Calculation of LTE Spectral Opacities for ICF Plasma Mixtures using an Average Atom Model

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Introduction

The accurate computation of radiative opacities is basic in several research fields such as astrophysics, or ICF target physics analysis. Radiation hydrodynamics codes for simulation of ICF targets need the use of detailed spectrally resolved opacity functions for each temperature and density condition. These calculations require a large computation time not only for high Z plasmas but in the case of mixtures as well. For this reason, simplified but accurate computation models are needed to be used in-line with hydrodynamic codes. We use the ATMED code to compute the opacity of plasma mixtures under LTE conditions in the average atom framework using a Screened Hydrogenic Model based on a new set of screened constants including the relativistic splitting of the energy levels. To validate the code we have carried out the computation of spectrally resolved and Rosseland and Planck mean opacities for several plasma mixtures of elements which are of interest for radiation driven imploding shells (ablators) of ICF capsules. The results are successfully compared with similar ones found in the literature.

Description of the model

The total spectral opacity of plasma $\kappa(\nu)$ is the combination of bound-bound, bound-free, free-free and scattering processes. The details of the model are presented in our previous work [6]. For a mixture the bound-bound and bound-free cross sections are weighted by the fraction number f_k of the N components of the mixture, in order to obtain the average cross section per ion [1].

$$\sigma_{mix}^{bb/bf} = \sum_k f_k \sigma_k^{bb/bf} \qquad (1)$$

where $\sum f_k = 1$. The bremsstrahlung absorption cross section has been computed with Kramer's

formula using the average value of the average ionization of each element in the plasma:

$$\langle \overline{Z} \rangle = \sum_k f_k \overline{Z_k} \quad (2)$$

The total spectral opacity of the mixture is given by the expression:

$$\kappa'(\nu) = \frac{n_i}{\rho}\left(\sigma^{bb}_{mix}(\nu) + \sigma^{bf}_{mix}(\nu) + \sigma^{ff}_{mix}(\nu) + \sigma^{scat}(\nu)\right) \quad (3)$$

where n_i is the average ion number density in the plasma and ρ is the mixture density. Each component of the mixture has its own ion-sphere radius r_{0k}, which determines a volume V_k and a partial density ρ_k:

$$\rho_k = \frac{m_k}{V_k N_A} \qquad m_k = \frac{f_k N_A}{A_k} \quad (4)$$

being m_k the mass fraction of the *k-th* component, A_k its molar mass and N_A, Avogadro's number. Since the volume of the mixture V is equal to the sum of the volumes occupied by the individual components of the mixture V_k, we have:

$$\frac{1}{\rho}\sum_k m_k = \sum_k \frac{m_k}{\rho_k} \quad (5)$$

Furthermore, under the conditions of thermodynamic equilibrium for systems in contact with diffusion, the chemical potentials μ_k should be equal. This condition together with eq. (5) has been used to obtain the partial densities ρ_k, following the algorithm explained in ref. [2].

Results and Discussion

To examine ATMED code several opacity calculations have been carried out for a beryllium-copper mixture, essential to describe the fusion ignition target compression [3] (Fig. 1). They have been compared with SPCTR code [3] and LEDCOP code [4] results. The spectral opacities for a Be(99.1%)-Cu(0.9%) mixture at several densities and temperatures are shown in Figs 2-5.

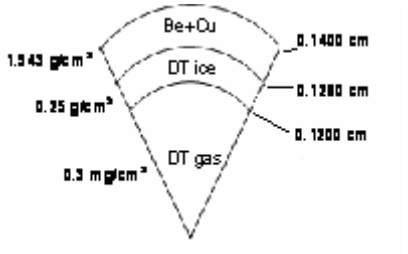

Fig. 1 Indirect driven fusion ignition NIF target design.

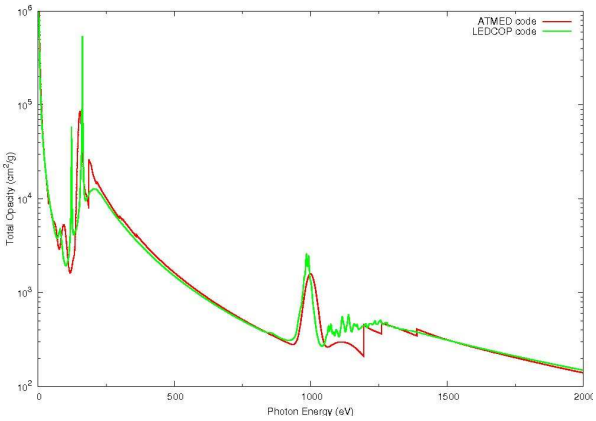

Fig 2. Spectral opacity for Be(99.1%) Cu(0.9%) at T=50 eV and ρ = 0.1 g/cm^3

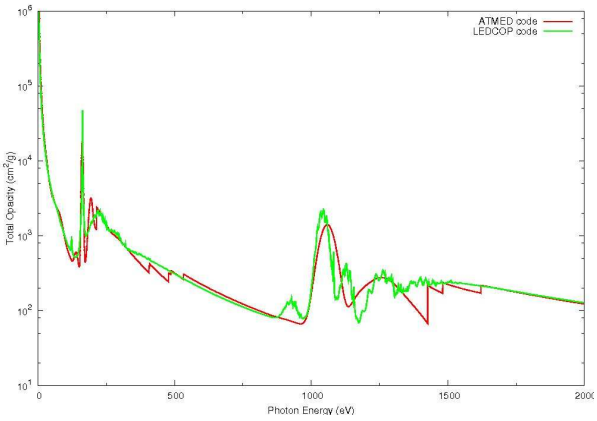

Fig 3. Spectral opacity for Be(99.1%) Cu(0.9%) at T=100 eV. and ρ =0.1 g/cm^3

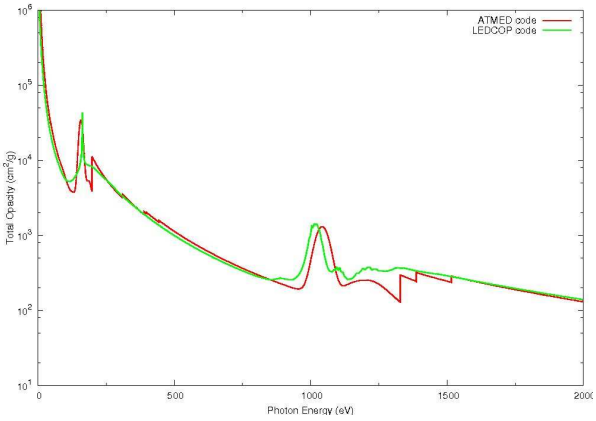

Fig 4. Spectral opacity for Be(99.1%) Cu(0.9%) T=100 eV and ρ =1 g/cm^3

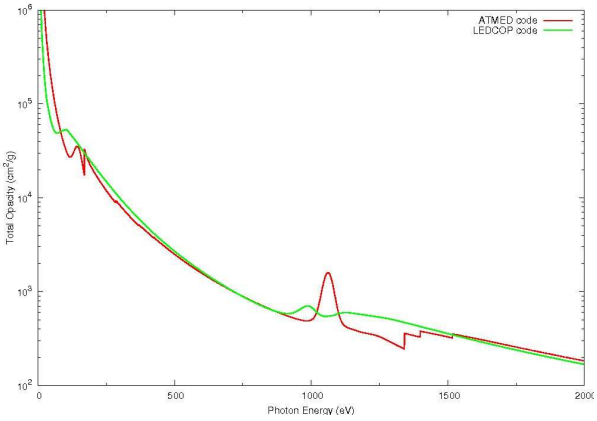

Fig 5. Spectral opacity for Be(99.1%) Cu(0.9%) T=100 eV and ρ =10 g/cm^3

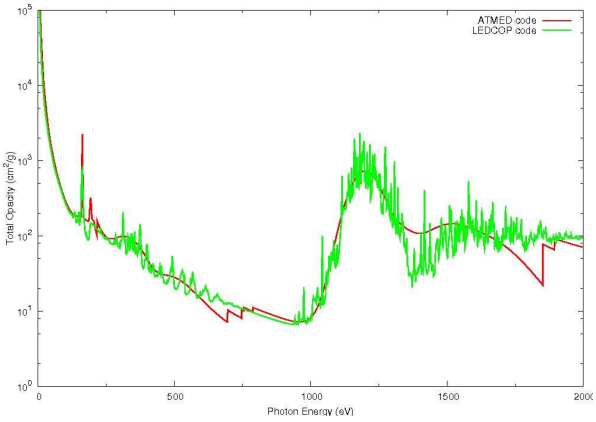

Fig 6. Spectral opacity for Be(99.1%) Cu(0.9%) T=250 eV and ρ =0.1 g/cm^3

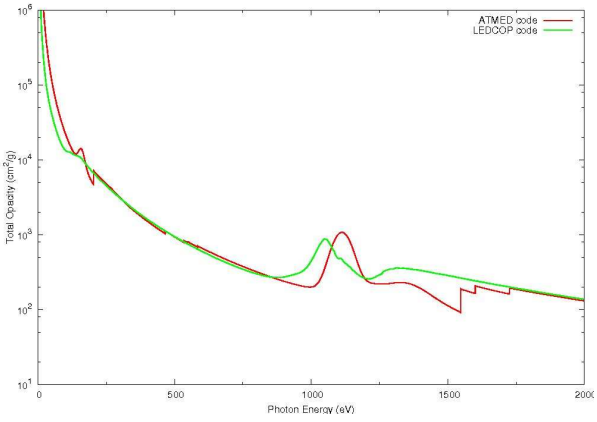

Fig 7. Spectral opacity for Be(99.1%) Cu(0.9%) T=250 eV and ρ =10 g/cm^3

As we can see there are good agreements between ATMED and LEDCOP in all the cases.

In Table 1 we compare our Rosseland mean opacities with those calculated by SPECTR code [3] for the same mixture and for temperatures from 40 eV to 360 eV and densities in the range from 10^{-3} to 10^{-1} g/cm^3. According as the temperature increases the opacity values obtained from ATMED are

closer to the SPECTR ones, since the atoms are more ionized and the screened hydrogenic model has a better behaviour.

Table 1. Comparison of κ_R (cm^2/g) calculated by our code with SPECTR [3]

ρ (g/cm^3)	40 eV		100 eV		250 eV		360 eV	
	SPECTR	**ATMED**	**SPECTR**	**ATMED**	**SPECTR**	**ATMED**	**SPECTR**	**ATMED**
10^{-3}	516.900	776.800	8.177	8.760	0.693	0.747	0.270	0.318
10^{-2}	2916.000	2905.000	66.700	61.240	4.286	3.653	1.066	1.044
10^{-1}	11430.000	8792.000	257.600	272.900	22.130	22.200	9.516	9.673
10^{0}	26810.000	17640.000	929.600	892.200	116.600	90.560	46.950	44.430

In order to check the values of the partial densities needed to obtain the mixture opacity, we have made a comparison with data from reference [5]. Table 2 shows atomic radii, R_0, in atomic units, number of bound electrons and chemical potentials computed for an Au-Gd mixture with the mass ratios of Au (70%) and Gd (30%) at a density $\rho = 100$ g/cm^3. As it can be seen the atomic radii are slightly different in all cases to those obtained from ref. [4], and the biggest differences occur in Ga radii at T = 100 eV and T = 400 eV.

Table 2. Comparison of atomic radius R_0, the number of bound electrons Z_b and the chemical potential μ for a mixture of Au (70%) and Gd (30%) at $\rho = 100$ g/cm^3.

		Ref [5]			**ATMED**		
T (eV)		**R_0 (ua)**	**Zb = ΣNnlj**	**μ**	**R_0 (ua)**	**Zb = ΣNnlj**	**μ**
100	Au	1.7023	57.6578	0.499	1.7174	60.2348	1.225
	Gd	1.6928	43.1651	0.499	1.6730	46.6543	1.225
400	Au	1.7194	46.4735	-24.409	1.7171	49.8126	-23.238
	Gd	1.6596	35.0587	-24.409	1.6737	36.9680	-23.238
800	Au	1.7163	37.7024	-71.828	1.7210	38.6356	-68.737
	Gd	1.6658	26.4722	-71.828	1.6640	27.5152	-68.737
1600	Au	1.7266	24.6219	-188.743	1.7257	24.9990	-183.000
	Gd	1.6450	17.3126	-188.743	1.6523	16.6006	-183.000
3000	Au	1.7263	14.6997	-437.644	1.7303	13.6380	-427.810
	Gd	1.6456	8.5978	-437.644	1.6405	8.2897	-427.810

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References

[1] S. J. Rose. *Calculation of the radiative opacity of laser-produced plasmas.* J. Phys B: At. Mol. Opt. Phys. 25 (1992)

[2] R.M.More et al. *A new quotidian equation of state (QEOS) for hot dense matter*. Phys. Fluids 31 (10) (1988)

[3] L.B. Samolovskikh et al. *Calculations of Spectral Opacities for Be-Cu plasmas using STA and Average Atom Models*. 31st EPS Conference on Plasma Phys. London, 28 June - 2 July 2004 ECA Vol.**28G**, P-2.019 (2004)

[4] TOPs Opacities. Los Alamos National Laboratory

[5] Jianmin Yuan. *Self-consistent average-atom scheme for electronic structure of hot and dense plasmas of mixture.* Physical Review E **66**, 047401 (2002).

[6] Rubiano et al. *Fast Calculations of Opacities for ICF Plasmas.* (2010)