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Modeling the population kinetics of NLTE plasmas based on approximations of nonrelativistic configurations

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Abstract
For the rapid calculation of population kinetics of high-Z nonlocal thermodynamic equilibrium (NLTE) plasmas, a collisonal–radiative model based on the nonrelativistic configurations approach was developed. The required atomic data about the collisonal and radiative processes such as photoexcitation, electron-impact excitation, photoionization, electron-impact ionization and autoionzation were obtained by using a set of analytical formulae. The population kinetics were determined by solving the rate equation in the steady-state approach. As illustrative results, experimental measurements of the average ionization degree and population distribution of Xe and Au plasmas were reproduced, and overall good agreement was found. The present model provides a useful tool for modeling the population kinetics of NLTE plasmas.

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1. Introduction

The population distributions of different ion stages in a plasma are required for the calculation of radiative properties of the plasma, which are needed in research areas such as astrophysics and inertial confinement fusion [1, 2]. At a very low electron density, the plasma is usually in coronal equilibrium (CE) and the populations of different ion stages can be obtained by solving the CE equation. When the electron density is high enough, the plasma can be in local thermodynamic equilibrium (LTE) and one can solve the Saha–Boltzmann equation to obtain the populations. Actually, the plasmas are usually in nonlocal thermodynamic equilibrium (NLTE) and the population kinetics are determined by the so-called collisonal–radiative (CR) model, which includes photoexcitation, electron-impact excitation, photoionization, electron-impact ionization and autoionization, as well as the inverse processes. The atomic data about these processes can be obtained by accurate line-by-line calculation. However, they become very difficult for the study of high-Z plasmas because of the large number of levels, which makes calculation impractical. Therefore, some statistical models based on approximations of detailed configurations, superconfigurations and average atom (AA) have been developed in recent years [3–11].

For example, Florido *et al* [8] developed a CR model and the ABAKO code by using analytical rates based on relativistic configurations. Chung *et al* [9] developed the FLYCHK code to calculate the radiative properties of NLTE plasmas, where the atomic data are obtained by using the screened hydrogenic formula. Wu *et al* [10, 11] developed a kinetic model where the atomic data are obtained based on the first perturbation theory and the configuration-averaged rate coefficients are used to solve the rate equation. An overview of the different codes for the CR model has been given by Florido *et al* [8].

For the rapid calculation of population kinetics of high-Z NLTE plasmas, a CR model using a set of approximations based on nonrelativistic configurations is presented in this paper. To check the validity of the present method, experiments for the Xe and Au plasmas are reproduced and a comparison between experiments and other theoretical results is made.

2. The theoretical method

Details of the theoretical method for the CR model can be found elsewhere [8] and we only give a brief outline here. In an NLTE plasma, the ionization balance is determined by all the microscopic processes, including radiation and collision. The population distribution is obtained by solving the following system of rate equations:

$$\frac{dN_{\Gamma_i}}{dt} = \sum_{\Gamma_i} N_{\Gamma_i} R_{\Gamma_i \to \Gamma_j} - \sum_{\Gamma_j} N_{\Gamma_j} R_{\Gamma_j \to \Gamma_i}, \qquad (1)$$

where N_{Γ_i} is the population of the state Γ_i, and $R_{\Gamma_j \to \Gamma_i}$ and $R_{\Gamma_i \to \Gamma_j}$ represent the atomic processes that contribute to populate and depopulate the state Γ_i, respectively. In the present model, the steady-state approximation is made, i.e. the left-hand side of equation (1) is equal to zero.

The present model is based on nonrelativistic configurations. For description convenience, the electric configuration is defined as a vector. For example, the configuration $(n_1 l_1)^{\omega_1}(n_2 l_2)^{\omega_2}\ldots(n_\lambda l_\lambda)^{\omega_\lambda}$ is marked as a vector of $(\omega_1, \omega_2, \ldots, \omega_\lambda)$, where ω_i is the number of bound electrons occupying on the shell $n_i l_i$. The configuration-averaged energy is defined as

$$E = \frac{\sum_J (2J+1)E^J}{\sum_J (2J+1)}, \qquad (2)$$

where E^J is the eigenenergy of the detailed level with the total angular momentum J belonging to the configuration. In the present calculation, the eigenenergy of the detailed levels is obtained by using the atomic structure code FAC [12] and then we averaged the energy of fine structure levels to obtain the configuration-averaged energy by using equation (2).

We take the spontaneous transition as an example. For a transition between the configurations i and j of the ion stage Γ, i.e. $\Gamma_i \equiv (\omega_1, \ldots, \omega_\xi, \ldots, \omega'_\xi, \ldots, \omega_\lambda)$ and $\Gamma_j \equiv (\omega_1, \ldots, \omega_\xi - 1, \ldots, \omega'_\xi + 1, \ldots, \omega_\lambda)$, the oscillator strength reads as

$$f_{ij} = \omega_\xi \left(1 - \frac{\omega'_\xi}{4l'_\xi + 2}\right) f(n_\xi l_\xi - n'_\xi l'_\xi), \qquad (3)$$

where $f(n_\xi l_\xi - n'_\xi l'_\xi)$ is the oscillator strength of the single-electron transition of $n_\xi l_\xi - n'_\xi l'_\xi$. The spontaneous decay rate reads as [8]

$$A_{\Gamma_j - \Gamma_i} = \frac{2\pi\alpha^3 g_i}{h I_H g_j} E_{ij}^2 f_{ij}, \qquad (4)$$

where α is the fine structure constant, h is the Planck constant and I_H is the Rydberg constant. E_{ij} is the transition energy, and g_i and g_j are the statistic weights of the initial and final states, respectively.

The cross-sections of electron-impact excitation are calculated by using the formula of van Regemorter [13], the photoionization by using Kramers' formula [14], the electron-impact ionization by using the modified semiempirical formula of Burgess and Chidichimo [15] and the autoionization rate by using the approximation made by Chung *et al* [9] and Florido *et al* [8]. The atomic data about the corresponding inverse processes are obtained by the principle of detailed balance. The rate coefficients for the processes with electrons involved are obtained by integrating the cross-sections over a free electron distribution, where the Maxwellian distribution is assumed. In the present model, the optic thin assumption is made, i.e. no radiation field is considered and the Debye–Hückel model ([16] and references therein) is applied to determine the ionization potential depression (IPD) of each ion stage in a plasma, which is expressed as (in atomic units)

$$\Delta\phi_i = Z^i_{\mathrm{eff}} \sqrt{4\pi n_e / kT}, \qquad (5)$$

where Z^i_{eff} is the effective charge of the ion i. Once the IPD has been obtained, a maximum principle quantum number $n_{\max}$ is determined for each ion stage. The configurations with the principal quantum number of the outermost electrons larger than $n_{\max}$ are considered to no longer exist and these configurations should be removed from the rate equation.

Table 1. Measured average ionization degree of the Xe plasma [17] and comparison with different theoretical methods.

Sources	$\bar{Z}$
Experiment [17]	27.4 ± 1.5
AVERROES: 450 eV [17]	26.8
SOSA: 400 eV [17]	26.5
ABAKO-a: 450 eV [8]	26.6
ABAKO-b: 450 eV [8]	27.1
This work: 375 eV	27.06
This work: 415 eV	27.40
This work: 450 eV	27.68

3. Results and discussion

To check the validity of the present model, the fraction distributions of high-Z plasmas (Xe and Au as examples) are calculated and compared with the experimental results. Chenais-Popovics *et al* [17] carried out a benchmark experiment on Xe, where the x-ray spectroscopy of a laser-produced gas jet Xe plasma was measured and used as a diagnostic tool of the ionization balance dynamics. The measured electron temperature is 415 ± 40 eV, the electron density is $(1.3 \pm 0.05) \times 10^{20}$ cm^{-3} and the average ionization degree is $\bar{Z} = 27.4 \pm 1.5$.

To reproduce the experimental results, the fraction distributions of Xe plasmas in the experimental condition are calculated. Large-scale configurations including the singly and doubly excited ones of Xe^{24+}–Xe^{31+} are included. As an illustrative example, the configurations of Xe^{27+} are included as follows: $[1s^2 2s^2 2p^6]3s^2 3p^6 3d^9$, $3s^2 3p^6 3d^8 nl$, $3s^2 3p^5 3d^{10}$, $3s^2 3p^5 3d^9 nl$, $3s^1 3p^6 3d^{10}$, $3s^1 3p^6 3d^9 nl$ $(n \leqslant 9,\ l = 0, 1, 2, \ldots, n-1)$, $3s^2 3p^6 3d^7 nln'l'$, $3s^2 3p^4 3d^9 nln'l'$, $3s^2 3p^5 3d^8 nln'l'$, $3s^1 3p^6 3d^8 nln'l'$, $3s^1 3p^5 3d^9 nln'l'$ and $3s^1 3p^5 3d^{10} n'l'$ $(n \leqslant 5,\ n' \leqslant 7,\ l = 0, 1, 2, \ldots, n-1,\ l' = 0, 1, 2, \ldots, n'-1)$. The total number of configurations for Xe^{24+}–Xe^{31+} is 9885. It should be noted that the detailed level calculation based on these configurations is impractical because the time of computation is impractically large.

Chenais-Popovics *et al* [17] applied an electron temperature of 450 eV for the code AVERROES and 400 eV for the code SOSA for the best fit with the measurement, where AVERROES is a method based on the superconfiguration concepts [18] and SOSA is a method considering the spin–orbit-split array [19]. The average ionization degree of the experiment and other theoretical methods is shown in table 1, where ABAKO-a and ABAKO-b

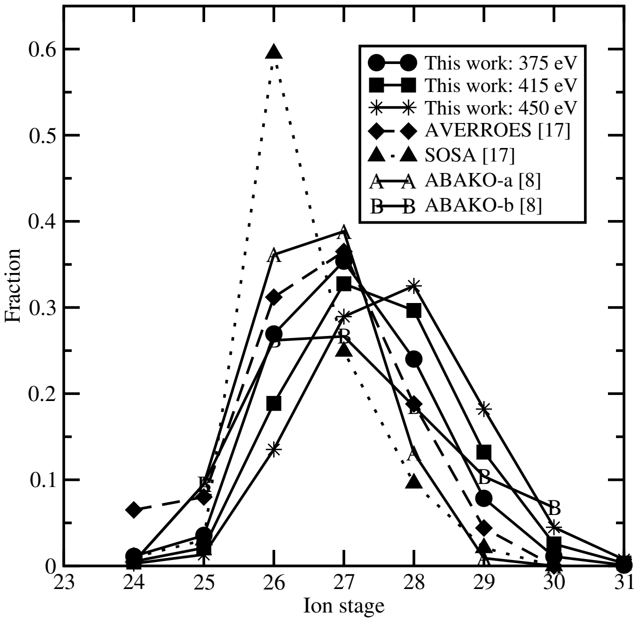

Figure 1. Fraction distribution of the Xe plasma. AVERROES and ABAKO assumed the electron temperature of 450 eV, and the SOSA assumes 400 eV.

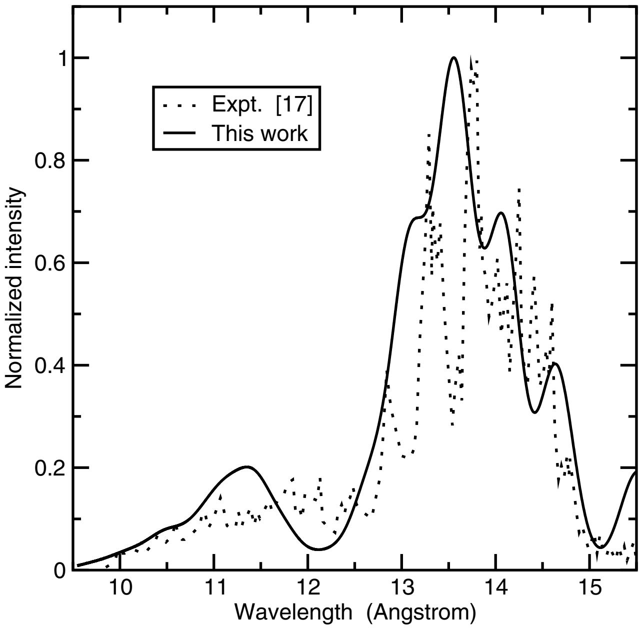

Figure 2. Emission spectra of the Xe plasma: comparison with the experiment. The present calculation was performed for the Xe plasma at $T = 450$ eV and $n_e = 1.3 \times 10^{20}$ cm^{-3}.

represent the results from the atomic data by using different methods [8]. From table 1, the best agreement with the experiment can be found for the result of ABAKO-b [8] and the present calculation at 415 eV. Other methods predict a relatively lower average ionization degree than the experiment. For the modeling of radiative properties of the Xe plasma, the fraction distribution of different ion stages is needed. For comparison, the fraction of ion stages of Xe^{24+}–Xe^{31+} of different theoretical methods is plotted in figure 1. It can be seen that the results of different calculations are generally in agreement except for the calculation of SOSA, which predicts a very large fraction of Xe^{26+} (about

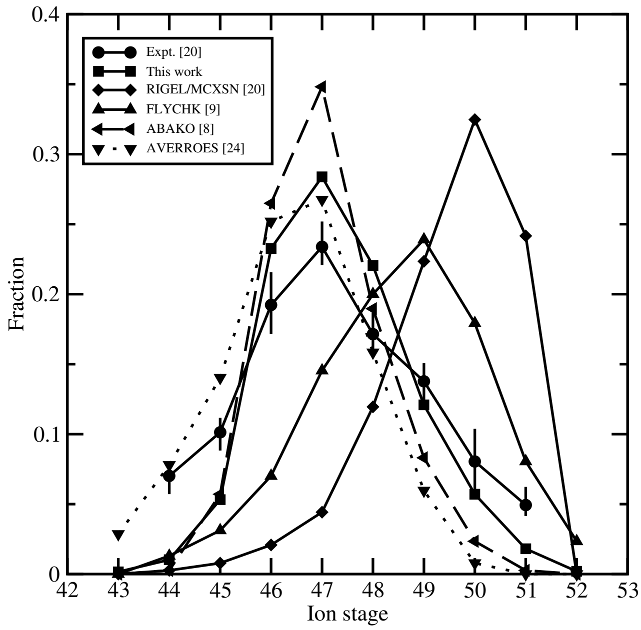

Figure 3. Fraction distribution of the Au plasma at 2500 eV and 1.0×10^{12} cm^{-3}.

Table 2. Average ionization degree of the Au plasma at (a) $T = 2500$ eV and $n_e = 1.0 \times 10^{12}$ cm^{-3} and (b) $T = 2200$ eV and $n_e = 6.0 \times 10^{20}$ cm^{-3}, respectively.

	Sources	$\bar{Z}$
(a)	Experiment [20]	46.8 ± 0.75
	This work	47.34
	RIGEL/MCXSN [20]	49.5
	MIST [20]	42.7
	Wu *et al* [11]	44.75
	ABAKO [8]	47.2
	AVERROES [24]	46.4
	FLYCHK [9]	48.5
(b)	Experiment [23]	49.3 ± 0.5
	This work	50.1
	RIGEL [23]	49.1
	ABAKO [8]	49.2
	AVERROES [25]	49.6
	FLYCHK [9]	49.6
	Wu *et al* [10]	46.79

60%). Figure 2 compares the emission spectra of Xe plasma of the present calculation with the experimental result, and one can see that the present result reproduces generally the strong emission around 13 Å.

Wong *et al* [20] determined the charge state distribution of a highly ionized gold plasma created in the Livermore electron beam ion trap EBIT-II through the measurement of spectral line emission. The electron temperature is 2500 eV and the electron density is 1.0×10^{12} cm^{-3}. The fraction distribution of gold ion stages and average ionization degree of the experimental and other theoretical results are shown in figure 3 and table 2(a), respectively. From figure 3, one can see that the present result agrees very well with the experiment. The results of ABAKO [8] and AVERROES [20] predict overall good agreement with the experiment, whereas other theoretical results predict distributions that shift to higher ion stages than the experiment. Accordingly, the average ionization degree of the present results agrees well with the

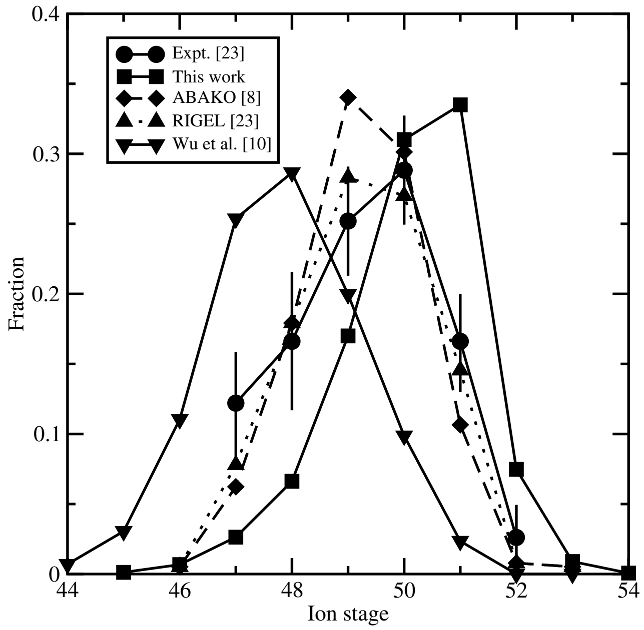

Figure 4. Fraction distribution of the Au plasma at 2200 eV and $6.0 \times 10^{20}\ \mathrm{cm}^{-3}$.

experiment, which can be seen in table 2(a), where REGIL is a Monte Carlo code [21] and MIST is a low-density tokamak impurity transport code [22].

Another experiment on a laser-produced gold plasma was carried out by Foord *et al* [23], where the electron density is $6.0 \pm 20\% \times 10^{20}\ \mathrm{cm}^{-3}$ and the electron temperature is about 2200 eV. The charge state distributions of the Au plasma of the experiment and theories are plotted in figure 4 and the average ionization degree is listed in table 2(b). From figure 4, one can see that the present result predicts a distribution toward higher ion stages compared to the experiment. As a consequence, the average ionization degree is a little higher than in the experiment, which can be seen in table 2(b).

4. Conclusion

In conclusion, a CR model based on nonrelativistic configurations was developed for the rapid calculation of population kinetics of high-Z NLTE plasmas. The atomic data about the basic atomic processes were obtained by using a set of formulae. To check the validity of the present method, experiments for the Xe and Au plasmas were reproduced. The average ionization degree and the fraction distribution of the experiments and other theoretical results were compared. Overall, good agreement was found. The present method can be applied to the modeling of the population kinetics of NLTE plasmas in experiments.

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