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LETTER TO THE EDITOR

Calculation of photoionized plasmas with an average-atom model

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Abstract
We use a simple average-atom model (NIMP) to calculate the distribution of ionization in a photoionization-dominated plasma, for comparison with recent experimental measurements undertaken on the Z-machine at the Sandia National Laboratory. The agreement between theory and experiment is found to be as good for calculations with an average-atom model as for those generated by more detailed models.

(Some figures in this article are in colour only in the electronic version)

Plasmas produced in the laboratory are, in general, far from local thermodynamic equilibrium (LTE). The distribution of ions in the plasma, both between and within ionization stages, is not described by the equations of statistical equilibrium (usually written as the Saha/Boltzmann equations). In this paper we are particularly interested in a steady-state plasma, far from equilibrium, formed by x-ray radiation from a Z-pinch for which, in addition to electron collisional processes, the ambient radiation field is important in determining the excitation and ionization in the plasma. Such photoionized plasmas are believed to occur in many astrophysical situations and the Z-pinch experiment has offered, for the first time, the opportunity to compare numerical models of photoionized plasmas with experiment.

The method usually employed to calculate the distribution of excitation/ionization in a non-LTE system is to solve the rate equations for all the important ionic states. For each of these states, the resulting coupled differential equations can be solved and, given a time history of the electron temperature and density, the time evolution of the different ionic states in the plasma can be evaluated. The steady-state solution can be arrived at by following the time evolution until the populations do not change with time. However, with lower temperatures and/or higher atomic number, the electronic structure of the ions involves open L-, M-, . . . shells. For these cases, following the time evolution of the number density of individual ionic states becomes very time consuming and the number of ionic states must be limited to provide detail in the area of particular interest. Plasmas containing such ions occur frequently in laboratory and in particular, laser-produced plasmas. As a consequence, Grasberger (1965, 1966) and Lokke and Grasberger (1977) extended the 'average-atom' model originally proposed for LTE plasmas by Mayer (1947) to the non-LTE case. The utility of the average-atom model comes about because instead of following the time evolution of individual ionic states, it follows the time evolution of principal quantum shell occupancies (or 'shell populations'), averaged over the distribution of ionic states. As a result, the shell occupancies are non integer. By following the shell populations in time the number of differential equations is reduced in comparison with what is needed for a model that follows individual ionic states. This results in a great saving of computer time (in the authors' experience average-atom models will run many hundreds of times more quickly than a detailed model, although this factor depends critically on how many levels are employed in the detailed model). Using an average-atom model also allows the possibility of tackling problems with complex atomic structure in a manner that, whilst not as accurate as detailed models, is more complete in its coverage of the levels involved. A fundamental approximation employed by the average-atom model that allows this simplification is that there is no statistical correlation between electrons occupying different shells.

The aim of this paper is to use an average-atom model of the excitation and ionization to calculate the distribution of ionization in a photoionized plasma and compare the predictions of this model with experiment. In a recent paper by Foord *et al* (2004), the distribution of ionization in a photoionized plasma produced in the laboratory was measured using high-resolution x-ray spectroscopy. The plasma, which contained fluorine, sodium and iron ions, was created using x-rays from a pinch at the Z-machine in Sandia, the x-ray flux acting both to heat and decompress the original foil and to subsequently bathe the plasma in a radiation field. Independent measurements of the density and radiation flux were made, which allowed comparison of the ionization distribution with different numerical models. Each of these models used a detailed description of the excitation and ionization as well as the plasma processes linking them. The electron temperature was derived from one of these models (CLOUDY) and is thereby the least certain of all the plasma parameters. However, Foord *et al* (2004) show that the distribution of ionization is not predicted to be very sensitive to the exact electron temperature.

The average-atom model employed here (NIMP) is very similar to that described by Djaoui and Rose (1992), which is itself derived from the work of Lokke and Grasberger (1977). However, it has been amended to include photoexcitation and photoionization (as well as their inverse rates) using a simple expression for the photoionization cross-section (Kramers 1923) convolved with the intensity of the ambient radiation field. The treatment of autoionization/dielectronic recombination (AI/DR) has also been amended from that described by Djaoui and Rose (1992). Instead of calculating a total DR rate we now calculate the AI/DR for each principal quantum level as described by Albritton and Wilson (1999, 2000), where the rates for the two-electron AI/DR processes were approximated by extrapolating the collisional excitation cross-section below threshold (More *et al* 1988).

To calculate the distribution of ions in a plasma from the level populations, we assume that the electrons are not statistically correlated (the fundamental assumption of the average-atom model). Then, using the binomial theorem, the probability, $P(\alpha)$, of finding a real 'configuration'

$$\alpha\colon \quad \{k_1, k_2, \ldots, k_{n\,\max}\}$$

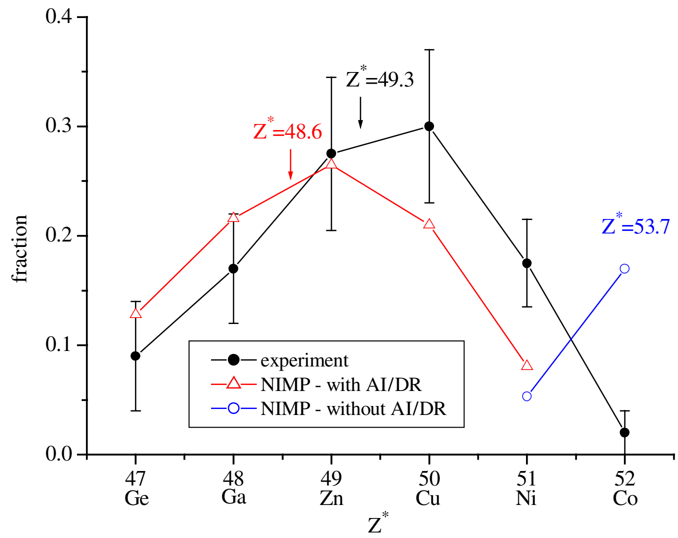

Figure 1. Comparison of the experimental ionization distribution for a gold plasma at an electron temperature of 2200 eV and an electron number density of 6×10^{20} cm^{-3} (Foord *et al* 2000a, 2000b) with calculations from the simple average-atom model NIMP, generated with and without the inclusion of autoionization/dielectronic recombination . For these calculations $n\,\mathrm{max} = 5$ is used in NIMP.

where k_n is the integer population of principal quantum number n, is given by

$$P(\alpha) = \prod_{n=1}^{n\,\mathrm{max}} \frac{2n^2!}{k_n!(2n^2 - k_n)!} \left[\frac{P_n}{2n^2}\right]^{k_n} \left[1 - \frac{P_n}{2n^2}\right]^{2n^2 - k_n}$$

where P_n is the average-atom (non-integer) population of principal quantum shell n. $n\,\mathrm{max}$ is the maximum principal quantum number used in the calculation. For the photoionized plasma calculations reported in this paper (figures 2, 3 and 4), the population in a particular ion stage is taken as that in the ground state of the ion. For the plasma densities concerned, this is a very good approximation.

Before we proceed to calculate the effect of the radiation field in modelling the experiment of Foord *et al* (2004), the accuracy of the modelling in the case of no ambient radiation field is assessed by comparing NIMP calculations with experimental data. Foord *et al* (2000a, 2000b) report the distribution of ionization for a gold plasma at an electron temperature of 2200 eV and an electron number density of 6×10^{20} cm^{-3}. The results are reproduced in figure 1 together with the calculated distribution from NIMP, with and without the effect of autoionization and dielectronic recombination. Inclusion of these two processes is seen to result in much better agreement with experiment (as is also found by Foord *et al* 2000b), emphasizing the need to include these processes in properly modelling plasmas well below solid density. The results in figure 1 also show that the method employed in NIMP for inclusion of AI/DR, whilst approximate, does produce in this case good agreement with experiment.

To model the photoionized plasma experiment of Foord *et al* (2004), the ambient radiation field is taken to be a Planckian at a temperature $T_r = 165$ eV, diluted by the geometrical factor α that accounts for the fact that the plasma is only irradiated by the Planckian over a relatively small solid angle. The factor α (which we take as 0.01 from Foord *et al* (2004)) enters each of the rates involving the Planckian radiation field as a multiplicative factor. Comparison between NIMP and experimental data is shown in figures 2, 3 and 4 for the three components

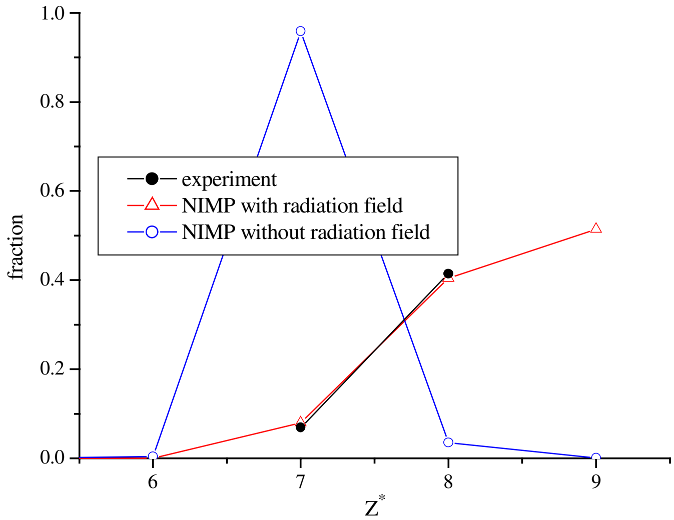

Figure 2. Comparison of the experimental ionization distribution for a fluorine plasma at an electron temperature of 150 eV and an electron number density of 2×10^{19} cm^{-3} (Foord *et al* 2004) with calculations from the simple average-atom model NIMP. The NIMP calculations include AI/DR and also the effect of a radiation field at a temperature of 165 eV, diluted with a geometrical reduction factor $\alpha = 0.01$. For these calculations $n\,\max = 10$ is used in NIMP. Experimental data are only available for two ionization stages and we plot the data here with the sum of the two ion fractions taken to be that predicted by NIMP.

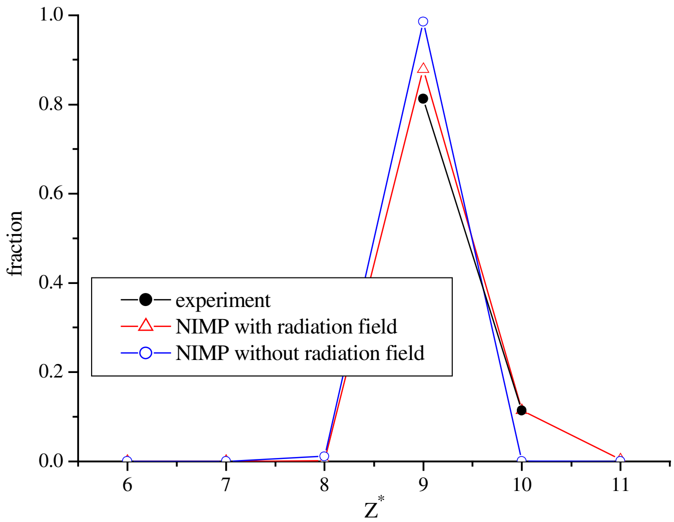

Figure 3. Comparison of the experimental ionization distribution for a sodium plasma at an electron temperature of 150 eV and an electron number density of 2×10^{19} cm^{-3} (Foord *et al* 2004) with calculations from the simple average-atom model NIMP. The NIMP calculations include AI/DR and also the effect of a radiation field at a temperature of 165 eV, diluted with a geometrical reduction factor $\alpha = 0.01$. For these calculations $n\,\max = 10$ is used in NIMP. Experimental data are only available for two ionization stages and we plot the data here with the sum of the two ion fractions taken to be that predicted by NIMP.

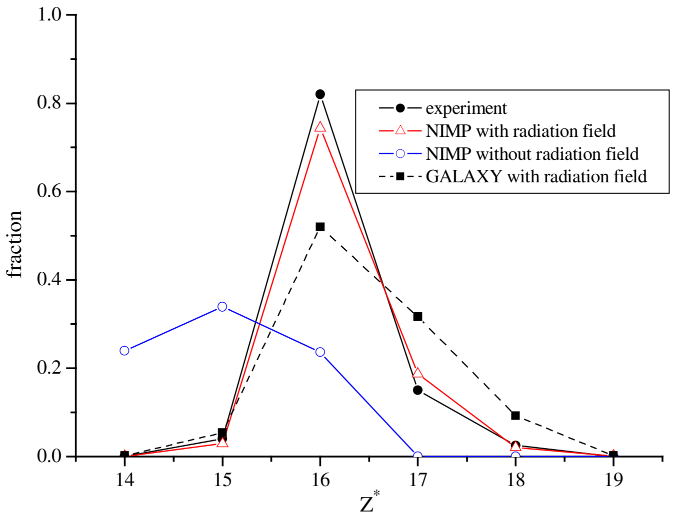

Figure 4. Comparison of the experimental ionization distribution for an iron plasma at an electron temperature of 150 eV and an electron number density of 2×10^{19} cm^{-3} (Foord *et al* 2004) with calculations from the simple average-atom model NIMP. The NIMP calculations include AI/DR and also the effect of a radiation field at a temperature of 165 eV, diluted with a geometrical reduction factor $\alpha = 0.01$. For these calculations $n\,\mathrm{max} = 10$ is used in NIMP. Also included are predictions from the detailed model GALAXY presented by Foord *et al* (2004) for the same conditions.

of the photoionized plasma: fluorine, sodium and iron. From Foord *et al* (2004) the electron temperature is taken as 150 eV and the electron number density is 2×10^{19} cm^{-3}. Calculations are shown with and without the inclusion of the ambient radiation field. In each case, very good agreement with experiment is found for the calculation that includes the radiation field, showing its significant influence in these experiments. NIMP also predicts that the effect of changing the electron temperature over the whole range (30–210 eV) considered by Foord *et al* (2004), results in a change of less than one in the ionization stage of the iron plasma. Thus NIMP results are even less sensitive to the exact electron temperature than those presented by Foord *et al* (2004). We intend to study these differences in future work.

We conclude that, on the basis of comparison with experimental data, the simple average-atom model NIMP can calculate with reasonable accuracy the distribution of ionization in a plasma both with and without an ambient radiation field. Comparison in figure 4 with the predictions of the code GALAXY (Foord *et al* 2004) shows that the results obtained with NIMP are at least as good (in the distribution of ionization) as those obtained using such a detailed model. Such validation of average-atom models is important, because they are used widely in radiation-hydrodynamic simulations of laboratory plasmas where the rate equations are coupled to the hydrodynamics both through collisional processes and through the radiation field.

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