High Energy Density Physics 20 (2016) 29–33

Contents lists available at ScienceDirect

High Energy Density Physics

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

The K x-ray line structures of the 3d-transition metals in warm dense plasma

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ARTICLE INFO

Article history:
Received 17 February 2016
Received in revised form 21 June 2016
Accepted 25 June 2016
Available online 29 June 2016

Keywords:
K x-ray lines
Outer-shell ionization
Plasma diagnostics
3d-transition metals

ABSTRACT

The shapes and positions of the Kα_1 and Kα_2 x-ray lines for 3d-transition metals can vary substantially as electrons are stripped from the outer-shells. This paper shows the detailed line shapes for nickel and zinc, obtained by calculations with a multiconfiguration Dirac–Fock method that includes Breit interaction and quantum electrodynamics corrections. The line shapes can be useful in interpreting hot, dense plasmas with energetic electrons for which the K x-ray lines are optically thin, as may be produced by pulsed power machines such as the plasma-filled rod pinch diode or the plasma focus, or in short-pulsed high power laser plasmas.

1. Introduction

X-ray spectra emitted by the dense plasmas created by pulsed power machines such as plasma focus PF-1000 device [1] are important in understanding the discharge dynamics, to determine the scaling laws that should help in designing larger fusion devices, and to identify other potential application. The anomalous effects that accompany the x-ray and neutron production in the later phase of a plasma focus implosion are a good example.

In the plasma focus, the peak emission of x-ray radiation is usually accompanied by energetic electron and ion beams, and affected by them. Energetic electrons are thought to be generated from the plasma micro-structures (hot-spots) in short time windows (7–10 ns), with energies within relatively narrow energy bands [2]. Mid-Z impurities from the electrodes, which can constitute 10^{-3} of the plasma's mass, interacting with the pulsed electron beams generate K x-ray spectra that provide rich and valuable information on the plasma parameters [3–9]. In particular, the K x-ray spectra from the impurities contain precise information on their charge state, and therefore the plasma temperature, during the short time of maximum K x-ray emission. For such studies, a particularly useful configuration is the plasma-filled rod pinch (PFRP) diode, a hot, dense plasma with a substantial non-thermal component of energetic electrons that can create inner-shell vacancies even in high-Z ions. In Ref. [9], the time and spatially averaged ionization distribution of a W plasma in the PFRP was determined from a single Lβ_2 line that could be measured with sufficient accuracy to be interpreted in terms of the ionization distribution. This was done by decomposing the broad and clearly asymmetric line into theoretically predicted, energy-shifted lines computed for the different ionization stages, without the need for plasma radiation kinetics codes or the complications from opacity.

The systematic computations on the energy and shape of characteristic x-ray lines positions in a series of papers [5–14] are done in large part to make such single lines valuable for plasma diagnostics. The intended application is for plasmas on the PF-1000 device (Institute of Plasma Physics and Laser Microfusion, Warsaw, Poland), and the PFRP diode (at the Naval Research Laboratory in Washington, USA), but the method should work for all plasmas that contain energetic electrons, notably the plasmas produced by short-pulsed lasers. The early papers [5,11] address the relatively smaller energy shifts in high-Z ions, e.g., the ~+10 eV increase in the ~60 keV photon energy of the Kα_2 transition of modestly (~17×) ionized iridium in the PFRP. This energy shift turned out to be consistent with a subsequent atomic physics studies, and with the ionization predicted from a simple model for this particular plasma [6,7,11,12]. More recent computations [13] on lower-Z ions show that outer-shell ionization has a particularly strong effect on the structure of the Kα_1 and Kα_2 x-ray lines for 3d elements such as copper.

The present paper deals with the Kα energies and line shapes for two other 3d-transition metal impurities, Ni and Zn, for a wide range of ionization stages that can be present in a dense (up to $n_e = 10^{20}$ cm^{-3}) and hot (up to $T_e = 2$ keV) plasma. Section 2 discusses the theoretical background; Section 3 contains the results.

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http://dx.doi.org/10.1016/j.hedp.2016.06.003
1574-1818/

Table 1
The energies of the KL_3 ($K\alpha_1$) and KL_2 ($K\alpha_2$) x-ray diagram lines for Ni, Cu, and Zn obtained in our computations, compared with the theoretical and experimental values in Deslattes et al. [20]. The values, their uncertainties (in brackets) and the differences Δ are all in eV.

Atom	Source	$K\alpha_1$ (eV)	Δ	$K\alpha_2$ (eV)	Δ
Ni (Z = 28)	Present	7478.79	+0.54	7461.81	0.78
	Theory	7477.72 (0.44)	–0.53	7459.96 (0.47)	–1.07
	Experiment	7478.2521 (0.045)	–	7461.0343 (0.045)	–
Cu (Z = 29)	Present	8048.01	0.19	8028.10	0.26
	Theory	8048.11 (0.45)	0.29	8028.38 (0.48)	0.54
	Experiment	8047.8227 (0.026)	–	8027.8416 (0.026)	–
Zn (Z = 30)	Present	8638.94	0.03	8615.72	–0.10
	Theory	8639.10 (0.45)	0.19	8616.22 (0.50)	0.40
	Experiment	8638.906 (0.073)	–	8615.823 (0.073)	–

2. Theoretical background

The calculations here use a fully relativistic multiconfiguration Dirac–Fock (MCDF) method, fully described in Refs. [15–19]. Its accuracy comes from including many effects beyond the kinetic and Coulomb energy, e.g., the Breit correction to the Coulomb repulsion operator, the two principal quantum electrodynamics corrections (self energy and vacuum polarization), and a finite size nucleus with a two-parameter Fermi charge distribution.

For an assessment of the computational accuracy, Table 1 compares the relatively perfect experimental data for Ni, Cu and Zn in the authoritative compilation of Deslattes et al. [20] with the energies computed there, and with the results here. For these important mid-Z elements the measurements are highly accurate, to within 0.08 eV or better, so that the computational accuracy can be gauged by its agreement with the measurements. Our computations seem to do slightly better than those in Ref. [20], even though both are sometimes outside the 1σ uncertainties (in brackets) claimed for the computations. The difficulties in deciding the computational accuracy ab initio is discussed in Ref. [20], and with a longer perspective in Ref. [21]. However, a code's approximation tends to affect the code output the same way, so that the effect or approximations may partly disappear from differences such as energy shifts. Therefore, we can also expect that the precision of our simulations for the satellite line shapes and positions is much more accurate. Especially, the energy shifts for studied 3d-transition metals is much more accurate, i.e., in the order of 0.05–0.1 eV.

3. Results and discussion

The detailed theoretical calculations with the MCDF method produce the line shapes and energies of the $K\alpha_1$ and $K\alpha_2$ x-ray lines in Figs. 1 and 2, for the two 3d-transition elements bordering copper: nickel (Ni; Z = 28) and zinc (Zn; Z = 30). Each panel is for the particular ionization stage with the electron configuration as indicated.

Fig. 1 shows the theoretical $K\alpha_{1,2}$ line structures for various electronic configurations of Ni, in two interesting ionization ranges. One is from Ni^{12+} to Ni^{16+} when ionization modifies the M-shell and the line energies remain close to the values for the neutral atom, ~ 7478 eV and ~7461 eV. The other range is for Ni^{20+} to Ni^{24+}, when ionization affects the L-shell. All these line energies are lower than the He-α resonance line at 7806 eV, where the Kα transition

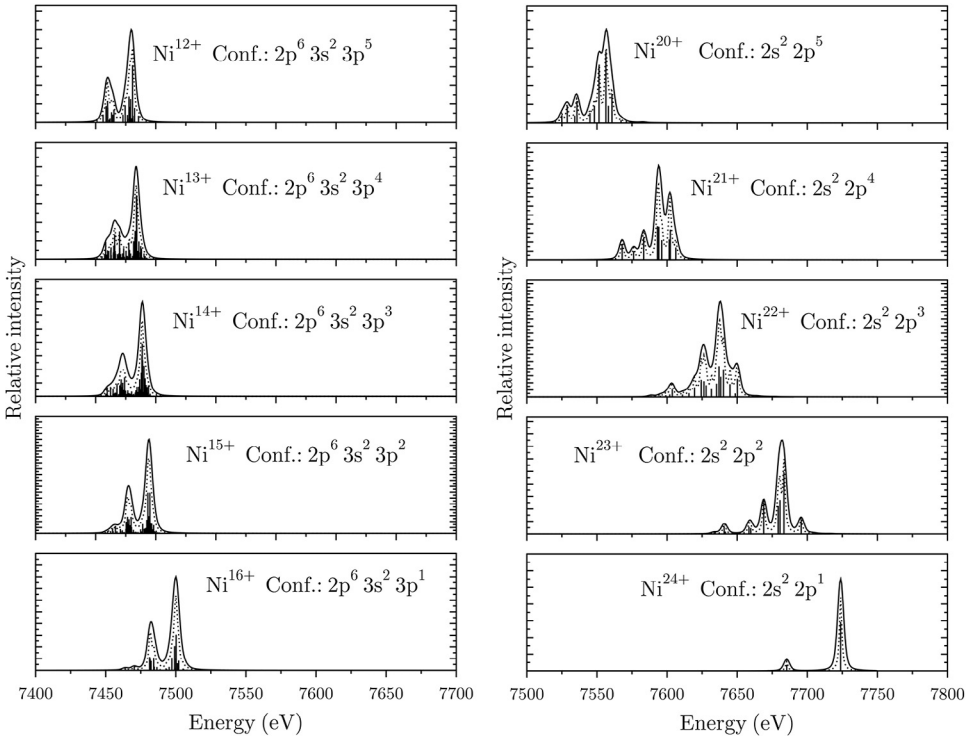

Fig. 1. Calculated stick (line positions and their relative intensities) and synthesized spectra for the $K\alpha_1$ and $K\alpha_2$ x-ray lines of Ni. The dashed curves describe the sum of the Lorentzian natural line shapes and the solid curves represent the convolution of the sum of Lorentzian natural line shapes with Gaussian instrumental response.