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Frequency-dependent opacity calculations for radiation transport simulations

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Abstract

We will present recent developments in the calculation of opacity 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 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.

1. Introduction and Objectives

- 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.
- However, 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.
- The challenge here is to find the correct balance between accuracy and computational cost. We will show recent improvements in the BiGBART opacity code [4] and study NLTE effects bias the improved RADIOM model.

2. Models implemented

- 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 [5,6] when possible or calculated with FAC. Ionization potential lowering is accounted using the modified Stewart-Pyatt formula [7].
  - Mixtures are treated consistently, iterating until both chemical potential and intrinsic densities converge.
- A Voigt profile is used for line broadening with Doppler [8] and UTA Gaussian widths, and natural [8] and colisional [9] Lorentzian widths.

3. NLTE effects

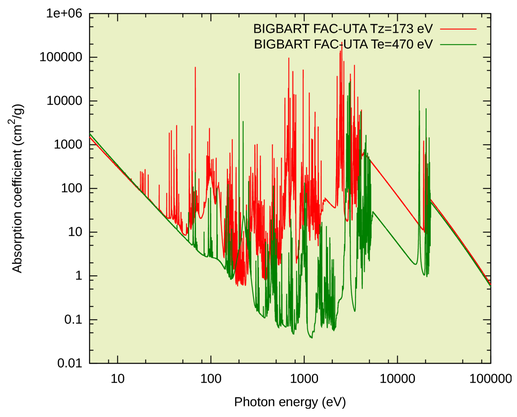
- The RADIOM model mimicks NLTE properties at Te (Z*, EOS, opacity) with LTE calculations at an equivalent temperature Tz.
- This is achieved by fitting the maximum of the charge state distribution in NLTE at Te in an extended Saha equation with the LTE value at Tz with the standard Saha equation.

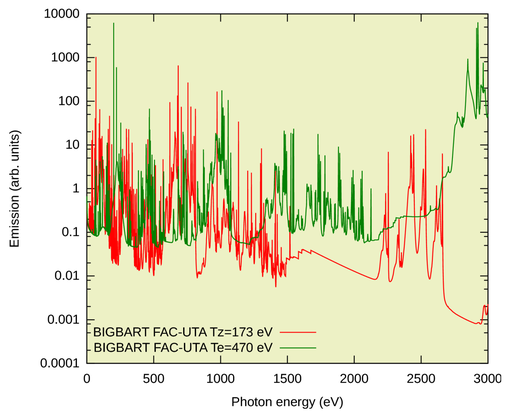
3. 1. Nb

Niobium at 260 µg/cc

LTE Te=470 eV : Z*=38.45

NLTE Tz=173 eV : Z*=30.52





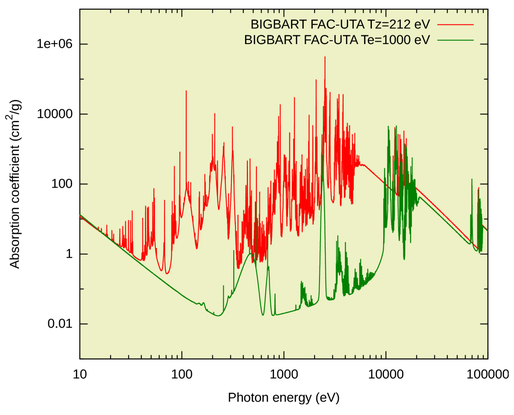
Lower NLTE effects
Tz/Te ~ 1/3

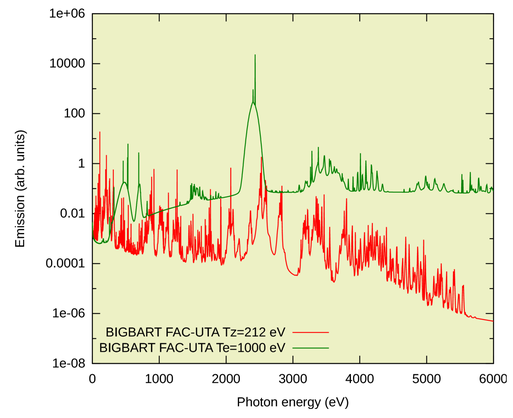
3. 2. Au

Gold at 19 µg/cc

LTE Te=1000 eV : Z*=70.42

NLTE Tz= 212 eV : Z*=50.22

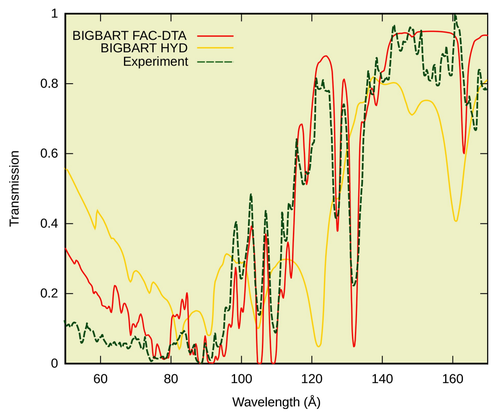




Stronger NLTE effects
Tz/Te ~ 1/5

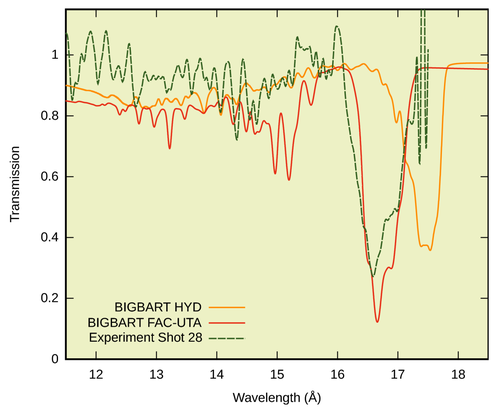
4. Experimental benchmark

4. 1. Al

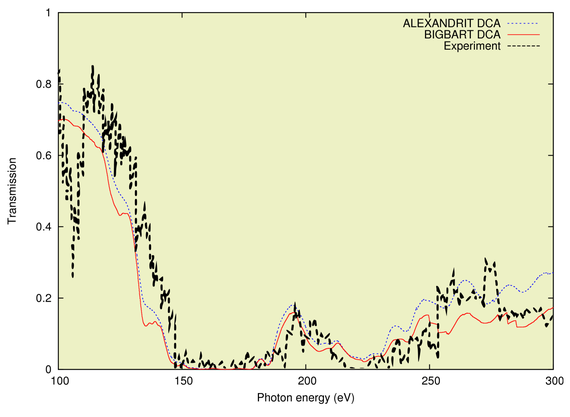


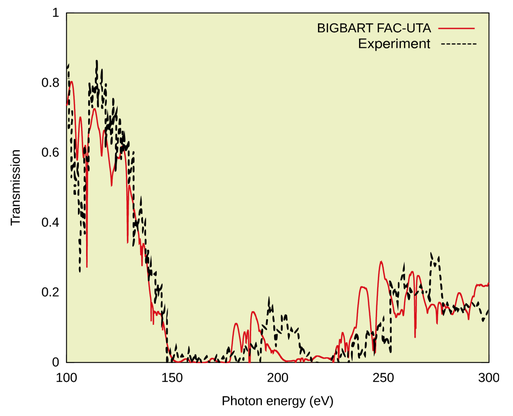
- Low Z aluminum [10] at 20 eV and 10 mg/cc. In this case we show detailed calculations due the tractable number of detailed levels in ionized Al. Good agreement can be seen with line positions of the partially resolved 2p–3s multiplets of Al^{4+} between 115 and 135 Å, and Al^{5+} between 100 and 112 Å. The hydrogenic approximation shows poor agreement, especially in the Al^{4+} 2p–3s transitions.
- Medium Z iron [11] at 22 eV and 4 mg/cc. With a single density–temperature point, BiGBART reasonably well reproduces the L-shell transitions, especially the main absorption window 2p–3d transitions, between 16 and 17.5 Å. The hydrogenic approximation is in worse agreement predicting a 2p–3d window shifted towards lower energies.

4. 2. Fe



4. 3. Fe Na F mixture





- In order to test mixtures calculations we have included a mixture of iron with sodium fluoride [12]. Conditions determined were 59 eV and 11.3 mg/cc. 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

- We have presented recent developments in models used in the Instituto de Fusión Nuclear to compute opacities, and shown the improvement from hydrogenic aproximation to self-consistent atomic databases.
- Future work will include testing the RADIOM model in simulations and developing a full NLTE module in BiGBART.

References

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