# ELECTRON DETACHMENT OF H-IONS IN HYDROGEN DISCHARGE

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**Abstract.** We present results of Monte Carlo simulation (MCS) for detachment rate coefficient for  $H^-$  ions in  $H_2$  and for modeling of spatiall dependence of apparent detachment excitation coefficient at very high E/N in a Townsend discharge.

## 1. INTRODUCTION

 $\rm H^-$  transport in discharges has an important role in plasma physics, ionospheric and flame chemistry and astrophysics. The transport is strongly affected by the large detachment cross section in the energy range of interest for those applications.

Negative ions in hydrogen discharges have been of particular interest as a source of ion beams that are to be neutralized to produce fast neutral beams that may be used for heating in fusion devices. However, hydrogen discharges have become interesting recently also for the etching of organic low-k dielectrics (Nagai et al. 2002) and possible conversion of negative ions to fast neutrals may be the origin of charging free plasma etching procedure for organic dielectrics. The mixtures containing H<sub>2</sub> are widely utilized as a working gas in different glow discharges for spectroanalytical sources, laser media, etc.

Goal of the present work is to model H<sup>-</sup> transport in Townsend discharges in H<sub>2</sub> when the main source of H<sup>-</sup> ion is not dissociative electron attachment (DEA) but heavy particle collisions. One may expect such situations at very high E/N where heavy particle excitation becomes dominant and mean electron energies are considerably larger than DEA threshold.

### 2. MONTE CARLO SIMULATION

Calculations were performed by using our Monte Carlo technique for electron transport that has been verified against all relevant swarm benchmarks (Raspopović et al. 2000, Petrović and Stojanović 1998). We followed between  $10^6 - 10^7$  electrons with the initial energy of 1 eV. Gas number density was  $3.54 \ 10^{22} \ m^{-3}$ . Nonequilibrium conditions for H<sup>-</sup> transport were selected from experimental results of (Petrović et al. 1992).



Figure 1: Cross section set for scattering  $H^-$  ions on  $H_2$  [3].

We assumed that negative ions are produced in fast H collisions with  $H_2$  according to probability given by Phelps (Phelps 1990) and assuming that  $H^-$  after collision is moving in the same direction as that of fast H before collision with  $H_2$ . Townsend discharge model at very high E/N based on heavy particles excitation is used (Phelps 2006) to calculate fluxes of  $H^-$  ions and production of electrons by electron detachment.  $H^-$  production was obtained by introducing cross section for  $H^-$  production. We also accounted for surface interaction of  $H^-$  ions in the same way as for  $H^+$  neutralization and reflection at the cathode surface (Stojanović et al. 2007). Note that according to the present model, the anode surface is not reflective for fast H and fast  $H_2$ . Approximately 60 % of  $H^-$  ions are reflected as fast H at the anode surface.

There is a large number of theoretical and experimental cross sections for  $H^-$  ions in  $H_2$ . The cross sections for  $H^-$  in  $H_2$  that have been evaluated and tested have been proposed in the review article of Phelps (1990). That cross section set frpm (Fig. 1) is used in our calculations.

#### 3. RESULTS

In Fig. 2 we show results for drift velocity obtained by Monte Carlo simulation. Splitting of flux and bulk values is a consequence of electron detachment which is one example of nonconservative collisions. Rate coefficients are calculated as a number of collisions per observation time divided by a number of electrons and gas density. In Fig. 3a) we show total rate coefficient and detachment rate coefficient as a function of E/N. Spatial excitation coefficient can be obtained by dividing rate coefficient with drift velocity of ion.



Figure 2: a) Drift velocity, b) Rate coefficient for  $H^-$  negative ion in pure  $H_2$  discharge.



Figure 3: a) Flux of H<sup>-</sup> ions in interelectrode space. b) Apparent detachment coefficient for H<sup>-</sup> ions in H<sub>2</sub>. E/N = 10 kTd, p = 145 mTorr.

At very high E/N between two plan-parallel plates H<sup>-</sup> ions exhibit non-equilibrium behavior similar to the positive ions (Stojanović et al. 2007). In order to calculate flux of negative ions we sum velocities whenever particle crossed a membrane (Stojanović and Petrović 1998) assuming positive ion fluxes towards cathode. Spatial dependent flux of H<sup>-</sup> ion is shown in Fig. 3.a). Maximum flux intensity is obtained in the middle between electrodes while fluxes of opposite sign were obtained close to the cathode and anode. Positive flux close to the cathode is a result of significant production of H<sup>-</sup> ions by the fast H neutrals. In the direction of the anode strong detachment rate is reducing intensity of H<sup>-</sup> flux. High energy H<sup>-</sup> ions are efficiently removed from the H<sup>-</sup> beam towards anode. One has to be aware that presented H<sup>-</sup> flux consist of two components, one due to the large flux of fast H in the direction of cathode and other due to the acceleration of H<sup>-</sup> ions in the direction of the anode.

Apparent detachment coefficient for  $H^-$  ions in  $H_2$  is shown in Fig. 3.b). Intensity is placed on the absolute scale by using normalization to the  $H^-$  detachment excitation coefficient at the anode (see Stojanović and Petrović 1998).

Total yield of secondary electrons produced in  $H^-$  collisions with  $H_2$  is proportional to detachment cross section so one may expect that maximum electron production due to the  $H^-$  detachment on  $H_2$  is close to the cathode.

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