ZERO-DIMENSIONAL CHEMICAL ANALYSIS OF POSITIVE COLUMNS IN Ar AND Ar-O_2 PLASMAS

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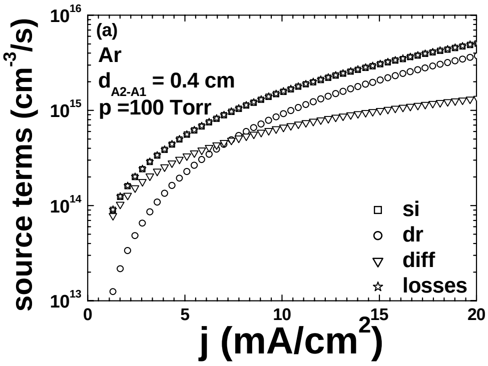
The purpose of this communication is to provide some estimates of the electrical properties and various species densities present in the high pressure positive column plasma generated in a 3-electrode microdischarge configuration – the MicroCathode Sustained Discharge (MCSD) [1]. Our analysis is based on a zero-dimensional formulation of the system of conservation equations coupled to a Boltzmann equation solver for the rate coefficients and an external circuit, as described below. More detailed 2D calculations [2] and companion experiments [3] are also underway as part of a larger project to quantify production of radical and excited species in the MCSD. The long-term goal of the 0D analysis described here is to provide a reduced chemical kinetic scheme suitable for incorporation in the 2D model.

For this purpose, we used a new computational library which is a quite universal tool and can be applied for a wide range of 0D plasmachemical simulations in various gas mixtures. This library is freely available on the web site of the LAPLACE laboratory. Existing solvers (like CHEMKIN, for example) are not always sufficiently flexible for plasma chemistry simulations where the kinetics of heavy species (neutral and charged ones) must be coupled with electron kinetics using Boltzmann equation. Moreover, standard solvers usually do not allow non-Arrhenius forms of rate coefficients, differences in the temperatures of heavy neutral species (gas temperature), or an external circuit – all of which are important for our application.

Our approach is based on a local approximation of the evolution of species densities by solving the conservation equation: d[n]/dt = S + L, where [n] is the density of the studied species, S and L are the source and loss terms, respectively. During the first step the list of species, reactions and corresponding rate coefficients in a simple user-friendly text format is transformed into a FORTRAN 90 module. This automatically generated module contains the definition of the problem, a simple explicit (for the moment) time-adaptive solver for the stiff problem and a set of supplementary routines. It includes as well an automated link to BOLSIG+ [4]**,** a Boltzmann equation solver, based on the two-term approximation, which provides the electron transport rates and the rates of electron-neutral collisions. The code yields the time evolution of the species densities, the reaction rates, the current in the discharge, the voltage and the reduced field for a given circuit (including only a series resistance).

We consider an uniform argon plasma column under the following conditions: pressures in the range of 100 torr, room temperature 300K and small space scale ~1mm (input needed to establish the electric field). These are the typical experimental conditions used in [3]. The species considered are Ar, Ar* (metastable), Ar^+, Ar_2^+ and electrons. Electrons, accelerated in the electric field, collide with the neutrals to produce ionization or excitation. Those new species will disappear by recombination, collisional deexcitation (with reactions rates increasing with pressure) or diffusion (with diffusion rates decreasing with increasing pressure). After a time of the order of 0,1 to 1 ms for our conditions, this system reaches its stationnary state where source terms for each species are exactly balanced by loss terms.

The first results obtained with the next code are consistent with expectations. For example, the three most important reaction rates at steady-state are presented in Figure 1 as a function of current density. We see on the graphs below that, as the current density varies, the plasma changes mode, from a diffusion driven mode for low current density to a dissociative recombination driven mode for high current density. When we change the pressure, the crossing point moves toward lower current densities, until disappearing for pressures higher than 300 torr (not represented here), because the importance of diffusion drops strongly with increasing pressure. The sum of the losses ("losses") is compensated exactly by two-step ionization, and we note the expected shift of the crossing point of the two loss curves with the pressure. These results and many other checks using analytical or semi-analytical test cases have been used to validate our code.



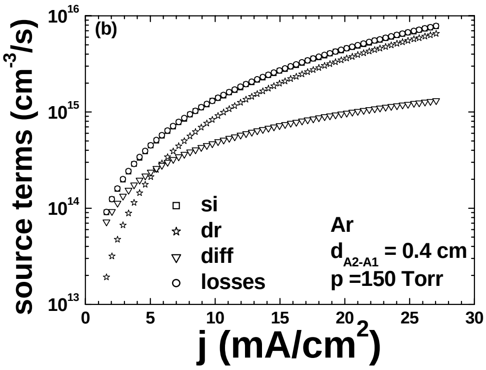


Fig. 1 Source/loss terms (for the electrons) corresponding to the loss due to diffusion (diffne), due to dissociative recombination (dr) and the gain by two-step ionization (si).

Another important result is shown in Figure 2. It represents the dependence of Θ, the power absorbed on average by an electron in the plasma volume, as a function of $p\times\Lambda$ (pressure times diffusion length). We clearly see that when the parameter $p\times\Lambda$ increases, the value of Θ increases as well. This is expected because the atomic to molecular ion conversion frequency increases with the square of the pressure, and the molecular ions recombine much more rapidly than atomic ions.

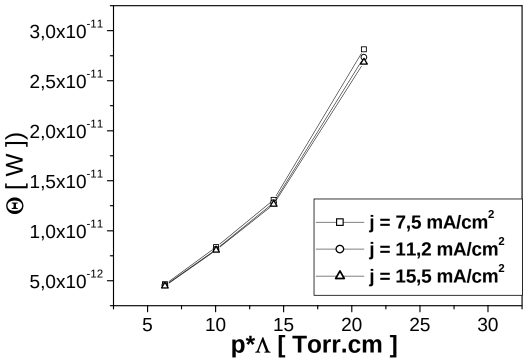


Fig. 2 Power used to maintain an electron as a function of the pressure times the diffusion length, for various current densities.

Further calculations are underway in Ar-O_2 mixtures where we are particularly interested in predicting the densities of the metastable $O_2(^1\Delta)$ number density in the context of the electric discharge pumped O_2/I_2 laser [3].

Reference

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