High Energy Density Physics xxx (2015) 1–4

Contents lists available at ScienceDirect

High Energy Density Physics

journal homepage: www.elsevier.com/locate/hedp

# The K X-ray line structures for a warm dense copper plasma

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ARTICLE INFO

*Article history:*
Received 11 March 2015
Accepted 11 March 2015
Available online xxx

*Keywords:*
Plasma diagnostics
K X-ray lines
High-resolution spectroscopy
Outer-shell ionization

ABSTRACT

Ionization affects the energy and shape of the characteristic X-ray lines that may be excited by energetic electrons in a partially ionized plasma. We present the first theoretical predictions for copper K-line spectra in different ionization states, one of a systematic series of computations on how ionization affects inner-shell X-ray lines. Detailed computations such as these may make it possible to use individual hard X-rays lines as diagnostics for warm, dense plasmas when high-resolution X-ray spectra are available.





## 1. Introduction

Under simplifying assumptions that are often reasonably well satisfied, the electrons in a hot, dense plasma have a Maxwellian electron energy distribution with a well-defined temperature, and the plasma ions are ionized to within a narrow range that reflects the temperature. Ionization by thermal electrons preferentially removes electrons from the ion's outer shells, hence such a plasma radiates X-rays with energies up to a few times higher than the electron temperature. Sometimes the plasma emits higher-energy X-rays, generated by energetic electrons that are not part of the thermal electron energy distribution. These X-rays can come from any higher-energy electron shell that is not affected by the thermal electrons. For plasmas from lower atomic number elements such as copper, the higher-energy lines can only come from the K-shell, but for higher atomic number plasmas the characteristic lines can be from the L-shell as well: tungsten is an example [1].

The harder X-rays may be able to leave the interesting plasma region unhampered by opacity, a plasma blanket, or even a solid window. Since the energy and line shape of the characteristic X-ray lines is affected by the immediate surroundings of the radiating ion, the harder radiation can be a unique diagnostic for a plasma that is otherwise inaccessible.

Well-known plasma radiation codes such as the Flexible Atomic Code (FAC) [2] and FLYCHK [3,4] contain the effect of ionization on the harder X-ray lines. However, computing the plasma together with the atomic physics demands compromises of one kind or another: to include the plasma, the atomic physics may use pre-computed data, or include fewer corrections than are contained in a more accurate code. In this paper the specific ionization stages in the plasma are taken as given, and the emphasis is on computing the energy shifts and line shapes of their higher-energy lines.

The absence in the literature of accurate predictions for the energy of the K-lines as function of ionization, needed in some of our work [5], initiated a detailed computation on the K$\alpha$ lines of higher atomic number elements. The small ($\simeq$10 eV) increase in energy of the $\simeq$63 keV K$\alpha_2$ line of iridium, obtained in the so-called Plasma-Filled Rod Pinch (PFRP) [6,7], turned out to be consistent with these computations and confirmed the plasma conditions already estimated earlier from a radiation mode. Further, the ionization energy shift observed for another element (Yb) could be understood later on, with additional computations [8–12] that were part of a systematic study about the influence of outer-shell electron stripping on the K and L X-ray lines by themselves. These papers show how outer-shell ionization affects the energy and shape of characteristic X-ray lines, with sufficient detail that a single line could contain enough information to find out about the plasma environment, around the radiating ion.

One example for which this could be done is a series of high-resolution X-ray spectra obtained by Zajac et al. [13] at the Plasma Focus (PF) on the ~ 1 MA PF-1000 device at the Institute of Plasma Physics and Laser Microfusion (IPPLM) in Warsaw. The spatially resolved and time integrated X-ray spectra in the photon energy range of 210 keV were measured by means of the X-ray

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http://dx.doi.org/10.1016/j.hedp.2015.03.005
1574-1818/© 2015 Published by Elsevier B.V.

focusing crystal spectrometer with spatial resolution in axial direction based on spherically bent crystal. The intensity of the radiation in Fig. 1 comes from four different plasma regions, as diffracted by a mica crystal. Rather than wave length or photon energy, the independent variable is the Bragg angle because the plasma contains two radiating species, ~3.5 keV photons from the PF's argon diffracted in the 4th order at the lower Bragg angles and the K$\alpha$ radiation from copper at ~8 keV from higher-order reflections.

The analysis done by Zajac et al. is primarily of the argon plasma in the different regions. The bottom spectrum is from the first region which is from radiation emitted close to the anode, the top spectrum is for the 4th region, which the farthest away from the anode. The highest intensity radiation is from He-like argon's resonance and intercombination lines, in the second region where a bright spot appears in the discharge; clearly the bright spot contains a high concentration of highly ionized Ar ions. The radiation from argon's lower ionization states in the first region indicates that the argon close to the anode is relatively cool.

The structures attributed to copper K$\alpha$, from the 9th order reflection at a Bragg angle of 54.5° and in 10th order at 64°, must come from evaporated anode material that mixes with the argon plasma. The single K$\alpha$ structure then represents two overlapping K$\alpha$ lines, whose peak energy and shape changes as the Cu moves into the hotter plasma further away from the anode.

Usually, the plasma is diagnosed from the argon spectrum as done in Ref. [13], but even if this spectrum were suppressed and Fig. 1 would only contain the harder copper K$\alpha$ radiation, information about the plasma could still be derived from the structure and energy of these lines. Besides a theoretical understanding of how the plasma affects the inner-shell lines, for a diagnostic it is only necessary that these lines exist the plasma with sufficiently small absorption so that the line shapes are not perturbed, and are intense enough for a high-resolution measurement. The PFRP fulfills these two requirements, very well for the tungsten L-shell radiation [1] and to a lesser degree for the iridium's K$\alpha_2$ line [6]. Plasmas produced by short-pulse lasers also have the energetic electrons needed to excite the harder X-rays.

Another example is a recently published [14] high-resolution copper K-line spectrum originating from a plasma produced by the Prague Asterix Laser System (PALS). It produces a 250 ps pulse at a wave length of 1.3 $\mu$m into 70 $\mu$m diameter spot, with 400 J per pulse. Irradiating a thin (1.4 $\mu$m) copper foil gives a time-integrated spectrum that can be reasonably well matched by a sum of K-lines generated by energetic electrons fluxes that change over time. The highly detailed spectra, in Sec. 3 and Fig. 2 can be very useful in refining the interpretation of the copper K-line spectra highlighted here [13,14].

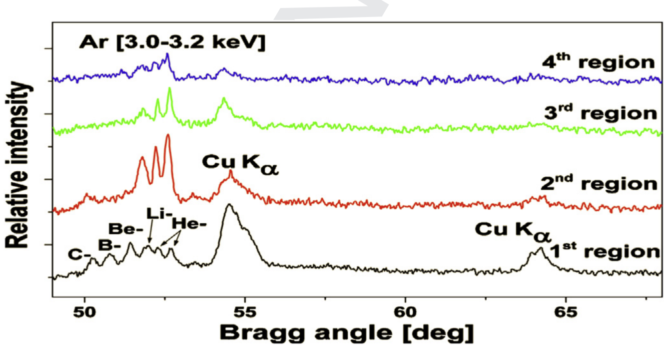


**Fig. 1.** High resolution spectra emitted from different areas of the plasma produced in the plasma focus device, PF-1000 [13].

## 2. The methodology of MCDF calculations

The computations performed use a code that implements the multi-configuration Dirac-Fock (MCDF) method, as discussed in many papers (see, e.g., [15–18]). The effective Hamiltonian for an atom with $N$ electrons is expressed by the Dirac-Fock operator,

$$H = \sum_{i=1}^{N} h_D(i) + \sum_{j>i=1}^{N} C_{ij}, \tag{1}$$

where $h_D(i)$ is the Dirac operator for the $i^{th}$ electron, and the terms $C_{i,j}$ account for electron–electron interactions. The latter are a sum of the Coulomb interaction operator and the transverse Breit operator. An atomic state function (ASF) with total angular momentum $J$ and parity $p$ is assumed in the form

$$\Psi_s(J^p) = \sum_m c_m(s)\Phi(\gamma_m J^p), \tag{2}$$

where $\Phi(\gamma_m J^p)$ are configuration state functions (CSF), $c_m(s)$ are the configuration mixing coefficients for state $s$, and $\gamma_m$ represents all information required to uniquely define a certain CSF. In addition to the transverse Breit interaction, the computation includes two additional QED corrections, for self-energy and vacuum polarization, and a finite nuclear size with a two parameter Fermi charge distribution [18].

The MCDF formalism is implemented in the GRASP [16] and GRASP2K codes [17] that are used here. The energy of a photon emitted in the transition of an electron in a higher-energy state to a vacancy in a lower-energy state is the difference between the two orbital energies. The radiative transition frequencies can be calculated in both the Coulomb [19] and the Babushkin [20] gauge.

## 3. Results

As an example of the detail obtainable from these MCDF predictions, Fig. 2 shows the K$\alpha_{1,2}$ X-ray lines of copper for a selection of ionization states. In all sub-figures the 'sticks' seen inside each spectrum are located at the center energy of the specific X-ray line; the height of the stick indicates the transition frequency, the inverse of the transition time.

The left side of the figure is for a modest ionization, from Cl-like $Cu^{12+}$ to Al-like $Cu^{16+}$, removing 3$p$ electrons one by one but leaving the neon-like core and the 3$s^2$ electrons unaffected. The two principal K$\alpha$ lines increase their energy as the ionization progresses, but it remains close to 8048 eV for K$\alpha_1$ and to 8028 eV for K$\alpha_2$ in the Cu bremsstrahlung spectrum. Removing an electron from Cu's 3$p$ subshell increases the energy of both K-lines by about 6 eV per electron, as discussed further in Ref. [21].

Besides the two principal lines, the K-shell spectrum has many lower-energy satellite lines that effectively widen the spectral structure beyond their Lorentzian natural width, which for cold materials is derivable from the level widths recommended in Ref. [22]; ~2 eV for cold Cu). The dotted line draped over the sticks is the sum of all these Lorentzians, with the widths defined by the code's transition frequency as computed by the code. For easier comparison with the experiment of Zajac et al. [13] below, the solid line will be a convolution of this theoretical spectrum with the Gaussian instrumental response having a width of 5.0 eV.

The right side in Fig. 2, for F-like $Cu^{20+}$ ionizing up to B-like $Cu^{24+}$ by removing 2$p$ electrons one by one from the Be-like core, shows a much stronger effect of the ionization on the spectrum. Besides an increase in energy of the most prominent K-L$_3$ transition reminiscent of the K$\alpha_1$ line, by about 45 eV per 2$p$ electron, the

Please cite this article in press as: K. Słabkowska, et al., The K X-ray line structures for a warm dense copper plasma, High Energy Density Physics (2015), http://dx.doi.org/10.1016/j.hedp.2015.03.005