Equation of State and opacities for warm dense matter

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HEDLA 2012, Tallahassee April 30th - May 4th

Introduction

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The HEDP group leaded by Pedro Velarde are formed by

- François de Dortan de Gaufridy (PostDoc)
- Manuel Cotelo Ferreiro (Professor assistant)
- David Portillo García (PhD student)
- Alberto García de la Varga (PhD student)
- Alfonso Barbas Espa (PhD student)
- Agustín González Fernández (PhD student)

Advances in EOS

- The starting point is an analytical EOS based on the Helmholtz free energy because it asures the thermodynamic consistency.
- Fitting of the EOS model to the avaliable experimental data using an empirical multiplier to the Helmholtz free energy
- We developed a new multiplier based on QEOS[1] model that includes dependency from the temperature and the density[2].
- We fit the EOS with shockwave data and *ab initio* MD[3]. simulations.

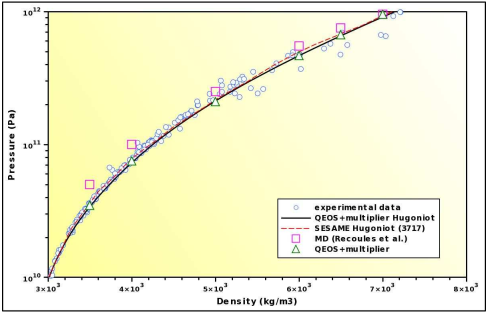

Figure: Alumnium Hugoniot

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[1] R. M. More et al. Phys. Fluids 31, 3059 (1988)

[2] M. Cotelo Astrophysics and Space Science, Volume 336, Issue 1, pp.53-5

[3] V. Recoules et al., Phys. Rev. B vol 72 pp. 104202 (2005)

Opacity calculations

Introduction

As many codes, BiGBART[4] can be divided in two main parts: population distribution and frequency dependent opacity/emissivity calculation.

Atomic data is generated using the FAC[5] atomic package.

- Population distribution
  - NLTE Collisional-radiative module
    - Specified radiation field
    - Optically thin
  - LTE Saha equation
  - RADIOM Pseudo-NLTE[6]. Inline calculations of NLTE radiation properties.
  - Stewart-Pyatt interpolated[7] continiuum lowering correction
- Frequency dependent opacity/emissivity
  - FAC photoexcitation/spontaneous decay transition energies and oscillator strenghts
  - Voigt profile with contribution from doppler, natural, collision and UTA widths
  - FAC photoionization/radiative recombination cross sections
  - Free-free bremsstrahlung absorption and emission.

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[4] A.G. de la Varga, HEDP 7, 163-168 (2011)

[5] M.F. Gu, Astrophysical Journal, 582, 1241 (2003)

[6] M. Busquet, HEDP 5 270-275 (2009)

[7] R.M. More, Applied Atomic Collision Physics, vol. 2 (1982)

LTE and NLTE data tables. Molybdenum

- For high compression and low temperatures (violet region) we get LTE conditions.
- We can see the shell effects of the NLTE model in the two regions in red

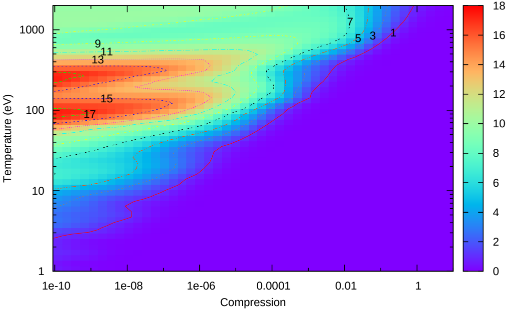
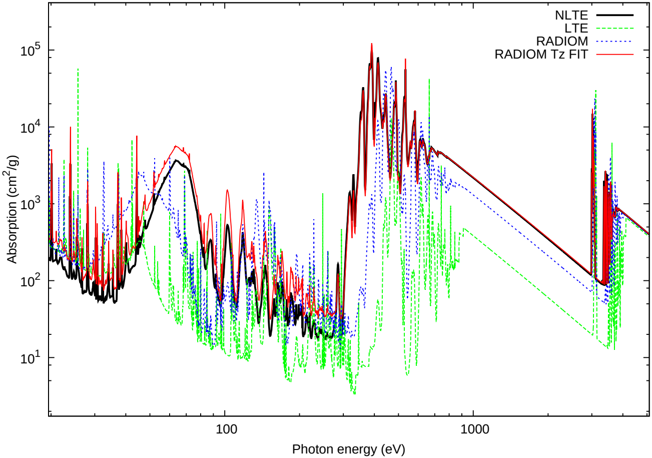


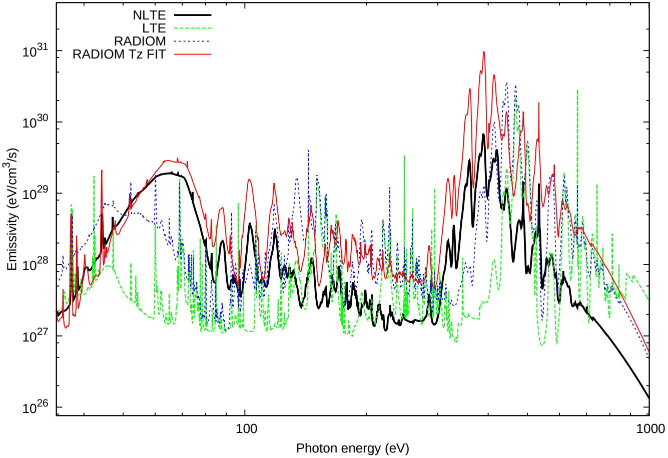
Figure: Difference of LTE average charge against NLTE charge: $\bar{Z}^{LTE} - \bar{Z}^{NLTE}$

Argon absorption coefficient: 100 eV and $8 \cdot 10^{19}$ e/cm^3, close to LTE conditions



The differences in the ionization states modifies the absorption due to the L shell between 1 keV and 3 keV approximately.

Argon emission coefficient close to LTE



The RADIOM+FIT reproduces the NLTE profile, but gives a higher emission coefficient.

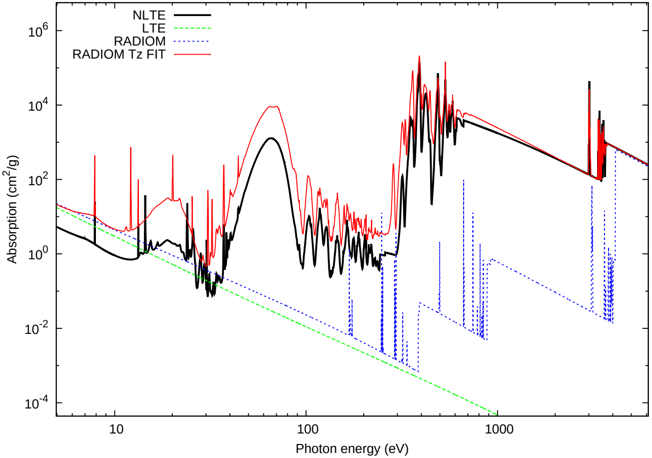
Resume of results for Ar close to LTE

- Great agreement of the RADIOM+FIT model for Plank opacity coefficient.
- LTE gives a 30% more ionization than NLTE models.

Model	T_z	$\bar{Z}$	Rosseland	Planck	Emission
NLTE	100	11.50	1.25[2]	7.55[3]	4.65[28]
LTE	100	15.33	1.85[1]	3.51[2]	5.06[28]
RADIOM	76	13.62	0.94[2]	3.03[3]	1.65[29]
RADIOM FIT	58	11.50	2.18[2]	7.40[3]	4.57[29]

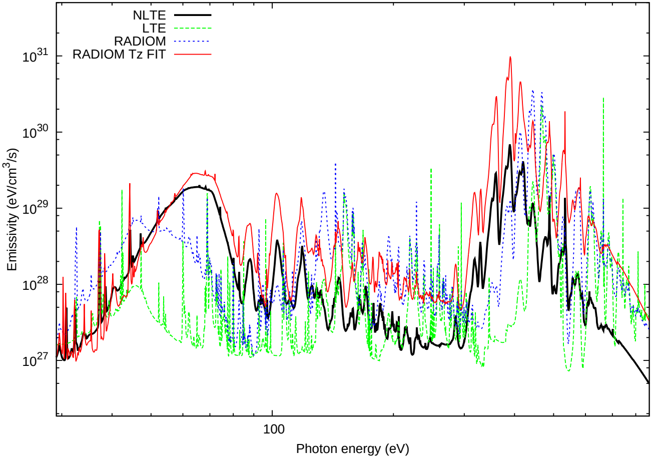
Argon absorption coefficient: 800 eV and $7.5 \cdot 10^{17}$ e/cm^3, far from LTE

Although we are far from LTE conditions, the RADIOM+FIT model still reproduces satisfactory the absorption coefficient.



Argon emission coefficient far from LTE

The RADIOM+FIT model still reproduces the profile of the absorption coefficient.

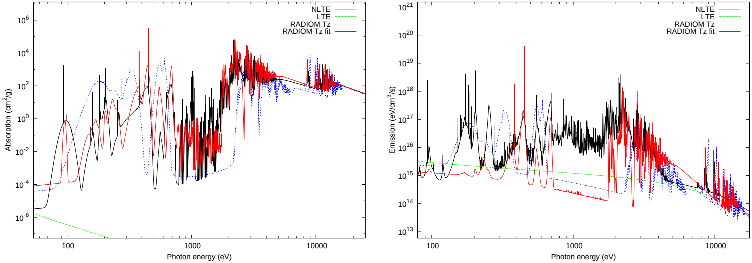


RADIOM+FIT give a reasonable estimation of the opacity and emission coefficients

LTE and simple RADIOM model overestimate the charge state in more than a 45% and then give poor estimations

Model	T_z	$\bar{Z}$	Rosseland	Planck	Emission
NLTE	800	10.98	2.24[2]	8.00[2]	5.64[23]
LTE	800	18.00	1.80[-1]	2.39[-5]	8.84[21]
RADIOM	130	16.00	3.83[-1]	8.33[1]	4.55[21]
RADIOM FIT	40	10.99	2.72[2]	1.00[3]	2.96[24]

Tungsten at 5 keV and 10^{14} e/cm^3



We have included some data taken from the 5th NLTE Workshop[8] to compare out NLTE results with other codes..

Model	T_z	$\bar{Z}$	Rosseland	Planck	Emission
Code 1	5000	47.43			
Code 2	5000	48.50			
Code 3	5000	47.61			
NLTE	5000	**47.69**	**2.11[1]**	**1.07[2]**	**1.07[15]**
LTE	5000	74.00	0.16[0]	1.07[-11]	9.25[13]
RADIOM	242	59.54	1.68[1]	1.19[2]	3.60[14]
RADIOM FIT	154	47.69	2.04[1]	1.36[2]	7.38[14]

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[8] C. J. Fontes et al. , HEDP 5, 15-22 (2009)

Radiative shocks

ARWEN: code description

We are using a 2D simulation code (ARWEN[9]). that couples hydrodynamics and full radiation transport using an AMR scheme based in BoxLib, a box library developed in Berkeley Lab[10].

Hydrodynamics:

- Unsplit high order Godunov method for XY and RZ coordinate systems
- Multimaterial fully conservative scheme

Radiation transport:

- Sn transport method
- Multigroups treatement with DSA and TSA[11].

Electron heat diffusion:

- Flux-limited diffusion
- Laser absortion with raytracing capabilities

Applications

- LA experiments[12].
- Fast ignition design[13].
- X-Ray lasers[14][15].

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[9] F. Ogando et al., Journal of Quantitative Spectroscopy & Radiative Transfer, v. 71, iss. 2-6, p. 541-550

[10] https://ccse.lbl.gov/BoxLib/index.html

[11] García Fernández, C et al. IEEE Transactions on Plasma Science, vol. 38, issue 9, pp. 2359-2366

[12] P. Velarde et al. Physics of Plasmas, Volume 13, Issue 9, pp. 092901-092901-10 (2006)

[13] P. Velarde et al., Laser and Particle Beams, vol. 23, Issue 1, p.43-46

[14] E. Oliva et al., Optics Letters, vol. 34, issue 17, p. 2640

[15] E. Oliva et al., Physical Review E, vol. 82, Issue 5, id. 056408

Sketch of the problem

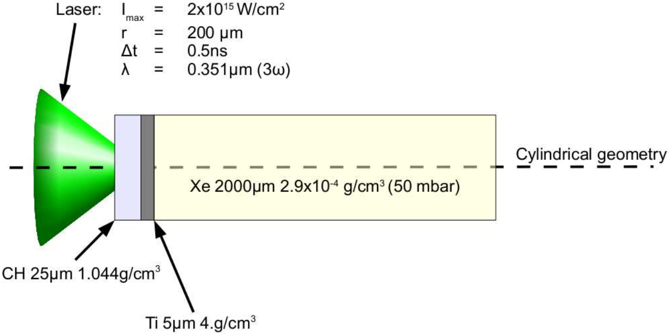

Figure: Sketch of the simulations done

First we have analyzed the effects of the wall in the evolution of the radiative shock.

As we can see in the next slide there are great differences due to shock interaction with the wall. We have done simulations in cartesian and cyclidrical coordinates.

Time evolution of the shock with and without wall boundary conditions

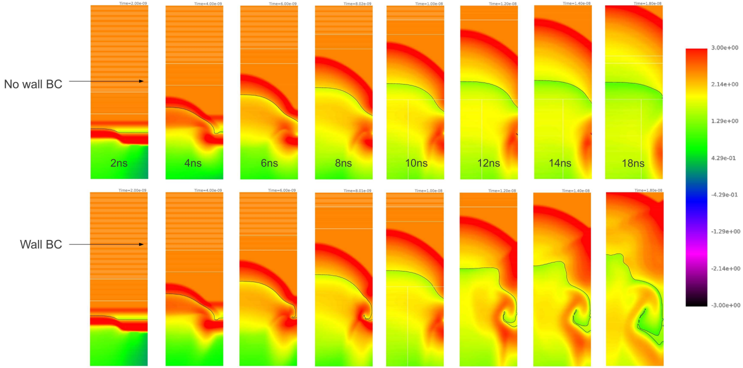

Figure: Effect of the tube wall in the shock, density color maps

In the case of no wall boundary conditions for 14 ns in advance, the material interface becomes almost planar while in the case of a wall it takes a complex shape.

Comparison for 12 ns

We present here a comparison for 12 ns. The shock reflected on the wall reaches the interface and changes its structure completely.

The velocity of the shock in the axis do not change.

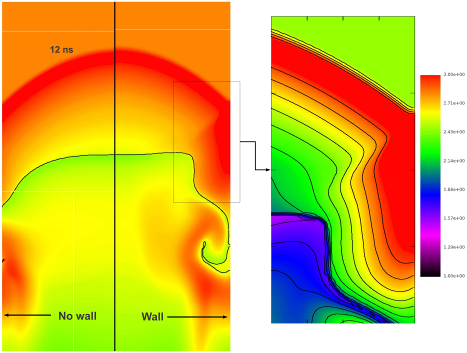

Figure: For 12 ns, we can see the differences in the density profile because of the different boundary conditions

Temperature profiles

The precursor signal is not clear because we are using a full radiation transport description.

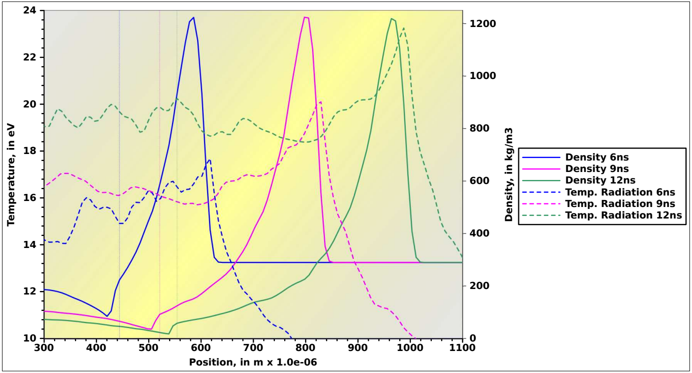

Figure: Radiation temperature versus density

Position of the shock

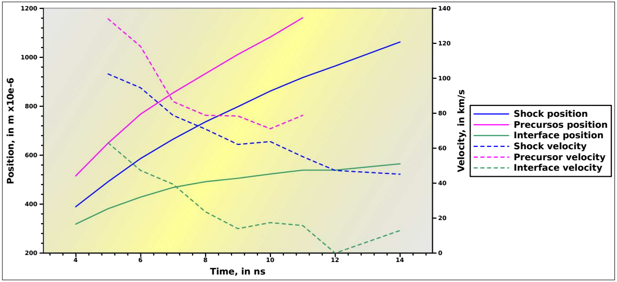

Figure: Position and velocity of the shock and the interface

At 10 ns we get a shock velocity of about 60 km/s and a precursor velocity of about 80 km/s.

Conclusions

Conclusions

- NLTE effects can have a strong impact in the radiation properties, specially in emission coefficients. Need to include better NLTE models in our radiation transport package
- The interaction of the radiative shock with the wall can have a great effect on the propagation of the precursos due to the reflected radiation.
- We need to continue investigating.

Conclusions

Thank you for your attention.