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Fusion tracer elements: atomic structure and spectroscopic properties of molybdenum

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Abstract: Near the thermonuclear burn in magnetic (MCF) and inertial (ICF) confinement fusion experiments temperatures of the order of 10 keV are envisaged. Densities, however, differ drastically, 10^{14} cm^{-3} for MCF whereas densities up to 10^{26} cm^{-3} are expected in ICF. The high density causes serious problems for diagnostics due to the perturbation of the Coulomb field and the large opacity of resonance lines. Relativistic atomic structure calculations and collisional-radiative simulations show, that a high Z tracer element like molybdenum is suitable for diagnostics in both cases. Spectra simulations developed for the dielectronic satellite emission near H-like Ly_α show interesting diagnostic properties.

I. Introduction

The achievement of the thermonuclear burn in ICF experiments is an important but critical issue. This is due to asymmetries in the implosion of the capsule and the generation of hot electrons. Therefore, diagnostic methods which provide information about 10 keV-temperatures and densities up to 10^{26} cm^{-3} are requested to control and optimise the fusion process. Usual tracer elements like argon are not suitable, because at some 10 keV, the argon ions are overionized and the perturbation of the line emission by micro fields is much too large for precise diagnostics. In the present work we propose the K-shell x-ray emission of high Z tracer elements like molybdenum for diagnostics in order to avoid too large perturbations of the ionic Coulomb field by the surrounding particles and obtain temperature sensitivities up to some 10 keV.

II. Atomic structure and diagnostic properties of molybdenum

In order to avoid too strong perturbations due to the plasma microfield, the ion Doppler effect should be smaller than the Stark shift. The Stark shift can be estimated according

$$\Delta E_{Stark} \approx \alpha_d F^2$$

where α_d is the dipole polarisability. For estimation, we calculate the Stark shift of the He-like resonance line 1s2p $^1P_1$ of Mo for $n_e = 10^{26}$ cm^{-3} and $kT_e = kT_i = 10$ keV:

$$\alpha_d(\gamma J) = 4 \sum_{\gamma' J'} \frac{f(\gamma J - \gamma' J')}{(E_{\gamma' J'} - E_{\gamma J})^2} \approx 4 \left\{ \frac{0.5732}{(1860/Ry)^2} + \frac{0.03855}{(153/Ry)^2} + \frac{0.00669}{(213/Ry)^2} \right\} = 1.8 \cdot 10^{-2}\ a.u.$$

Assuming $F = 2F_0$, where F_0 is the Holtzmark field

$$F_0 \approx 2.603 \frac{N^{2/3}}{a_0^2} \approx 15\, a.u.$$

we obtain a Stark shift of

$$\Delta E_{Stark} \approx -2 \alpha_d F_0^2 \approx -8.4\, eV .$$

The Doppler width is $\Delta E_{Doppler} \approx 14\, eV$. We therefore expect sufficient stability of the ionic Coulomb field of Mo against the micro field even for densities being achieved for the highest compression.

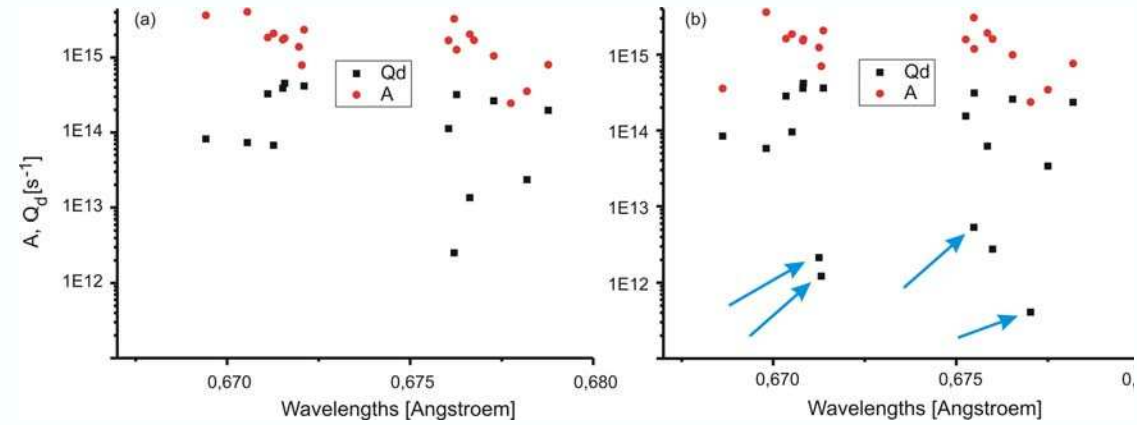

Figure 1: Radiative decay rates A and dielectronic satellite intensity factors Q_d of 2l2l'-configurations of He-like molybdenium calculated with different methods: a) multi-configuration Z-expansion MZ, b) multi-configuration-Dirac-Fock MCDF. The arrows indicate transitions arising from relativistic effects.

For temperature diagnostics we consider the dielectronic satellite emission near H-like Lyman-alpha. The satellite intensity achieved by dielectronic capture only is given by

$$I(satellite) \approx 1.656 \cdot 10^{-22}\, n_e\, n_{1s} \frac{Q_d}{g_{1s}} \frac{\exp(-E_S / kT_e)}{(kT_e)^{3/2}}$$

where the dielectronic satellite intensity factor Q_d is given by

$$Q_d = \frac{g_j \Gamma_{jk} A_{ji}}{\sum A + \sum \Gamma} .$$

For large Z like Mo (Z_n = 42), relativistic effects become important for the atomic structure and the corresponding diagnostic applications. Figure 1 shows the radiative decay values A and dielectronic satellite intensity factors Q_d for the 2l2l'-satellites calculated with the Multi-Configuration-Z-Expansion (MZ) and the Multi-Configuration-Dirac-Fock (MCDF) method employing the MZ-code [1] and the RATIP-code [2]. Figure 1 shows the comparison between the two methods. It can be seen, that both data sets show rather good agreement except for the transitions indicated by arrows. This is due to the fact, that the autoionising rate of the $2p^2\ ^3P_1$ configuration arises from the Breit-interaction only which is not included in the MZ simulations.

III. MARIA-simulations: dielectronic satellite emission of Mo

Spectra simulations for molybdenum are carried out with the MARIA-code [3]: a multi-level, collisional radiative simulations for transient optically thick plasmas.

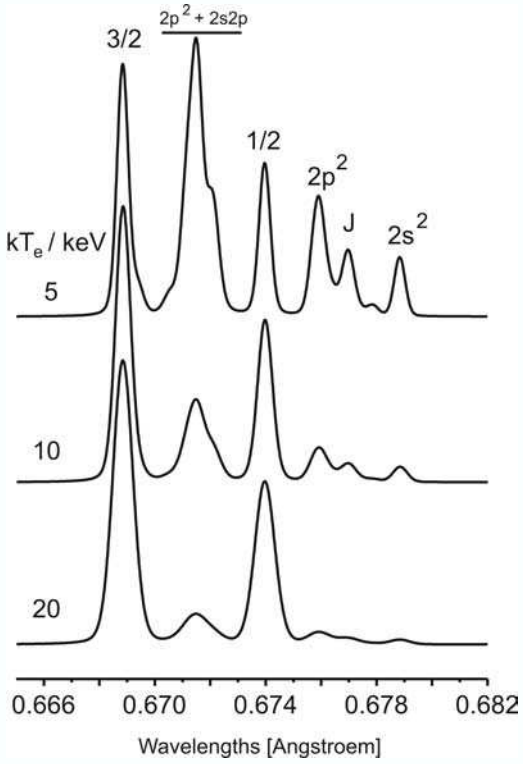

Figure 2: MARIA-simulations of the temperature sensitivity of He-like dielectronic satellites 2l2l' near Ly_α, Z_n = 42.

Figure 2 shows the temperature sensitivity of the dielectronic satellite emission near H-like Lyman-alpha of molybdenum, $n_e = 10^{23}$ cm^{-3}. Indicated are the Lyman-alpha lines "3/2" and "1/2", the J-satellite $2p^2\ ^1D_2$ – $1s2p\ ^1P_1$ and some other configurations for prominent line groups: $2p^2$+2s2p, $2p^2$ and $2s^2$. Despite the high density, collisional redistribution effects between the autoionising levels 2l2l' are not yet important. The simulations show, that a strong temperature sensitivity is obtained up to temperatures of about 20 keV.

We note, that even for kT_e = 20 keV, Mo is still not over ionized. Unlike low Z-elements, a strong emission between the Ly_α-components originates from the 2l2l'-satellites. Also

remarkable is the strong emission of the two-electron emission: $2s^2\ ^1S_0 - 1s2p\ ^3P_1$ which arises from the configuration interaction of the $2s^2\ ^1S_0$ and $2p^2\ ^3P_0$-levels.

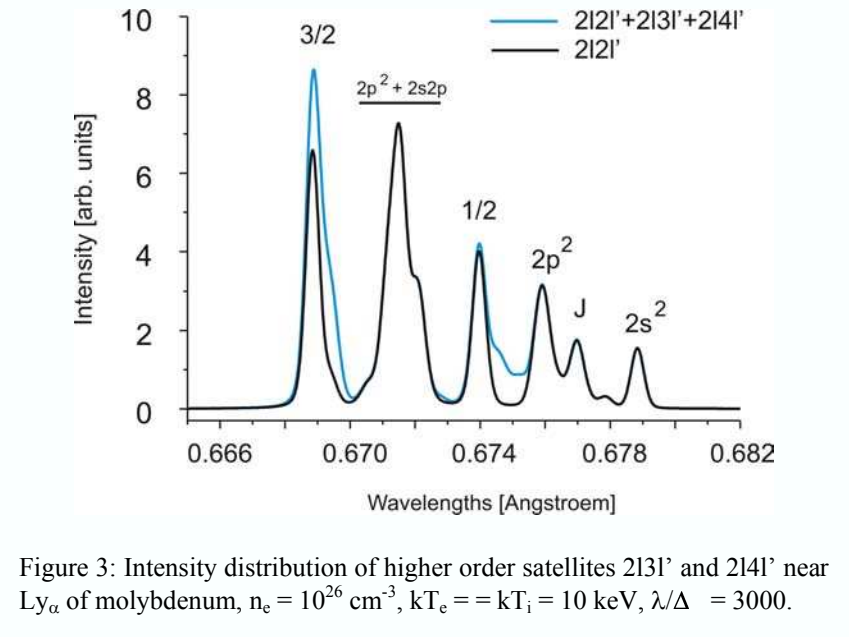

Figure 3: Intensity distribution of higher order satellites 2l3l' and 2l4l' near Ly_α of molybdenum, $n_e = 10^{26}$ cm^{-3}, $kT_e = = kT_i = 10$ keV, $\lambda/\Delta = 3000$.

Figure 3 shows the higher order satellite contributions, 2l3l' and 2l4l' near Ly-alpha. It can be seen, that the higher order contributions leads to a line overlapping near the 3/2-component rising their peak intensity. This effect is important when considering the intensity ratio of the Lyman-alpha doublet for diagnostic purposes. Also line overlapping between the 1/2-component and the $2p^2$- group takes place, being important when analysing line profiles.

IV. Conclusion

We have proposed Mo as a tracer element for parameters near the thermonuclear burn in MCF and ICF experiments. The stability of the ionic Coulomb field against micro field perturbations makes Mo a good choice even for densities up to 10^{26} cm^{-3}. Spectra simulations for the dielectronic satellite emission near H-like Lyman-alpha were developed and large temperature sensitivities up to 20 keV were demonstrated.

V. References

[1] Vainshtein & Safronova, ADNDT **21**, 49 (1979).

[2] S. Fritzsche et al.,Computer Physics Communications **124**, 340 (2000).

[3] F.B. Rosmej, J. Phys B Lett., **30**, L819 (1997).