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Magnetic-dipole lines in 3d^n ions of high-*Z* elements: identification, diagnostic potential and dielectronic resonances

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Abstract
We present a review of measurements and analyses of extreme-ultraviolet magnetic-dipole (M1) lines in 50–60 times ionized atoms of tungsten, hafnium, tantalum and gold with an open 3d shell. The spectra were measured with the electron beam ion trap at the National Institute of Standards and Technology. Large-scale collisional–radiative modeling was instrumental in line identification and in analysis of their diagnostic potential. The M1 line ratios are shown to be an accurate and versatile tool for studying the LMN dielectronic resonances in 3d^n ions.

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(Some figures may appear in colour only in the online journal)

1. Introduction

Highly charged ions (HCI) of heavy elements are a subject of ongoing research due to their importance in magnetic and inertial confinement fusion, laser-produced plasmas and astrophysics. Elements such as tungsten and gold are routinely used in fusion environments, and their spectra provide important diagnostic information on plasma parameters (e.g. [1]). Moreover, complex spectra of high-*Z* elements offer a challenge to advanced theoretical methods due to strong relativistic and quantum-electrodynamic effects that greatly affect ion properties [2].

One of the most notable characteristics of HCI emission is the presence of forbidden transitions that are barely seen in light elements. Forbidden lines generally show a very strong dependence of their rates on ion charge, and therefore they are less subject to collisional damping and thus can be relatively easily recorded in low-density plasmas. At the National Institute of Standards and Technology (NIST), we continue a research program on the study and identification of extreme-ultraviolet (EUV) spectra from HCI of high-*Z* elements. Various forbidden lines are often the most prominent features in such spectra [3–6]. This paper reports on progress in analysis of magnetic-dipole (M1) lines from the ions of Hf, Ta, W and Au with an open 3d shell.

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2. Measurements and line identifications

Measurements of EUV spectra were performed with the electron beam ion trap (EBIT) at NIST. A typical electron density of about 10^{12} cm^{-3} in an EBIT is low enough not to quench forbidden lines in high-*Z* elements. A flat-field grazing-incidence spectrometer [7] equipped with a charge-coupled device (CCD) was used to measure spectra between 4 and 26 nm with a resolving power of about 400. Ions of metals under investigation were injected into the trap by using the metal vapor vacuum arc ion source, while the neutral gases used for calibration were loaded through the gas injection system. Calibration of the measured spectra was performed with known lines from C, N, O, Fe, Kr and Xe. The typical wavelength measurement uncertainty was about 0.003 nm.

An example of our measurements is presented in figure 1 where the spectra of Ta ions (in atomic-to-digital units of CCD) are shown for the beam energies between 4000 and

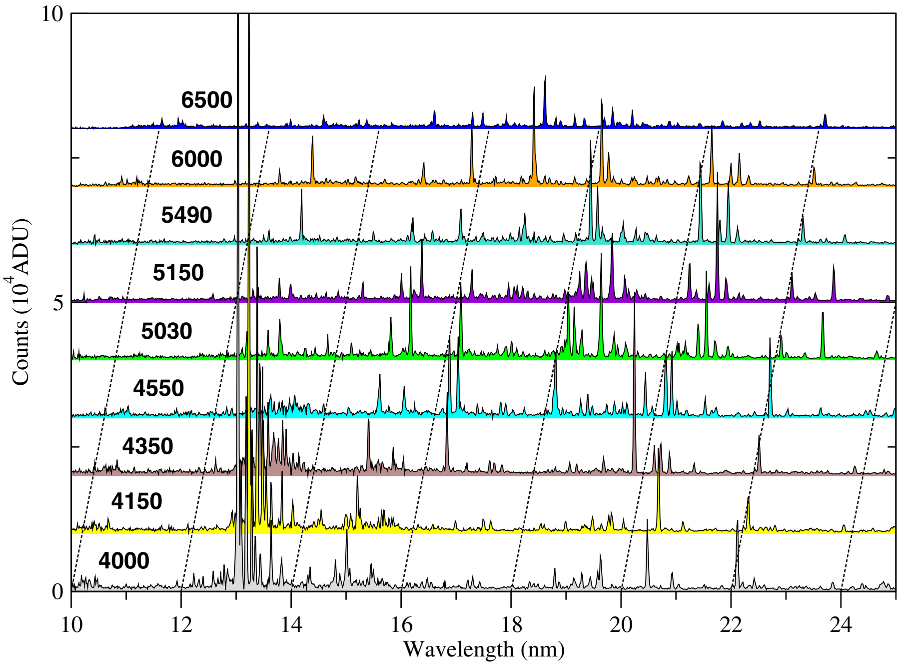

Figure 1. Measured spectra (in analogue-to-digital units of CCD) of Ta for beam energies between 4000 and 6500 eV.

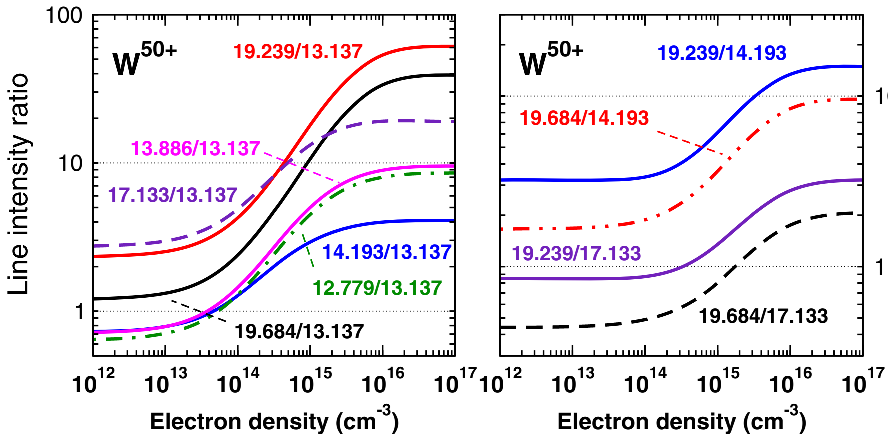

Figure 2. Calculated line intensity ratios for Cr-like tungsten. The line wavelengths are given in nm.

6500 eV. The observed lines are generally well resolved, and the impurities (e.g. the Ar XV line at 22.115 nm) are clearly identifiable.

The measured spectra were analyzed with the non-Maxwellian collisional–radiative (CR) code NOMAD [8]. The required atomic data, e.g. energy levels, radiative and autoionization transition probabilities, and electron-impact cross sections, were calculated with the relativistic-model-potential flexible atomic code (FAC) [9]. The effect of charge exchange with neutrals in the trap on the ionization balance was accounted for as well. We developed a hybrid model that combines a detailed representation of low excited states (for instance, the $n = 3$ complex in $3d^n$ ions) with a condensed description of high excited states [10]. Thus, the states that are responsible for the observed M1 emission are described as accurately as possible and, on the other hand, the computation times are significantly reduced without a loss of accuracy.

In total, 170 new forbidden (primarily M1) spectral lines from W^{48+} to W^{55+} [10], Hf^{44+} to Hf^{54+}, Ta^{45+} to Ta^{57+} and Au^{51+} to Au^{60+} were identified between 9 and 25 nm. Most of the new lines represent transitions within the $3d^n$ ground configurations.

3. Plasma diagnostics with M1 lines

The M1 lines from W and other high-*Z* elements can be used for fusion plasma diagnostics. Since these lines appear within a rather narrow spectral window, their relative intensities are not very sensitive to spectrometer efficiency. Furthermore, a mere appearance of specific lines from different ions may give reasonable estimates of plasma temperature from the ionization balance considerations. Finally, the M1 lines represent a good spectroscopic tool for measuring electron density n_e in low-density hot plasmas of magnetic confinement fusion. A typical procedure for density diagnostics includes comparison of intensities of two (or more) spectral lines that have different radiative decay rates and therefore respond differently to collisional damping.

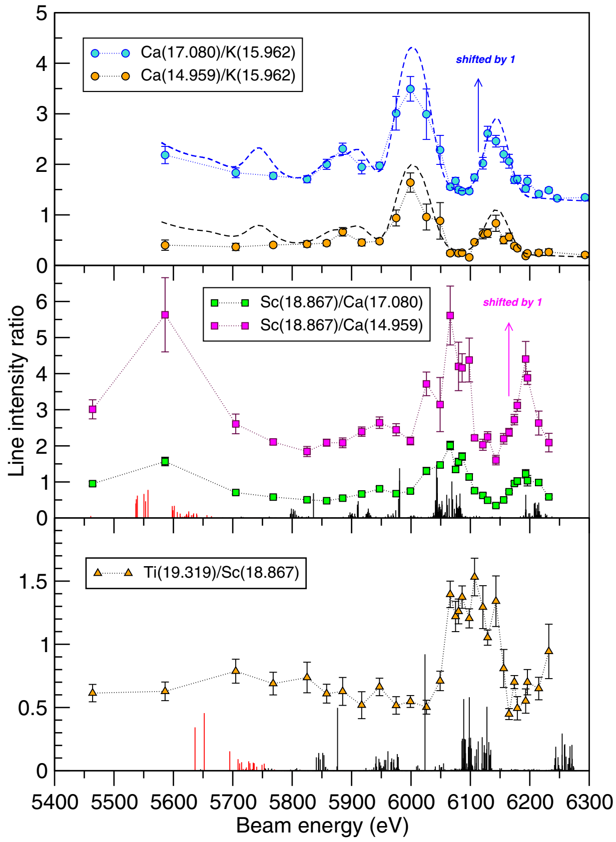

Figure 3. Measured ratios of M1 lines in W ions. Results of CR modeling are shown by dashed lines in the top panel. The wavelengths (in nm) of spectral lines are shown in the legends. The relative strengths of LMM (red) and LMN (black) resonances are shown in the middle and bottom panels for the Sc-like and Ti-like ions, respectively.

A ratio of resonance to intercombination lines in He-like ions is one of the well-known examples. The calculated transition probabilities for the M1 lines in the $3d^n$ ions of W were found to vary by about two orders of magnitude, between 4×10^4 and $5 \times 10^6\ s^{-1}$. Our CR simulations show that some line pairs are sensitive to electron density at $n_e = 10^{13}$–$10^{16}\ cm^{-3}$. An example for lines of the Cr-like tungsten is presented in figure 2. The ratios of such lines as e.g. 19.239 and 13.137 nm change by more than an order of magnitude between low- and high-density limits.

The M1 lines from the other high-Z elements considered here should also exhibit similar dependences on n_e. Since the transition probabilities for Hf and Ta are smaller than those for W and for Au are larger than those for W, the sensitivity ranges shift to lower densities for the former elements and to higher densities for Au.

4. Inner-shell dielectronic resonances

One of the common techniques to study dielectronic resonances (DRs) in EBITs utilizes beam energy ramping from the values of high abundance for a specific ion down to the energy region of DRs. Due to their energy structure, the $3d^n$ ions provide an opportunity to perform direct measurements of inner-shell DRs without beam ramping [11, 12]. Extensive calculations with FAC show that the LMN resonances, which correspond to excitation of a $2p_{3/2}$ electron into the 3d subshell with simultaneous capture of a beam electron into the N shell, can be produced with beam energies of the order of 6 keV. Since DRs shift the ionization balance between the neighboring ion stages, this change in ion distribution is expected to be revealed through intensity ratios of the corresponding M1 lines.

To test this hypothesis, we performed a series of EUV measurements scanning beam energies between 5.7 and 6.3 keV. Figure 3 presents the measured intensity ratios for several pairs of M1 lines. Two [Ca]/[K] ratios are shown in the top panel, the middle panel presents two [Sc]/[Ca] ratios, and the bottom panel contains the [Ti]/[Sc] line ratio. One can see that, indeed, the plots do show the presence of strong resonance structures in line ratios.

A CR model for Ca- and K-like ions was developed with about 10 500 levels including approximately 1200 autoionizing $2p^5 3s^2 3p^6 3d^2 4l$ levels in the Ca-like ion. To account for the anisotropic energy distribution of beam electrons that leads to non-statistical populations of magnetic sublevels, correction factors were introduced to dielectronic capture cross sections and autoionization probabilities. The results of anisotropic CR modeling are shown by dashed lines in the top panel of figure 3. Clearly, the agreement with the measured line ratios is very good. As the available computational resources do not allow development of a CR model with DRs for more complex $3d^n$ ions, we only show the relative calculated strengths of the corresponding DRs (red LMM, black LMN). The positions of resonances and their strengths agree with the measurements.

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