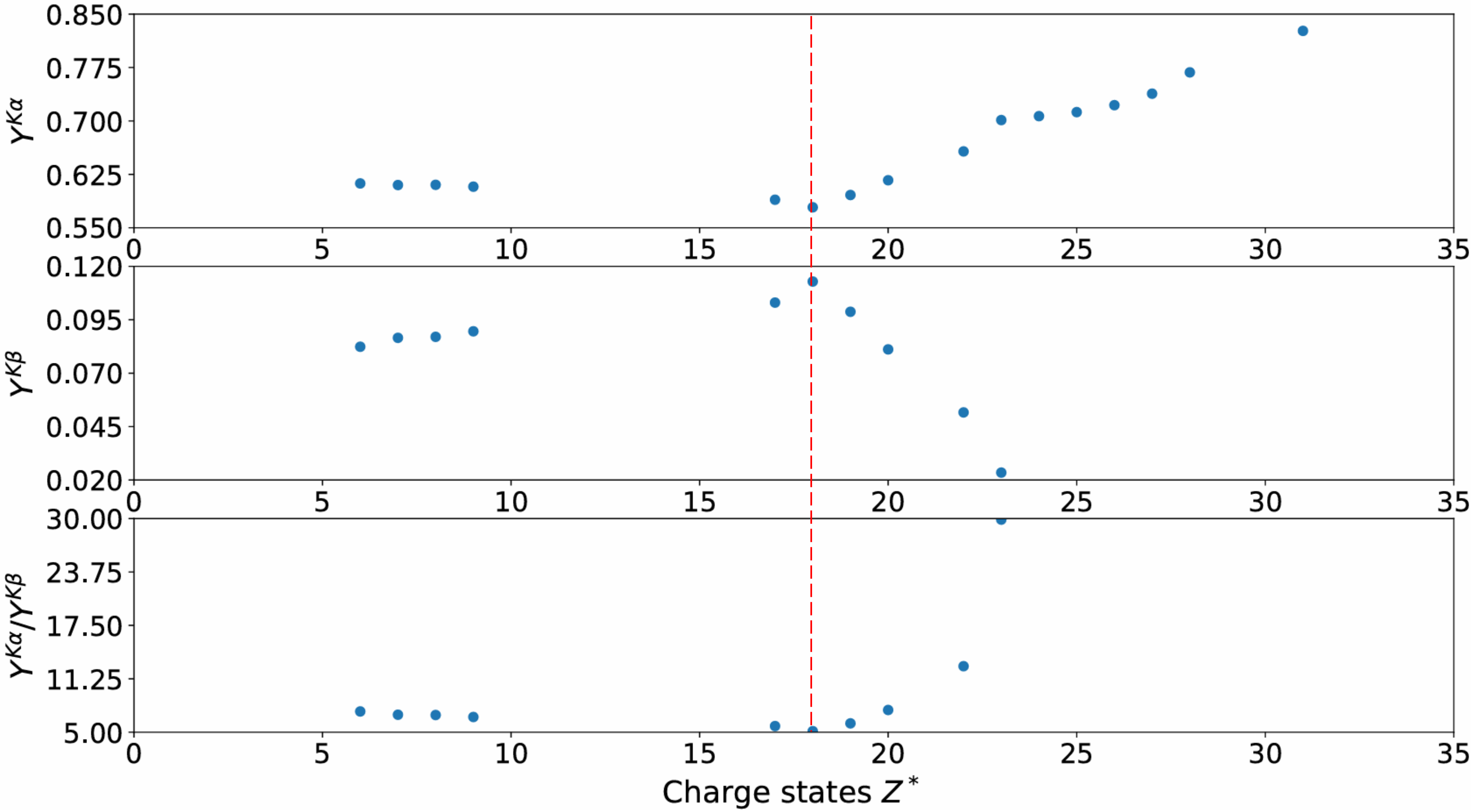
K-line emission

$3p^6$	$3p^5 3d$
$[1s]3d$	$3p^5 4s$
$[1s]4s$	$[1s]3p^5 3d^2$
$[2s]3d$	$[1s]3p^5 3d4s$
$[2s]4s$	$[1s]3p^5 4s^2$
$[2p]3p^5 3d^2$	$[2s]3p^5 3d^2$
$[2p]3p^5 3d4s$	$[2s]3p^5 3d4s$
$[2p]3p^5 4s^2$	$[2s]3p^5 4s^2$
—	$[2p]3d$
—	$[2p]4s$

Auger effect

KLL		*KLM*		*KMM*	
Configuration	ε (Ry)	Configuration	ε (Ry)	Configuration	ε (Ry)
$3p^4 3d$	—	$3p^4 3d$	—	$3p^4 3d$	—
$[3s]3p^6$	—	$[3s]3p^6$	—	$[3s]3p^6$	—
$[3s2]3d$	—	$[3s2]3d$	—	$[3s2]3d$	—
$[2p]3p^5 3d$	—	$[2p]3p^5 3d$	—	$[2p]3p^5 3d$	—
$[1s]3p^6$	—	$[1s]3p^6$	—	$[1s]3p^6$	—
$[2s^2]3p^6 \varepsilon s$	671.436	$[2s3s]3p^6 \varepsilon s$	796.787	$[3s^2]3p^6 \varepsilon s$	918.411
$[2s^2]3p^6 \varepsilon d$	671.436	$[2s3s]3p^6 \varepsilon d$	796.787	$[3s^2]3p^6 \varepsilon d$	918.411
$[2s^2]3p^6 \varepsilon g$	671.436	$[2s3s]3p^6 \varepsilon g$	796.787	$[3s^2]3p^6 \varepsilon g$	918.411
$[2s2p]3p^6 \varepsilon p$	688.121	$[2s]3p^5 \varepsilon p$	802.239	$[3s]3p^5 \varepsilon p$	924.469
$[2s2p]3p^6 \varepsilon f$	688.121	$[2s]3p^5 \varepsilon f$	802.239	$[3s]3p^5 \varepsilon f$	924.469
$[2s2p]3p^6 \varepsilon h$	688.121	$[2s]3p^5 \varepsilon h$	802.239	$[3s]3p^5 \varepsilon h$	924.469
$[2p^2]3p^6 \varepsilon s$	702.920	$[2p3s]3p^6 \varepsilon p$	812.778	$3p^4 \varepsilon s$	929.851
$[2p^2]3p^6 \varepsilon d$	702.920	$[2p3s]3p^6 \varepsilon f$	812.778	$3p^4 \varepsilon d$	929.851
$[2p^2]3p^6 \varepsilon g$	702.920	$[2p3s]3p^6 \varepsilon h$	812.778	$3p^4 \varepsilon g$	929.851
—	—	$[2p]3p^5 \varepsilon s$	818.359	—	—
—	—	$[2p]3p^5 \varepsilon d$	818.359	—	—
—	—	$[2p]3p^5 \varepsilon g$	818.359	—	—

K_α and K_β fluorescence yields



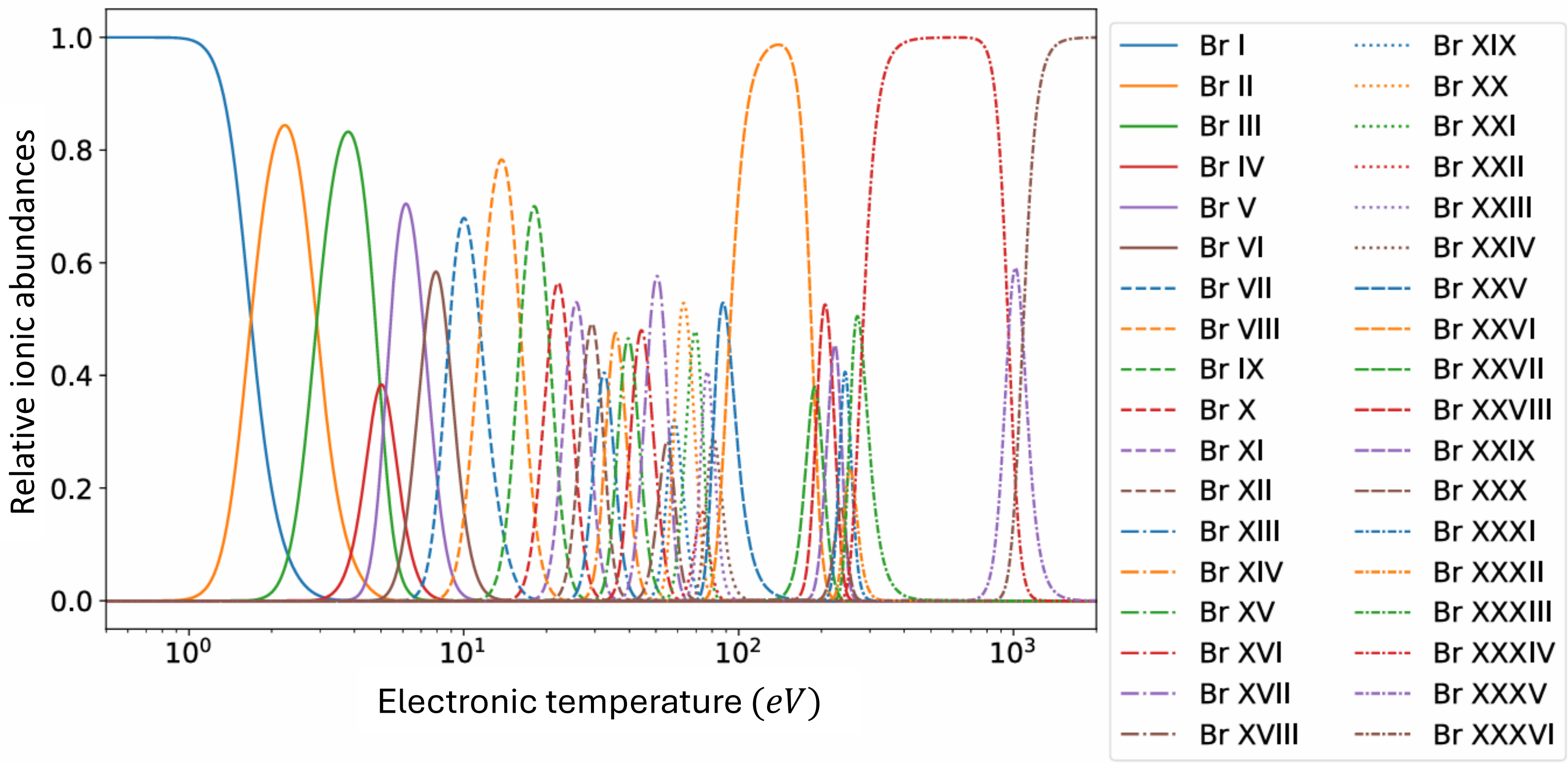
For Br XIX (18+) ([1s]$3p^6$), $Y^{K\alpha}$ reaches a minimum while $Y^{K\beta}$ starts to decrease due to the opening of the 3p subshell

$Y^{K\alpha}$ more sensitive after $Z^* > 23$ while $Y^{K\beta}$ is expected to be a good diagnostic for plasma temperature for low and moderate charged Br ions ($Z^* \leq 23$)

The K_α/K_β ratio for temperature diagnostics in laser-plasma experiments

- From the Saha equation: $\frac{n_{Z^*+1}n_e}{n_{Z^*}} = 2\,\frac{U_{Z^*+1}(T)}{U_{Z^*}(T)}\left(\frac{m_e k_B T}{2\,\pi\hbar^2}\right)^{3/2}\exp(-\frac{E_{Z^*,g\infty}}{k_B T})$,

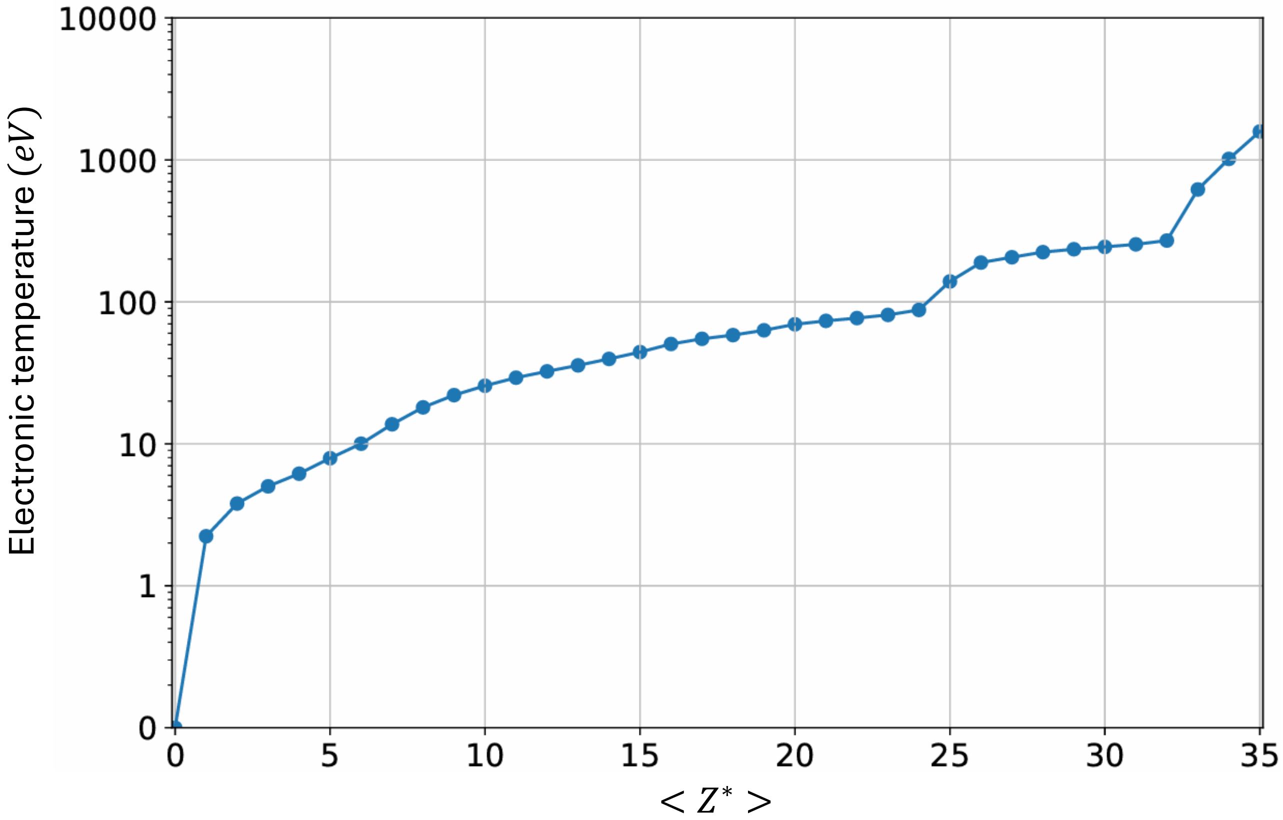
where $U_{Z^*}(T) = \sum_{i=g}^{\infty} g_{Z^*}(i)\exp\left[-\frac{E_{Z^*}(i)-E_{Z^*}(g)}{k_B T}\right]$



The K_α/K_β ratio for temperature diagnostics in laser-plasma experiments

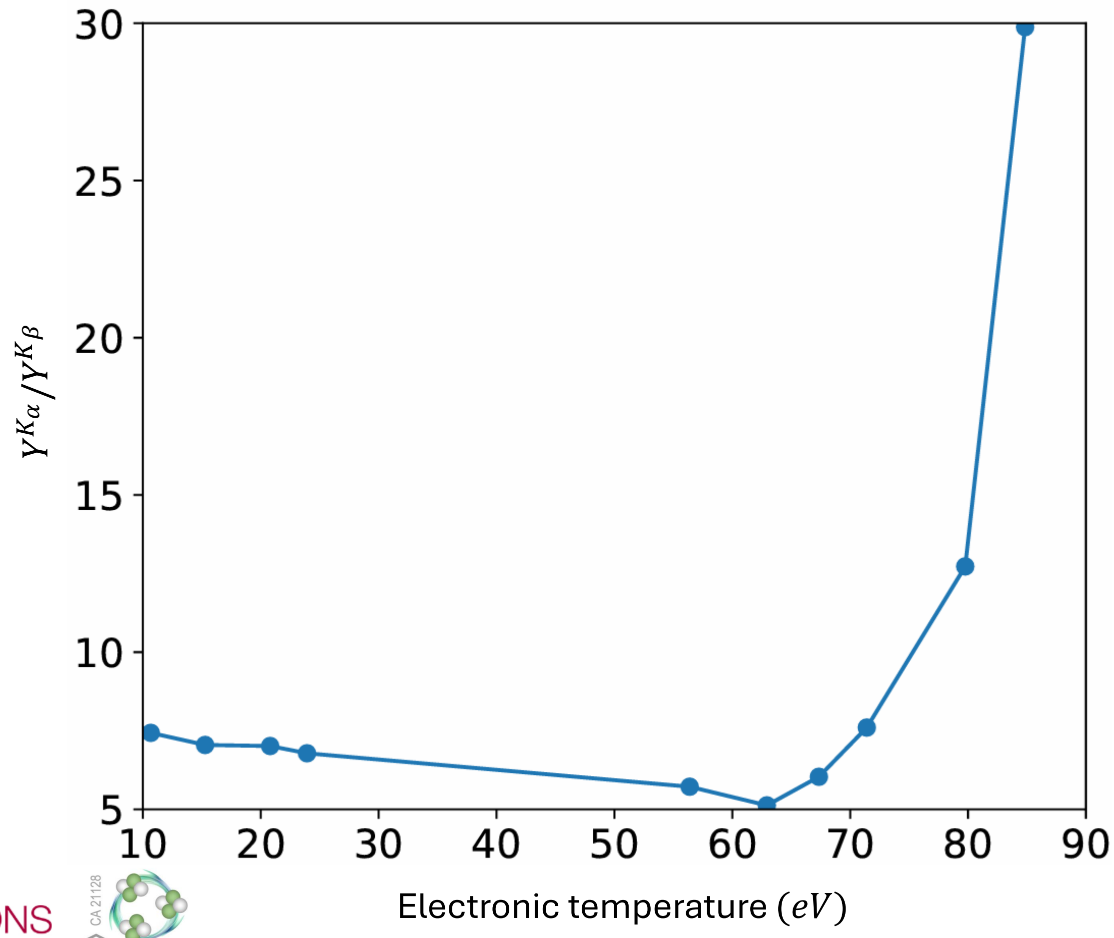
- From the Saha equation: $\frac{n_{Z^*+1} n_e}{n_{Z^*}} = 2\,\frac{U_{Z^*+1}(T)}{U_{Z^*}(T)} \left(\frac{m_e k_B T}{2\,\pi\hbar^2}\right)^{3/2} \exp(-\frac{E_{Z^*,g\infty}}{k_B T})$,

where $U_{Z^*}(T) = \sum_{i=g}^{\infty} g_{Z^*}(i) \exp\left[-\frac{E_{Z^*}(i)-E_{Z^*}(g)}{k_B T}\right]$



The K_α/K_β ratio for temperature diagnostics in laser-plasma experiments

- From the figure $K_\alpha/K_\beta \sim Z^*$ and T $\sim < Z^* >$, if we assume that the ratio does not depend on the average realistic ion distribution as it was confirmed in previous studies for Cu by Palmeri *et al.* (2015b)



The K_α/K_β ratio can give an estimation of the plasma temperature up to nearly 85 eV

Conclusion

- In laser-solid experiments, the K-shell EII cross section and fluorescence yields are important atomic parameters for modeling the K-shell emission as well as the K-line formation processes
- The total KEII cross sections for all bromine ions have been computed with the FAC atomic code and extrapolated to higher relativistic energies of the incident electrons with the MRBEB+DEF model
- The K_α and K_β fluorescence yields have been estimated from the HFR method for some particular bromine ions
- The K_α/K_β ratio provides an estimation of the plasma temperature up to 85 eV for laser-solid applications

Outlooks

- Calculations of fluorescence yields for other bromine ions with HFR but also with FAC to have an independent comparison of the results
- Other dopants used in ICF can be useful for plasma diagnostics, for example germanium (Ge, Z=32) (Regan *et al.*, 2012)
- To probe higher plasma temperature in laser-solid experiments, need higher Z dopant

THANK YOU !

UMONS
University of Mons

CA 21128
PROBONO

Physique Atomique et Astrophysique

Faculty of Science

Badziak, J. et al. (2008). « The effect of high-Z dopant on laser-driven acceleration of a thin plastic target ». In : Applied Physics Letters 92.21, p. 211502.
Batani, D. (2024). « Inertial confinement fusion : Recent results and perspectives ». en. In : EPJ Web of Conferences 310. Sous la dir. de L. Cifarelli et al., p. 00013.
Cowan, R. D. (1981). The Theory of Atomic Structure and Spectra. en. Berkeley : California Uni versity Press, Berkeley.
Davies, J. R. et al. (2013). « Copper K-shell emission cross sections for laser–solid experiments ». en. In : Physics of Plasmas 20.8.
Gu, M. F. (2002a). « The Flexible Atomic Code : I. Atomic Structure ». In : Cambridge, MA : Center for Space Research, Massachusetts Institute of Technology.
Gu, M. F. (2002b). « The Flexible Atomic Code : V. Electron Impact Ionization ». In : Cambridge, MA : Center for Space Research, Massachusetts Institute of Technology.
Guerra, M. et al. (2012). « Modified binary encounter Bethe model for electron-impact ionization ». In : International Journal of Mass Spectrometry 313, p. 1-7.
Palmeri, P. et al. (2015a). « Copper fine-structure K-shell electron impact ionization cross sections for fast-electron diagnostic in laser-solid experiments ». In : Atomic Data and Nuclear Data Tables 102, p. 1-5.
Palmeri, P. et al. (2015b). « Copper fine-structure K-shell electron impact ionization cross sections for fast-electron diagnostic in laser-solid experiments ». In : Atomic Data and Nuclear Data Tables 102, p. 1-5.
Palmeri, P. et al. (2015c). « Vanadium fine-structure K-shell electron impact ionization cross sections for fast-electron diagnostic in laser–solid experiments ». In : Atomic Data and Nuclear Data Tables 105-106, p. 1-8.