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Measurement and Modeling of Molecular Ion Concentrations in a Hydrogen Reflex-arc Discharge

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The production of the molecular hydrogen ions H_2^+ and H_3^+ is expected to play an important role in a wide variety of plasmas, such as planetary ionospheres [1], neutral beam sources [2], and the edge and divertor regions of magnetic fusion devices [3]. Many of the collision rate coefficients relevant for H_2^+ and H_3^+ creation and destruction have been calculated (*e.g.* Ref [4]); however, there has been little experimental validation for many of these calculations. Here, equilibrium molecular ion concentrations are measured under typical hydrogen gas discharge conditions ($N_e \approx 10^{11}$-10^{12} cm^{-3}, $N_{H2} \approx 10^{13}$-10^{15} cm^{-3}, $T_e \approx 2 - 10$ eV). Over this parameter range, the molecular ion concentration is found to vary between 0.1 and 1. The observed concentrations can be modeled reasonably well (typically within about 25%) using currently available rate coefficients, provided that the molecular hydrogen vibrational temperature T_{vib} is included. Neglecting T_{vib} typically results in the equilibrium molecular ion concentration being underestimated by a factor of 2 – 5.

A schematic of the University of California, San Diego PISCES-A reflex-arc discharge is shown in Fig. 1. The experimental apparatus has been described previously [5]. The dominantly H^+ plasma created in the source region passes through a floating copper baffle tube before entering the target chamber. This baffling allows the target pressure region pressure to be varied over the range $P_{target} \approx 0.5 - 30$

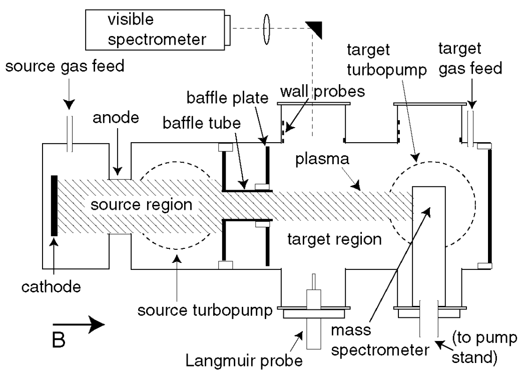

Fig. 1. Layout of experiment showing source region, target region, and principal diagnostics

mTorr while maintaining constant source conditions (typically, $P_{source} \approx 2$ mTorr). Hydrogen is used as a working gas in both source and target regions.

The main diagnostics used in these experiments are a reciprocating radially-scanning Langmuir probe, fixed wall probes, a visible spectrometer, and an omegatron-type mass spectrometer. The reciprocating probe is used to obtain the electron density N_e, while the visible spectrometer, together with N_e, is used to obtain the electron temperature T_e (from the measured Hα intensity). Also, visible spectroscopy can be used to estimate the H_2 vibrational and rotation temperatures T_{vib} and T_{rot} [6,7]. The molecular ion concentrations are measured using the mass spectrometer [8]. The neutral hydrogen molecule density N_{H2} is obtained from the measured neutral gas pressure (assuming T_{H2} = 300 K since the neutral-ion mean free path is longer than the plasma dimensions). The mean ion lifetime is obtained from the axial flux to the mass spectrometer plus the radial flux measured using the wall probes [9].

To model the ion concentrations in this experiment, a zero-dimensional model is developed for solving the system of rate balance equations for ion and gas species. The model solves for the 5 unknowns (the three ion densities, the atomic hydrogen density, and the H^+ inflow rate) given measured values of N_{H2}, N_e, T_e, T_{vib}, and the ion lifetime τ_i. The atomic and molecular processes believed to be important for molecular hydrogen ion production and destruction have been discussed previously [10,11]. Vibrationally-resolved rate coefficients are used for H_2^+ and H_2, but are not available for H_3^+. The vibrational temperature of H_2^+ is assumed to be half of that measured for H_2, because of the factor 2 increase in vibrational constant. For the purposes of calculating velocity averages $\langle \sigma v \rangle$, the neutral velocities are assumed to be negligible compared with the ion and electron velocities. The ion temperatures are taken to be $T_j = T_e^{0.9}$, as this is found to provide a reasonably good smooth fit to the measured temperatures. To include atomic hydrogen H in the model, we assume a probability of 0.9 for an H atom to be reflected from the wall [12].

The variation of measured relative ion concentrations is plotted as a function of neutral density N_{H2} in Fig. 2 for plasmas with $T_e \approx 2.6$ eV, $N_e \approx 1.3\times10^{11}$cm^{-3}, and $\tau_i \approx 40$ μs. Not shown in Fig. 2 is the measured vibrational temperature,

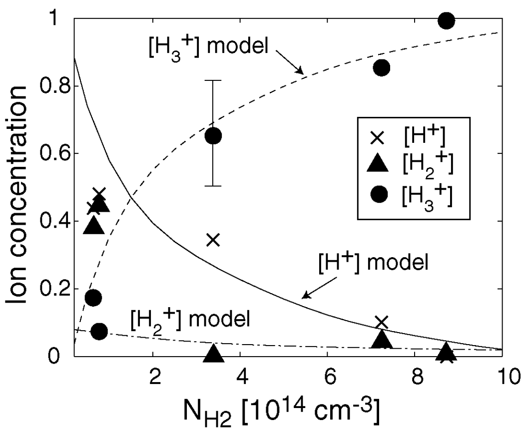

Fig. 2. Measured relative ion concentrations as a function of neutral density N_{H2} for plasmas with electron temperature T_e = 2.6 eV, electron density $N_e = 1.3\times10^{11}$ cm^{-3}, ion confinement time τ_i = 40 µs, and vibrational temperatures T_{vib} = 3000 – 5000 K.

which is found to drop smoothly from about 5000 K to about 3000 K as a function of increasing N_{H2}. A line fit through the T_{vib} data is used to create the smooth model curves shown in Fig. 2.

The variation of the measured and predicted ion concentrations with electron density is shown in Fig. 3 for plasmas with $T_e \approx 2.5$ eV, $N_{H2} \approx 4\times10^{14}$cm^{-3}, and $\tau_i \approx 70$ µs. As before, a linear fit to the T_{vib} measurements is used to create the model curves. In this case, we observe a T_{vib} which varies between 3500 and 4000 K.

These measurements demonstrate that inclusion of the vibrational temperature T_{vib} is important for accurate modeling of hydrogen molecular ion production. Modeling of the vibrational excitation of H_2 in these plasmas is thus a logical extension of this work. There is also good evidence that H_2 rotational excitation can affect relevant reaction rates [13,14], so inclusion of rotational temperature into the model is another important goal. To qualitatively illustrate the significant degree to which vibrational and rotational temperature can change in these experiments, the observed T_{vib} and T_{rot} are plotted as a function of electron pressure $P_e = N_eT_e$ in Fig. 4.

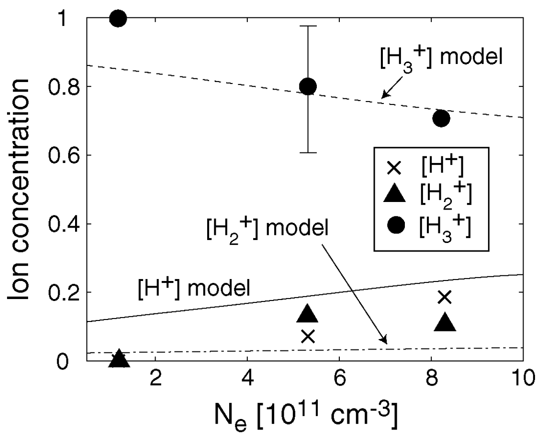

Fig. 3. Measured relative ion concentrations as a function of electron density N_e for plasmas with electron temperature T_e = 2.5 eV, neutral density $N_{H2} = 4\times10^{14}$ cm^{-3}, ion confinement time τ_i = 70 µs, and vibrational temperatures T_{vib} = 3500 – 4000 K

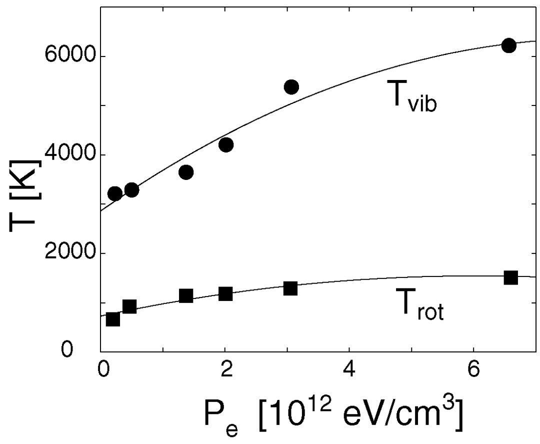

Fig. 4. Measured vibrational and rotational temperatures as a function of electron pressure P_e for plasmas with $N_{H2} = 4\times10^{14}$ cm^{-3}.

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