Modeling of the M X-ray line structures for tungsten and L X-ray line structures for molybdenum

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Abstract. Modeled within the Collisional-Radiative approach, for parameters relevant to plasmas in the centre of JET, the M X-ray line structures for tungsten and L X-ray line structures for molybdenum both occur in the wave length range 5.0-5.35 Å; and, their strengths are comparable. Therefore, the spectra obtained with the upgraded high-resolution X-ray spectrometer KX1 on JET should include both tungsten and molybdenum in their interpretation. The same will be true for the high-resolution X-ray diagnostic on tokamaks such as WEST and ITER, where tungsten plasma-facing components will be implemented.

1. Introduction

The theoretical background for the future high-resolution X-ray diagnostics of tokamak plasmas is an active topic of research [1-5]. The urgent need for such studies comes primarily from the choice of tungsten as a plasma facing component in the future ITER fusion reactor. Highly charged tungsten ions appearing in the central plasma due to the plasma-wall interaction [6] are therefore a natural source of X-rays for high-resolution X-ray diagnostics that monitor ion temperature, rotational velocity and W impurity level in tokamak fusion reactors. The structures of tungsten X-ray spectra emitted over a wide wave length range are extremely complex, and require exhaustive theoretical and experimental studies that provide guidance for X-ray diagnostics of the plasma planned for next-generation tokamaks.

In this work we present the results of modeling of the M X-ray line structures for tungsten in the 5.0-5.35 Å wavelength range, and the L X-ray line structures for molybdenum in the same wave length range, expected from high-temperature plasmas with parameters relevant to the centre of the plasma in JET, and the outside plasma expected on ITER (r/a=0.8-0.9). The simulations are performed using the Flexible Atomic Code (FAC) package, within the framework of Collisional-Radiative Model (CRM) approach [4, 7, 8]. FAC calculates the atomic structure with a fully relativistic Dirac-Fock-Slater method and the configuration interaction method. The modeling performed assumes a plasma electron temperature of 4.5 keV and electron density of 6x1013 cm−3. For tungsten this predicts ions will be ionized from W+44 to W+47 and their X-rays are primarily from the M-shell, in the 5.0-5.35 Å wavelength range. For molybdenum the ions will be mostly from Mo+30 to Mo+35 and these primarily emit L-shell radiation, which happens to be in the same wave length range.
2. Theory - Flexible Atomic Code

The simulations have been performed using the FAC package within the framework of CRM approach [4, 7, 8]. In the package the full-relativistic Dirac-Fock-Slater iteration method and the configuration interaction method are used to calculate of the atomic structures, and the distorted-wave approximation method is used for electron collision cross sections. Briefly [7], the energy levels of an atomic ion with $N$ electrons are obtained by diagonalizing the relativistic effective Hamiltonian $H$. In atomic units this reads

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

where $h_D (i)$ is the single-electron Dirac Hamiltonian for the potential due to the nuclear charge. The basis states $\Phi_\nu$, which are usually referred to as configuration state functions (CSF), are antisymmetric sums of products of $N$ one-electron Dirac spinors $\varphi_{n\kappa\sigma}$

$$\varphi_{n\kappa\sigma} = \frac{1}{r} \left( P_{n\kappa} (r) \chi_{\kappa\sigma} (\theta, \phi, \sigma) \right),$$

where $\chi_{\kappa\sigma}$ is the usual spin-angular function. $n$ is the principal quantum number, $\kappa$ is the relativistic angular quantum number, which is related to the orbital and total angular momentum.

The FAC code not only computes atomic data, such as energy levels and transition probabilities for radiative transitions and auto-ionization, but also cross sections for excitation and ionization by electron impact and the inverse processes (e.g., radiative recombination and dielectronic capture). With these data, and within the approximations of the CRM (e.g., [9]), FAC can also compute fractional ionizations and the resulting X-ray spectrum, with rates computed for specific electron energy distributions.

3. Results

The preliminary results in this paper are done for an initial interpretation of the X-rays emitted by the plasma in the JET tokamak operated in the ITER-like wall configuration, as registered by the upgraded high-resolution crystal spectrometer (KX1) [10, 11]. Below we present some results for the X-ray spectra for tungsten and molybdenum, with electron temperature and density relevant to central JET; these parameters are similar to those expected for high-radius ITER plasmas. Therefore, based on the shape of X-ray spectrum registered KX1 spectrometer on JET [12] we established a line width in Figure 1 and Figure 2 equal to 2 eV. It should be emphasized that in our simulation we applied original distribution of tungsten and molybdenum ions predicted by the most advanced version of CR model applied in FAC package.

3.1 M X-ray spectra for tungsten

Figure 1 presents the M X-ray line structures for tungsten in plasmas with electron temperature of 4.5 keV and electron density of $6 \times 10^{13}$ cm$^{-3}$. The modeling includes the weak $4d \rightarrow 3p$ and other low intensity transitions in tungsten ions from W$^{+44}$ to W$^{+47}$ that occur in the 5.0-5.35 Å wavelength range. Their intensity is about 20-30 times lower than for the most intense lines M$\alpha_1$ and M$\beta_1$ (i.e. for $4f \rightarrow 3d$ transitions). However, for higher electron temperature, e.g. 7.0 keV, the M X-ray line structures will contain significant contributions of the much stronger M X-ray lines M$\alpha_1$ and M$\beta_1$ that originate from the more highly ionized tungsten ions W$^{+48}$ to W$^{+52}$ [13].

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Figure 1. M X-ray line structures of tungsten ions (from W$^{+44}$ to W$^{+47}$) for electron temperature of 4.5 keV and electron density of $6 \times 10^{13}$ cm$^{-3}$.

3.2. L X-ray spectra for molybdenum

Figure 2 shows the corresponding results for the L X-ray line structures for molybdenum ions from Mo$^{+30}$ to Mo$^{+35}$ expected in this same plasma (4.5 keV electron temperature, $6 \times 10^{13}$ cm$^{-3}$ electron density). Over the entire wavelength range the spectrum may be less complicated than for W, but is still sufficiently complex to be potentially confusing.

The upgraded KX1 spectrometer [10, 11] almost always finds that the JET plasma emits these molybdenum spectra. One of the possible molybdenum sources is the marker made from molybdenum tile installed as an inner vertical divertor target [12]. Therefore, both elements (tungsten and molybdenum) should be taken into account in the analysis of high-resolution X-ray spectra in this wave length regime. Moreover, presented in Figure 1 and Figure 2 results should reliably reproduce the measured KX1 spectrometer spectra.
4. Summary and conclusions

In this work we present the results of modeling of the M X-ray line structures for tungsten in the 5.0-5.35 Å wavelength range, and the overlapping L X-ray line structures for molybdenum, for an electron temperature and density that is relevant to central JET and high-radius ITER plasmas. The L X-ray spectra for molybdenum have a significant spectral contribution in the same wavelength region as the M X-ray spectra for tungsten, hence both elements should be included in the interpretation of the high-resolution X-ray spectra registered on JET. The obtained results are equally useful for the high-resolution X-ray diagnostics on the ITER and WEST tokamaks, where tungsten X-ray spectra will overlap the radiation emitted by other plasma facing components that will most likely include molybdenum as well.

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