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Part A

DISTRIBUTIONS OF H^+, H_2^+ AND H_3^+ IONS IN TOWNSEND DISCHARGE AND DETERMINATION OF THEIR COLLISION CROSS SECTIONS

J. Bretagne, T. Šimko*, G. Gousset
Laboratoire de Physique des Gaz et des Plasmas (UA CNRS),
Université Paris-Sud, 91405 Orsay Cedex, France

M. V. V. S. Rao, R. J. Van Brunt, Y. Wang, J. K. Olthoff
National Institute of Standards and Technology, Gaithersburg, MD 20899, USA

B. L. Peko, R. L. Champion
Department of Physics, College of William & Mary, Williamsburg, VA 23187, USA

Introduction

Experimental and theoretical investigations of hydrogen discharges are complicated by coexistence of three dominant ionic species (H^+, H_2^+ and H_3^+) and their mutual interconversion by collisions with neutral gas molecules. A recent cross-section set for collisions of H_n^+ ions ($n = 1, 2, 3$) with H_2 based on extrapolations to low energies [1] is highly uncertain, especially for H_3^+/H_2 with moderate collision energies (10 to 1000 eV), and this uncertainty can be reflected in predicted ion-energy distributions.

In this work, an attempt is made to deduce a consistent set of H_n^+/H_2 cross sections by comparing experimental and theoretical investigations of ion-energy distributions and fluxes in low-pressure Townsend discharges.

Experimental

The cross sections for destruction of vibrationally cool H_3^+ ions of energies from 15 to 400 eV have been measured by Peko *et al* using an ion-beam technique with an electrostatic trap [2]. These results which indicate a much higher total H_3^+ destruction cross section when compared to [1], are used in the model calculations discussed here.

Measurements of flux-energy distribution functions of H_n^+ ions striking the cathode in a plane-parallel Townsend discharge have been performed by the NIST group in an experimental setup similar to [3]. Typical operating parameters were: room-temperature, gas pressure ranging from 40.0 Pa to 93.3 Pa, interelectrode gap from 1 to 3 cm, and reduced electric field E/N from 0.5 to 20 kTd (1 Td $\equiv 10^{-21}$ Vm^2).

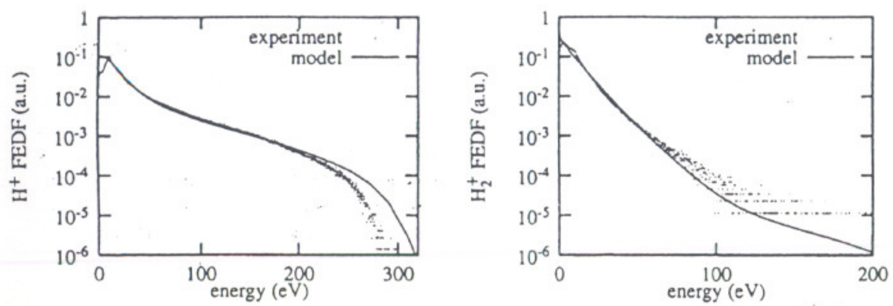
Simulation

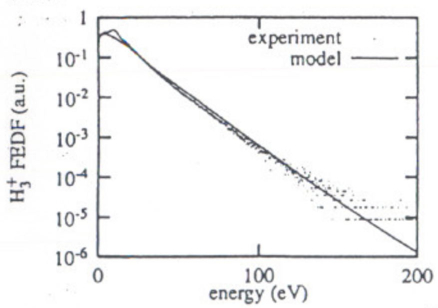
Flux-energy distribution functions (FEDFs) at the cathode were simulated by Orsay group using a 1D Convective Scheme model [4]. The possible shortcomings of 1D simulation approach were studied by ion Monte Carlo simulation. For E/N less than 600 Td, this approach was also used [5], to determine transport coefficients and to adjust elastic cross sections.

The H_n^+/H_2 cross-section set is primarily that given in [1] except for H_3^+/H_2 destruction cross sections as mentioned above. Possible influence of internal vibrational energy of H_3^+ ions has been accounted for by multiplying corresponding cross sections by factors of about 2. Inelastic H^+/H_2 collisions were treated as anisotropic with an empirically chosen angular dependence.

Results

As an illustration of the results, Fig. 1 shows the comparison of experimental and calculated FEDFs for 1 kTd Townsend discharge. Fairly good agreement was found for E/N values up to about 2 kTd (Fig. 1). The situation is worse for E/N values above 5 kTd, for which additional experimental and theoretical work is needed. Fig. 2 shows the relative contribution of the three ionic species to the total ion flux at the cathode over the whole range of E/N. Increasing role of H_2^+ species at high E/N results from rapid breakup of high-energy H_3^+ ions mainly into energetic H^+ ions that are efficiently converted to H_2^+ through charge transfer.





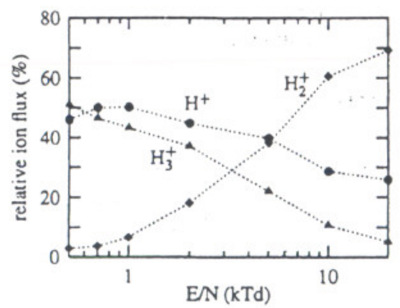


Figure 1. Flux-energy distribution functions of H^+, H_2^+ and H_3^+ at the cathode for $E/N = 1$ kTd, 62 Pa and 2 cm gap space.

Figure 2. Relative contributions of ionic species to the total ion flux as a function of E/N. Experimental results (1 Td $\equiv 10^{-21}$ Vm^2).

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*Permanent address: Dept. of Plasma Physics, Comenius University, Mlýnská dolina F2, 84215 Bratislava, Slovakia