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# Ionization-potential depression and other dense plasma statistical property studies - Application to spectroscopic diagnostics.

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**Abstract.** The radiative properties of an emitter surrounded by a plasma, are modified through various mechanisms. For instance the line shapes emitted by bound-bound transitions are broadened and carry useful information for plasma diagnostics. Depending on plasma conditions the electrons occupying the upper quantum levels of radiators no longer exist as they belong to the plasma free electron population. All the charges present in the radiator environment contribute to the lowering of the energy required to free an electron in the fundamental state. This mechanism is known as ionization potential depression (IPD). The knowledge of IPD is useful as it affects both the radiative properties of the various ionic states and their populations. Its evaluation deals with highly complex n-body coupled systems, involving particles with different dynamics and attractive ion-electron forces. A classical molecular dynamics (MD) code, the BinGo-TCP code, has been recently developed to simulate neutral multi-component (various charge state ions and electrons) plasma accounting for all the charge correlations. In the present work, results on IPD and other dense plasma statistical properties obtained using the BinGo-TCP code are presented. The study focuses on aluminum plasmas for different densities and several temperatures in order to explore different plasma coupling conditions.

## 1. Introduction

For various purposes, it is necessary to simulate virtual plasma composed of electrons and ions in different ionization states. Depending on the plasma conditions, e.g. when they are such that the electron-ion interactions are strong or those generated by direct target interaction with intense laser beams, it is required to account, in the simulations, for bound states as well as quantum mechanical processes to create and destroy them. This permits to avoid non-physical Coulomb collapse and to extend the applicability of classical MD simulations, which are ideally suited for fully-ionized, non-degenerate plasma, to a widest range of plasma conditions. Various methods have been developed and proposed by different groups. Among them, one can mention the methods based on the density functional theory (DFT) such as the quantum Molecular Dynamics method (QMD) [1] which is widely used to provide benchmark data but is limited to low temperature or the orbital free density functional theory molecular dynamics (OF-DFT-MD) [2] which has been developed to extend QMD to higher temperatures. Other methods exist which do not use DFT but simulate interacting classical ions and electrons incorporating some quantum mechanical effects through the interaction pseudo-potential between ions and electrons [3, 4].

We have also chosen to simulate the ions and electrons as classical particles and to incorporate a minimum of quantum information through a regularized potential allowing to model collisional ionization and recombination processes. The BinGo-TCP code has been designed to deal with neutral mixtures composed of ions of the same atom with different charge states and electrons [5, 6]. Within the limits of classical mechanics, all charge-charge interactions are accounted for in the particle motion. In this article, after a brief recall of the modeling basis, the importance of such a model to get a good understanding in correlation effects will be emphasized through a study of the ionization potential depression (IPD) and some other statistical properties in dense plasmas. In particular, some results obtained on aluminum plasmas at various conditions of densities and temperatures, corresponding to different conditions of coupling parameter, will be presented and analyzed.

## 2. Modeling

A classical multi-component plasma molecular dynamics (MD) code, the BinGo-TCP code, has been developed to follow the evolution of plasmas involving ions of various charge states and electrons. The overall structure of the BinGo-TCP code is consistent with that of a standard code of classical MD simulation. Non-relativistic point-like charged particles are simulated in a cubic box. The system inside the simulation box is neutral. The periodic boundary conditions are used together with the minimum image convention and the Newton's equations are solved using a Velocity-Verlet algorithm. A molecular dynamics simulation requires the definition of the potential function that governs interactions between the particles inside the simulation box.

### 2.1. Soft potentials

The electron-electron or ion-ion interactions are taken to be screened Coulomb:

$$V_{ii,ee} = Z_{i,e}^2 e^2 e^{-r/\lambda}/r, \quad (1)$$

where the screening length,  $\lambda \simeq s/2$ , with  $s$  the box size, is chosen large enough not to affect the simulated results. Simulating ions and electrons together can be performed provided that an ion-electron potential finite at short distances avoid electron-ion collapse. Such effective regularized potentials are designed to approximately account for known quantum properties appropriate for the kind of investigated plasma. Here, the ion-electron regularized potential depends on  $Z_i$ :

$$V_{ie}(r) = -Z_i e^2 e^{-r/\lambda} (1 - e^{-r/\delta(Z_i)})/r, \quad (2)$$

with the regularization distance  $\delta$  chosen to reproduce the ionization energy  $E_i$  of the unperturbed ion of charge  $Z_i$  in the ground state when the electron is located at the ion ( $r = 0$ ).

$$\delta(Z_i) = -Z_i e^2 / E(Z_i) \quad (3)$$

In other words, an electron located at an ion ( $r = 0$ ) occupies the fundamental state of the ion whose charge is  $Z$  with a nucleus charge  $Z + 1$ .

### 2.2. Ionization/recombination protocol.

In the simulation, the particle motion is followed with very small time-steps  $\sim 10^{-20}$ s appropriate for the description of the micro motion of electrons around ions. These time steps required by the simulations are small compared to typical collision rates, thus any statistics on collisional events are expensive. The setting up of the population of electrons temporary trapped in the ion wells, i.e. the reaching of the required equilibrium state, depends on collisional events between electrons, and thus, is a very slow process. The choice of the previous soft ion-electron potential

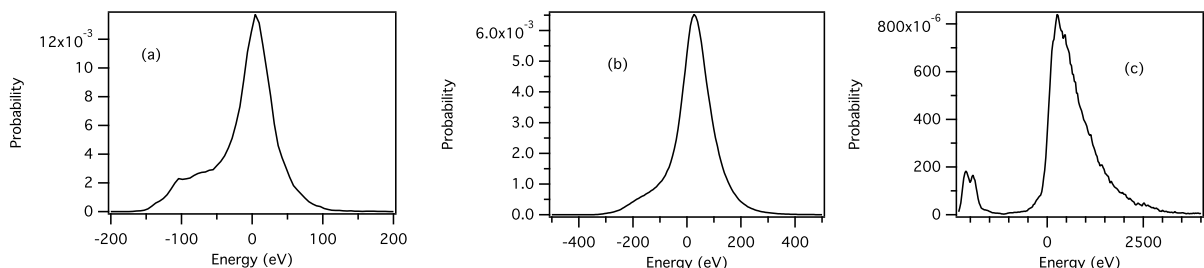
allows to implement a ionization/recombination protocol to control the plasma ion charge distribution and the trapping of electrons in the ion wells. Usually, the ionization-recombination mechanisms rely on an approximate analysis of collisional events between one ion and 1 or 2 electrons. In dense plasmas, the concept of collisions is not straightforward as the interactions involve all the particles within the screening length. To design a ionization/recombination protocol the definition of a collisional process is crucial but necessarily empirical. An analysis of the local environment of a given ion is performed to evaluate if the ion is susceptible to be ionized or recombined. The location of the two nearest neighbor electrons together with the sign of their total energy is used to evaluate if locally the plasma, at one step of its evolution, is favorable to an ionization (in case of positive energy) or a recombination (in case of negative energy) of the ion. When the local environment is favorable to an ionization, the ion of charge  $Z$  is changed to an ion of charge  $Z + 1$  with an electron located on it. This pre-ionization state will give rise to an effective ionization if the interactions of the trapped electron with the surrounding plasma, permit it.

A preparation phase of the particle set (into the simulation box) before extracting any sampling from simulations, is necessary. At the end of the preparation phase the system follows a quasi stable evolution with stationary trapped and free electron populations. The ionization/recombination process implemented in the code has two fundamental functions. It allows the evolution of the charge state population towards a stationary state depending on temperature, density and composition of the plasma and it favors the setting up of a population of electrons temporary trapped in the ion wells.

With this model, one gains the ability to describe the ion-electron coupling accounting for mixtures of ions undergoing changes of their ionization stages. It is important to note that the coupling of electrons with radiation is ignored and that the notion of discrete energy for the ionic excited states is here replaced by its continuous equivalent.

### 3. Some plasma properties.

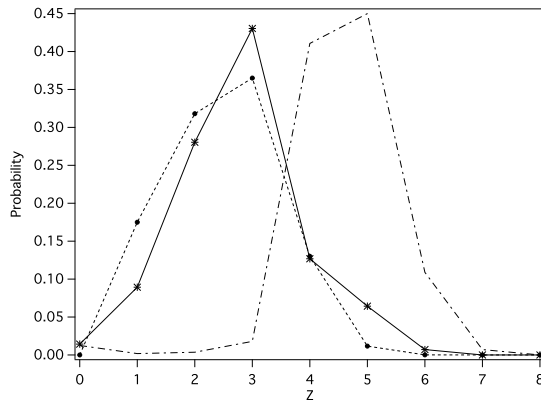
Depending on its total energy and its nearest neighbor ion, an electron is either trapped or free. An illustration is given by the electronic total energy distribution functions measured in aluminum plasmas for various conditions.



**Figure 1.** Electronic total energy distribution function measured in aluminum plasmas at (a)  $T_e=T_i=20\text{eV}$  and  $\rho = 0.65\text{g.cm}^{-3}$ , (b)  $T_e=T_i=50\text{eV}$  and  $\rho = 2.7\text{g.cm}^{-3}$  and (c)  $T_e=T_i=550\text{eV}$  and  $\rho = 6.5\text{g.cm}^{-3}$ .

The analysis of these distribution functions together with the knowledge of the electron number in the simulation box, allows to infer the proportion of free electrons and thus the mean charge value. During a simulation run, various charge states of the same ion exist. The distribution function of these charge states is not representative of the plasma equilibrium

as some electrons are trapped in the ion wells (revealed by the negative part of the energy distribution functions, cf. Figure 1). Therefore, to estimate the equilibrium charge states distribution function, a detailed examination of the electrons around each charge state has to be performed. The ionic charge state distribution function obtained for an aluminum plasma at



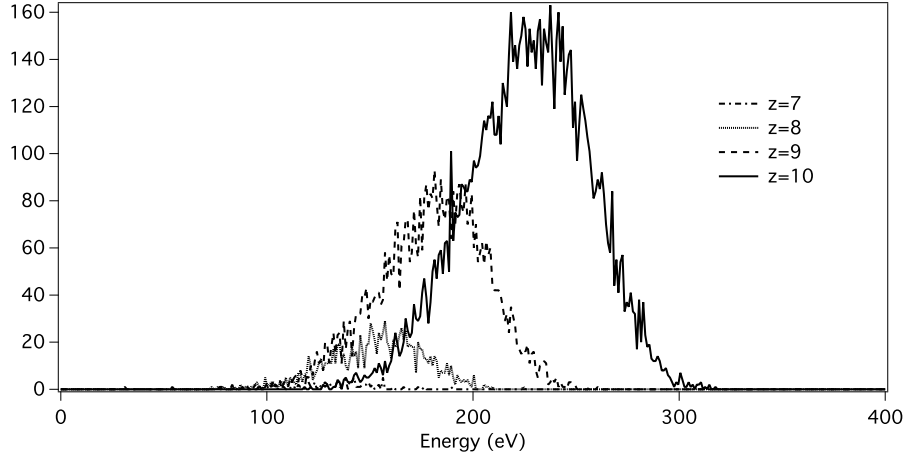
**Figure 2.** Charge state distribution function in an aluminum plasma at  $T_e=T_i=20\text{eV}$  and  $\rho = 0.65\text{g.cm}^{-3}$  measured with (full line and stars) and without (dot-dash line) accounting for trapped electrons compared with the Flychk result (dash line and dots).

$T_e=T_i=20\text{eV}$  and  $\rho = 0.65\text{g.cm}^{-3}$ , is shown in Figure 2. It can be seen that the result which accounts for the trapped electrons, compares quite well with the one obtained with the Flychk code [7].

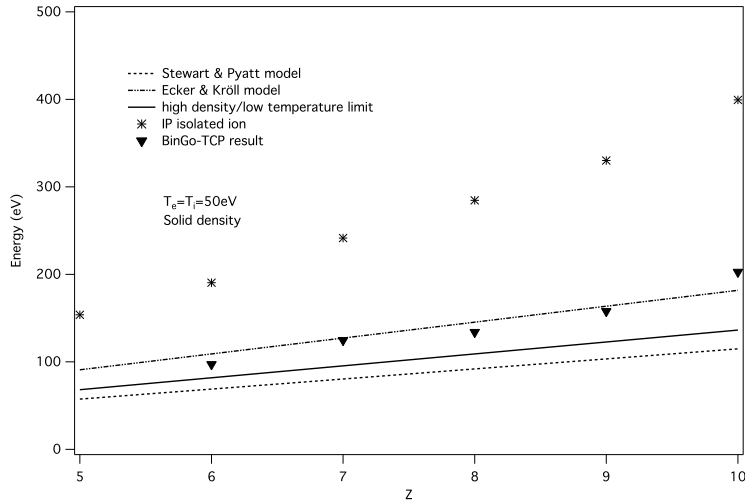
#### 4. The ionization potential depression.

Due to its environment, an ion embedded in a dense plasma will undergo a potential significantly different from the one experienced by the same isolated ion. This plasma-dependent potential will lower the energy required to free a bound electron. This mechanism which is known as the ionization potential depression (IPD), will affect the number of bound states and consequently the radiation emitted by the system.

The evaluation of the IPD has important implications for dense plasma physics and in particular for the detailed prediction of the dense plasma equation of state and radiative opacity in stellar interiors, inertial confinement fusion research, or planetary interiors. Recent experiments [8, 9] leading to IPD measurements in situ has renewed interest for this issue (see for example [10, 11, 12, 13, 14, 6]). Taking advantage of the particular design of the ionization protocol in the BinGo-TCP code, it is possible, when the ion is in a pre-ionization state, to measure the necessary energy to free an electron in the ground-state of a given ion and this, by accounting for all the interactions with the surrounding plasma. Figure 3 shows the distribution of this energy for four charge states existing in an aluminum plasma at  $T_e=T_i=50\text{eV}$  and  $\rho = 2.7\text{g.cm}^{-3}$ . The curves are not normalized and their relative intensities reflect the number of pre-ionization events for each ion of charge  $Z$ . It can be seen that due to a fluctuating local environment of the ions, the ionization energy is characterized by a distribution function. If one compares the mean energies deduced from these distribution functions with the corresponding energies of the isolated ions, it is possible to infer the ionization potential depression due to the interactions with the environment. The results are shown in Figure 4 with the results obtained with two theoretical IPD models, the Stewart-Pyatt (SP) [15] and the Ecker-Kröll (EK) [16] model, which apply across a wide range of densities. In those conditions of plasma, the electron



**Figure 3.** Distribution of the ionization energy of an electron in the ground state of an ion of charge  $Z$  in an aluminum plasma at  $T_e=T_i=50\text{eV}$  and  $\rho = 2.7\text{g.cm}^{-3}$ .



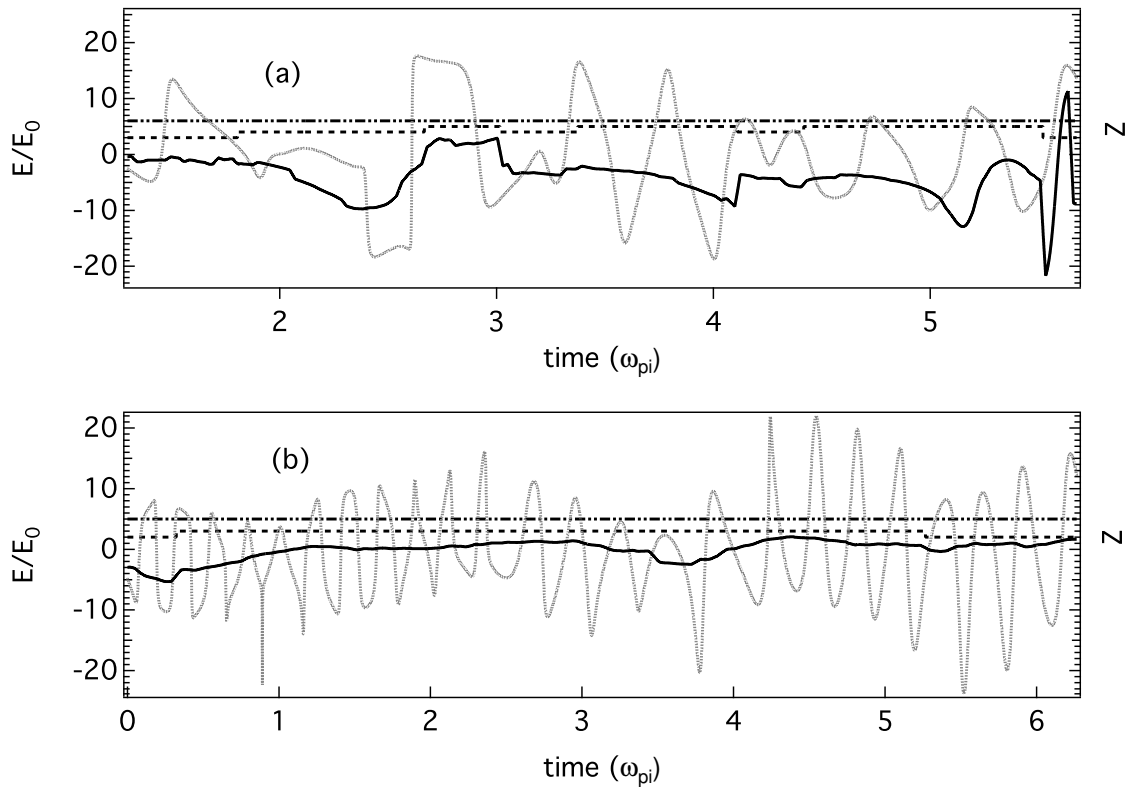
**Figure 4.** The ionization potential depression obtained with the BinGo-TCP code (down triangles) for an aluminum plasma at  $T_e=T_i=50\text{eV}$  and  $\rho = 2.7\text{g.cm}^{-3}$ , compared with the IPD calculated with the SP (dot line) and EK (dot-dash line) models for the same conditions. The high density/low temperature limit of the SP model is also plotted (full line) for comparison.

coupling plasma parameter is  $\Gamma_e = 0.35$  and the measured mean charge is  $Z_b = 7.4$  leading to an ion coupling plasma parameter,  $\Gamma_i = 9.96$ . The effects of the charge correlations on the lowering of the necessary energy to free an electron are very strong and cannot be ignored. The comparisons with the theoretical models show that for these conditions, our results are in better agreement with the EK model than with the SP model. Other results obtained for other conditions of plasma (aluminum plasmas at  $T_e=T_i=20\text{eV}$  and  $\rho = 0.65\text{g.cm}^{-3}$  and  $T_e=T_i=550\text{eV}$  and  $\rho = 6.5\text{g.cm}^{-3}$ ), not presented here, show a good agreement with the SP model and thus, one cannot conclude on the relevance of one or the other model.

## 5. Discussion.

Due to the specific implementation of the ionization/recombination protocol, our classical MD method gives access to the potential surrounding an ion accounting for the influence of the free electrons and neighboring ions. By comparison with the ionization potential of the equivalent isolated ions, the ionization potential depression can be estimated. Our simulations provide data for further discussion on IPD models.

Moreover, the local electric fields produced by the electrons and ions of the plasma, which derived from the force calculations on individual charges, can be measured by accounting for all the interactions between charges. Characterizing properly these electric fields is very important for spectroscopic diagnostics as they interact with the emitters and modify the radiated spectra. The TCP simulation is well designed to obtain time sequences of electric field. These can be used in the resolution of the Schrödinger equation describing the time evolution of the emitter wave functions in the time-dependent field, or to infer, via a statistical analysis, the field distribution and correlation functions, characterizing the contributions of ions or electrons, or both [17]. As



**Figure 5.** Ionic charge and field histories in an aluminum plasma at  $T_e=T_i=20\text{eV}$  and  $\rho = 0.65g.cm^{-3}$ . Bare ionic charge - dot dash line -; Ionic charge accounting for trapped electrons (effective charge)- dash line-; Electronic electric field measured at the bare ionic charge - dot line -; Electronic electric field seen by effective charges - full line -

it has been mentioned previously, it is possible to identify, during a simulation run, the trapped and free electrons and thus to measure the electric fields at a given charge. Examples of two electronic electric field histories measured at two different bare ionic charges ( $Z = 6$  and  $Z = 5$ ) are shown in Figure 5(a) and (b), respectively, for the same plasma conditions as Figure 2. The dot line corresponds to the total electronic electric field at the ion and the full line corresponds

to the electronic electric fields without the trapped electrons then accounted in the ion charge. It is also shown the value of the bare ionic charge (dot-dash line) and the ionic charge accounting for trapped electrons, the effective charge (dash line). A statistical analysis of the field histories at the effective charges will give access to statistical properties of electric fields, such as field distribution or correlation functions in plasmas composed of various ionic charges and electrons. The same field histories used in the resolution of the emitter evolution equation will permit to infer the influence of correlations on spectral line shapes. And finally, a statistical analysis of the ionization and recombination events will be performed to evaluate the corresponding rates. This work is in progress.

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