Algorithm of calculating the passive signal of tokamak edge plasma for CXRS diagnostics

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1. Introduction. Active spectroscopic diagnostics is widely used in modern tokamaks to measure such important plasma parameters as the concentration and distribution of impurities, the profiles of the ion temperature and the rotation speed of the plasma. CXRS Edge diagnostics on ITER will be located in the third equatorial port plug and will take measurements for the outer part of the plasma, from the plasma entry point to the middle of the plasma's small radius. The general scheme of charge exchange process (state-selective charge transfer):

$$A^{z+} + B^0 \rightarrow A^{(z-1)+}(n, l) + B^+. \tag{1}$$

Plasma ion A^{z+} interacts with the neutral atom B^0 and captures its electron. Usually, the electron is captured in the excited state $A^{(z-1)+}(n, l)$, where n, l are the principal and orbital quantum numbers, respectively. The excitation relaxes by emission of radiation, which is collected by the optical system and delivered to the spectrometers.

Passive signal in CXRS diagnostics is formed by charge exchange of the ions in the tokamak plasma periphery on neutral hydrogen isotopes atoms coming from the vacuum chamber first wall during the recycling process. Predictive modeling of passive signal remains a problem, as it requires a number of theoretical tasks to be solved together, which need sophisticated numerical modeling.

2. Passive signal modelling algorithm.

2.1. Algorithm general description. For the modeling of passive signal in CXRS Edge diagnostics we developed an algorithm (see Fig. 1) that includes: (i) using the data of modeling the SOL (and divertor) plasma with account of impurities to be diagnosed with the CXRS Edge diagnostics (such data are accumulated and being extended; for ITER see simulations with the SOLPS (B2-EIRENE) [1] and OSM+EIRENE+ DIVIMP [2] codes); (ii) using the data for cross-sections of charge exchange reactions, which produce highly-excited atomic states of H-like impurity ions from collisions of impurity nuclei with hydrogen isotopes neutral atoms (including their low-lying excited states) of background plasma; (ii-a) evaluation of charge

exchange cross sections not covered by the existing databases; (iii) calculation of the rates of the above-mentioned reactions for essentially non-Maxwellian velocity distributions function (VDF) of hydrogen isotopes neutral atoms (the VDF data may be generated, e.g., by stand-alone EIRENE code [3] simulations using the background SOL plasma data of item "i"); (iv) calculation of the photon emission coefficients (PEC) data for interested impurity visible-light spectral lines in the case "iii" which is beyond the available data in ADAS and similar sources (these data may be generated, e.g., with the code [4], similarly to evaluation of CXRS active signal in [5]).

2.2. Charge exchange cross sections and rates. In existing databases (e.g., OPEN-ADAS [6], ALADDIN [7]) the most of available information about charge exchange cross sections (item (ii) in Fig. 1) covers the range of energies, interesting primarily for the calculations of the active signal, i.e. for diagnostic neutral beams with energies of tens or hundreds of keV. At the same time, for estimations of the passive charge exchange signal, when the energy of

Fig. 1. General scheme of passive signal modelling algorithm.

coming from the wall neutral atoms is tens or hundreds of eV, the data is not enough. Therefore, additional theoretical calculations of the cross sections may be necessary (item (ii-a) in Fig. 1) for the charge exchange reactions of interest.

The rate of quantum state $A^{(z-1)+}(n, l)$ population due to charge exchange is given by

$$\langle v\sigma_{nl}\rangle \equiv \langle\langle v_{AB}\sigma_{nl}\rangle_{v_A}\rangle_{v_B} = \int d\boldsymbol{v}_A \int d\boldsymbol{v}_B \ f_A(\boldsymbol{v}_A)f_B(\boldsymbol{v}_B)v_{AB}\sigma_{nl}(v_{AB}). \qquad (2)$$

Here $\boldsymbol{v}_A$ is the velocity of ions A, $\boldsymbol{v}_B$ is the velocity of neutral atoms B, $v_{AB} \equiv |\boldsymbol{v}_A - \boldsymbol{v}_B|$ is the relative velocity of ions and neutral atoms, $f_A(\boldsymbol{v}_A)$ is ions' VDF, $f_B(\boldsymbol{v}_B)$ is neutral atoms' VDF, σ_{nl} is charge exchange cross section, which depends only on the relative velocity v_{AB}; n and l are the principal and orbital quantum numbers of that atomic state which electron is captured to after charge transfer.

In Fig. 2 it is shown the comparison of $\langle v\sigma_{nl}\rangle$ calculated by Eq. (2) with the data available in OPEN-ADAS for the reaction $C^{6+} + H^0(1s) \rightarrow C^{5+}(n = 4) + H^+$. It should be noted that in this case, in order to compare with the data from OPEN-ADAS, the charge exchange cross section
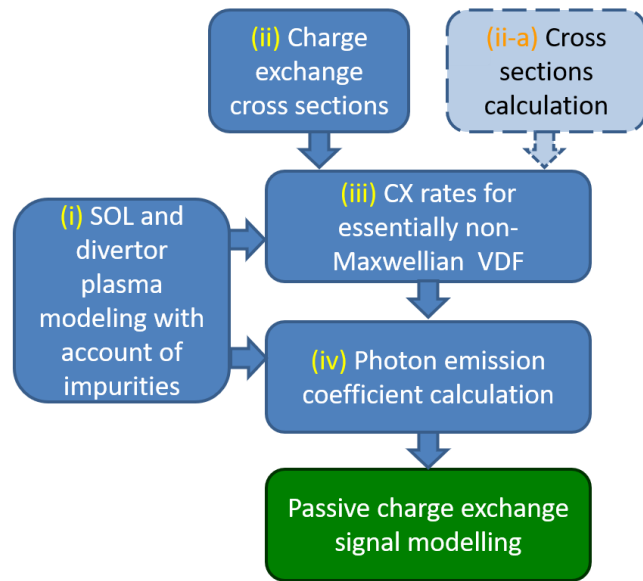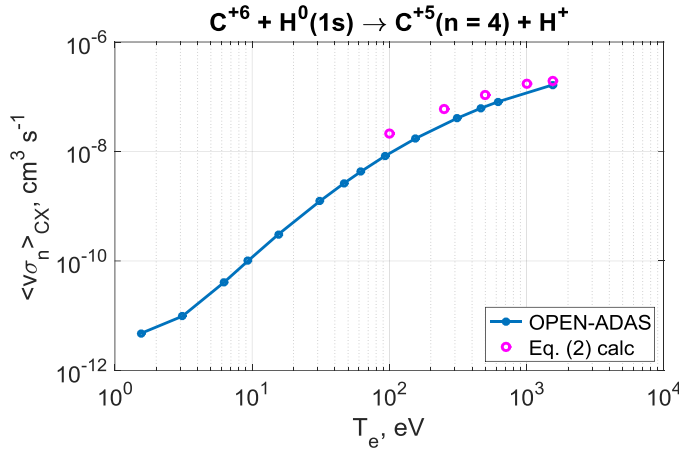
Fig. 2. The comparison of $\langle v\sigma_{nl}\rangle$ calculated by Eq. (2) (purple circles) with the data available in OPEN-ADAS (blue curve) for the reaction $C^{6+} + H^0(1s) \rightarrow C^{5+}(n = 4) + H^+$.

calculations were conducted assuming the Maxwellian VDF of hydrogen atoms with the temperature corresponding to the mean energy of deuterium atoms from EIRENE code simulations of the divertor and SOL operation scenario in ITER. In general, for calculating the rate (2) one should use the VDF of atoms calculated by EIRENE, and then the result will not be a universal function, but a functional which depends on the spatial profiles of all plasma parameters throughout the SOL (i.e. on the operation scenario of the diverter and SOL) rather than the coordinates only.

2.3. Photon emission coefficient calculation. For calculation of photon emission coefficients (PEC, see item (iv) in Fig. 1) the previously developed code *nl*-KINRYD [4] is used. This code is based on the quasi-classical model of the radiative-collisional cascade of a highly-excited bound electron in a hydrogen-like ion in plasmas.

Quantum kinetic equation for the radiative-collisional cascade in *nl*-space has the form

$$[\hat{L}_c + \hat{L}_r^q]f(n, l) + q(n, l) = 0, \tag{3}$$

where $f(n, l)$ is the population distribution function in the two-dimensional space of *n* and *l* quantum numbers, $\hat{L}_c f(n, l) = \sum_{n',l'} [W(n', l' \rightarrow n, l)f(n', l') - W(n, l \rightarrow n', l')f(n, l)]$ is the operator of collisional transitions, $\hat{L}_r f(n, l) = -A(n, l)f(n, l) + \sum_{n',l'} A(n', l' \rightarrow n, l)f(n', l')$ is the operator of radiative transitions, $A(n, l) = \sum_{n',l'} A(n', l' \rightarrow n, l)$ is the total rate of radiative decay of *nl*-level, $q(n, l)$ is the source of atomic state population.

The iterative solution method [4] is used:

$$\hat{L}_c f_k(n, l) - A(n, l)f_k(n, l) + q_k = 0, \tag{4}$$

$$q_k(n, l) \equiv \sum_{n'=n+1} \sum_{l'=l\pm 1} f_{k-1}(n', l') A(n', l' \rightarrow n, l). \tag{5}$$

Such a method is used to allow for the non-local coupling between states for the two-dimensional distribution. The function *f* is presented in the form of a series $f = f_0 + f_1 + f_2 + \ldots + f_k + \ldots$, that corresponds to the successive emission of photons. Each term f_k of this series can be determined from the Eqs. (4)-(5) using f_{k-1} calculated at the previous step, while f_0 can be found by substituting the original source. For highly excited electrons the collisional operator

may be reduced to a differential operator of the diffusion type in nl-space. For $n^2 << l^3$ ($l < n$) the radiative operator is reduced to a differential operator, describing a continuous classical flow of electron in nl-space. An example of nl-KINRYD calculations results is shown in Fig. 3: the population distribution function of bound atomic electron in Be^{+3} as a function of the principal (n_Z) and orbital (l_Z) quant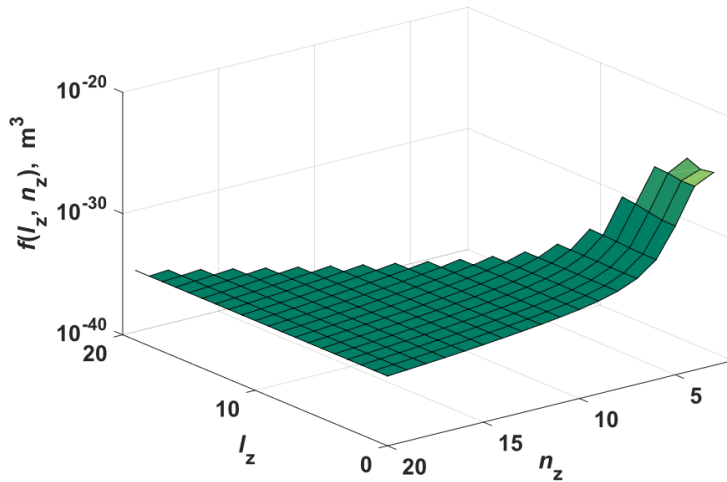um numbers for the source produced by populating the levels $n = 3$ and $n = 4$ by the charge exchange collisions of Be^{+4} on the neutral deuterium atoms in the ground states. The result corresponds to Be^{+3} level population per one atom of Be^{+4} and one atom of deuterium. Results are given for a deuterium plasma with electron and ion densities $N_e = N_i = 4.5 \cdot 10^{19}$ m^{-3} and temperatures $T_e = T_i = 2$ keV; effective temperature of neutral deuterium is 800 eV.

Fig. 3. The population distribution function of bound atomic electron in Be^{+3} as a function of the principal (n_Z) and orbital (l_Z) quantum numbers.

3. Conclusions. The algorithm for the modeling of passive signal in CXRS Edge diagnostics of tokamak plasma periphery was developed. This algorithm includes: (1) using the predictive SOL and divertor plasma simulation data with impurities taken into account; (2) calculation of charge exchange rates for essentially non-Maxwellian velocity distribution functions (VDF) of neutral hydrogen isotope atoms; (3) calculation of photon emission coefficients (PEC) for spectral lines in the visible part of the spectrum of impurities, which, at least because of neutral hydrogen non-Maxwellian VDF, are outside the data available in ADAS or similar sources.

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