Modeling in Ar/H_2 discharge

Ž. Nikitović , V. Stojanović and Z. Lj. Petrović

Institute of Physics, University of Belgrade, POB 68, 11080 Belgrade, Serbia
zeljka@ipb.ac.rs

In this work we present transport coefficients for electrons in Ar/H_2 mixtures for the conditions used in plasma assisted technologies for semiconductor production i.e. in moderate and very high *E/N*. We used a two term numerical solution of Boltzman equation at lowest *E/N* and mean energies and Monte Carlo simulation technique at moderate and high *E/N*. We show that a good agreement with experimental data exists for low and moderate *E/N* and that based on the tests for pure H_2 and Ar we can model properly the high *E/N* development. Results are in abundances of H_2 from 1% to 30%, which are necessary in kinetic models for this mixture.

Argon is a typpical buffer gas in a number of technologies. It allows control of electron temperature (mean energy may be quite high and one may support the selected processes with high threshold. Mixtures with hydrogen in rf plasmas may be useful for ashing of photoresists in microelectronic processing but may be used in a broader range of procedures.

In this paper we study the kinetics of electrons in *E/N* by using Monte Carlo simulations that have been well tested for similar discharges in [Ar, H_2 and N_2]. As electrons have a special role in plasmas and in high *E/N* discharges we focus on them leaving out heavy particle collisions which will be dealt with separately. Another motivation is to provide the transport data for the electrons in the mixtures of Ar and H_2 for modeling of such plasmas and also to point out the need to employ a more detailed kinetic modeling in sheath regions. These results can be used as the basis for modeling of anomalously broadened Doppler profiles which are particulary pronounced in Ar-H_2 mixture [1], fast neutral plasma etchers for organic dielectrics and the whole range of plasma ashing/cleaning devices.

The MC code used in our analysis is based on the null collisions method, applied to model stationary Townsend discharge and it consists of four codes. The first follows the motion of electrons from the cathode the other one follows the motion of ions created in collisions of electrons and atoms of the gas the third follows the motion of electrons created by the ions. By analyzing all three parts it is possible to get the space distribution of the emission and the excitation coefficients [2]. The fourth MC code is used to follow the electrons reflected from the surface and the secondary electrons created at the surface. This code is completely independent from the code for simulation of the electrons from the cathode, and it can be included but also excluded from the simulation. In this paper we have used data for the steel and graphite electrodes [3].

For a limited range of calculations in this paper we have used a two term computer code ELENDIF [4] to solve Boltzmann's equation. This is in fact the finite difference method which allows for such a formulation of the Boltzmann equation in which many processes as well as the time evolution of the distribution function can be included. The code has limitations due to inherent approximations, but they are well known and have been studied [5, 6]. The two term code has been used to extend calculations to low *E/N* where two term theory is valid and also to give indication of the failure of the two term theory as it is used often without testing it in plasma modeling. For non-equilibrium (non-local) conditions this code is not applicable.

We use the argon cross sections from our calculations for argon electron (and ion) swarms [2]. For hydrogen we use the data defined in the data base of Phelps [1]. Both sets are based on accurate low energy cross sections that were tested aginst the best swarm data at low *E/N* and have been tested against the emission profiles at high *E/N* and energy distribution functions. Thus there is no reason to question application of such set for the mixture of two gases.

Figure 1 shows electron drift velocity in the mixture Ar/H_2 as a function of *E /N*. Even a smallest addition of H_2 completely changes the shape of the drift velocity and induces effect of negative differential conductivity. The range of negative differential conductivity is however reduced by a further increase of hydrogen concentration and is eventually lost beyond 15% of added hydrogen. In drift velocity curves we have also used a Two Term theory (TTT) to calculate the drift velocity at lower energies where Monte Carlo simulation becomes inefficient (in higher H_2 abundance lower

energies extend to higher *E/N*). Agreement with experimental results of Engelhardt and Phelps [7] (EXP) confirms that a well-chosen set of sections is used to describe the behavior of electrons in Ar/H_2 mixtures.

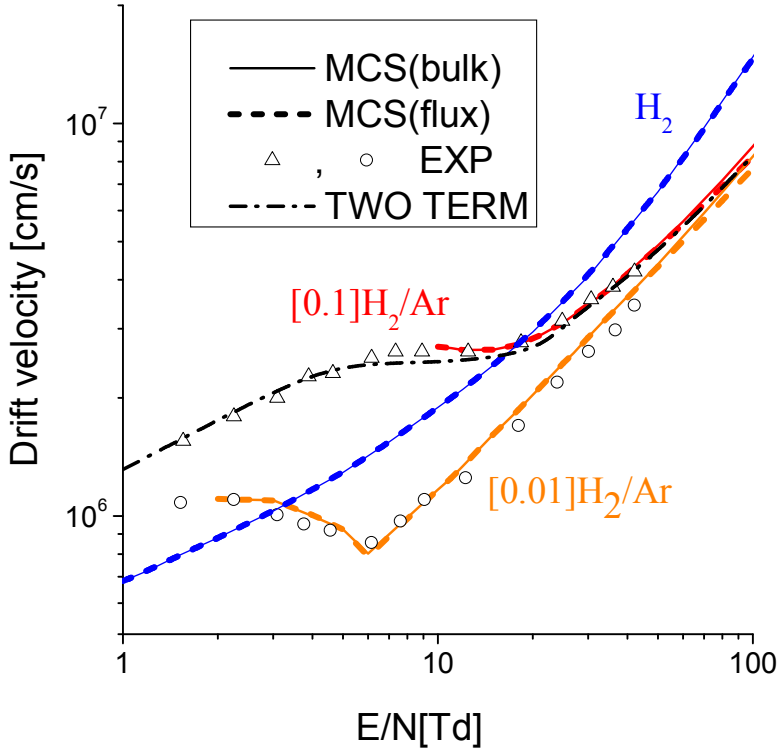

Fig. 1: Electron drift velocity for the mixture of Ar and H_2.

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