Equation of State and Opacities for Warm Dense Matter

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Abstract. We will present recent developments in the calculation of opacity and equation of state tables suitable for including in the radiation hydrodynamic code ARWEN [1] to study processes like ICF or X-ray secondary sources. For these calculations we use the code BiGBART to compute opacities in LTE conditions, with self-consistent data generated with the Flexible Atomic Code (FAC) [2]. Non-LTE effects are approximately taken into account by means of the improved RADIOM model [3], which makes use of existing LTE data tables. We use the screened-hydrogenic model [4] to derive the Equation of State using the population and energy of the levels avaliable from the atomic data.

1 Introduction

The complete study of an ICF target couples a great variety of physical effects that must be accounted to get meaningfull results. At first we need to know the properties of matter at the states reached during the ICF process. This means to cover a wide range of temperatures that reaches several keV and densities from 1 mg/cm^3 to several times the solid density.

The radiation hydrodynamic codes like ARWEN [1], have to be supplied with thermodynamic and radiative data. The accuracy of this properties is a key to get results close to the experiments. For locar thermodynamic equilibrium (LTE) this data is arraged as functions of two state variables of our system. For hydrodynamics the most common used state variables are density and internal energy, while for radiation transport the most meaninful variables are density and temperature.

To be able to solve the hydrodynamics a relation between pressure and the state variables density and internal energy is needed. This relation is the Equation of State (EOS) which tell us the compressibility of a material and then have a great influence on the hydrodynamics of the plasma.

The matter at high temperature like the plasma formed in the ICF targets emits a large amount of energy in form of electromagnetic fields. In general, radiative properties of plasmas are important in the study of high energy density matter. With more accurate radiative properties the physical picture we obtain in simulations will be closer to reality.

Here is described a methodology to obtain EOS and opacity tables with consistent data between thermodynamics and atomic calculations. The challenge is to find the correct balance between accuracy and computational cost. We will show recent improvements in the BiGBART opacity code [5] and study non-local thermodynamic equilibrium (NLTE) effects bias the improved RADIOM model and also derive an EOS from atomic calculations.

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2 Radiative Model

Calculating these properties is a formidable task. Main difficulties come from the transition from LTE models to full NLTE models, where a myriad of transitions between levels are needed for solving a colisional-radiative system, with the increasing complexity of ions with increasing Z. The simplest codes assume an average atom and calculates transitions between average orbitals. Other models merge close configurations to obtain configuration-averages reducing the amount of levels to treat.

In order to reduce computational cost as much as possible BiGBART now uses modified FAC binary files to reuse the atomic data generated. Energy levels, radiative transitions and photoionization cross-sections are calculated under request and stored in indexed binary files. This way, when generating opacity tables, the data generated in a temperature-density point is used, accessing and extracting necessary self-consistent data.

Energy levels are applied in a full Saha system that yields the fractional ionization occupancies. Ionization potentials are taken from literature [6,7] when possible or calculated with FAC. Ionization potential lowering is accounted using the modified Stewart-Pyatt formula [8]. Mixtures are treated consistently, iterating until both chemical potential and intrinsic densities converge.

A Voigt profile is used for line broadening with Doppler [9] and UTA Gaussian widths, and natural [9] and colisional [10] Lorentzian widths.

2.1 NLTE effects

The RADIOM model mimicks NLTE properties at temperature $T_e = T_e(Z^*, EOS, opacity)$ with LTE calculations at an equivalent temperature T_z. This is achieved by fitting the maximum of the charge state distribution in NLTE at T_e in an extended Saha equation with the LTE value at T_z with the standard Saha equation.

In figure 1 is shown the absorption coefficient and the emission of gold at 1000 eV for LTE and NLTE using the radiom model, both pictures uses the UTA model with FAC atomic data. The absorption coefficient for NLTE is higher than in LTE and the emission in NLTE is lower, as spected because in NLTE the excited states of the atom are more populated than in LTE and then emission is lowered.
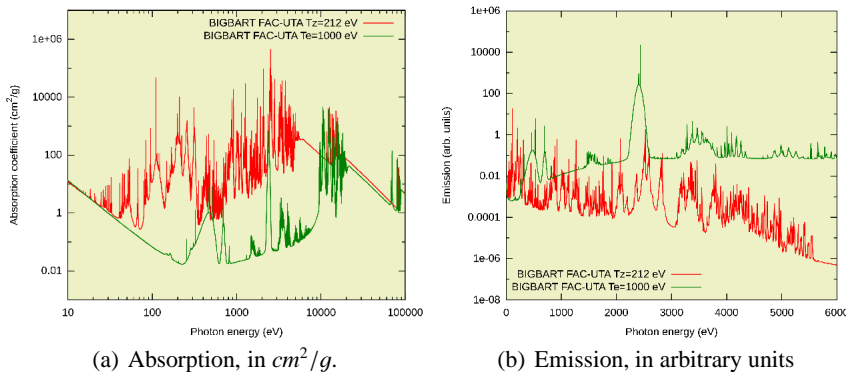

(a) Absorption, in cm^2/g. (b) Emission, in arbitrary units

Fig. 1. Radiative properties for Au at $19\mu g/cm^3$ and temperature of 1000 eV (LTE data in green, NLTE data in red).

3 Equation of State

EOS is computed using the screened-hydrogenic model (SHM) described in [4] for LTE. This model gets the Helmholtz free energy $F = F(\rho, T)$ from the electronic configuration of the average atom. A thermodynamic consistent EOS can be derived from the free energy F.

In the figure 2(a) we compare the results from our EOS (full lines) using the SHM against the Thomas-Fermi (TF) theory (dashed lines). In the TF model the chemical potential is the key variable. We compare the pressure using the chemical potential from our SHM and from the TF model. Great differences found at low temperatures.

Finally it is possible to improve our analytical EOS using an empirical correction as described in [12] to make the thermodynamic data as close as possible to experimental data and ab initio MD simulations, as it is shown in the figure 2(b) where a corrected EOS model is compared against the avaliable data. In this figure is ploted the aluminum Hugoniot curve computed using the QEOS model [14] using a pressure multiplier against experimental data and other models like the SESAME aluminum table and *ab initio* molecular dynamics data [13].
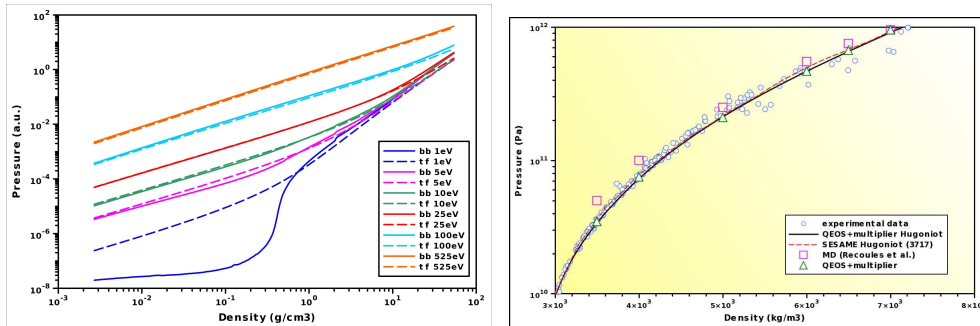
(a) Comparison between the Thomas-Fermi (tf, dashed line) model and the screened-hydrogenic model (bb, full line) derived from BiGBART for Al.

(b) Hugoniot curve for Al.

Fig. 2. EOS data for Al with several models and copared to experimental shock wave data

4 Comparison to experimental data

In order to test mixtures calculations we have included a mixture of iron with sodium fluoride [11]. Conditions determined were 59 eV and 11.3 mg/cm^3. We include non-relativistic (ALEXANDRIT DCA) and relativistic (BIGBART DCA) hydrogenic calculations from older versions used in the Instituto de Fusión Nuclear.

The new FAC-UTA calculation shows in general a better fit, especially in the $100 - 150\,eV$ range, showing the absorption peak above $100\,eV$ which do not appear in the hydrogenic calculations.

5 Conclusions and future work

The methodology and models used to compute EOS and opacities in the Instituto de Fusión Nuclear have been presented in this work. This data are stored in tables suited to be used in radiation hydrodynamic codes like ARWEN. This methods can obtain accurate atomic properties for several materials using well-known models and with a very fast algorithm.

Future work will include testing of RADIOM model in simulations and developing a full NLTE module in BiGBART and also developing an EOS consistent with the atomic calculations for NLTE. Also a time-dependent ionization routine has been developed [15] to get the charge state evolution including NLTE effects and then corrections to the opacities and EOS must be applied to account this NLTE effects.
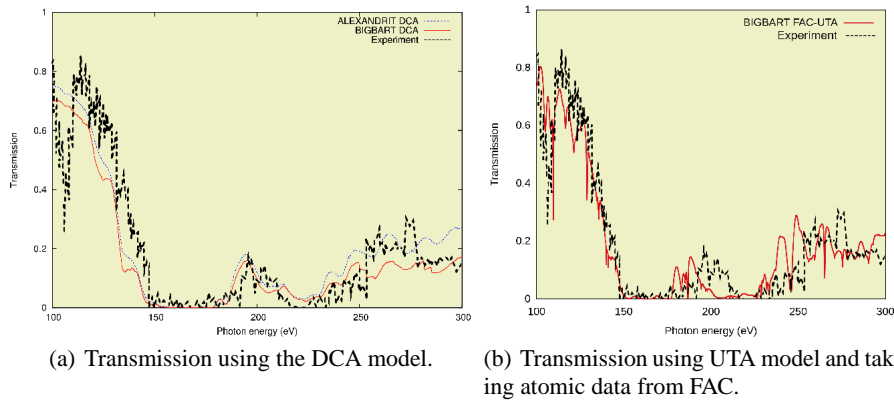
(a) Transmission using the DCA model.

(b) Transmission using UTA model and taking atomic data from FAC.

Fig. 3. Spectral transmision for a mixture of Fe and NaF at plasma conditions of 59 eV and density of 11.3 mg/cm^3. The equivalent areal density is 339 $\mu g/cm^2$.

Acknowledgments

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