

3D Self-Consistent Full-Wave PIC Models for Investigating Space-Resolved ECR Plasma Properties







B. Mishra, A. Galatà, A. Pidatella, G. Torrisi, C. Salvia, G.S. Mauro, E. Naselli, R. Ràcz, S. Biri and D. Mascali

Department of Physics and Astronomy "Ettore Majorana", University of Catania and INFN-LNS

PhD candidate under the supervision of David Mascali

ECR Ion Sources and PANDORA



Schematic of ECRIS operation and global electron properties [1]



ECR magnetic trap to study nuclear astrophysics in a plasma.

- Modification of β-decay rates of radio-isotopes relevant to s-process nucleosynthesis
- 2. Opacity of heavy elements for modelling kilonovae light curves relevant to rprocess nucleosynthesis

Schematic of PANDORA ECR plasma trap surrounded by HpGe detectors and diagnostics systems

The shape and size of plasma chamber, pressure, RF power and frequency strongly influence

- Beam magnitude and current
- Plasma density and temperature distribution
- Susceptibility to instabilities

PANDORA - Plasmas for Astrophysics, Nuclear Decay Observations and Radiation for Archaeometry

Ion CSD and LPD control the decay rates and opacity of radio-isotopes in the plasma

Talk by Eugenia Naselli on Sep 21!

[1] D. Mascali et al., Eur. Phys. J. A 53, 145 (2017).

Measurement and Modelling Strategy Simulations can be a powerful tool to predict 3D space-resolved properties of ECR plasma for fundamental and applied studies THEORY **EXPERIMENT** Steady state electron simulations X-ray spectroscopy Secondary y-detection Optical spectroscopy lon current Steady state ion simulations X-ray emissivity maps Opacity maps y emissivity maps Injected neutral particle β -decay rates and heavy element opacity [2, 3]and 1⁺ beam dynamics X-ray emissivity maps

[2] K. Takahashi and K. Yokoi, Nucl. Phys. A 404, 1983 [3] A. Pidatella *et al*, Frontiers in Astronomy and Space Science 9:931744

Full-Wave Electron Kinetics



[4] A. Galatà et al, Frontiers in Physics 10:947194, 2022

Full-Wave Electron Kinetics: Hot Electron Tensor

Wave-plasma coupling self-consistently modelled using "cold electron" approximation

• Electron speed << phase velocity of waves

Warm electron contribution to dielectric tensor substantial in ECR plasma

• Efforts underway to switch from cold electron to hot electron dielectric tensor





Self-Consistent Ion Kinetics

Vlasov-Maxwell equations + Fokker-Planck Collisions + Balance Equation



Till convergence...

Self-Consistent Ion Kinetics: Modules



MONTE CARLO SAMPLING

Formalism for sampling from multiple competing processes

$$\begin{array}{ll} \nu_{CEX} = n_0 \sigma_{CEX} v_i & \text{Effective reaction frequency} & P_{ion} = \frac{\nu_{ion}}{\nu_{tot}} (1 - e^{-\nu_{tot}\Delta T}) \\ \nu_{ion} = n_e \sigma_{ion} v_e & \nu_{tot} = \nu_{ion} + \nu_{CEX} & P_{CEX} = \frac{\nu_{CEX}}{\nu_{tot}} (1 - e^{-\nu_{tot}\Delta T}) \\ \end{array}$$

CSD AND DENSITY SCALING

ION NUMBER DENSITY

$$\oint_{V} n_{e} dV = K_{3} \left[(1 - k_{1 \rightarrow 2} + 2k_{1 \rightarrow 2}k_{2 \rightarrow 1} + k_{1 \rightarrow 2}k_{2 \rightarrow 3}k_{3 \rightarrow 2}) \oint_{V} n_{1} dV + \frac{2k_{1 \rightarrow 2}(1 - k_{2 \rightarrow 3} - k_{2 \rightarrow 1} + k_{2 \rightarrow 3}k_{3 \rightarrow 2})}{\text{Transfer}} \int_{V} n_{2} dV + \frac{3k_{1 \rightarrow 2}k_{2 \rightarrow 3}(1 - k_{3 \rightarrow 4} - k_{3 \rightarrow 2})}{3k_{1 \rightarrow 2}k_{2 \rightarrow 3}(1 - k_{3 \rightarrow 4} - k_{3 \rightarrow 2})} \int_{V} n_{3} dV + \frac{4k_{1 \rightarrow 2}k_{2 \rightarrow 3}k_{3 \rightarrow 4}}{4k_{1 \rightarrow 2}k_{2 \rightarrow 3}k_{3 \rightarrow 4}} \int_{V} n_{3 \rightarrow 4} dV \right]$$

Conservation of total charge

[5] B. Mishra *et al*, Frontiers in Physics 10:932448, 2022 [6] B. Mishra, EPJ Web of Conferences 275, 02001, 2023
[7] A. Galatà *et al*, PSST 25, 045007, 2016 [8] A. Galatà *et al*, Rev. Sci. Instrum. 91, 013506, 2019

Model Predictions: CSD and Ion Current



Regions of peak occupancy of each charge state (top) and 3D distribution of mean charge state of plasma [6] (bottom)

[5] B. Mishra *et al*, Frontiers in Physics 10:932448, 2022 [6] B. Mishra, EPJ Web of Conferences 275, 02001, 2023

[9] S. Biri *et al*, Rev. Sci. Instrum. 83, 02A431, 2012

Model Predictions: X-Ray Emissivity Maps





Model Predictions: **B**-Decay Rate Maps

Vlasov-Maxwell equations + Fokker-Planck Collisions + Balance Equation



Model Predictions: Neutral Particle Dynamics

1.6

1.4





Deposition of injected neutral particles on the plasma wall, indicating regions of capture from different processes [13]

See poster by Angelo Pidatella!

[13] A. Pidatella *et al*, Metal evaporation dynamics in Electron Cyclotron Resonance Ion Sources: plasma role in the atom diffusion, conversion to ion, and transport, submitted to PPCF

Conclusions and Perspectives

- ECR ion sources are useful for generating ion currents with tunable magnitude and charge states, but their internal plasma structure is complicated
- Full-wave PIC codes which evolve density with EM field distribution can furnish spaceresolved maps of electron density and energy
- The algorithm is now being updated to shift from cold to hot electron tensor
- PIC-MC codes which solve ion balance equation self-consistently with electron charge distribution can furnish space-resolved maps of CSD and excitation levels
- Together these maps are powerful predictive tools to study numerous ECR plasma phenomena like X-ray emission, heavy element opacity and neutral particle dynamics
- These simulations can improve fundamental understanding of the operation of ECR ion sources (instabilities, current generation) as well as for applications involving them (PANDORA facility)



Sandor Biri Richard Rácz



David Mascali Domenico Santonocito Angelo Pidatella Eugenia Naselli Giorgio Finocchiaro Giuseppe Torrisi Giorgio Mauro Claudia Salvia

ISI INFN Istituto Nazionale di Fisica Nucleare Laboratori Nazionali di Legnaro

Alessio Galatà

Alessandro Cardinali



Dipartimento di Ingegneria Astronautica Elettrica ed Energetica



THANK YOU FOR YOUR ATTENTION!!!



E. Naselli et al, Condens. Matter 1, 0 (2021).

SDD volumetric spectrum from Debrecen 2014 (left) and spectrum from CCD pixel from Debrecen 2018 (right)

$$T = 300 \rho_e \rho_i \omega_{K\alpha} \varepsilon_g \varepsilon_q \int_{3.205}^{\infty} \sigma_{K,ion}(E) v(E) f(E) dE$$

Electron and ion density – free parameter







Schematic of experimental setup showing usefulness of collimator in filtering out emission from the walls/extraction plate





Contribution from bremsstrahlung, Ar fluorescence (confined electrons) and Cr/Fe fluorescence (escaping electrons)

Line Emissivity Density (Ar ions)

$$J_{theo,2.96} = \frac{h\nu_{2.96}}{\Delta E} \rho_e \rho_i \omega_{2.96} \int_{3.205}^{\infty} \sigma_{K,ion}(E) v_e(E) f(E) dE$$
$$J_{theo,3.19} = \frac{h\nu_{3.19}}{\Delta E} \rho_e \rho_i \omega_{3.19} \int_{3.205}^{\infty} \sigma_{K,ion}(E) v_e(E) f(E) dE$$



$$\sigma_{K,ion} = a_K q_K rac{\ln arepsilon/I}{arepsilon I} \{1 - b_K ext{exp}[-c_K(arepsilon/I-1)]$$

Pseudo-Voigt profile for line broadening

$$D_{PV}(x-x_0,f)=\eta L(x-x_0, au_L)+(1-\eta)G(x-x_0,\sigma_G)$$

$$J_{theo,line,plasma}(h
u) = [J_{theo,2.96}D_{PV}(h
u - 2.96, f_{2.96}) + \ J_{theo,3.19}D_{PV}(h
u - 3.19, f_{3.19})]\Delta E$$



Lotz cross-section for Ar superposed on Maxwell EEDFs at different temperatures [6]



Electron Diagnostics – X-Ray Spectroscopy - Volumetric



[6] B. Mishra et al, Phys. Plasmas, (2021)

Objective: Launch electron simulations for higher energy ranges and compare model-generated maps with experiment again

SECOND ATTEMPT DATA: Debrecen 2018







Qualitative EEDF fit of ROI 2 – best function Maxwellian+Druyvesteyn



Electron Diagnostics – X-Ray Spectroscopy - Fluorescence



Schematic of multi-collimator CCD-pinhole setup used in Debrecen 2018 [9]

collimator (top) and with multi-collimator (bottom) - enhanced screening and resolution
 3D space-resolved charge density and EEDF
 K-shell ionisation cross-section

Local geometrical efficiency calculated using the ray-tracing Monte Carlo method without multi-



Local geometrical efficiency

Electron Diagnostics – X-Ray Spectroscopy - Fluorescence



Grid of 1024 x 1024 points Map photon to nearest neighbour grid points (1st order approximation)



Electron Diagnostics – X-Ray Spectroscopy - Fluorescence





0th order projection

- 50



Conclusions:

New method for resolving plasma non-homogeneity established, allowing quantitative study of EEDF on a ROI-by-ROI basis

Match between experiment and model much better for Debrecen 2018 as compared to Debrecen 2014 – electron density on correct order of magnitude, general features reproduced

Some aspects not reproduced – notably the hole in the centre – can be attributed to incompleteness of electron simulations

Only 3 magnetic branches visible in experiment – may be attributed to ion density distribution, incomplete implementation of clusterisation



[9] S. Biri et al, JINST 16, P03003 (2021)

Objective: Develop Particle-in-Cell code to model 3D CSD and LPD profile of ions



Buffer Ion PIC Code – Preliminary Benchmarks



Buffer Ion PIC Code – Preliminary Electrostatic Field





400 400

1D profile of double layer field along solenoid axis [10]

-After 2

INFN

Plasmas for Astrophysics

rchaeometry

Nuclear Decay Observation and Radiation for

Upgrades underway:

• Self-consistent evaluation of electrostatic field and potential dip

