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# SIMULATION OF PHA SOFT X-RAY SPECTRA EXPECTED FROM W7-X

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**ABSTRACT:** A computer code named RayX has been developed for checking the performance of a spectroscopy system and optimizing individual parts, like detectors and filters for the pulse height analysis (PHA) diagnostic system designed for the stellarator W7-X. Using the code, the intensity and shape of the X-ray spectra are simulated for different plasma scenarios characterized by varying the temperature and density profiles as well as the electron cyclotron resonance heating (ECRH) power over a wide range. In the simulations of the recorded spectra, the influence of geometrical configuration changes of the diagnostic system (pinhole size, detector size, location of each diagnostic component), of the timing of data collection, as well as of the type and thickness of filters are being investigated. The atomic processes of free-free (bremsstrahlung), free-bound (recombination radiation), and bound-bound emission (line radiation) are considered. For the impurities fractional abundancies of 3% carbon (C), 0.5% oxygen (O) and 0.002% iron (Fe) are taken into account. Information about the number of photons which reach the detector and the current generated inside the detector is given. It is shown that the distance between pinhole and detector has a larger impact on the registered spectra (intensity and total number of photons) than the distance between plasma and pinhole. Based on the results of the simulations, the expected optimal positions of the individual components (pinholes, detectors) were defined for the PHA W7-X diagnostic system.

**KEYWORDS:** stellarator; plasma spectroscopy; pulse-height-analysis, soft x-ray spectra

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## Contents

<b>1.Introduction.....</b>	.....
<b>2.Description of the RayX code.....</b>	.....
<b>3.Exemplary results</b>	
<b>4.Conclusion.....</b>	.....

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## 1. Introduction

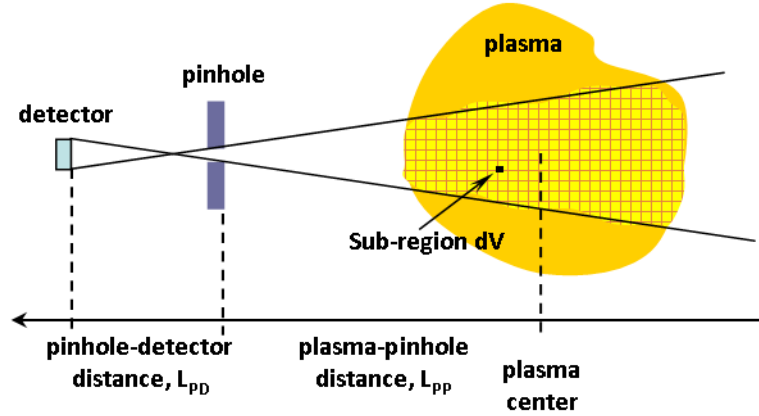
High temperature plasmas, apart from electrons and hydrogen isotopes, contains impurity ions which have significant influence on fusion plasma properties. This makes monitoring of the impurity density very important and special diagnostic tools for such measurements must be present in existing and future fusion devices.

Identification of the line radiation from impurities present in a plasma and determination of their concentration is one of the key issues in the way to a commercial thermonuclear reactor. One of the diagnostics which delivers such an information is a Pulse Height Analysis (PHA) system, currently constructed for the stellarator W7-X. It is one of the commonly used system for measurements of soft X-ray spectra [1-3]. Analysis of the slope of the hydrogen and low-Z continuum radiation is used to determine the central electron temperature of the plasma while the intensity of the continuum radiation along with additional spectroscopic data are used to assess  $Z_{\text{eff}}$  values in the plasma center.

To design the PHA diagnostic system, a special numerical code, named RayX has been developed in Delphi [4]. It is equipped with modules that are responsible for simulation of soft X-ray emission in both, tokamaks or stellarators. It takes into account the geometry of diagnostic port and the type of applied detectors.

## 2. Description of the RayX code

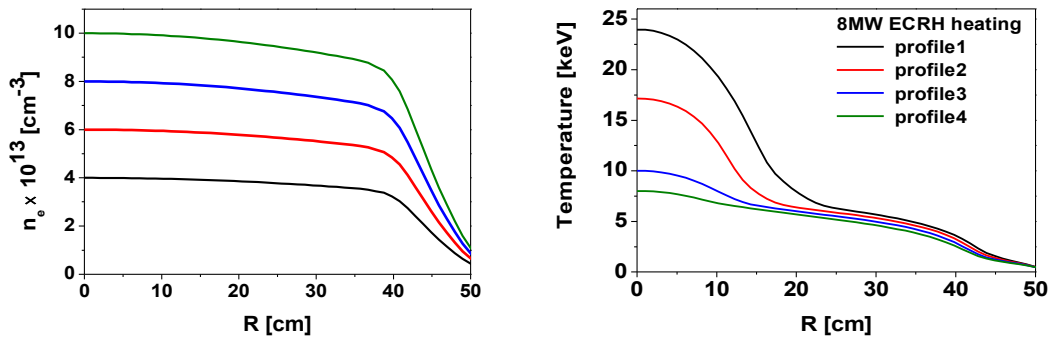
The RayX code makes it possible to analyse the soft X-ray emission, taking the plasma scenarios (distribution of  $n_e$  and  $T_e$ ), the port geometry and the position of the individual elements of the diagnostic system into account. In the code it is possible to consider the real cone of the plasma view for each detector and compute the number of quanta reaching the sensor. It is possible to establish the correct pinhole-detector distance, pinhole size, plasma-pinhole distance for developing the optimum diagnostic configuration which ensure the required energy resolution. The computation idea is demonstrated in fig.1. Each cone of view is divided into small sub-regions ( $dV=1 \text{ mm}^3$ ), where constant values of the electron temperature as well as electron and ions density is assumed.



**Fig.1** Computation scheme.

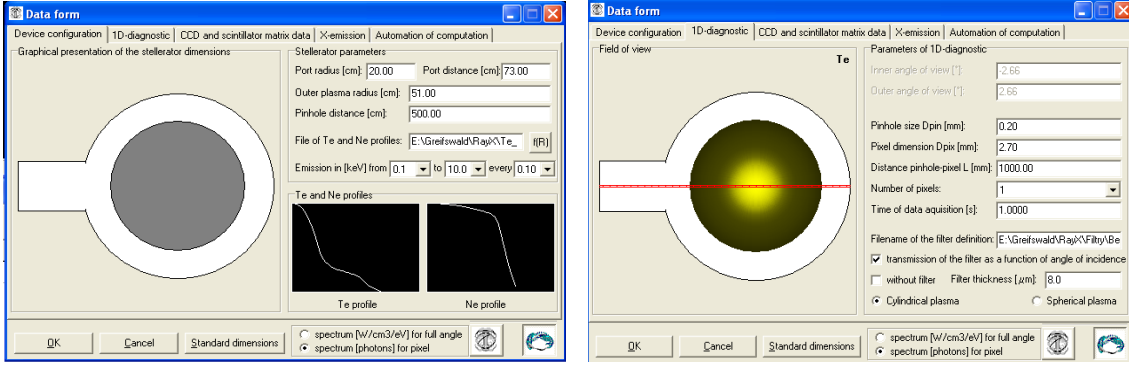
Next, the contribution of each sub-area into the total value of X-rays reaching the detector is calculated. X-ray emission from each sub-region is dependent on a local electron temperature ( $T_e$ ) and, local electron and ions densities ( $n_e, n_i$ ).

It is planned that the super conducting stellarator W7-X will run pulses of up to 30 min duration. The main heating method for steady-state operation is Electron Cyclotron Resonance Heating (ECRH). In the operation phase a heating power of 8-10 MW is planned to be used. In the chosen simulations plasma scenarios for 8MW of ECRH, presented in fig.2, have been taken into account [5].



**Fig.2** Scenarios planned for the W7X device. Electron temperatures -left, electron densities -right.

The user interfaces of RayX are presented in fig.3. They are foreseen to set system parameters, like geometry of the diagnostic port, plasma scenarios as well as type of detectors and content of plasma including impurities.



**Fig.3** The user interface for setting of the plasma device parameters.

In order to simulate a full range of mechanisms of soft X-ray emission it is necessary to take into account several components like:

- ⤴ free-free emission (bremsstrahlung);
- ⤴ free-bound emission (recombination radiation);
- ⤴ bound-bound emission (line radiation);
- ⤴ de-excitation after radiative recombination (additional mechanism for free-bound emission);
- ⤴ de-excitation after dielectronic recombination (additional mechanism for free-bound emission);
- ⤴ electron impact excitation (additional mechanism for bound-bound emission);
- ⤴ de-excitation after CX recombination.

The RayX code includes only first three of these components because they have the largest influence on the registered spectra. Moreover, for detector test purpose they are the most important. A more elaborate description of the X-rays emission from plasma was made in the code IONEQ by A. Weller [6].

In the case of free-free emission, radiation is emitted by free electrons, which are accelerated in the electric field of charged particles. Both, the initial and final states of the electron are free. This explains its continuous spectrum. If the free electrons are scattered by the plasma ions, the bremsstrahlung emission energy  $E_{ff}$  per unit frequency  $\omega$ , temporal interval  $dt$  and unit volume  $V$ , averaged over the Maxwell velocity distribution is:

$$\frac{dE_{ff}}{d\omega dt dV} = \sum_j \frac{16}{3} \left( \frac{2\pi}{3} \right)^{1/2} \left( \frac{e^2}{4\pi \epsilon_0 c} \right)^3 \frac{n_e n_j Z_j^2}{m_e^{3/2} (k_B T_e)^{1/2}} \bar{G}_{ff} e^{-\frac{\hbar\omega}{k_B T_e}} \quad (1)$$

where it is summed over all species of ions;  $m_e$ ,  $v$ ,  $T_e$  are the electron mass, velocity and temperature,  $\hbar\omega$  is the emitted photon energy,  $n_j$  is the ion density with the charge  $Z_j$ , and  $\bar{G}_{ff}$  is the Maxwell-averaged Gaunt factor.

Recombination radiation differs from bremsstrahlung in the final state of the electron, which is bound. Radiative recombination emission term is represented by the equation similar to that for bremsstrahlung:

$$\frac{dE_{ff}}{d\omega dt dV} = \sum_j \frac{16}{3} \left( \frac{2\pi}{3} \right)^{1/2} \left( \frac{e^2}{4\pi \epsilon_0 c} \right)^3 \frac{n_e n_j Z_j^2}{m_e^{3/2} (k_B T_e)^{1/2}} e^{-\frac{\omega}{k_B T_e}} \times \left[ \frac{\chi_{j-1}}{k_B T_e} \bar{G}_{fb}(n) \frac{\xi}{n^3} e^{-\frac{\chi_{j-1}}{k_B T_e}} + \sum_{\mu=n+1}^{\infty} \bar{G}_{fb}(\mu) \frac{Z_j^2 \chi_H}{\mu^2 k_B T_e} \frac{2}{\mu} e^{-\frac{Z_j^2 \chi_H}{k_B T_e}} \right] \quad (2)$$

$\chi_{j-1}$  is the ionization potential of the final ion with charge  $j-1$ ,  $n$  is the main quantum number of this state,  $\xi = 2n^2$  is the total number of places in the shell with the main quantum number  $n$ , and  $\bar{G}_{fb}(\mu)$  is the Gaunt factor for the recombination to the  $n$ th shell. The spectrum of radiative recombination has a continuous character with discrete edges.

Line radiation originates from the transitions of electrons between the bound states of atoms or ions.

$$\frac{dE_{bb}}{dt dV} = 2.56 \cdot 10^{-22} n_e n_Z \sum_j f_j \bar{G}_{ex} \frac{(E_{ph,j} / kT_e)^{1/2}}{kT_e^{3/2}} E_{ph,j} \quad (3)$$

where:  $f_j$  is an oscillator strength,  $\bar{G}_{ex}$  is an averaged Gaunt factor for emission bound-bound,  $n_e$ ,  $n_Z$  are electron and ion densities,  $T_e$  is an electron temperature and  $E_{ph,j}$  is the energy of the X-ray photon.

Data for the computations were taken from [7-10].

As it is seen, all equations are dependent on temperature as well as on the concentrations of electrons  $n_e$  and ions  $n_Z$ . These parameters are connected with the geometry of the devices taken into account during simulations. RayX is able to use realistic  $T_e$ ,  $n_e$  and  $n_Z$  profiles from a tokamak or a stellarator. The ionic compositions for all kinds of impurities are calculated by solving a set of kinetic-equations with assumption of the coronal plasma model [11] (Elvert thermodynamic equilibrium model). In this model different ways for ionization and recombination are assumed. The process of ionization by radiation as well as the process of recombination on the way of collisions between two electrons and one ion, is not allowed here. An example for the Li ions is presented below.

ionization	recombination	equilibrium equations
$\text{Li}^0 + e \rightarrow \text{Li}^{1+} + 2e$	$\text{Li}^{1+} + e \rightarrow \text{Li}^0 + h\nu_1$	$k_1^{01} n_0 n_e = k_1^{10} n_0 n_e \Rightarrow K_1 = n_1 / n_0$
$\text{Li}^{1+} + e \rightarrow \text{Li}^{2+} + 2e$	$\text{Li}^{2+} + e \rightarrow \text{Li}^{1+} + h\nu_2$	$k_2^{12} n_0 n_e = k_2^{21} n_0 n_e \Rightarrow K_2 = n_2 / n_1$
$\text{Li}^{2+} + e \rightarrow \text{Li}^{3+} + 2e$	$\text{Li}^{3+} + e \rightarrow \text{Li}^{2+} + h\nu_3$	$k_3^{23} n_0 n_e = k_3^{32} n_0 n_e \Rightarrow K_3 = n_3 / n_2$

where:  $n_0, n_1, n_2, n_3, n_e$  are densities of the ions  $\text{Li}^0, \text{Li}^{1+}, \text{Li}^{2+}, \text{Li}^{3+}$  and electrons,  $k_1^{01}, k_2^{12}, k_3^{23}$  are ionization coefficients and  $k_1^{10}, k_2^{21}, k_3^{32}$  are recombination coefficients for low density plasma. In the case of high density plasma we have another coefficients connected with the other type of ionization and recombination in plasma (for example ionization by radiation).

$$\frac{n_1}{n_0} = K_1 \quad \frac{n_1}{n_0} \frac{n_2}{n_1} = \frac{n_2}{n_0} = K_1 K_2 \quad \frac{n_2}{n_0} \frac{n_3}{n_2} = \frac{n_3}{n_0} = K_1 K_2 K_3 \quad (5)$$

$$\frac{n_1 + n_2 + n_3}{n_0} = K_1 + K_1 K_2 + K_1 K_2 K_3 \quad (6)$$

Finally, the equations for  $n_1, n_2, n_3$  can be rewritten in the form of:

$$\begin{aligned} \frac{n_1}{n_1 + n_2 + n_3} &= \frac{1}{1 + K_2 + K_2 K_3} \\ \frac{n_2}{n_1 + n_2 + n_3} &= \frac{K_2}{1 + K_2 + K_2 K_3} \\ \frac{n_3}{n_1 + n_2 + n_3} &= \frac{K_2 K_3}{1 + K_2 + K_2 K_3} \end{aligned} \quad (7)$$

An integral part of the RayX code consists of modules responsible for calculation of the influence of the applied filters for X-rays quanta reaching the detector as well as for simulation of the detector sensitivity. In the case of using filters, the code is able to compute the attenuation of the X-rays based on data read from a file. In such files, values of the quanta transmission as a function of the quanta energy are collected. For detectors, there are four predefined choices of absorption of quanta by a detector. These are: the ideal CCD (all photons are detected), back illuminated CCD, front illuminated CCD and front illuminated deep depletion CCD. In the case of PHA will be used silicon diode type detectors instead of CCD detectors. Diode detectors can be compute by loading the data from the file, when is chosen option ‘‘Definition of CCD or scintillator from file’’. The relevant interface is presented in fig.5

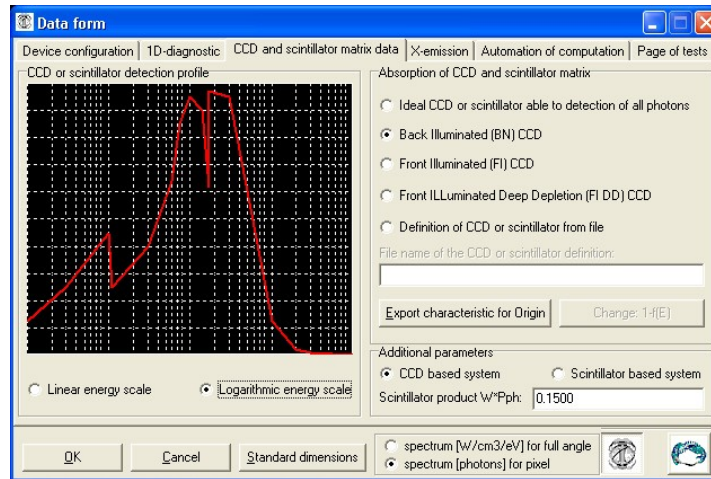


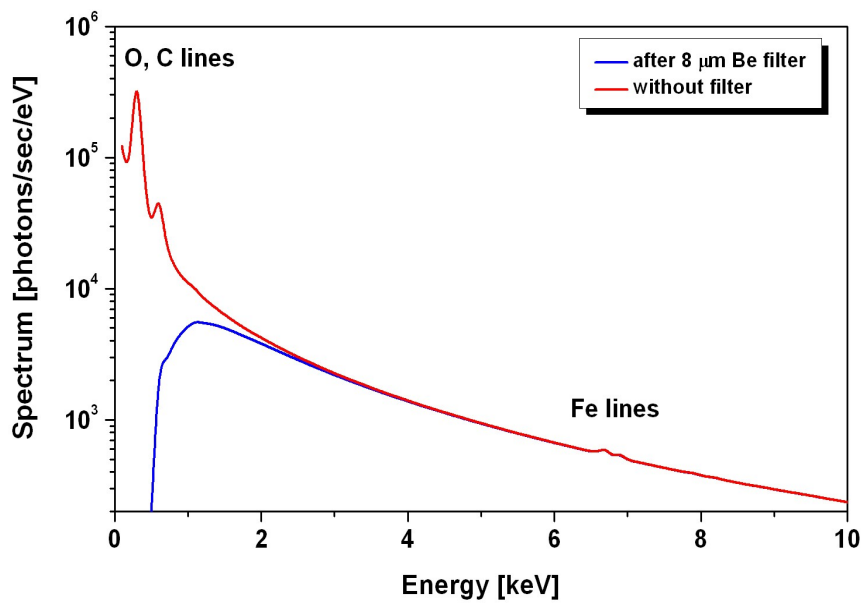
Fig.5 The user interface for setting of the detectors parameters.

### 3. Exemplary results

A number of simulations have been done and the results allowed to determine the position of the particular diagnostic components [11]. Example of spectra were received for the following input parameters: plasma scenario-profile 1 for 8MW ECRH (presented in fig.2), hydrogen plasma with impurities: carbon 3 %, oxygen 0.5 %, iron 0.02 %, 8 $\mu$ m Be filter, distance between pinhole-plasma equal to 6.5 m, distance pinhole-detector equal to 1 m,

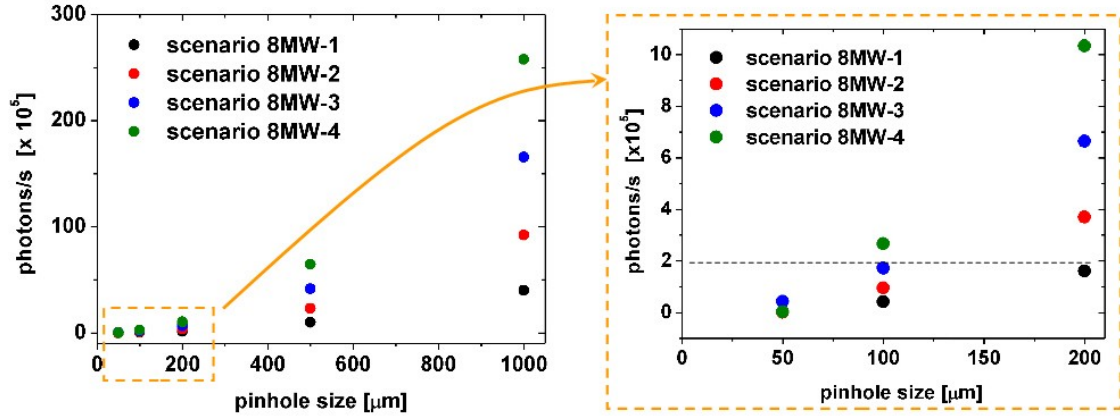


detector size of  $2.7 \text{ mm}^2$ , pinhole size  $200\mu\text{m}$ , presented in fig. 6. The total number of quanta per second which reach the detector is 146915. This value is very important to obtain a good energy and time resolution. Usually, the producer of detectors provides the dependence of the energy resolution (FWHM full width at half maximum) on the input count rate. This indicates the limit of the number of photons for the requested energy resolution. In case of the PHA system for W7-X it is planned to use SDD (Silicon Drift Detectors) from PNDetectors where the energy resolution is almost constant up to  $2 \times 10^6$  input counts per second, and this is equivalent to  $132\text{eV}@5.9\text{keV}$ .



**Fig.6** Spectrum calculated using RayX for W7-X assuming C 3%, O 0.5 %, Fe 0.002 %  
 $L_{PP}=6.5 \text{ m}$ ,  $L_{PD}=1 \text{ m}$ , detector size =  $2.7 \text{ mm}$ , pinhole  $200 \mu\text{m}$ .

Other computation results are presented in fig. 7 which shows the number of photons which reach the detector dependent on the pinhole size. It is clearly seen that for the applied input parameters, distance plasma and pinhole equal to 5 m and distance between pinhole and detector equal to 1m, the pinhole size should be not larger than  $200\mu\text{m}$  to ensure the best energy resolution.



**Fig.7** Number of quanta reaching the detector as a function of the pinhole size. Contents of impurities: C - 3 %, O - 0.5 %, Fe - 0.02 %, pinhole-plasma distance: 5 m, pinhole-detector distance: 1 m.

Finally, taking into account also the influence of the magnetic field on the turbo-molecular pump, in the PHA system for W7-X, the pinhole has been located at 6.5 m from the plasma centre, and the distance between pinhole and detector has been set to 1 m. Moreover, simulations show that the distance between detector and pinhole has higher impact on spectra (number of photon which reach the detector) than the distance between pinhole and plasma centre. To ensure a good energy resolution of registered spectra, changeably pinholes with piezo drives have been installed to allow handling of the expected high dynamic range of the X-ray flux.

#### 4. Conclusion

The code RayX proved to be useful tool for optimizing of the detecting systems working in the X-ray range of photons generated by the plasma inside the stellarator. A basic description of code modules was presented as well as exemplary results. The code was used for developing of the PHA system for use on the W7-X stellarator [12,13].

#### Acknowledgments

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