On the reaction rates in the low pressure nitrogen discharge

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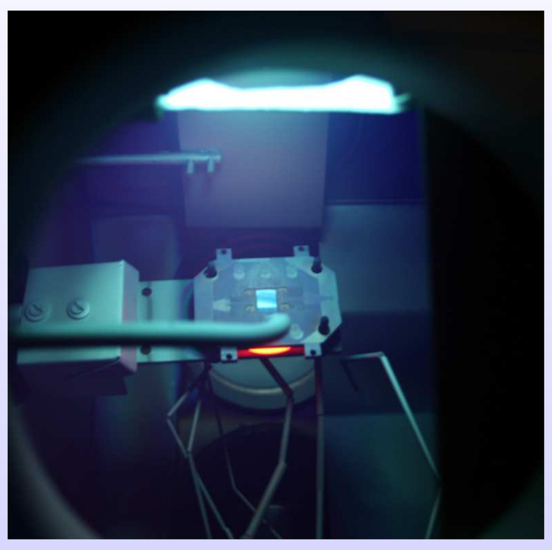

Introduction

- A global (volume averaged) model is applied to study a low pressure (1 - 100 mTorr) high density nitrogen discharge in the steady state.
- Based on a previous model of the O_2/Ar discharge (Gudmundsson and Thorsteinsson, 2007)

The global (volume averaged) model

- In addition to electrons the nitrogen discharge consists of molecular nitrogen in ground state $N_2(X^1\Sigma_g^+, v=0)$, vibrationally excited molecular nitrogen $N_2(X^1\Sigma_g^+, v=1-6)$, metastable molecular nitrogen $N_2(A^3\Sigma_u^+)$, atomic nitrogen in ground state $N(^4S)$, metastable atomic nitrogen $N(^2D)$ and $N(^2P)$, and the positive ions N^+, N_2^+, N_3^+ and N_4^+.
- A comprehensive reaction set has been developed that includes roughly 450 interactions of the discharge species.
- Electrons are assumed to have a Maxwellian-like energy distribution in the range 1 – 10 V.
- The collisional energy loss per electron-ion pair created is defined as

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

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.

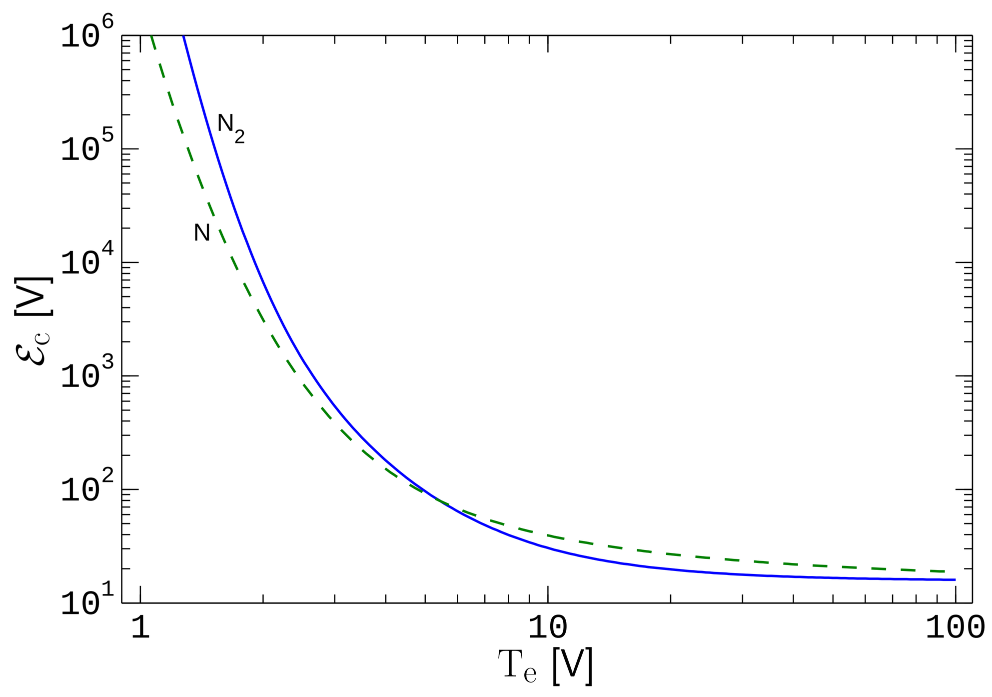

Figure 1: The collisional energy loss versus electron temperature for the ground state nitrogen molecule $N_2(X^1\Sigma_g^+, v=0)$ and the ground state nitrogen atom $N(^4S)$. The electron energy distribution is assumed to be Maxwellian-like.

Results and discussion

- The surface recombination coefficient for atomic nitrogen in assumed to be 0.07 (Singh et al., 2000a).
- The gas temperature is assumed to have a linear dependence on the absorbed power, $T_g = 0.17 \times P_{abs} + 387$ K.
- The density of neutral species versus pressure is shown in figure 2. The atomic density decreases above 10 mTorr whereas the molecular density increases monotonically with pressure.
- Vibrationally excited ground state molecules $N_2(X^1\Sigma_g^+, v>1)$ are important at intermediate and high pressure, but negligible at 1 mTorr.
- Density of charged species versus pressure is shown in figure 3(a). The density of N^+ is comparable to the N_2^+ density at 1 mTorr, but decreases rapidly with presssure above 10 mTorr.

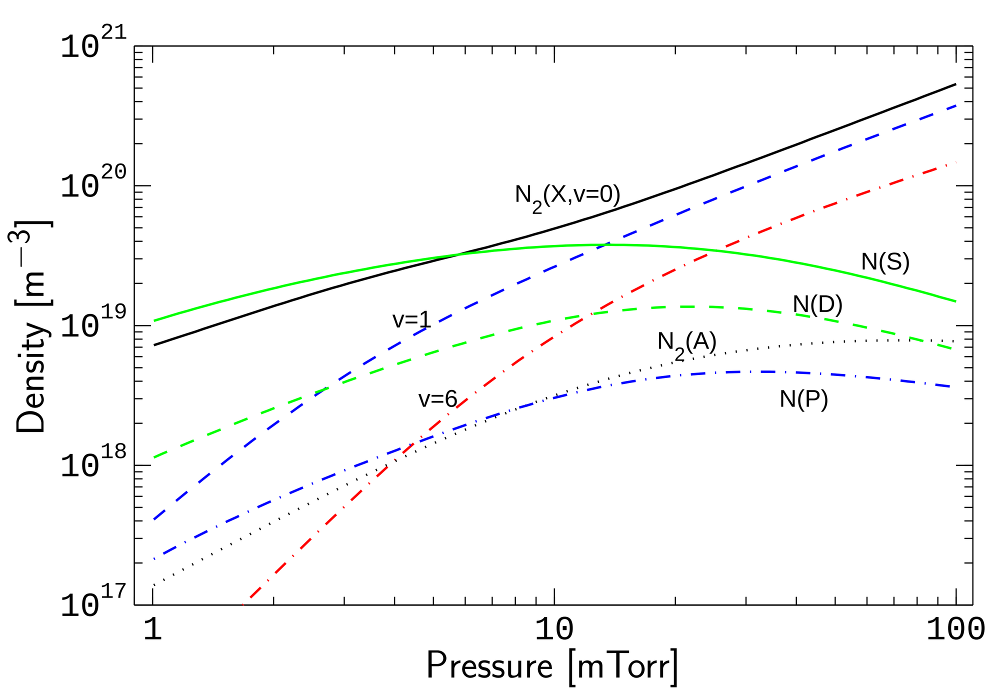

Figure 2: The density of neutral nitrogen species versus discharge pressure. The absorbed power is 500 W, the gas flowrate is 50 sccm and the chamber has the dimensions $R = 10$ cm and $L = 10$ cm.

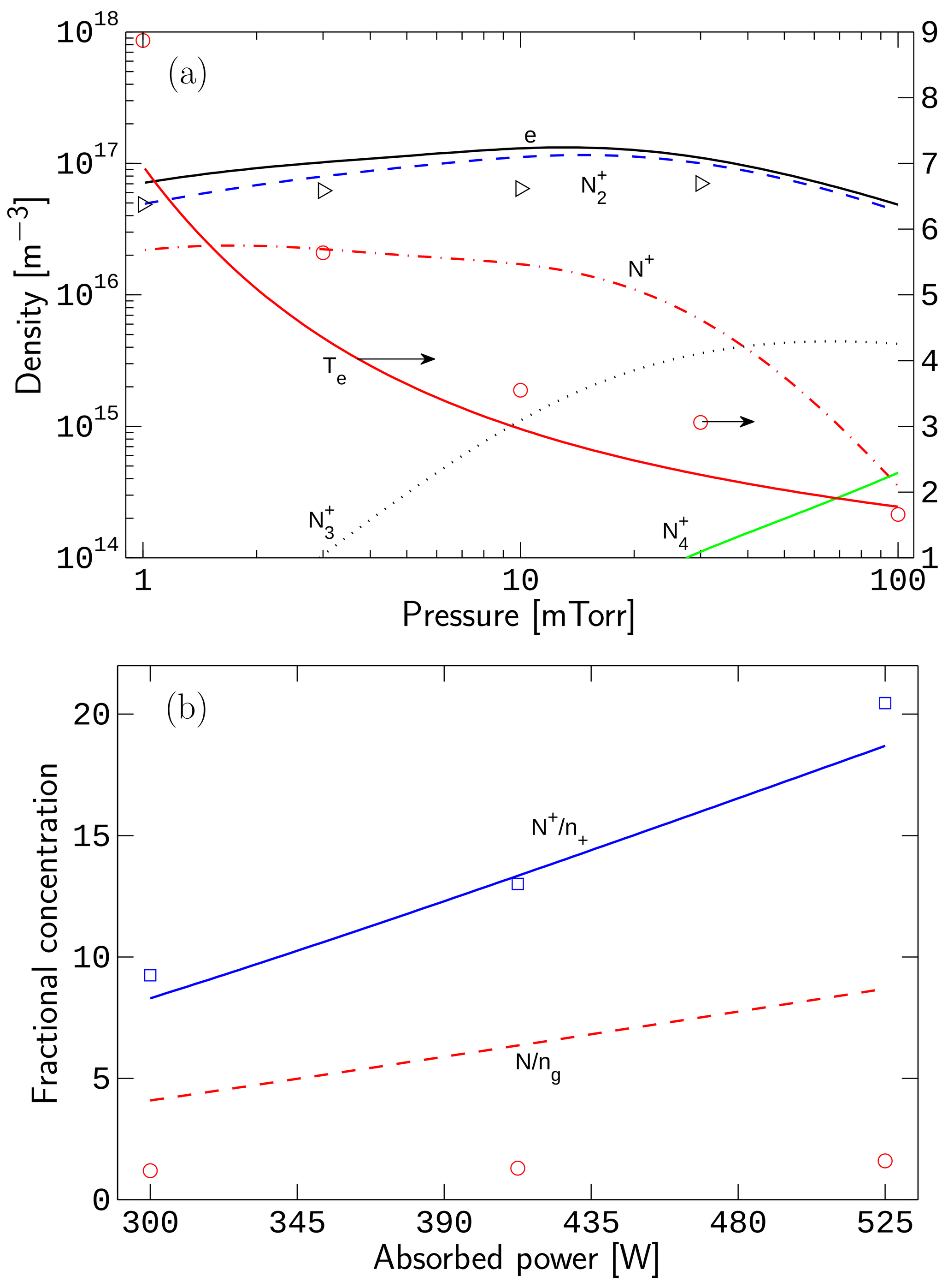

Figure 3: Comparison of the calculations with measurements. (a) ▷ the electron density and ○ the electron temperature measured by Singh and Graves (2000b) as a function of discharge pressure. The absorbed power is 240 W. (b) □ the fraction of the N^+ density versus the total ion density and ○ the fractional dissociation measured by Singh and Graves (2000c) as a function of absorbed power ($P_{abs} \simeq 0.75 \times P_{rf}$). The discharge pressure is 30 mTorr. Other conditions are as in figure 2.

- Relatively good agreement with measured electron temperature and electron density is shown in figure 3(a).
- The measured dissociation fraction is much lower than the calculated value despite the excellent agreement with the measured N^+ ion fraction.

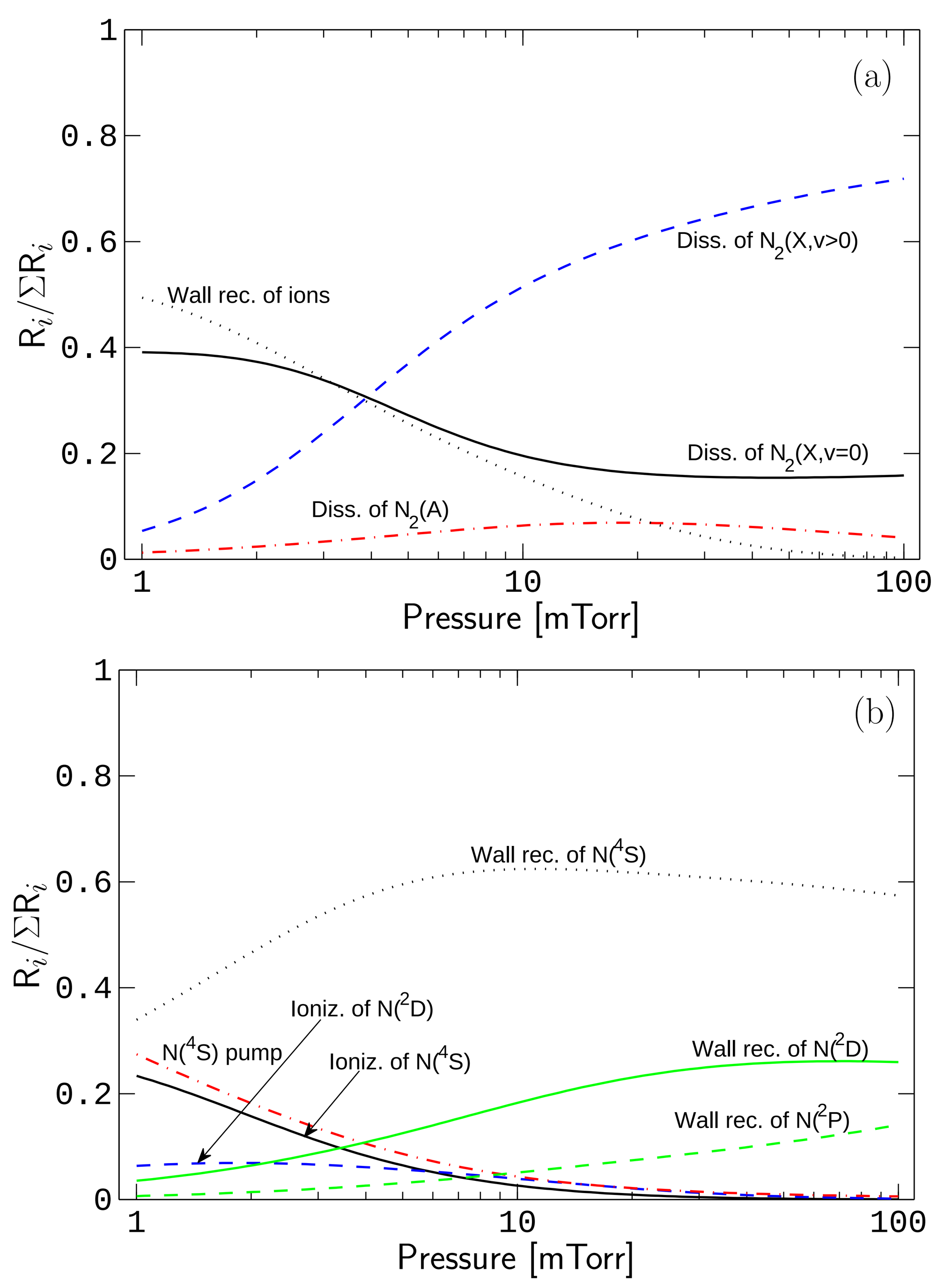

Figure 4: The reaction rates for (a) the overall creation and (b) the overall destruction of neutral nitrogen atoms versus discharge pressure. Conditions are as in figure 2.

- Neutral atoms are mostly created by electron impact dissociation of $N_2(X^1\Sigma_g^+, v>0)$ at high pressure but by recombination of N^+ on the wall and dissociation of $N_2(X^1\Sigma_g^+, v=0)$ at low pressure.
- Nearly all neutral atoms are generally lost by recombination on the wall, with electron impact ionization and pumping of species out of the chamber being important only at low pressure.

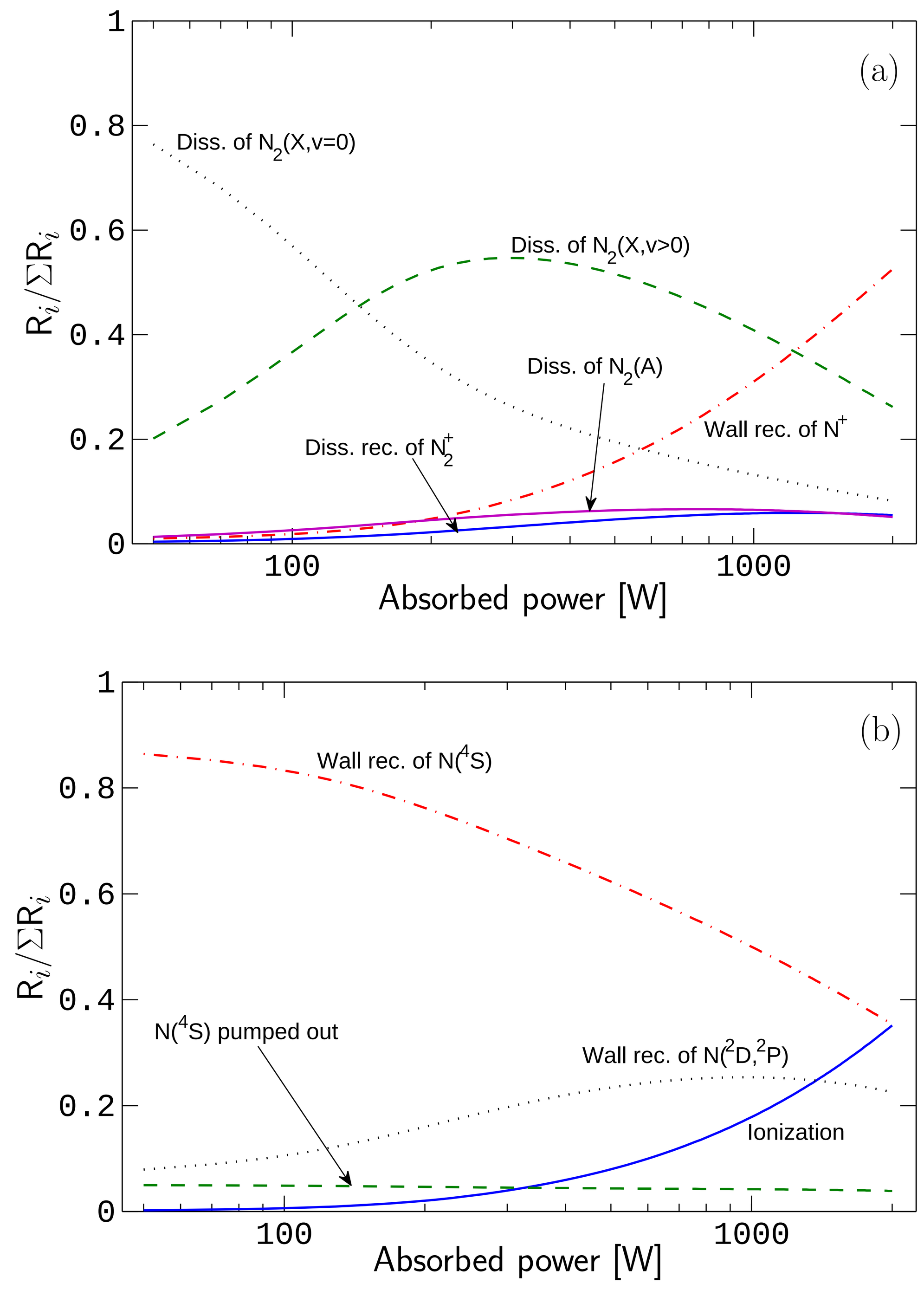

Figure 5: The reaction rates for (a) the overall creation and (b) the overall destruction of neutral nitrogen atoms versus absorbed power. Conditions are as in figure 2.

- Neutral atoms are created mostly by electron impact dissociation of $N_2(X^1\Sigma_g^+, v=0)$ at low power, by dissociation of $N_2(X^1\Sigma_g^+, v>0)$ at intermediate power and by wall recombination at high power.
- Wall recombination of neutral atoms is responsible for almost all of their loss, although electron impact ionization accounts for roughly 35 % of the loss at 2000 W.
- The ions N^+ and N_2^+ are almost entirely created by electron impact ionization of their neutral atomic and molecular counterparts.
- Wall recombination is the dominating loss mechanism for both ions at low and intermediate pressures, whereas resonant charge transfer and dissociative recombination are the most important processes at 100 mTorr for the loss of N^+ and N_2^+, respectively.

Conclusions

- The discharge is essentially atomic at low pressure but is dominated by molecular nitrogen at high pressure.
- Electronically and vibrationally excited species become more important with increasing pressure. The density of $N_2(X^1\Sigma_g^+, v=1-6)$ is comparable to the $N_2(X^1\Sigma_g^+, v=0)$ density above 10 mTorr.
- Although the calculated dissociation fraction is much larger than measurements, the agreement with the other measured plasma parameters is good.
- Electron impact dissociation and recombination of atoms on the wall are generally the dominant pathways for the creation and the destruction of neutral atoms, respectively.
- Wall recombination of the N^+ ion is important for the creation of neutral atoms at low pressure and high power.
- Electron impact ionization is important for the destruction of neutral atoms at low pressure and high power.

Acknowledgments

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References

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