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 - 10 mTorr) high density H₂/Ar discharge in the steady state.
• Based on a previous model of the H₂/Ar discharge (Thorsteinsson and Gudmundsson, 2009).

The global (volume averaged) model

• In addition to electrons the discharge consists of ground state atoms (H, Ar), molecules (H₂), positive ions (H⁺, H₂⁺, Ar⁺, ArH⁺) negative ions (R⁻), vibrationally excited molecules (H₂v (v = 1 - 14)), electronically excited atoms (Ar(4π), metastables (Ark, 1s)), radiatively coupled states (Ar¹(1s and 1s)) and radiatively coupled states (Ar²(1s and 1s)).
• Electrons are assumed to have a Maxwellian energy distribution in the range 1 - 10 eV.
• The collisional energy loss per electron-ion pair created is defined as

\[ \Delta E = \varepsilon_i + \sum_{j} \frac{k_{ij} m_j}{m_i} \delta_{ij} \delta_{ij} \]  

where \( \Delta E \) is the ionization energy, \( \varepsilon_i \) is the threshold energy and \( k_{ij} \) is the rate coefficient for the i-j excitation process and \( \delta_{ij} \) is the ionization rate coefficient for single-step ionization.

Results and discussion

• The surface recombinant 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 \( \frac{[H_2]}{[H]} \) 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.
• \( \lambda_h \) is the dominant positive ion in the discharge for pressures below 14 mTorr, for higher pressure \( \lambda_e \) becomes the dominant positive ion.
• For very low pressures (\( p < 2 \) mTorr) there is a significantly higher density of \( \lambda_e \) and \( \lambda_h \) than the \( \lambda_e \) ion. The density of \( \lambda_e \) ions increases with increasing pressure.
• The density of \( \lambda_h \) increases with pressure at first, peaking at roughly 9 mTorr but then it decreases again with increasing pressure.

Figure 1: The calculated collisional energy loss \( \Delta E \) per electron ion pair created as a function of the electron temperature \( T_e \) for atomic and molecular hydrogen and the argon atom.

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

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, \( T_e = 500 \) K and \( P_{inlet} = 600 \) 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 1.96 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 \( \lambda_h \) molecule.

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

• The atom transfer reaction

\[ \text{H} + \text{Ar} \rightarrow \text{H} + \text{Ar}^+ \]  

is most effective in the creation of \( \lambda_h \) at all pressures, having almost 80% contribution at best at 1 mTorr.
• Dissociation on the walls and the proton transfer reaction

\[ \text{H}_2 + \text{Ar} \rightarrow \text{H} + \text{Ar}^+ \]  

are the main contributors to the loss of \( \lambda_h \).

Conclusions

• The effects of dissociative attachment on the creation of the negative ion \( \lambda_h \) resulting from vibrationally excited states were explored, showing that dissociative attachment from the \( \text{H}_2 \rightarrow \lambda_h \) state contributes the most to the creation of \( \lambda_h \) with 10%.
• 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 \( \lambda_h \) ion and the role of the direct electron impact vibrational excitation is negligible in comparison.
• The density of the \( \lambda_h \) is large, in particular in the pressure range 2-30 mTorr, and it plays a crucial role in the destruction of the \( \lambda_h \) ion in this pressure range.

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References


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