The LisbOn KInetics Boltzmann Solver

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Introduction

Predictive tools for non-equilibrium low-temperature plasmas should properly describe the kinetics of electrons, which are responsible for inducing plasma reactivity. A microscopic description of the electron kinetics provides essential information for global / fluid models, such as electron impact rate coefficiients and macroscopic electron transport parameters. It also provides the power transferred from the electric field to the different electron collisional channels.

Here, we focus on plasma-based environmental and biological applications, which have recently attracted the interest of pure and applied research. In this context, we have launched a research project for delivering a KInetic Testbed for PLASMa Environmental and Biological Applications (KIT-PLASMEBA) [1] that includes a simulation tool, the LisbOn KInetics (LoKI), with a Boltzmann solver (LoKI-B).

Code implementation

LoKI-B is a simulation tool, developed under MATLAB® with an object-oriented design, that describes the electron kinetics by solving the homogeneous and stationary electron Boltzmann equation under the classical two-term approximation, for continuous or high-frequency applied electric fields. It includes:

a) inelastic direct/stepwise and superelastic collisions with all types of excited states (electronic, vibrational and rotational), with distributions defined in a proper and user-friendly way;

b) the continuous approximation for rotations with a Chapman-Cowling corrective term, simplifying the handling of rotational inelastic/superelastic collisions for some gases [2];

c) secondary electrons born in ionization events, allowing for an electron density spatial or temporal growth, with an energy sharing described by a single differential cross section or one of the limiting cases "equal energy sharing" or "no energy sharing";

d) electron-electron collisions (impact upon the isotropic part only).

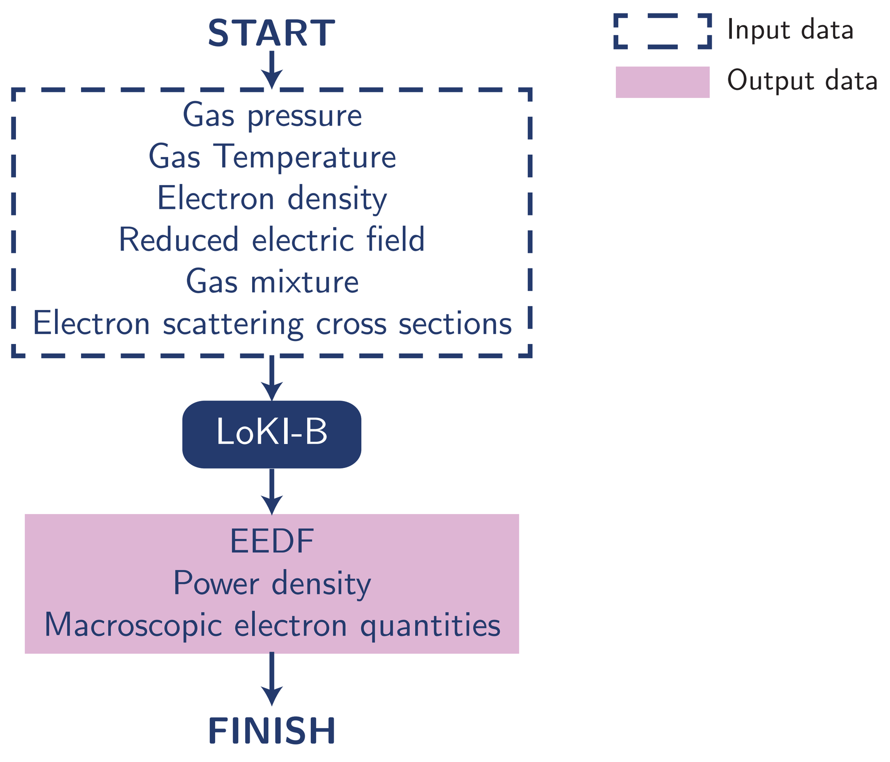
Alternatively, LoKI-B can consider a generalized prescribed EEDF, ranging in the limits of the Maxwellian and the Druyvesten EEDFs.

We are currently engaging verification and validation procedures, to ensure the quality of the tool and the results it provides, before its public release (late 2018) as an open-source tool. LoKI-B can be used as a standalone tool, but it can also be easily coupled to macroscopic global / fluid models [3].

Input / Output

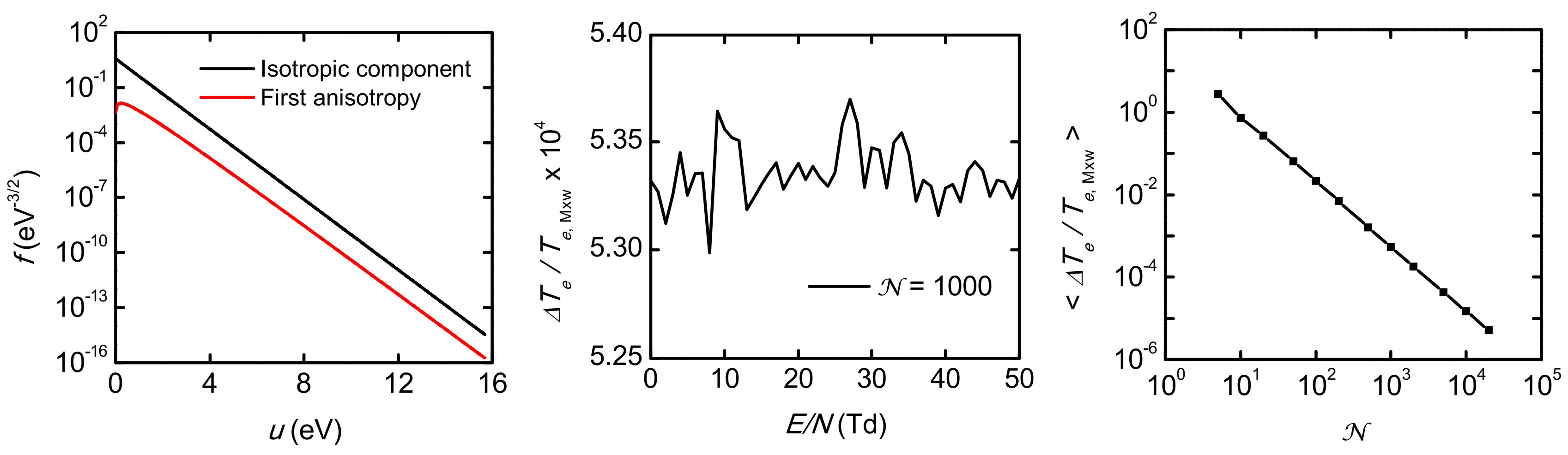
LoKI-B users must provide as input: the working conditions, the electron scattering cross sections (directly obtainable from the open-access platform LXCat [4]), some atomic and molecular data, and the populations of the different excited states present in the gas mixture.

On output, LoKI-B yields: the electron energy distribution function (EEDF) and the corresponding first anisotropy, the electron macroscopic quantities (rate coefficients and transport parameters) and a detailed description of the power density transferred to the different electron collisional channels.

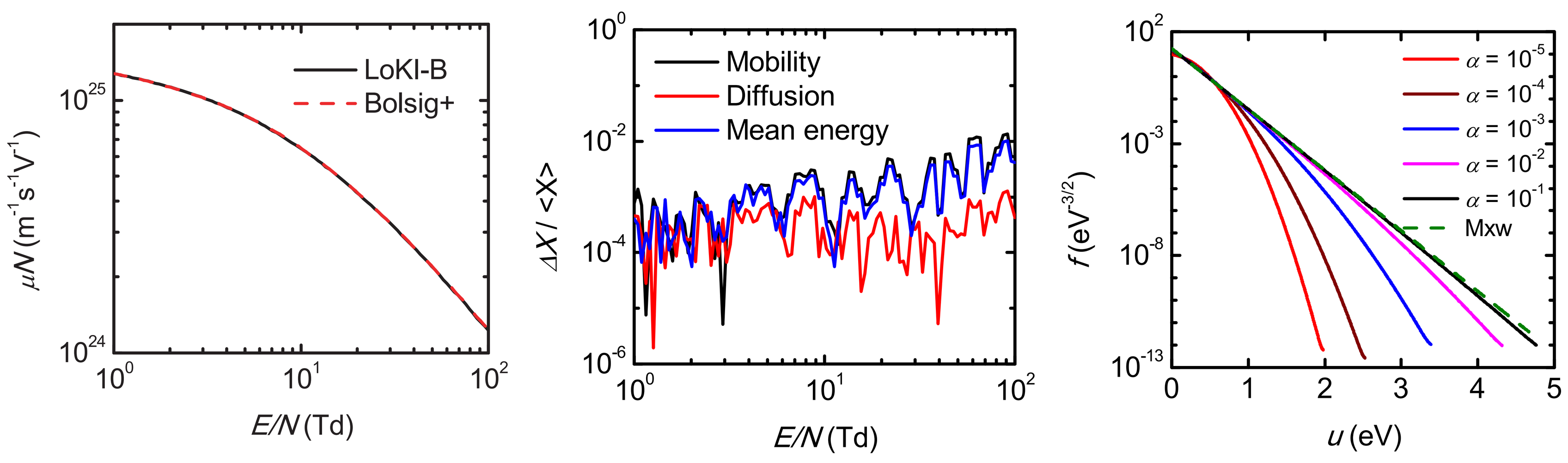


Verification / benchmark tests (model gases)

LoKI-B was verified using a model gas where the sole electron scattering mechanism are elastic collisions with neutrals, at constant momentum-transfer collision frequency. In this case, the analytical solution of the electron Boltzmann equation is a Maxwellian EEDF at a know temperature. Good agreement was obtained between the analytical / numerical results, the latter showing good scaling properties with the number of energy steps, $\mathcal{N}$.



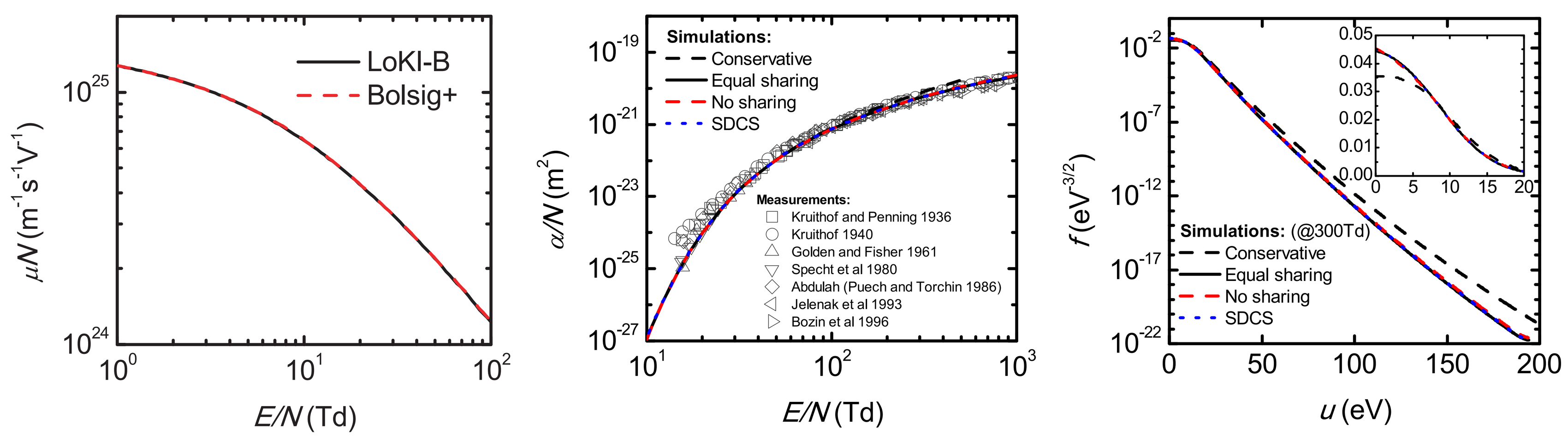
LoKI-B was benchmarked against Bolsig+ [5], using a Reid's ramp model gas. We have found a good agreement between both codes. For this same model gas, we can also see the effect of e-e collisions upon the EEDF.



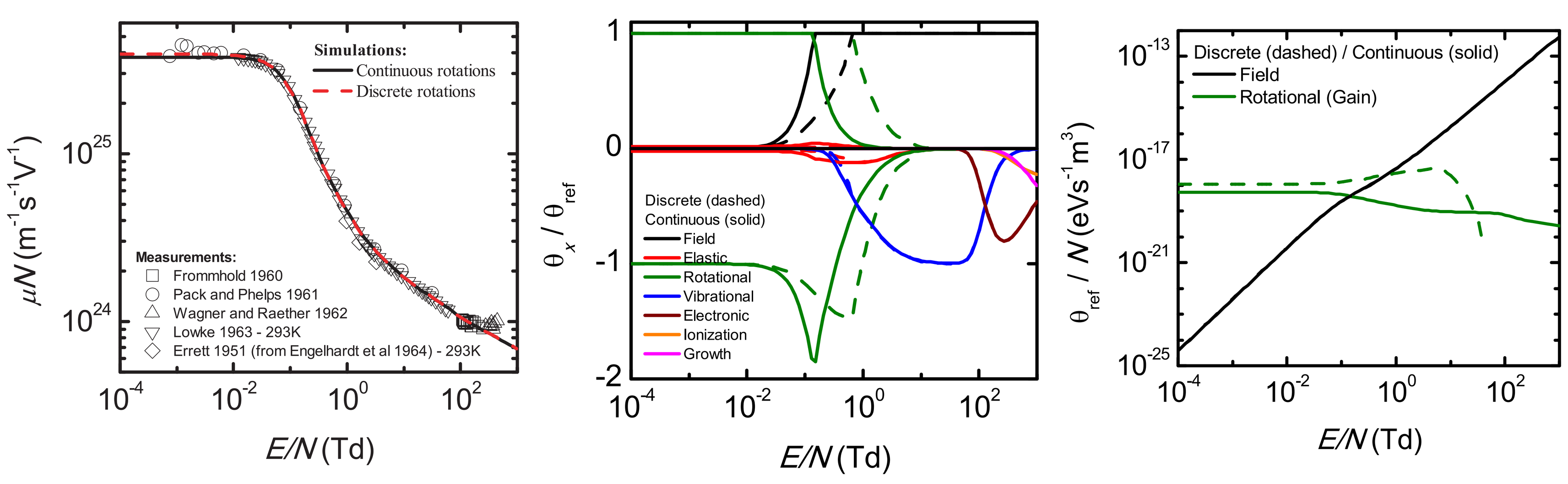
Validation (real atomic / molecular gases)

LoKI-B has been validated by performing swarm analysis, using complete sets of cross sections from the IST-Lisbon database on LXCat [4].

Taking Argon as an example for an atomic gas, very good agreement was found between simulations and measurements. In this case, we can also observe the effect on the results of the ionization model considered in the simulations.

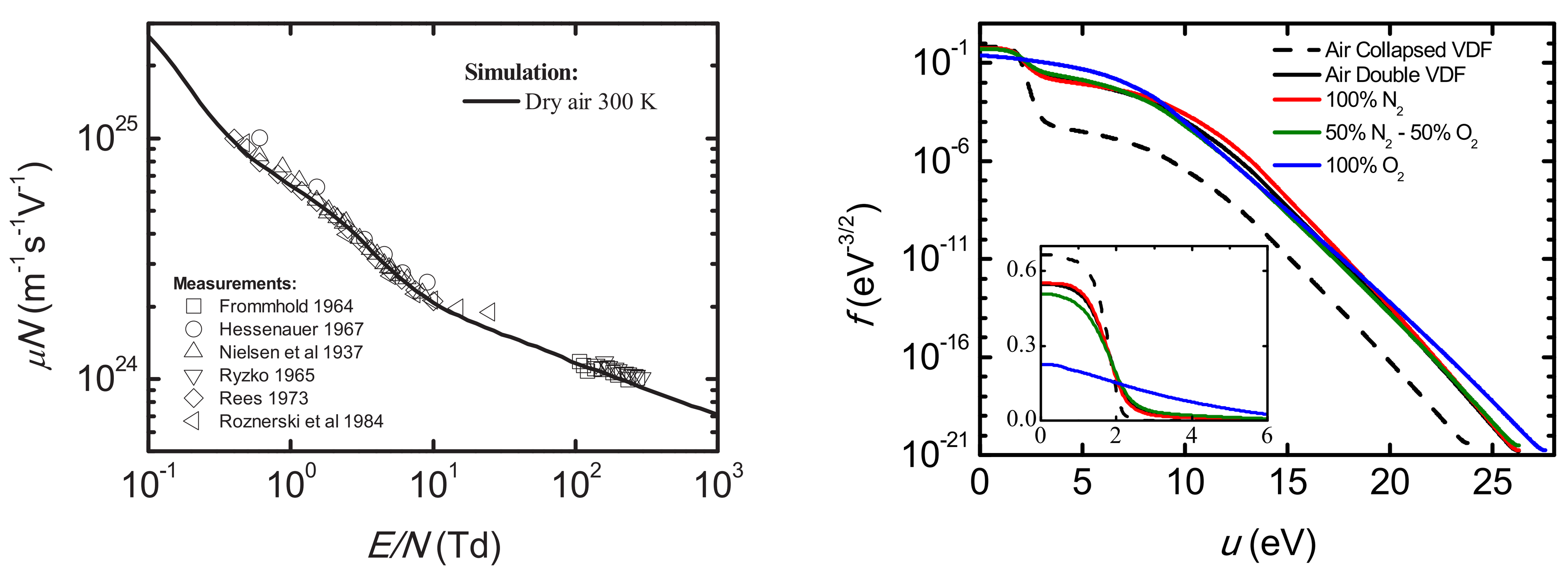


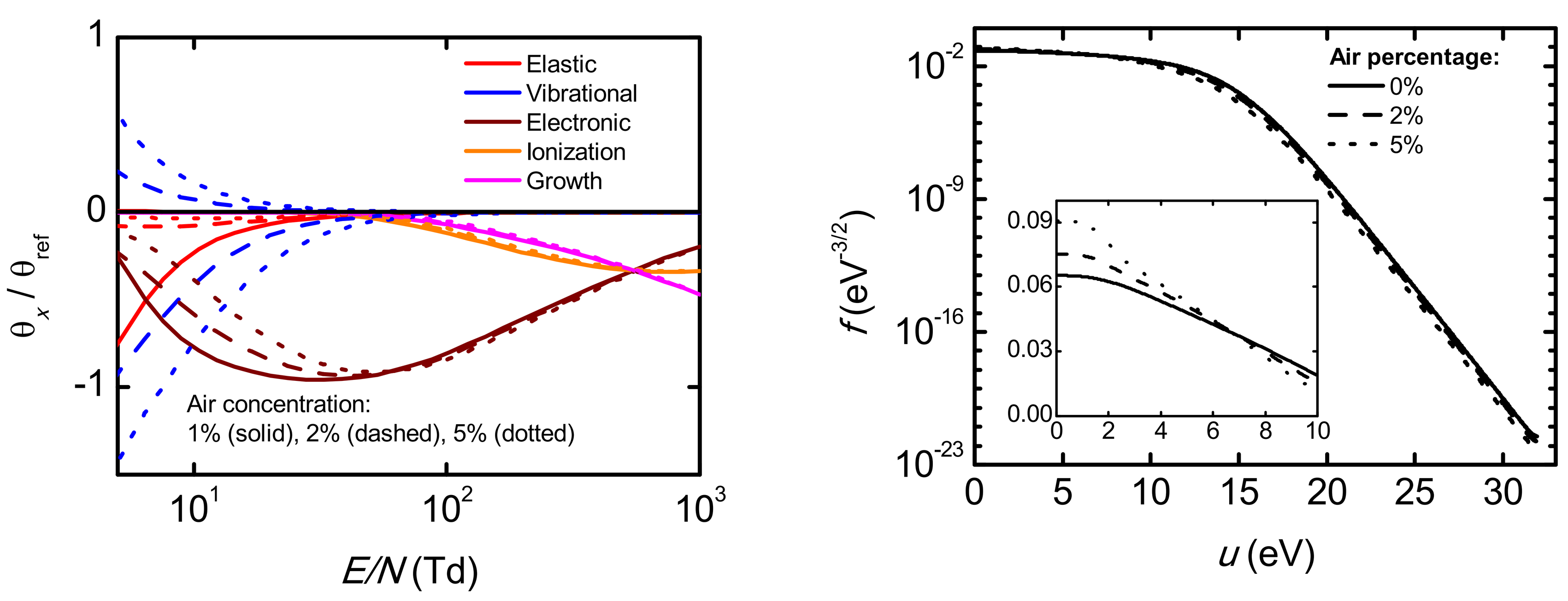
When molecular gases are considered, the populations of the internal states must be properly accounted for. In Nitrogen, as an example for a molecular gas, we described rotational transitions with a discrete description or a continuous operator with a Chapman-Cowling correction. Very good agreement was found between both descriptions and with measurements. In this case, we have also analysed the fractional power transferred to the different electron gain / loss energy channels.



Validation (gas mixtures)

The flexibility of LoKI-B has been tested with simulations for different gas mixtures. We have performed a swarm analysis for dry air (80% N_2 - 20% O_2), monitored the effect upon the EEDF of including vibrational distributions for N_2 and O_2, and analysed the influence in results of considering different admixtures of dry air in a pure Ar plasma.





Conclusions

LoKI-B is a user-friendly, scalable and upgradable open-source tool, that enable researchers to easily study the electron kinetics for any gas mixture. This work discussed its current status of development, presenting basic structure, evidencing functionality and introducing test cases along with first results of benchmarking. LoKI-B development will continue focusing on its graphical user interface and on the introduction of verification and validation procedures. The tool will be publicly released by the end of 2018.

References

[1] KIT-PLASMEBA project webpage: http://plasmakit.tecnico.ulisboa.pt.
[2] M A Ridenti et. al., *Plasma Sources Sci. Technol.*, **24**, 035002 (16pp) (2015)
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[4] LXCat webpage: http://www.lxcat.net.
[5] G. J. M. Hagelaar and L. C. Pitchford, *Plasma Sources Sci. Technol.*, **14**, 722-733 (2005)

Acknowledgments

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