Modeling of Excitation by Heavy Particles in Pure H_2 Discharges at High E/N

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H_α emission profiles were calculated for the high E/N (electric field E to gas density N ratio) Townsend discharges in pure hydrogen. Heavy particle collisions including the fast neutrals and interactions with the cathode surface are also included. The basic data were chosen to be in accordance with those used by Phelps. Monte Carlo simulation technique employing null collision method was used to follow electrons and heavy particles between collisions with H_2 or with surface for the conditions of a high E/N. Trajectories of reaction fragments are followed after the collision until their neutralization or thermalization down to the threshold of H_α excitation. We obtained spatially resolved emission profiles and the Doppler broadened line profiles for the conditions of the experiment of Petrović and Phelps. Intensity of the Doppler profile wing showing H_α emission of particles emerging from the cathode direction is obtained assuming that the reflection coefficient of the fast H atoms depends on the incident angle and on energy of the incident particle.

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1. Introduction

Fast neutral etching is the leading candidate to reduce charging induced damage in etching of high aspect ratio holes in dielectrics. It also reduces the roughness of etched surfaces allowing extension of plasma related technologies below 22 nm. Thus control of fast neutrals in gas discharges is of considerable importance.

Following the first observation, the anomalously Doppler broadened H_α lines have attracted numerous explanations. One example of the early studies is that of Benesch and Li [1], who observed symmetric broadened wings in the side-on profile but very asymmetric far wings in the end-on observation. Experiments in dc fields with observation along the axis of the field are rare [1]. The idea of Petrović et al. to make measurements in the Townsend regime [2, 3] where electric field is uniform allowed exact modeling of absolute values. Thus it became possible to test quantitative predictions of different proposed mechanisms. Most observations in plasmas are made at the right angle to the electric field and invariably these results show symmetric lines. The model proposed in [2] proved to be valid in all conditions (even with different combinations of gases) where this effect was observed.

This gives an explanation that the broadening of the central line is caused by dissociative excitation [4] or dissociative recombination. High energy excited species in the far line wings are due to acceleration of ions in the field and their conversion to fast neutrals by charge transfer collisions. At the same time, the wing that corresponds to the particles moving against the acceleration by the external field is assumed to be produced by the fast neutrals reflected from the cathode in either reflection of fast neutrals or neutralized ions. After losing some energy, this component of the line is narrower but still may have a higher integral value than the "direct" component [2, 3].

We used cross-section sets of Phelps [5]. Surface collisions of heavy particles are accounted for by using reflection coefficients from [5] and cosine angular distribution of reflected fast H.

2. Discussion of the simulation procedure and results

We use a Monte Carlo code that follows electrons, ions and fast neutrals and has been tested in a number of papers on high E/N transport [6, 7]. The code is based on null collision technique and is valid in the swarm limit, but it follows all relevant particles in the discharge. It is possible to establish spatially resolved profiles of flux, energy distribution and other sample properties. While limited attempts to predict the Doppler broadened profiles were made in the literature, to our knowledge none of these included spatial dependence of the profile. We release a large number of initial particles (500 000) electrons and follow them while maintaining recordings of the

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transport of resulting ions, fast neutrals and secondary electrons.

Reflection with dissociation, energy losses and neutralization was modeled by using the same model as given by Phelps [5]. The same reference was the source for the reflection of fast neutrals and all collisions.

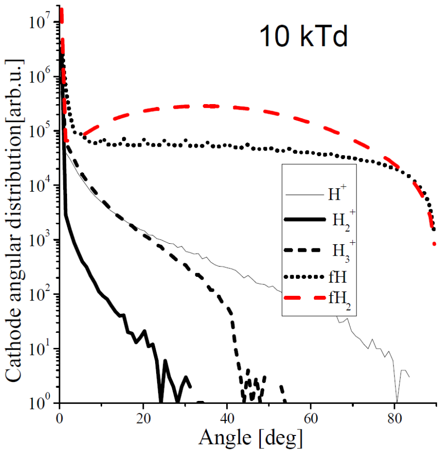

Fig. 1. Townsend discharge in pure hydrogen. Angular distribution of particles arriving at the cathode at $E/N = 10$ kTd ($E = 500$ V/cm, $N = 0.5 \times 10^{16}$ cm^{-3}).

In Fig. 1 we show angular distribution of all heavy particles in the simulation arriving to the cathode. Thus presented distribution is integrated over particle energy. Selection of the arriving particle angle is with respect to the field axis. One can see a very large degree of anisotropy especially for fast H which is the dominant agent of excitation. The anisotropy is introduced by the nature of collisions and acceleration of ions by electric field. The particles at high scattering angles are due to momentum transfer collisions and lead to side-on broadening.

In Fig. 2 we show profiles of lines observed at 90° to the field (side-on). One may see a large central peak due to all the fast particles aligned with the electric field, and also the broad wings due to scattered fast neutrals gaining some perpendicular momentum. The wide wing component increases rapidly towards the cathode.

The observation of symmetric side-on profile is just a projection of random momentum transfer collisions and by no means implies isotropy in the processes leading to the Doppler broadening [8] which would be perhaps applicable for electron induced excitation.

Figure 3 shows that the profiles due to fast neutrals in the direction of the field (end-on spatial distribution of Doppler) are quite asymmetric. The profile obtained for particles moving in forward direction (towards the cathode) increases with distance. Profile in the backward direction is insignificantly attenuated since beam of particles consists mostly of fast H with the origin at the cathode.

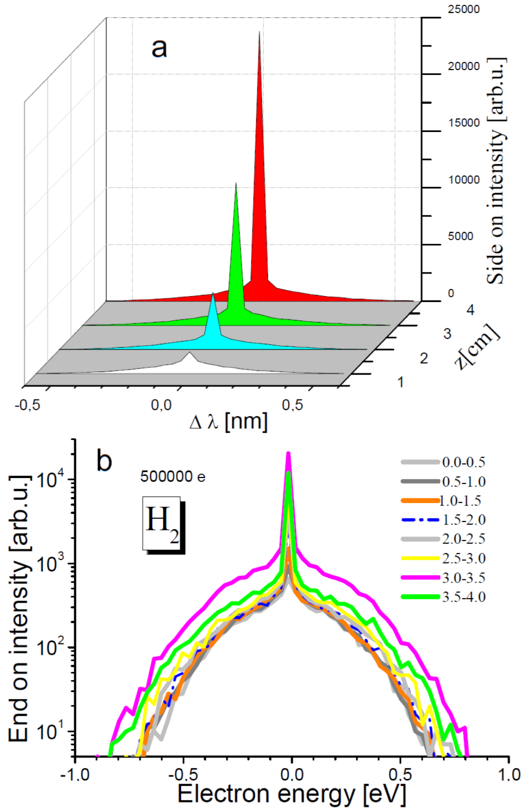

Fig. 2. Spatial distribution of side-on Doppler broadened H_α profile in Townsend discharge of H_2 at $E/N = 10$ kTd ($E = 500$ V/cm, $N = 0.5 \times 10^{16}$ cm^{-3}). The cathode is at 4 cm: (a) linear, (b) log scale.

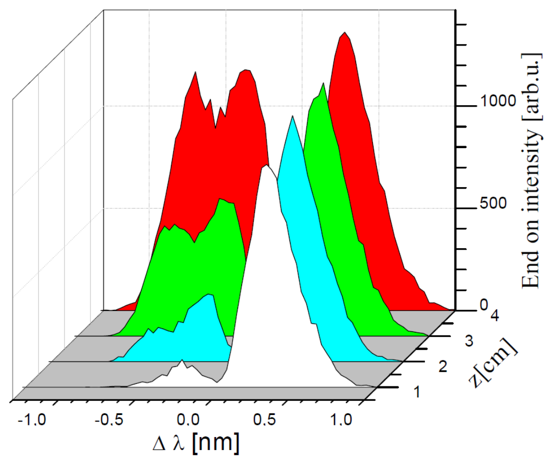

Fig. 3. Spatial distribution of end-on Doppler broadened H_α profile in Townsend discharge of H_2 at $E/N = 10$ kTd ($E = 500$ V/cm, $N = 0.5 \times 10^{16}$ cm^{-3}). Negative values are for particles moving toward cathode while positive for those moving away from the cathode. The cathode is at 4 cm.

3. Conclusion

Anisotropy of anomalously broadened H_α lines in a low current Townsend discharge in hydrogen was shown to be considerable and their origin is in ion acceleration by electric field, reflection at surfaces and nature of collisions. Monte Carlo simulation based on the best available data was used to predict angular distributions of heavy particles and spatial dependence of line profiles due to heavy particle excitation at 10 kTd. The results show that for a range of E/N which overlaps with realistic discharges one needs to consider detailed kinetic representation of ions and fast neutrals in addition to a similar treatment of electrons [9–11].

It may be interesting to check whether kinetic phenomena arising from fast ions and neutrals may be employed to achieve fast neutral etching, show runaway effects due to the ions and neutrals, show heavy particle effects in the cathode of glow discharges and thus be employed in elementary particle detectors. The Doppler broadened lines are in any case a useful diagnostic technique for checking the fast neutrals and their role in gas discharges [12].

Acknowledgments

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