Publ. Astron. Obs. Belgrade No. 84 (2008), 87 - 90 *Contributed Paper*

THE EFFECT OF ANISOTROPY OF THE SCATTERING OF HEAVY PARTICLES ON MODELLING OF THE DOPPLER PROFILE IN PURE H_2 DISCHARGE

V. D. STOJANOVIĆ, Ž. D. NIKITOVIĆ and Z. Lj. PETROVIĆ

Institute of Physics, Pregrevica 118, 11080 Zemun, Serbia
E–mail: zeljka@phy.bg.ac.yu

Abstract. The Effect of anisotropy of vibrational excitation by heavy particle scattering (fast H_2, H^+ and H_2^+) on Doppler profile and spatial distribution of emission in pure H_2 is studied by Monte Carlo technique by using simple differential cross sections (DCS) in the center of mass system (CMS). Electron and heavy particle collisions are represented by the latest cross section sets compiled by Phelps. For the conditions of very high reduced electric fields nonequilibrium electron transport should necessarily be modelled by anisotropic scattering.

1. INTRODUCTION

The first interpretations of unusually high Doppler broadening of hydrogen lines in non-equilibrium plasmas were based on possible dissociative processes, recombination and excitation (Capelli et al. 1985). The experiments, especially the experiments performed at dc fields revealed a large asymmetric component with energies exceeding the energy available from the repulsive potentials of the dissociating molecules (Barbeau and Jolly 1990, Konjević and Kuraica 1992). The explanation of such results was found in a specially designed high E/N swarm experiment (Petrović et al. 1992, Petrović and Phelps 1991) which gave a proof that, to the largest degree the excitation is due to collisions of fast neutrals formed in charge transfer collisions of the feed gas with fast ions. At high E/N, which can only be achieved under breakdown conditions at the left branch of the Paschen curve, the mean free paths are sufficiently high to allow large energy gain by ions and consequently formation of very fast neutrals with comparable energies. In addition it is possible to have reflection and neutralization of ions with reflection as fast neutrals, which leads to different components in blue and red wings of the Doppler profile (Petrović et al. 1992).

Some alternative explanations of anomalous Doppler profiles were offered in the literature (Mills et al. 2002), but all reliable measurements performed so far (Jovićević et al. 2004, Tatarova et al. 2007a, Tatarova et al. 2007b) do not require more than a combination of ionization and acceleration of the resulting ions in high fields leading to heavy particle (predominantly fast neutral) excitation. High, DC, E/N swarm experiment (self sustained discharge operating in the Townsend regime) may be modeled directly and exactly as it does not require self consistent calculation of the electric field and is thus open to a simple Monte Carlo simulation (MCS) that may include maximum complexity in the representation of collisions.

Vibrational excitation is a significant momentum and energy loss process for H^+ in H_2 at energies between 10 and 100 eV and potentially important process for H_2^+ in H_2 and H_2 in H_2 (Phelps 1990). Usual assumption for plasma models treating vibrational excitation is that scattering anisotropy for vibrational excitation by heavy particles is forward scattering although precise calculations (Krstić and Schultz 1999) exist. For both proton and neutral atom impact the scattering angles following vibrational excitation are shifted significantly towards larger values in comparison with the data due when only elastic scattering is involved.

In this paper we show results of simple modeling of heavy particles induced spatially resolved emission intensity or the Doppler profile in pure H_2 discharge when scattering anisotropy is included in the model.

2. DATA AND SIMULATION TECHNIQUE

The Monte Carlo code (Petrović and Stojanović 2008) based on null collision technique was used to follow electrons and heavy particles (H^+, H_2^+, H_3^+, fast H and fast H_2) between collisions with H_2 or with the cathode surface for the conditions of high electric field (E) to gas density (N) ratios E/N. We followed trajectories of all reaction fragments until they neutralized or thermalized below the H_α excitation energy. Conditions of simulation are appropriate for very high E/N (E/N =10 kTd, p =145 mTorr, interelectrode distance is d =4 cm) and are selected from experimental Townsend discharges in pure H_2 (Petrović et al. 1992). Effect of anisotropy of vibrational excitation by heavy particle scattering (fast H_2, H^+ and H_2^+) on Doppler profile, and spatial distribution of emission in pure H_2, is studied by using differential cross sections (DCS) in the center of mass system . One model of vibrational excitation was chosen to be isotropic below 30 eV in CMS and forward for the energies over 30 eV (this combination was marked as VA in this text) the other as forward scattering at all energies. All other processes have the same anisotropy as the model of Phelps (1990).

3. RESULTS AND DISCUSSION

Simulations are performed for the cases with vibrational excitation is included or excluded in the cross section set and when we use different models of scattering anisotropy. We used the model of Phelps (Phelps 2006) which includes vibrational excitation only by H^+ ions on H_2 from Phelps (1990) as the starting point and in that model at all energies forward scattering is assumed. Results obtained with these data compared to experimental results and other calculations are shown by dashed lines in Figs. 1. and 2. In both figures the same factor (F) is used to fit the intensity from the MCS to EXP. Effect of anisotropy of vibrational excitation by H^+ ions obtained by using VA differential cross section is shown in Fig. 1 by the thin solid line. If vibrational excitation proceeds with the VA model for H^+ ions than the Doppler peak due to particles moving towards the cathode is significantly shifted towards lower energies and so is the backward peak (reflected from the cathode). If one wants to compare these results to scale with experiment (EXP) than normalization factor

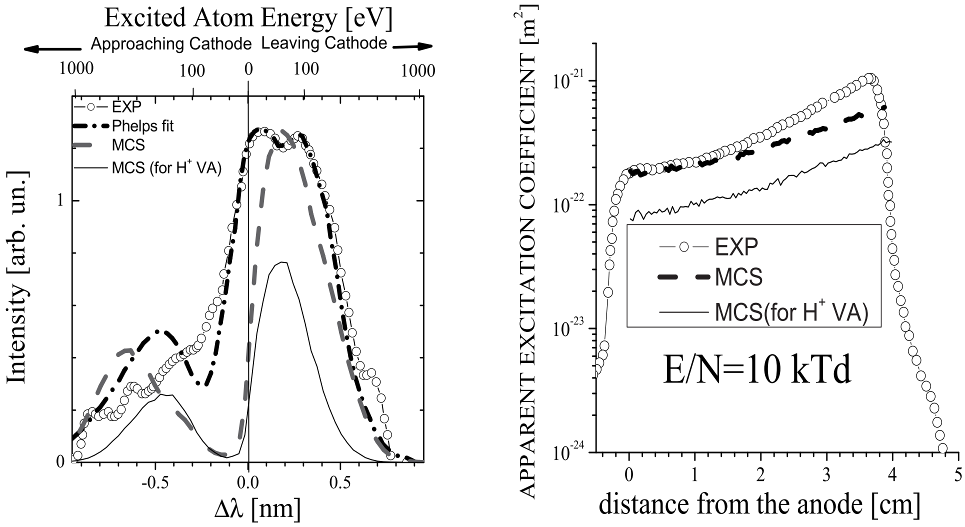

Figure 1: a) Doppler broadened profile, b) spatial distribution of emission, at very high E/N. "Phelps fit" and "EXP" are results published by Petrović et al. (1992).

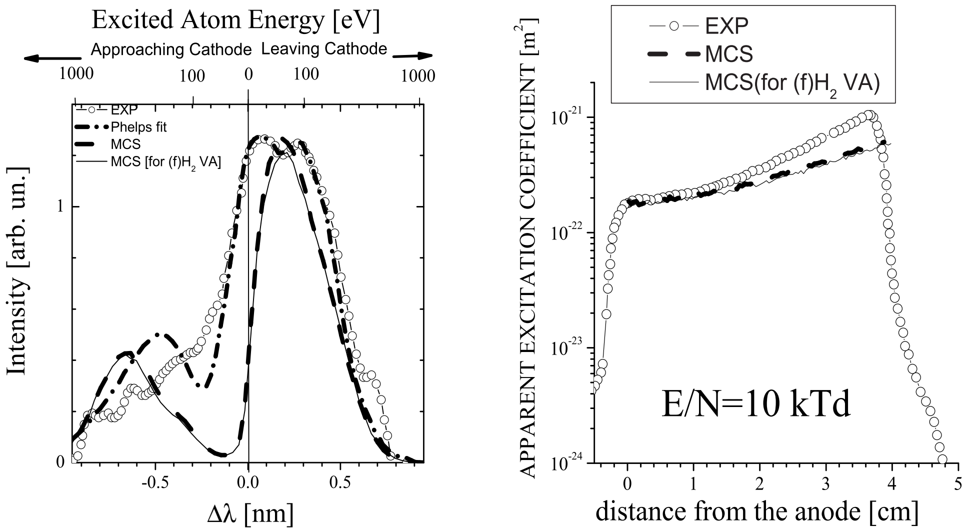

Figure 2: a) Doppler broadened profile, b) spatial excitation coefficient. "for (f)H_2" - MCS results for case where cross section for vibrational excitation by (f)H_2 from Phelps (1990) is included in the model while vibrational excitation for other heavy particles on H_2 is excluded.

F*1.7 (thin line in Fig 1.) should be applied. At the same time vibrational anisotropy shifts down the results for spatially resolved emission by a factor of two.

Introduction of vibrational excitation by H_2^+ and/or (f)H_2 collisions with buffer gas molecules with forward scattering (Phelps 1990) into our Monte Carlo simulation affects neither Doppler profile nor spatial profile of H_α emission intensity. Only minor changes can be observed with VA scattering anisotropy. Results for the e case where only vibrational excitation by (f)H_2 (Phelps 1990) is taken into account are shown in Fig. 2. MCS results are fitted to EXP by the same normalization factor.

Acknowledgments

Work at the Institute of Physics is supported by the MNRS, under grants 141025.

References

Barbeau, C., Jolly, J.: 1990, *J. Phys. D*, **23**, 1168.
Capelli, A. I., Gottscho, R. A., Miller, T. A.: 1985, *Plasma Chem. Plasma Process*, **5**, 317.
Jovicević, S., Ivković, M., Konjević, N., Popović, S., Vušković, L.: 2004, *J. Appl. Phys.*, **95**, 24.
Konjević, N., Kuraica, M.: 1992, *Phys. Rev. A: At. Mol. Opt. Phys.*, **46**, 4429.
Krstić, P. S., Schultz, D. R.: 1999, *J. Phys. B: At. Mol. Opt. Phys.*, **32**, 2415.
Mills, R. L., Raz, P. C., Dhandapani, B., Mayo, R. M., He, J.: 2002, *J. Appl. Phys.*, **92**, 7008.
Petrović, Z. Lj., Jelenković, B. M., Phelps, A. V. : 1992, *Phys. Rev. Lett.*, **68**, 325.
Petrović, Z. Lj., Stojanović, V. D.: 2008, AIP CP938, Spectral Line Shapes in Astrophysics-VI-Serbian Conference (VI SCLSA) ed. By L.Č. Popović and M.S. Dimitrijević, p. 237.
Petrović, Z. Lj., Phelps, A. V.: 1991, *Proc. of the Internatonal Seminar on Reactive Plasmas*, **E-3**, 351.
Phelps, A. V.: 2006, unpublished
Phelps, A. V.: 1990, *J. Phys. Chem. Ref. Data*, **19**(3), 653.
Tatarova, E., Dias, F. M., Ferreira, C. M., Puač, N.: 2007a, *J. Appl. Phys.*, **101**(6), 063306.
Tatarova, E., Dias, F. M., Puač, N., Ferreira, C. M.: 2007b, *Plasma Sources Sci. Technol.*, **16**, S52.