Low pressure hydrogen discharges diluted with argon

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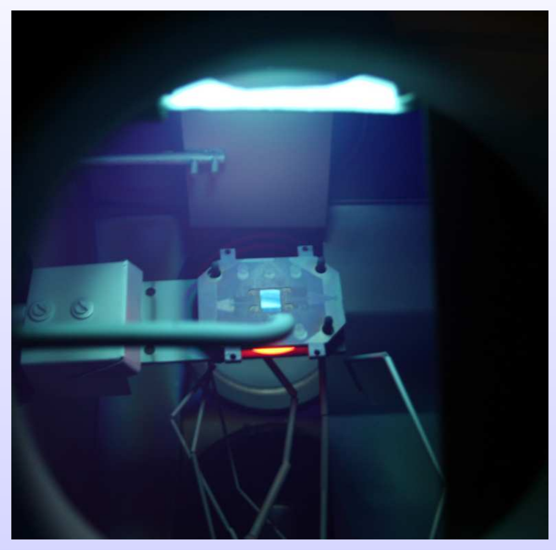

Introduction

- A global (volume averaged) model is applied to study a low pressure (1 - 100 mTorr) high density H_2/Ar discharge in the steady state.
- Based on a previous model of the Cl_2/Ar discharge (Thorsteinsson and Gudmundsson, 2010)

The global (volume averaged) model

- In addition to electrons the discharge consists of ground state atoms (H, Ar), molecules (H_2), positive ions (H^+, H_2^+, H_3^+, Ar^+, ArH^+) negative ions (H^-), vibrationally excited molecules ($H_2(v = 1-14)$), electronically excited atoms (Ar(4p)), metastables (Ar^m ($1s_5$ and $1s_3$)) and radiatively coupled states (Ar^r ($1s_4$ and $1s_2$)).
- Electrons are assumed to have a Maxwellian energy distribution in the range 1 – 10 V.
- The collisional energy loss per electron-ion pair created is defined as

$$\mathcal{E}_c = \mathcal{E}_{iz} + \sum_i \mathcal{E}_{ex,i}\frac{k_{ex,i}}{k_{iz}} + \frac{k_{el}}{k_{iz}}\frac{3m_e}{m_i}T_e \quad (1)$$

where $\mathcal{E}_{iz}$ is the ionization energy, $\mathcal{E}_{ex,i}$ is the threshold energy and $k_{ex,i}$ is the rate coefficient for the i-th excitation process and k_{iz} is the ionization rate coefficient for single step ionization.

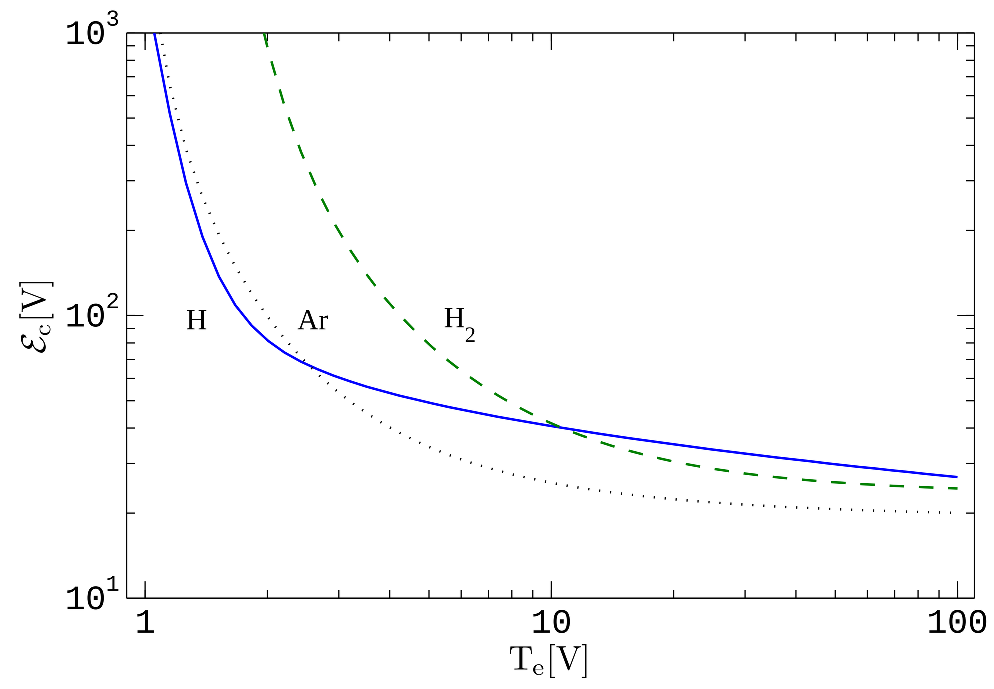

Figure 1: The calculated collisional energy loss $\mathcal{E}_c$ per electron-ion pair created as a function of the electron temperature T_e for atomic and molecular hydrogen and the argon atom.

Results and discussion

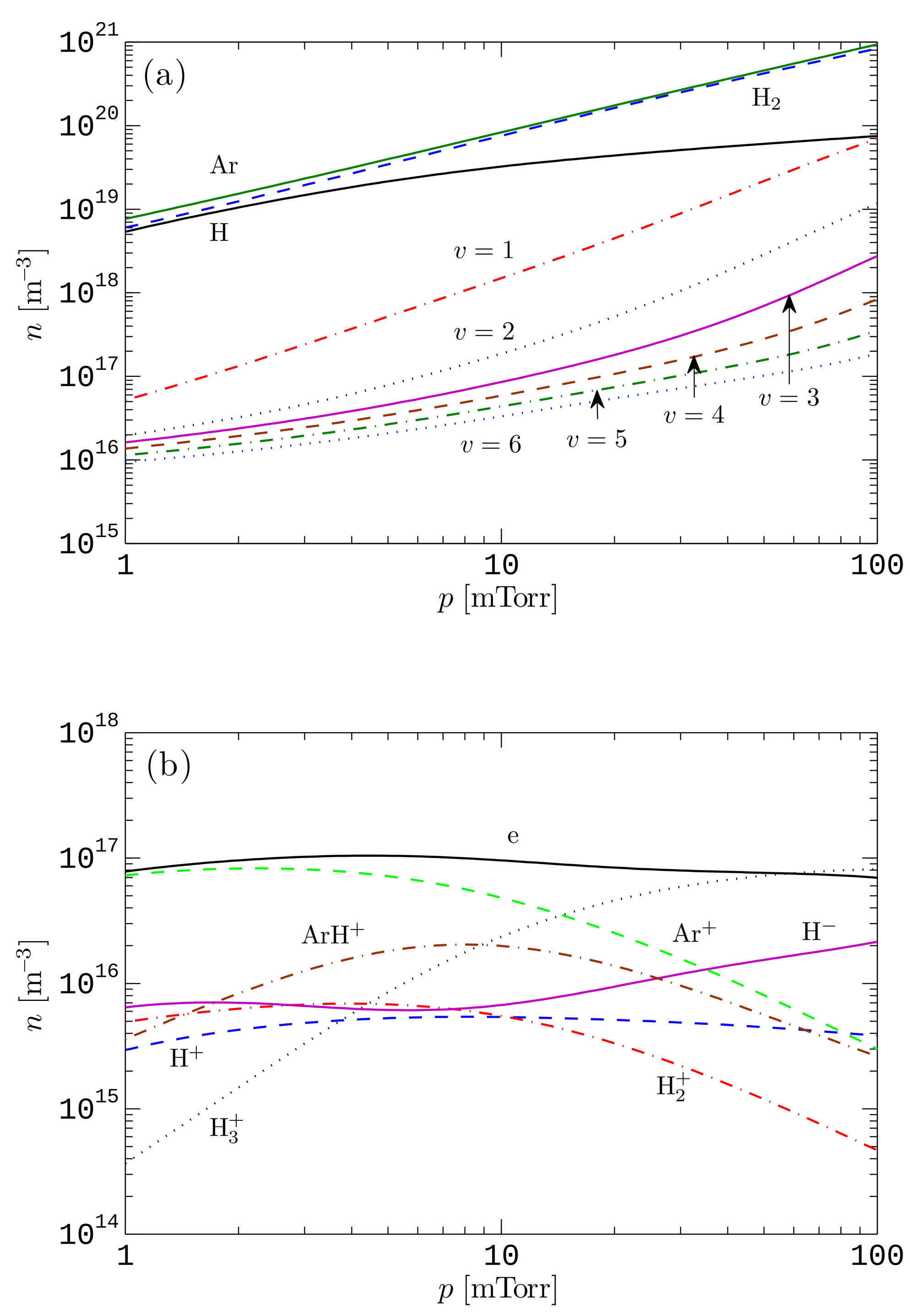

Figure 2: The (a) neutral particle densities and (b) the charged particle densitiesversus pressure at R = 15.24 cm, L = 7.62 cm, Q = 50 sccm, P_{abs} = 600 W, T_g = 500 K and 50% Ar dilution.

- The surface recombination coefficient for atomic hydrogen is assumed to be 0.023 (Curley et al., 2010) and the gas temperature is assumed to be T_g = 500 K.
- The atomic and molecular hydrogen densities are similar at 1 mTorr, but at 100 mTorr the atomic density is an order of magnitude lower.
- The $[H_2(v > 0)]/[H_2(v = 0)]$ ratio increases from 0.026 to 0.1 when the pressure is increased from 1 to 100 mTorr.
- The density of H^- is relatively small over most of the pressure range of interest but increases with increasing discharge pressure.
- Ar^+ is the dominant positive ion in the discharge for pressures below 14 mTorr, for higher pressure H_3^+ becomes the dominant positive ion.
- For very low pressures (p < 2 mTorr) there is a significantly higher density of H_2^+ and H^+ ions than the H_3^+ ion. The density of H_3^+ ions increases with increased pressure.
  The density of ArH^+ increases with pressure at first, peaking at roughly 8 mTorr but then it decreases again with increasing pressure.

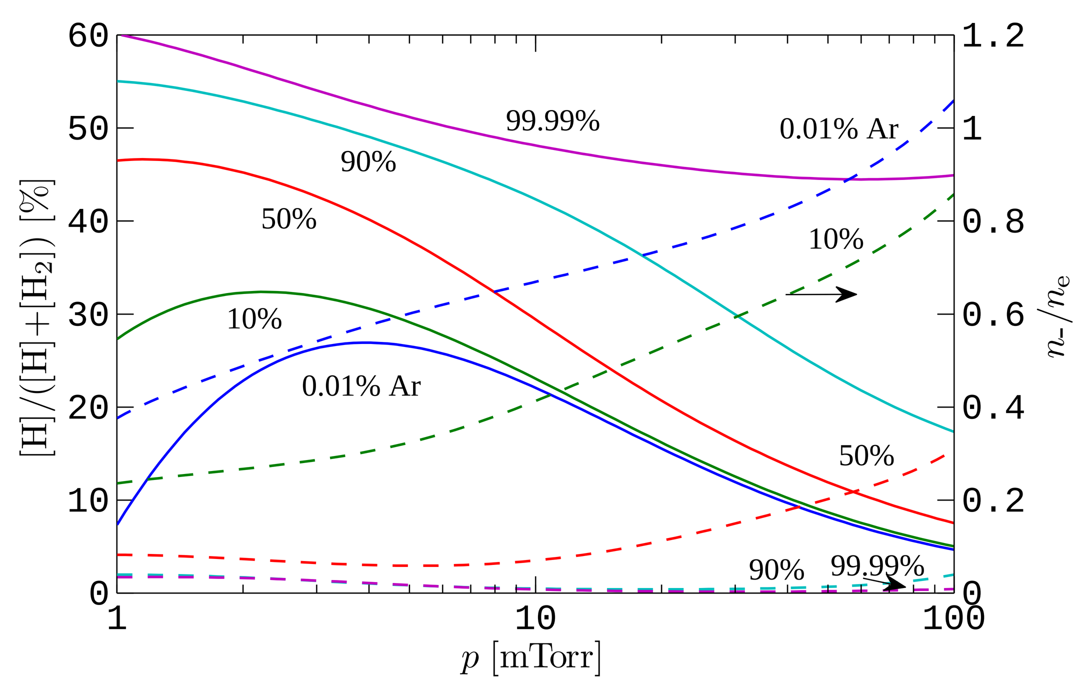

Figure 3: The dissociation fraction (solid lines) and electronegativity (dashed lines) versus pressure at R = 15.24 cm, L = 7.62 cm, Q = 50 sccm, T_g = 500 K and P_{abs} = 600 W..

- The dissociation fraction increases as the argon content increases.
- The electronegativity is low and decreases with increased argon content but increases with increased discharge pressure. It is at a maximum of 1.06 in a pure hydrogen discharge at 100 mTorr.
- It is well known that the dissociative attachment of hydrogen molecules is important in creating negative ions, in particular from the higher vibrational levels of the H_2 molecule.

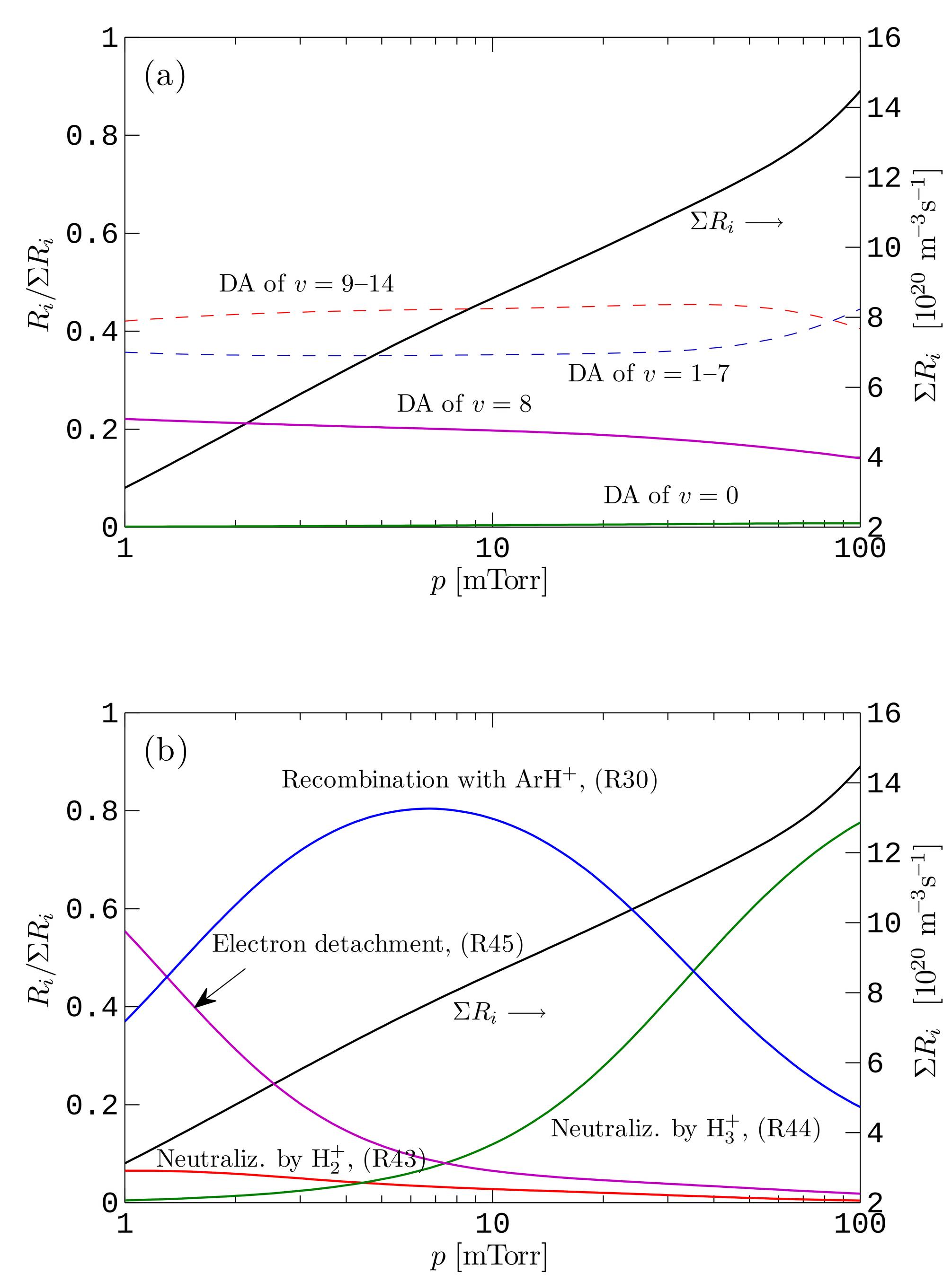

Figure 4: The absolute and relative reaction rates for (a) creation and (b) loss of H^- versus pressure at R = 15.24 cm, L = 7.62 cm, Q = 50 sccm, T_g = 500 K, P_{abs} = 600 W and 50% argon dilution.

- The cross section for dissociative attachment increases significantly when the molecule is vibrationally excited and the threshold decreases.
- Dissociative attachment of the v=8 vibrationally excited molecule is generally the most dominant individual contributor to the creation of H^- with 22% contribution at 1 mTorr.
- Dissociative attachment of $H_2(v = 7)$ and $H_2(v = 9)$ are also effective, contributing around 18% and 14%, respectively.
- The ion-ion recombination reaction

$$H^- + ArH^+ \longrightarrow H_2 + Ar \quad (R30)$$

dominates the loss of H^- in the pressure range 1–36 mTorr, reaching 80% contribution at roughly 7 mTorr.

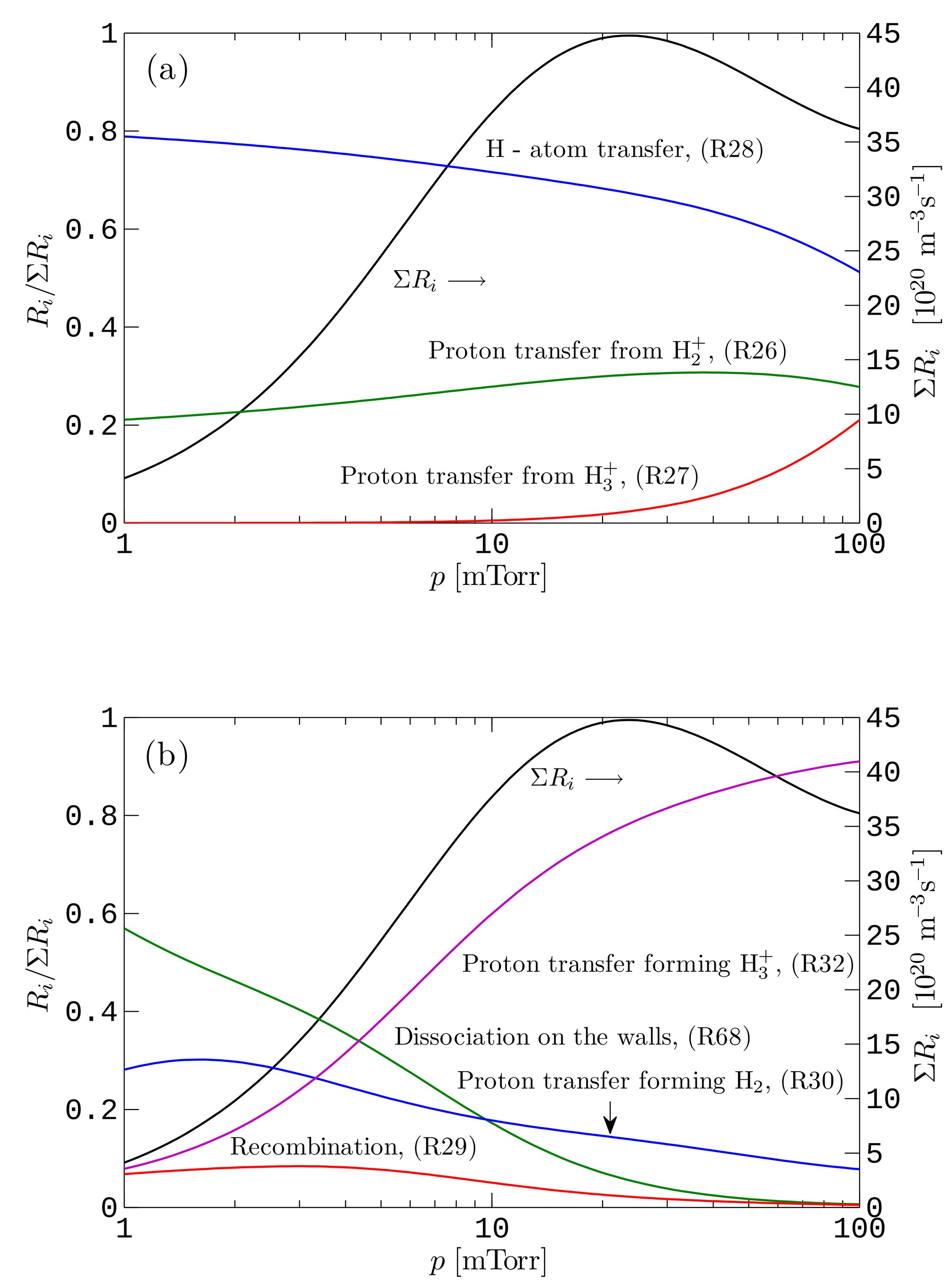

Figure 5: The absolute and relative reaction rates for (a) creation and (b) loss of ArH^+ versus pressure at R = 15.24 cm, L = 7.62 cm, Q = 50 sccm, T_g = 500 K, P_{abs} = 600 W and 50% argon dilution.

- The atom transfer reaction

$$H_2 + Ar^+ \longrightarrow H + ArH^+ \quad (R28)$$

is most effective in the creation of ArH^+ at all pressures, having almost 80% contribution at best at 1 mTorr.
- Dissociation on the walls and the proton transfer reaction

$$H_2 + ArH^+ \longrightarrow H_3^+ + Ar \quad (R32)$$

are the main contributors to the loss of ArH^+.

Conclusions

- The effects of dissociative attachment on the creation of the negative ion H^- resulting from vibrationally excited states were explored, showing that dissociative attachment from the v = {7–9} states contributes the most to the creation of H^- or about 50%.
- The contribution of the electron impact singlet excitation followed by a radiative decay to a vibrationally excited state is the most significant in the creation of the H^- ion and the role of the direct electron impact vibrational excitation is negligible in comparison.
- The density of the ArH^+ is large, in particular in the pressure range 2–30 mTorr, and it plays a crucial role in the destruction of the H^- ion in this pressure range.

Acknowledgments

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References

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