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Modelling of N_2-H_2 capacitively coupled radio-frequency discharges

M. Jiménez-Redondo[1], L. Marques[1,2], N. Carrasco[3], G. Cernogora[3], L. L. Alves[2]

[1]*Centro de Física das Universidades do Minho e do Porto, Universidade do Minho, 4710-057, Braga, Portugal*
[2]*Instituto de Plasmas e Fusão Nuclear, Instituto Superior Técnico, Univ. Técnica de Lisboa, Lisboa, Portugal*
[3]*Université Versailles St-Quentin, CNRS, LATMOS, 11 blvd d'Alembert, 78280 Guyancourt, France*

In this work, we present the results of simulations carried out for N_2-H_2 low pressure, low power capacitively coupled radio-frequency discharges, for amounts of H_2 up to 5%. Simulations are performed using a hybrid code that couples a two-dimensional time-dependent fluid module, describing the dynamics of the charged particles, to a zero-dimensional kinetic module, that solves the Boltzmann equation and describes the production and destruction of neutral species. The model accounts for the production of several excited states, and contains a detailed surface chemistry that includes recombination processes and the production of NH_x molecules. Simulations show that surface production of NH_3 plays a key role in the neutral and ion kinetics of the discharge.

1. Introduction

Capacitively coupled radio-frequency (ccrf) discharges in nitrogen-containing mixtures have been used in planetary studies to simulate, in laboratory environment, the reactivity of ionospheres. The present work is part of a research strategy, involving both simulations and experiment, to analyse the N_2-CH_4 ionospheric chemistry of Titan, the biggest satellite of Saturn. The first step was the study of ccrf discharges in pure N_2 [1], and now continues with the analysis of N_2-H_2 discharges.

2. Modelling

The simulations run at low pressures (0.6–1.2 mbar), for 30–100 sccm gas flows and 5–20 W coupled powers, in N_2-H_2 mixtures with hydrogen concentrations up to 5%.

The model consists of a hybrid code that couples a two-dimensional (*r*,*z*) time-dependent fluid-type module, which describes the transport of the charged particles, to a very complete zero-dimensional kinetic module for the nitrogen-hydrogen mixture. The fluid module solves the continuity and the momentum transfer equations for electrons, positive ions N_2^+, N_4^+, H^+, H_2^+, H_3^+, HN_2^+, NH^+, NH_2^+, NH_3^+ and NH_4^+, and negative ions H^- and NH_2^-, the electron mean energy transport equations, and Poisson's equation for the rf electric potential. The space-time map of the electron transport and rate coefficients are obtained from the electron mean energy profile, using the local mean energy approximation [1,2]. The kinetic module solves the two-term homogeneous and stationary electron Boltzmann equation (accounting for inelastic collisions from ground-state molecules and atoms, and inelastic and superelastic collisions involving vibrationally excited states) and the rate balance equations of the ground-state vibrational excited states of N_2 and H_2, the most relevant electronic excited states for N_2 and N, H, and the most important crossed-species NH_y (y=1-3) and N_2H_y (y=2-4) resulting from interactions within the N_2/H_2 systems [2,3]. An extended surface chemistry is considered, taking in account adsorption, surface association and heterogeneous reactions, which are key to the formation of NH_3. The electron impact chemistry of hydrogen has been updated using the latest set of cross sections available from the IST-Lisbon database of LXCat [4,5].

3. Results

Simulations show that significant amounts of NH_3 are produced in the discharge, with a high dependence on the parameters for the surface kinetics. The abundances of positive ions are greatly affected by the neutral composition, with NH_4^+ quickly becoming the major ion when sufficient NH_3 is present.

4. Acknowledgments

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5. References

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