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OPACITY CALCULATIONS OF MEDIUM AND HIGH Z DENSE PLASMAS FOR ICF

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Abstract

A code has been developed for calculating opacities of hot dense plasmas. This uses the average atom model and a new relativistic screened-hydrogenic model to calculate energy levels and occupation numbers in order to obtain opacities with contributions from bound-bound, bound-free, free-free and scattering processes under LTE conditions.

1. Introduction

In calculating hot-dense plasmas properties a detailed atomic structure of ions is needed. As the use of the Hartree-Fock model or Density Functional Theory requires time-consuming calculations, the screened-hydrogenic model (SHM) is widely used in plasma physics since it calculates the atomic structure in a timely manner. The SHM, used along with the average atom model, allows to calculate easily the occupation number of ions, the opacity and the emissivity of the plasma, both in LTE and in NLTE conditions.

We have developed a code for calculating plasma opacity in LTE by means of the average atom model based on a new relativistic screened-hydrogenic model (NRSHM). In the next sections we describe the outlines of the code and we present a comparison of our results with other codes.

2. LTE-relativistic screened-hydrogenic average-atom model

The atomic model is based on a new set of universal screening constants including *j*-splitting, which are obtained from the fit to a wide database of atomic energies. This database was built with both energies compiled from the NIST database of experimental atomic energy levels [1], and energies calculated with the Flexible Atomic Code (FAC) [2].

The energy of an electronic configuration $\{P_k\}$ is given by:

$$E_T = \sum_{k=1}^{k_{max}} P_k \left\{ m_e c^2 \left[1 + \left(\frac{\alpha Q_k}{n - j - \frac{1}{2} + \sqrt{\left(j+\frac{1}{2}\right)^2 - (\alpha Q_k)^2}} \right)^2 \right]^{-1/2} - 1 \right\} \qquad (1)$$

being m_e the electron mass, c the light speed, α the fine structure constant, P_k the occupation number of subshell k (k means {n_k, l_k, j_k}) and Q_k the screened nuclear charge experienced by an electron belonging to the k subshell. It is written as [3]:

$$Q_k = Z - \sum_{k'=1}^{k_{max}} \sigma_{kk'} \left(1 - \frac{\delta_{kk'}}{D_k^0} \right) P_{k'} \qquad (2)$$

where Z is the nuclear charge, $\delta_{kk'}$ is the Kronecker symbol, $\sigma_{kk'}$ the screening constants and

$$D_k^0 = 2j + 1 \qquad (3)$$

is the integer electronic degeneracy of the subshell k in the isolated ion.

The fractional occupation numbers P_k are computed, minimizing, at fixed mass density ρ, electronic temperature T_e, and nuclear charge Z, the electronic Helmholtz free energy per ion of the plasma [3], by means of the following expression:

$$P_k = \frac{D_k}{1 + e^{\beta(\varepsilon_k + \Delta I - \mu_e)}} \qquad (4)$$

In order to take into account dense plasma effects, the electronic degeneracy of a subshell in the isolated ion, D_k^0, has been reduced using a function that depends smoothly on density [4]:

$$D_k = \frac{D_k^0}{1 + \left(a \frac{r_k^0}{R_0} \right)^b} \qquad (5)$$

where r_k^0 is the relativistic expression of the inverse of the expectation value of $1/r$, R_0 is the ion-sphere radius and a and b are free parameters which are calculated in a relativistic frame as described in reference [3]. In the denominator of equation (4), $\beta = 1/k_B T_e$ is the electronic inverse temperature, ε_k is the one-electron energy of subshell k obtained from the energy E_T of an electronic configuration, written as [3]:

$$\varepsilon_k = \left. \frac{\partial E_T}{\partial P_k} \right|_{(P_i)} \qquad (6)$$

ΔI is a continuum lowering correction to the energy levels [3],

$$\Delta I = c_{ZM} \frac{9}{5} \frac{\bar{Z} e^2}{R_0} \qquad (7)$$

Here, $\bar{Z}$ is the average ionization of the plasma, e is the electron charge and c_{ZM} is a constant, $c_{ZM} \in [0,1]$. Finally, μ_e is the chemical potential, which is determined using the condition of electroneutrality of the plasma:

$$\sum_k P_k + \overline{Z} = Z \qquad (8)$$

The average ionization $\overline{Z}$ is [3]:

$$\overline{Z} = \frac{4}{\sqrt{\pi}} \frac{A}{\rho N} \left(\frac{m_e k_B T_e}{2\pi\hbar^2} \right)^{\frac{3}{2}} f_{1/2}(\eta_e) \qquad (9)$$

where A is the molar mass, N the Avogadro number, ρ the mass density of the plasma, m_e the electron mass, k_B the Boltzmann constant, T_e the electronic temperature, η_e the reduced chemical potential and $f_{1/2}(\eta)$ the Fermi-Dirac integral of order ½.

The total spectral opacity of plasma $\kappa(\nu)$ is the combination of bound-bound, bound-free, free-free and scattering processes. The line absorption cross section calculation has been computed using a new analytical expression for oscillator strengths based on relativistic screened-hydrogenic wave functions. The lineshape includes natural width, Doppler line broadening and electron collisional broadening [5]. The bremsstrahlung absorption cross section has been computed with Kramer's formula and for photoionization and scattering processes expressions from reference [6] have been used.

3. Results and Discussion

In this section, we compare our code results (ATMED) with other codes from WorkOp-III:94 [7]. Table 1 compares the average ionization $\overline{Z}$ with OPAL, CORONA and THERMOS codes for several elements and different conditions. There are good agreements among the four models.

Table 1: Comparison of $\overline{Z}$ for different elements and condition

	ρ (g/cm³)	T (eV)	ATMED	OPAL	CORONA	THERMOS
Al	1.00	500.0	11.90	12.31	12.14	12.28
Al	1.00	1000.0	12.71	12.88	12.80	12.88
Fe	1.00	500.0	22.39	22.53	21.96	22.35
Fe	1.00	1000.0	23.89	23.86	23.67	23.91
Fe	7.90	200.0	14.22	13.37	13.22	14.13
Ge	0.01	500.0	29.85	29.82	29.83	29.82

In figure 1 we show the spectrally resolved opacity is plotted in Fig. 1 for a plasma of iron at ρ=0.1 g/cm^3 and T=100 eV and we compare it with results computed with the DCA code ANALOP [8]. In figure 2, our results for a Zn plasma at ρ=20 g/cm^3 and T=1000 eV, are compared with data obtained from the LANL TOPS data base [9]. As it can be seen, overall features match on the whole range of photon energies and it is remarkable that the peaks overlap, which means that NRSHM transition energies agree with more accurate models. However, there are peaks too high since oscillator strengths are not correct on the whole range of energies. Using a WKB approximation could improve them.

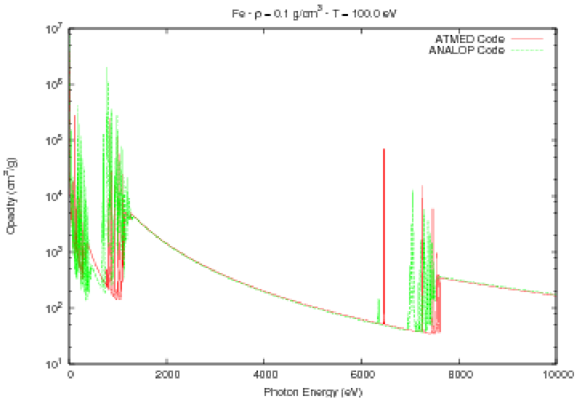

Fig.1. $\kappa(\nu)$ for Fe $\rho = 0.1$ g/cm^3, T =100 eV

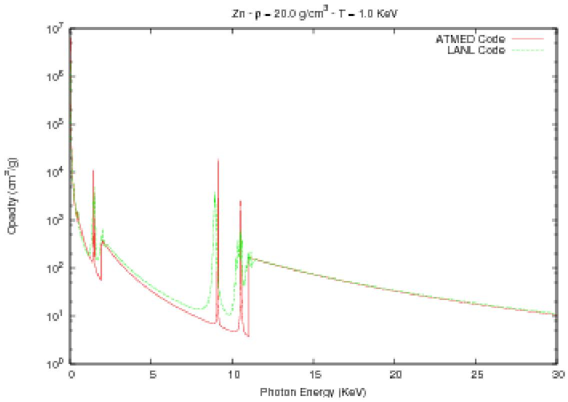

Fig.2. $\kappa(\nu)$ for Zn $\rho = 20$ g/cm^3, T =1 keV

In table 2 we compare the Planck and Rosseland mean opacities, κ_P and κ_R, provided by our model with TOPS Opacities offered by Los Alamos National Laboratory. In spite of its simplicity, the model gives the magnitude order of the values correctly, so it can be used to model radiative transport phenomenon in hydrodynamic codes, in an approximate way. Nevertheless, we can improve the value by using detailed configurations from calculated from the average atom model and by adding UTA formalism.

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Table 2: Comparison of κ_R and κ_P with TOPS (LANL)

	ρ (g/cm^3)	T (eV)	κ_R (cm^2/g)	TOPS κ_R (cm^2/g)	κ_P (cm^2/g)	TOPS κ_P (cm^2/g)
Al	0.27	100.0	1.028E+03	1.414E+03	3.241E+03	5.256E+03
	0.27	125.0	3,585E+02	4.965E+02	1.528E+03	2.446E+03
	0.27	150.0	1.442E+02	2.024E+02	7.785E+02	1.166E+03
Ar	1.00	200.0	5.820E+02	7.075E+02	1.492E+03	2.429E+03
	1.00	500.0	1.278E+01	1.839E+01	1.085E+02	1.395E+02
	1.00	1000.0	4.054E+00	6.242E+00	2.250E+01	5.406E+01
Fe	1.00	500.0	5.467E+01	7.493E+01	2.171E+02	2.813E+02
	1.00	1000.0	2.114E+00	3.322E+00	2.429E+01	2.872E+01
	10.00	1000.0	1.207E+01	2.192E+01	8.525E+01	1.140E+02
	50.00	1000.0	2.979E+01	6.239E+01	2.430E+02	2.690E+02

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