Model of opacity and emissivity of non-equilibrium plasma

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Abstract. In this work the model describing absorption and emission properties of the non-equilibrium plasma is presented. It is based on the kinetics equations for populations of the ground, singly and doubly excited states of multi-charged ions. After solving these equations, the states populations together with the spectroscopic data, supplied in the special database for a lot ionization stages, are used for building the spectral distributions of plasma opacity and emissivity in STA approximation. Results of kinetics simulation are performed for such important X-ray converter as gold, which is investigated intensively in ICF- experiments.

1. Introduction

When simulating the interaction of power laser pulse with a matter resulted in a plasma generation, one of the main problems is how to describe correctly the efficiency of laser energy transformation into X-ray radiation, spectral distribution and transport of this radiation. It is well known that due to the atomic processes of photorecombination and lines emission the approximation of local thermodynamic equilibrium does not hold, as a rule, for laser plasma. So, the ability to absorb and emit the X-ray quanta may be very susceptible to the degree of plasma ionization balance deviation from the Saha-Boltzman law.

The most self-consistent approach of description of the non-equilibrium plasma radiative properties is based on kinetics simulation of the populations of bound electron configurations under influence of some ionizer. Numerical realization of such approach meets great difficulties, so some simplifications are used. In the works [1,2], for example, the ionization balance of non-equilibrium plasma is inferred from the Saha-Boltzman distribution with, so called, ionization temperature. This temperature is estimated when the coronal balance, dictated by the processes of photorecombination and collision ionization between adjacent ionic stages dominating in the plasma, is equal to the equilibrium one. The work [3] implements more sophisticated approach within the framework of which the ionization balance is defined by the system of steady-state kinetics equations for the most populated superconfigurations in the plasma. Populations of separate electron configurations belonging to the same superconfiguration mixture are distributed in accordance with the Boltzman law for some effective temperature differing from the temperature of free electrons.

Here we present the version of collision-radiative kinetics model similar to that from [3] but without specifying different temperatures for each superconfiguration. It is realized in the code TARAN [4] and can operate as a 1-D non-stationary postprocessor to hydrodynamics calculations.

2. Description of the model.

Our kinetics model specifies the set of generalized ionic states (superconfigurations) such as the ground, singly and, in the case of sufficiently dense plasma, doubly excited states for all appreciable
ionization stages. They are classified with the total number of bound electrons \( I \), number of electrons on the ground level \( N_\text{g} \), principal quantum number of optical electron level \( n = \tilde{n} \ldots N_{\text{max}}, \quad n_{\text{max}} = 8 \). It is assumed that the fine structure components of excited electronic levels are populated proportionally to their statistical weights. The populations of the ground states configurations are defined by the ratios of collision- radiative excitation and deexcitation rates at given free electron temperature and plasma density.

The kinetics matrix coefficients connecting generalized states are derived from configuration averaging of the single electron transitions rates for calculation of which, in one’s turn, some spectroscopic characteristics are required. The single- electron ionization potentials of bound electron shells are the most important characteristics. They are calculated with Cowan code [5] in Hartree-Fock- Slater approximation including the splitting of each \( n \)-th level by orbital momentum \( l \)- number. The levels with \( n = 2, 3, 4 \) are split additionally by total momentum \( j \)- number. Corresponding energy values \( \varepsilon_q (q = \{nl\} \text{ or } \{nlj\}) \) as well as the lines strengths and Slater integrals have been calculated for a lot of matters and for all their ionic abundances from neutral atoms to hydrogen-like ions and systematized in special database.

Before solving the kinetics equations the configuration analysis is carried out. First of all, averaging on configurations gives the effective numbers of electrons \( \Phi_q \) in each \( q \)- subshell, through which the ionization potentials of generalized states \( n \)-th levels are expressed:

\[
\bar{\varepsilon}_n = \sum_{i,j} \Phi_{q} \varepsilon_{q} \sum_{i,j} \Phi_{q} , \quad q = \{nlj\}
\]

Then the energies of single- electron line transitions between \( q, q' \) subshells are defined by averaging the differences of these subshells total energies all over the possible configurations of each ion ground state. The lines widths are treated as the mean- square deviations of \( q - q' \) transitions energies relatively to the mean values in different configurations. Additionally, the multiplet broadening of lines is considered in the Moszkowski approximation.

Calculation of the ionic states populations at known plasma parameters such as density, electron, ion and photon temperatures, allows determination of the spectral absorption coefficient and emissivity of the plasma. They can be represented as superpositions of contributions from free- free, free- bound and bound- bound radiative transitions in different spectral ranges.

Main peculiarities of the model are connected with description just of the third contribution corresponding to inter- configuration lines amount of which may be enormous. Due to principal narrowness lines emission is assumed to be distributed over Voigt spectral profiles characterized with the peak absorption coefficients and source functions. Depending on line type, these characteristics are expressed through complex combinations of generalized states populations reflecting the non-equilibrium degree of plasma.

Some additional assumptions are made for the lines not considered directly by kinetics matrix. For example, non-equilibrium decreasing of the source functions on transitions between fine structure sublevels of the same superconfiguration is treated by means of the ratios of spontaneous radiative decays and collision deexcitations rates. On the contrary, such decreasing is neglected for transitions induced by dielectronic recombination process when electrons from the ground levels fill inner vacancies.

3. Dielectronic recombination for ions with partially filled M-, N- shells.

Analysis of the multi- charged ions spectroscopic characteristics shows that the higher is the principal quantum number \( \tilde{n} \) of ground states of the ions dominating in the plasma, the stronger is the effect of dielectronic recombination on plasma average ionization. As to the estimations, the rate of free electron capture with simultaneous excitation of one of an inner shell electrons and subsequent radiation decay into the vacancy may exceed the rates of single- electron photorecombination captures in dozens of times for the ions with partially filled M-, N- shells (\( \tilde{n} =3, 4 \)).
The problem is that the accurate consideration of the autoionization processes and inverse processes of dielectronic recombination in the kinetics matrix for all ionic abundances is too difficult. Hence, we use the simplification implying increase of the Kramers- like photorecombination rates on the transitions between ground levels of adjacent ions by means of the renormalization multipliers being proportional to the rates of corresponding dielectronic captures. The latter are estimated from the detail balance relations, which assume that the autoionization state of \( I \)-th ion with \( N_{\tilde{n}} + 1 \) electrons on the ground level and a vacancy on the inner one with \( n = \tilde{n} - 1 \) can decay both radiatively and by autoionization process. For multi- charged ions with \( \tilde{n} = 3, 4 \) of all matters, even such heavy as the gold, the autoionization decay is most rapid. It means that dielectronic recombination rate depends in fact only on the rate of single- electron radiative decay from the \( \tilde{n} \)-th to the \( \tilde{n} - 1 \)-th level, which is accurately calculated by use of Hartree- Fock- Slater dipole lines strengths.

The comparison of tabulated lines strengths for different \( l, l' \) shows that the dominating radiative transitions filling the vacancies are \( 2p - 3d \) and \( 3d - 4f \) for \( \tilde{n} = 3 \) and 4 respectively. Considering this we obtain the expression for renormalization multipliers depending only on plasma temperature \( T_e \) and ground levels numbers:

\[
\alpha_{\tilde{n}} = 1 + \gamma \frac{(\varepsilon_{\tilde{n}-1} - \varepsilon_{\tilde{n}})^3}{T_e \varepsilon_{\tilde{n}}^2} e^{-(\varepsilon_{\tilde{n}-1} - 2\varepsilon_{\tilde{n}})/T_e} \left( \frac{2\tilde{n}^2}{N_{\tilde{n}}} \beta_{\tilde{n}} - 1 \right),
\]

where

\[
\gamma = \begin{cases} 0.4, & n_l = 3 \\ 0.9, & n_l = 4 \end{cases}
\]

The coefficient \( \beta_{\tilde{n}} \) is taken to be 1 for the \( \tilde{n} = 3 \) and \( \beta_{\tilde{n}} = 1 - \prod_{k=0}^{N_{\tilde{n}}-1} \frac{18-k}{32-k} \) for \( \tilde{n} = 4 \). This coefficient is used to allow for the fact that dielectronic capture is possible not into all \( l \)-subshells of the \( \tilde{n} \)-th level for ions with the partially filled N-shell. Hartree-Fock-Slater ionization potentials for N-shell ions demonstrate that the condition for dielectronic capture \( \varepsilon_{\tilde{n}-1} - \varepsilon_{\tilde{n}'} - \varepsilon_{\tilde{n}''} > 0 \) with 3d- electron excitation is strictly valid if only excited and captured electrons go into 4f-subshell (\( l' = l'' = 3 \)). Nevertheless, the value of \( \alpha_d \) may be significant; for Cu-like ions it achieves \( \sim 30 \). When \( \tilde{n} = 3 \) dielectronic recombination condition is satisfied for all possible \( l', l'' \); hence, \( \beta_3 = 1 \).

4. Test calculations.

The model described was tested when analyzing the golden plasma non-equilibrium ionic abundances and emissivity at thermodynamical parameters typical for power laser irradiation conditions. First of all, we investigated the dielectronic recombination effect on the average ionization \( \langle Z \rangle \) of optically thin plasma. Corresponding temperature dependences in fig. 1 for relatively low density \( \rho = 0.001 \) g/cc demonstrate that accounting for dielectronic recombination prevents ionic abundances from shifting to the M-shell ions; \( \langle Z \rangle \) varies weakly and doesn't exceed 50 up to \( T_e \sim 3 - 4 \) keV.

Figure 2 compares emissivity from TARAN and AVERROES [2] calculations for \( \rho = 0.004 \) g/cc and \( T_e = 2.2 \) keV. In our case \( \langle Z \rangle \sim 48.9 \) that is close, respectively, to 49.5 published. However, the spectral emissivity profile disagrees in some parts of the spectrum that is primarily the result of differences in the definition of the widths of inter-configuration line transitions. The AVERROES calculations implemented the convolution procedure, which essentially smoothed the spectrum and united a lot of separate lines in wide bands.
5. Simulation of the X-ray radiation spectra for non-equilibrium plasmas.

Knowing spectral distributions of absorption coefficient and emissivity, one can simulate and interpret the experimental spectra of the X-ray radiation emitted by different plasma objects. We perform such simulations for golden plasma jet obtained under conditions of ISKRA facility laser experiment [6].

The golden target was irradiated by a 0.46 ns, 400J pulse at wavelength 1.38 μm and peak flux \( \sim 10^{14} \text{W/cm}^2 \). Time integrated X-ray radiation spectrum was recorded with the transmitting grating under the angle \( \theta_0 = 45^\circ \) to the target surface in spectral range 0.2 – 1.5 keV. Efficiency of pulse absorption was estimated \( \sim 0.5 \).

Kinetics and spectral simulations postprocessed results of the 2-D calculations by three-temperature code TIGR-3T [7] describing hydrodynamics behavior of the plasma jet. Final simulated spectrum is given in fig. 3. It demonstrates reasonable agreement with the experimental curve. Of course, calculated spectrum is more jagged, but its integral over quantum energies estimates the total radiation energy losses closely to the measured value \( \sim 10 \text{ J/sr} \).

Analysis of the simulation results gave some information useful for understanding of the thermodynamical state of golden plasma jet. It became clear that X-ray radiation from the jet was essentially non-equilibrium and was generated in conditions of ionic abundances non-stationary distribution. In spite of high peak temperatures inside the plasma \( \sim 2 \text{ keV} \), ionization inertia and dielectronic recombination prevent the appearance of ions with partially open L- and M- shells during laser pulse. Only lines emission of N-shell ions gives the main contribution to the spectrum recorded. Contribution of the continuum radiation does not exceed 10%. Then, calculations of the optical depths for all lines show that plasma jet is optically thin and produces X-ray radiation as a volumetric source. Spectral distribution of such radiation is very susceptible to plasma non-uniformities, errors of spectroscopic constants and details of the bound states fine structure. We consider that this is the main reason of observed discrepancies.

References

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