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Detailed-level-accounting approach calculation of radiative properties of aluminium plasmas in a wide range of density and temperature

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Abstract. In this work it is accomplished a study of radiative properties of aluminium plasmas. It is analyzed the calculation of spectrally resolved and mean opacities both under NLTE and LTE approaches. Furthermore, the effect of the re-absorption of the radiation in these magnitudes is also examined. The calculations were performed into the detailed-level-accounting approach including configuration interaction among the levels belonging to the same non-relativistic configuration.

1. Introduction

Radiative properties of hot dense plasmas remain a subject of current interest since they play an important role in the inertial confinement fusion (ICF) research as well as in stellar physics [1]. In particular, the understanding of ICF plasmas requires emissivities and opacities both for hydrosimulations and diagnostics [2]. Hence, the emission spectra from plasmas under non local thermodynamic equilibrium (NLTE) may be used for plasma diagnostics or the spectrally integrated emissivity for determining the evolution of the electronic and radiation temperatures in a hydrodynamic simulation [3]. Furthermore, as an essential contribution to the energy transport in hot dense plasma is caused by the radiation, modeling of such plasmas strongly relies on radiative opacities. During the past two decades, aluminum plasmas have been of particular interest and much experimental investigation [4-7] has been made. Theoretically, several studies were carried out to simulate the opacities and the transmission spectrum [9-13]. However, most of these works have been developed assuming LTE conditions. Furthermore, the theoretical calculation of plasma radiative properties is very complex and it is necessarily to use approximations. For these reasons, there is still a lack of complete understanding of these magnitudes and their investigation is always welcomed. In this work it is accomplished a study of radiative properties of aluminum plasmas in a wide range of plasmas density and temperature. This analysis covers situations where either LTE or NLTE conditions are found. The calculations were performed into the detailed-level-accounting (DLA) approach. Configuration interaction is included among the levels belonging to the same nonrelativistic configuration. In the next section it is presented the theoretical framework in which this work has been developed. In section three results and main remarks are presented.

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2. Theoretical model

The atomic data employed in this work were obtained using FAC code [13] into the DLA approach. The standard jj coupling scheme has been used and configuration interaction among levels belonging to the same non-relativistic configuration has been included. The configuration selected has been those proposed by Zeng et al. [13]. With these configurations the authors reproduce quite well the transmission experiment in [6]. Plasma effects are taken into account through the continuum lowering [14]. In order to obtain the level populations and radiative properties we have employed ABAKO-RAPCAL code. ABAKO is an improvement of ATOM3R code [15] and it solves a level-by-level collisional-radiative-steady-state (CRSS) model. The processes included are the following: collisional ionization, three-body recombination, collisional excitation, collisional deexcitation, spontaneous decay, dielectronic recombination and autoionization. Therefore, no induced atomic processes are explicitly considered. ABAKO can handle plasmas of any atomic number, in a wide range of density and temperature, and in optically thin and thick situations. For the latter, the escape factor formalism [16] for basic geometries –plane, cylindrical and spherical- is used to take into account bound-bound opacity effects. Finally, ABAKO uses a sparse iterative method to invert the CR matrix. This code has been successfully tested with other kinetic codes in the last Kinetic Code Comparison Workshop [17]. RAPCAL [18] is a module implemented in ABAKO code to determine radiative properties such as spectrally resolved and mean emissivities and opacities, intensity, transmission and radiative power loss. Complete redistribution is assumed. A Voigt profile is employed including natural, Doppler and electron collisional broadenings. Line overlapping is considered. Photoionization cross section is evaluated in the distorted wave approximation without including resonances and free-free spectra are calculated using Kramer's formula.

3. Results

Due to space needs, we have restricted ourselves to perform an analysis of the variations of the opacities with density and temperature. With this purpose, we have selected an isothermal sequence (40 eV) and a sequence with a fixed free electron number density $(10^{21} \text{ cm}^{-3})$. Firstly, we have studied the optically thin situation. For a given temperature, we have obtained that the spectrally resolved opacities increase with the density (see figures 1 and 2). This fact is due to the diminution of the average ionization.



Both Rosseland and Planck mean opacities increase as density does (see figure 3). This increase is larger in Rosseland mean opacity than in the Planck one. The latter depends mainly on the differences in the position of the peaks but, in this sequence, they are rather small since there are little variations in the average ionization. On the other hand, Rosseland mean opacity also depends strongly on the line width. For a fixed temperature, the Doppler width remains constant, but the collisional one increases

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with the density, which will change more the Rosseland mean opacity than the Planck one. For a given density, the behaviour with the temperature is a little more complex. It is observed a shoulder both in the Rosseland and Planck opacities (see figure 4). The increase of the mean opacities at low temperatures is due to the fact that the maximum of the spectrally resolved opacity is approaching to the maximum value of the Planck and its first derivative functions. For higher temperatures, the average ionization increases and, therefore, the mean opacities diminish. Great changes are observed in both mean opacities. These changes are basically due to the considerable shifts of the maximum values of the opacities toward higher photon energy because of the increase of the average ionization.



Figure 3. Behaviour of the mean opacities with the plasma density.

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Figure 4. Behaviour of the mean opacities with the plasma temperature.

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In the figures 1 to 4, we also show the discrepancies in the opacities when plasma is not really under LTE conditions. They are appreciable even for near LTE conditions as it happens in the case of figure 2. Since Saha-Boltzmann equations overestimate the average ionization with respect to the CRSS calculations, the mean opacities in the latter model are always greater than in the former. This is displayed in table 1, where we have also listed the results given by [12] assuming LTE approach.

Table 1.	Planck	(κ_P)	and Ro	sseland	(κ_R)	mean o	pacities in	cm	² /g for sev	eral de	ensities
$(gcm^{-3}).$	SAHA	and	CRSS	denote	the	model	employed	to	calculate	them.	Mean
opacities	calcula	ted in	n [12] a	ssuming	LT	E condit	tions are al	so s	hown.		

2. .

ρ	к _Р [15]	к _р (SAHA)	к _Р (CRSS)	к _R [15]	к _R (SAHA)	к _R (CRSS)
10-4	4236	3484	18540	68	66	248
4×10^{-4}	8130	7301	17214	316	419	755
10^{-3}	11380	10018	17449	845	1091	1494
4×10 ⁻³	15900	16220	20375	3435	3746	4013

We have also studied the changes in the opacities introduced by the plasma re-absorption. As it is known, the re-absorption produces an increase of the average ionization with respect to the optically thin situation. Therefore, both the Rosseland and Planck mean opacities will decrease (see tables 2 and 3). We can observe significant variations between optically thin and thick situations, even when the modifications in the average ionization are small. We have obtained that the relative differences between optically thin and thick calculations of the mean opacities are weakly dependent of the temperature. However, the dependence with the density is more noticeable. We have observed that the relative differences for the Planck case increase with the density and decrease with the temperature being the behaviour for the Rosseland case just the opposite. This can be understood taking into

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account the dependence of the Rosseland and Planck mean opacities with the temperature and the density which was explained before.

Table 2. Effects of the re-absorption in plasma average ionization (*Z*) and Planck (κ_P) and Rosseland (κ_R) mean opacities (cm²/g) for several densities (gcm⁻³) at 40 eV. 0 μ m is the optically thin situation

	_	0 µm	_	15 µm		50 μm			
ρ	Ζ	κ _P	κ _R	Ζ	κ _P	κ _R	Ζ	κ _P	κ _R
0.0001	7.555	18540	248	7.609	17690	118	7.687	16854	108
0.004	7.340	20375	4013	7.539	17507	3875	7.603	16867	3830

Table 3. Effects of the re-absorption in plasma average ionization (\overline{Z}) and Planck (κ_P) and Rosseland (κ_R) mean opacities (cm²/g) for several temperatures (eV) at 10²¹ cm⁻³. 0 µm is optically thin situation

		0 μm		· ·	15 μm			50 µm		
Т	Ζ	к _Р	κ _R	Ζ	КP	κ _R	Ζ	κ _P	κ _R	
80	10.266	3611	262	10.505	2269	196	10.543	2066	180	
120	10.849	439	38	10.886	286	27	10.895	247	24	

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