Opacity calculations for ICF target physics using the ABAKO/RAPCAL code

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Abstract: In this work we present a set of atomic models (called ABAKO/RAPCAL), and its validation with experiments and with other NLTE models. We consider that our code permits the diagnosis and the determination of opacity data. A review of calculations and simulations for the validation of this set is presented. As an interesting product of these calculations, we can obtain accurate analytical formulas for Rosseland and Planck mean opacities. These formulas are useful for the use as input data in hydrodynamic simulations of targets where the computation task is so hard that in line computation with sophisticated opacity codes is prohibitive. Analytical opacities for several Z-plasmas are presented in this work.

1.- Introduction.

In the plasmas generated in ICF targets the calculation of radiative properties is a difficult task due to the huge number of levels and transitions involved, even for low Z elements. In particular, the understanding of ICF plasmas requires emissivities and opacities both for hydro-simulations and diagnostics. To assist in these calculations, the code ABAKO/RAPCAL has been developed \cite{1} which can determine populations, radiative properties, spectrally resolved opacities and emissivities, and perform K-shell spectroscopic diagnostics to infer both the average electron density and the temperature of the plasma in LTE and non–LTE (NLTE).

The atomic structure model used in this code follows a relativistic detailed configuration-accounting (DCA) scheme, where relativistic electronic configurations are determined by solving the mono-electronic Dirac equation, using parametric analytical potentials developed by our group in the last years \cite{2-6}. The non–local thermodynamic equilibrium (NLTE) system of rate equations is solved assuming steady-state, and analytical formulas are used to compute rate coefficients. The code provides good results in a wide range of temperatures and densities, reproducing the Coronal and Saha results in the limits of low and high density, respectively. Optically thin and thick plasmas can also be treated.

2.- Spectroscopic diagnostic.

ABACO/RAPCAL has been used to analyze several laser produced plasmas. In this way, an experimental study to measure the opacity and emissivity of bound-bound transitions in laser-shocked dense hot aluminium plasma was carried out at the LULI laser facility \cite{7}. A database of emergent intensities in the photon energy from 1700 to 2400 eV was computed, producing a 20 x 20 grid of
electron temperatures and densities. An optically 80 µm thick aluminium plasma was assumed, which matches with the thickness of the aluminium layer of the target.

The electron temperature and density for a given spectra is performed by researching in the database the synthetic spectrum that yields the best fit to the data. Following in this way with the application of this procedure, each of the spectral line outs in the recorded film results in a spatial profile of electron temperature and density.

3.- Relativistic screening hydrogenic model.

In ABAKO/RAPCAL, analytical potentials are used to solve the Dirac equation avoiding self-consistency. Detailed multifrequency apacities are determined creating a database for any element. However a simpler approach consists in calculate energy levels using the analytical expressions of the hydrogenic atom.

This approach has been widely used in plasma physics and is the basic for a family of closely related models called screened hydrogenic model (SHN). This relativistic model [8] is able to obtain fast and accurate computation of detailed opacities with a reduced computational time, and it has the advantage that can be coupled to hydrodynamic codes.

Planck and Rosseland mean opacities obtained with our model are compared (Table 1) with those from TOPS Opacities [9] given by Los Alamos National Laboratory, for several elements. Inspite of its simplicity, the model gives the magnitude order of the values correctly.

Table 1: Comparison of $k_R$ and $k_P$ with TOPS (LANL)

|       | $\rho$ (g/cm$^3$) | $T$ (eV) | TOPS $k_R$ (cm$^2$/g) | TOPS $k_P$ (cm$^2$/g) |
|-------|-------------------|----------|-----------------------|-----------------------|
| Al    | 0.27              | 100.0    | 1.028E+03             | 3.241E+03             |
|       | 0.27              | 125.0    | 3.585E+02             | 1.528E+03             |
|       | 0.27              | 150.0    | 1.442E+02             | 7.785E+02             |
| Ar    | 1.00              | 200.0    | 5.820E+02             | 1.492E+03             |
|       | 1.00              | 500.0    | 1.278E+01             | 1.085E+02             |
|       | 1.00              | 1000.0   | 4.054E+00             | 2.250E+01             |
| Fe    | 1.00              | 500.0    | 5.467E+01             | 2.171E+02             |
|       | 1.00              | 1000.0   | 2.114E+00             | 2.492E+01             |
|       | 10.00             | 1000.0   | 1.207E+01             | 8.525E+01             |
|       | 50.00             | 1000.0   | 2.979E+01             | 2.430E+02             |

4.- NLTE analytical mean opacities.

In the simulation of ICF targets, radiation hydrodynamics codes need the use of thousands of spectrally resolved opacity points for each temperature and density mesh point. A usual approach consists of weighting these opacities in only one group, using the Rosseland and Planck mean opacities. For this reason, analytical expressions for the Rosseland and Planck mean radiative opacities of several low Z plasmas in a wide range of temperature and densities are determined. These formulas are obtained fitting the analytical expression proposed to mean opacities data computed by using the code ABAKO / RAPCAL.
Analytical expressions used to model Rosseland and Planck mean opacities were proposed to match LTE data, but there are no values for a wide range of density and temperature conditions where NLTE assumptions are important. In order to extend those expressions for NLTE, a new one is proposed

\[ \mu_{\alpha\beta}(\text{cm}^{-1}) = \rho \mathcal{K}_{\alpha\beta} = e^{--T} \rho a^2 f(x, y) \]

with

\[ f(x, y) = \left[ \exp(a_3xy + a_4x + a_5y) \right] \]

where \( x = \log(T) \) and \( y = \log(\rho) \).

The variation of Planck and Rosseland mean absorption coefficient in cm\(^{-1}\) for lithium in the range of 1 to \(10^{-3}\) eV for temperature and \(10^{-10}\) to \(10^{-1}\) g cm\(^{-2}\) for density are shown in figure 1.

5. – Conclusions

ABAKO/RAPCAL can determine spectrally resolved opacities under LTE and NLTE conditions, that can be used as a database for radiation hydrodynamic codes to simulate ICF targets. Also, we have used this code to measure, experimentally, opacity an emissivities of hot dense plasmas created with laser.

With the analytical potentials used in ABAKO/RAPCAL, we have developed a new relativistic screening hydrogenic models that give successful results and can be compiled to radiation hydrodynamic codes for getting on-line detailed opacities.

Finally, we have obtained NLTE analytical mean opacities, using data from ABAKO/RAPCAL fitting with an analytical formula coefficients most important elements used in ICF targets.

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Figure 1. For a Li plasma: (a) Planck absorption coefficients in cm$^{-1}$ with ABAKO, (b) fit using analytical expressions, (c) Rosseland absorption coefficients in cm$^{-1}$ with ABAKO, (d) fit using analytical expressions.