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Multifrequential and mean opacity calculation of carbon plasmas in a wide range of density and temperature

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Abstract. The purpose of this work is to calculate the multifrequential and mean opacity of optically thin carbon plasmas in a wide range of density and temperature, where corona equilibrium, local thermodynamic equilibrium and non-local thermodynamic equilibrium regimes are present.

1. Introduction

In several research fields of current interest such as astrophysics or inertial fusion confinement the knowledge and the understanding of the interactions between the photons and the plasma particles, i.e. plasma optical properties, result essential. Carbon is one of the most important elements under investigation, since it is likely to be a major plasma-facing wall component in ITER [1] and that means that radiation rates from carbon impurities must be known. Moreover, some laser experiments have focused on spectrally resolved emission from hydrocarbon systems. As a consequence, the study of carbon plasmas is a subject of current interest and many efforts are headed. In particular, recent NLTE workshops [2] have focused on comparisons of modeling calculations for specific cases that allow testing the models since there are very few experimental measurements for carbon plasmas.

The purpose of this work is to calculate the multifrequential and mean opacity of optically thin carbon plasmas in a wide range of density and temperature, where local thermodynamic equilibrium and non-local thermodynamic equilibrium regimes are present. Moreover, in this work is briefly analyzed the changes introduced in the mean opacities when the plasma is considered optically thick. This study is performed under the detailed-level-accounting approach using as atomic data those provided by FAC code [3]. All the calculations presented in this work were performed using ABAKO which is an improvement of ATOM3R code [4] and it also integrates the RAPCAL code [5]. The first one solves a level by level collisional-radiative steady state equations, and the second one determines the radiative properties, such as the spectrally resolved and mean opacities.

2. Description of the ABAKO Code

ABAKO is composed of three modules: atomic data, level populations and optical properties. The first one is very flexible module which can work using different two complementary levels depending on the atomic number or the ionization degree of the element under consideration. For low-Z or highly ionized medium and high-Z plasmas we use a detailed level description provided by the FAC code in which the bound states of the atomic systems are calculated with convenient specification of jj-coupling schemes and including configuration mixing. On the other hand, for lowly ionized intermediate and high-Z plasmas this detailed calculation becomes impracticable and a detailed relativistic configuration accounting approach is chosen. In particular, ABAKO works using a set of analytical potentials developed by us which can model both isolated ions [6] and ions immersed into plasmas [7] including plasma effects and single and core excited configurations [8]. Even for situations wherein more celerity is desired, the code can perform the atomic calculations using a relativistic screened hydrogenic model [9].

The second module is devoted to determinate the ionic state distributions and level populations by solving a colisional-radiative steady state (CRSS). The populations can be computed with a reasonable accuracy for plasmas of any element in a wide range of conditions both for optically thin and thick plasmas, and in the last case, the radiation transport is modeled through the escape factor formalism [10]. The processes included in the CRSS model are the following: collisional excitation and de-excitation; spontaneous decay; collisional ionization and three body recombination; radiative recombination; autoionization and electronic capture, being the majority of the rate coefficients evaluated by analytical formulas that can be found in the literature. In order to solve the set of rate equations, we employed the technique of sparse matrix to storage the non-zero elements. This implies substantial savings in computing time and memory requirements and it also allows us to include a large amount of ionic configurations in our calculations. Finally, in the third module, the spectrally resolved and mean emissivities and opacities are determined making use of the populations and the atomic data given in the previous modules. Bound-bound opacity and emissivity are calculated by using Voigt profile for all the lines and assuming complete redistribution of the photons. In this Voigt profile, there are included natural, Doppler and Stark widths, using a simplified semiempirical method for obtaining the last one. The bound-free cross section can be calculated from quantum mechanically procedure or from Kramer´s formula. Finally, the free-free spectrum has been obtained employing the Kramer's formula for the cross section (corrected by the gaunt factor).

3. Results

In this work all the atomic data were obtained using FAC code including configuration interaction. Thus, the total number of levels and line transitions included has been 24700 and $7 \cdot 10^5$, respectively. These numbers can change due to the Stewart and Pyatt continuum lowering model has been used. The bound-free and free-free cross section have been calculated from Kramer´s formula.

In table 1 we show some calculations of the mean opacities in LTE obtained from ABAKO and they are compared with those provide by LEDCOP(new) code [11] in which a self-consistent Hartree-Fock calculations with relativistic corrections is used to generate both single configuration LS term energies. Discrepancies from 3% at 10 eV and 10^{-3} gcm^{-3} to 60% at 20 eV and 10^{-1} gcm^{-3} are founded.

Table 1. Mean opacities in LTE obtained from ABAKO code (a) and LEDCOP(new) code (b).

T,ρ	$\kappa^{(a)}_{Planck}$	$\kappa^{(a)}_{Rosseland}$	$\kappa^{(b)}_{Planck}$	$\kappa^{(b)}_{Rosseland}$
$10,10^{-5}$	$1.6928 \cdot 10^{3}$	$1.1874 \cdot 10^{2}$	$1.3291 \cdot 10^{3}$	$1.6335 \cdot 10^{2}$
$20,10^{-5}$	43.30	4.07	63.15	4.81
$10,10^{-3}$	$4.6255 \cdot 10^{4}$	$1.7580 \cdot 10^{4}$	$5.1471 \cdot 10^{4}$	$1.8083 \cdot 10^{4}$
$20,10^{-3}$	$1.7802 \cdot 10^{3}$	$2.2131 \cdot 10^{2}$	$2.3661 \cdot 10^{3}$	$3.6264 \cdot 10^{2}$
$10,10^{-1}$	$2.3535 \cdot 10^{5}$	$8.5105 \cdot 10^{4}$	$1.6991 \cdot 10^{5}$	$6.9015 \cdot 10^{4}$
$20,10^{-1}$	$2.6211 \cdot 10^{4}$	$2.5031 \cdot 10^{3}$	$3.2825 \cdot 10^{4}$	$6.5728 \cdot 10^{3}$

In a previous work the change in the average ionization and level populations was analyzed when the calculations were obtained from Saha equation (LTE) or CRSS [12]. For example it was found NLTE regime at 75 eV and 10^{20} cm^{-3} (electron density) and the average ionization obtained from Saha equation and CRSS at this plasma conditions were respectively 5.92 and 4.98. In Figure 1 we can see discrepancies in the opacity. Planck and Rosseland mean opacities (in cm^2/g) and obtained were 2.89510^2 and 0.903 respectively in LTE while it was obtained 5.341 10^3 and 2.153 in NLTE.

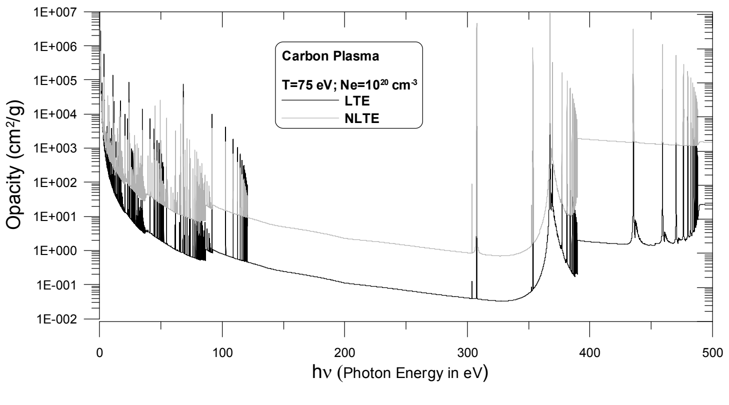

Figure 1. Multifrequency opacity obtained from ABAKO code in LTE and NLTE

In Figure 2 we present the Planck and Rosseland mean opacities in a wide region of plasma conditions and in NLTE. In general we can see that the mean opacity arise when the matter density decrease. More complex behavior is found on the temperature. Also, we have found at this plasma conditions that the discrepancies with the LTE calculations arise when the temperature decrease a the temperature arise.

Finally, we have calculated the opacity at 70 eV and 10^{19} cm^{-3} for optically thick carbon plasma assuming planar geometry and for 0, 50 and 100 μm. The average ionization obtained are 4.89, 4.99 and 5.04 respectively, and for example, the Rosseland mean opacity (in cm^2/g) obtained are 0.6533, 0.6241 and 0.6138 respectively. If we consider infinite medium, we obtain 5.75 and 0.4902 respectively.

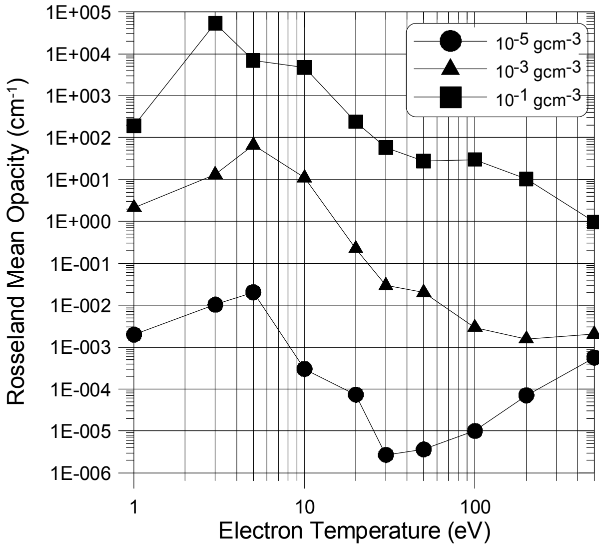

Figure 2. Rosseland mean opacity obtained from ABAKO code in NLTE.

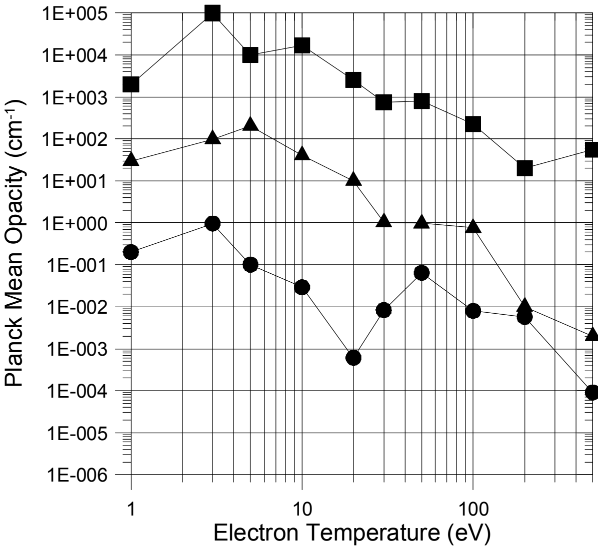

Figure 3. Planck mean opacity obtained from ABAKO code in NLTE.

Acknowledgments

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