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MONTE CARLO MODELING OF ELECTRONS AND HEAVY PARTICLES IN PURE H₂ DISCHARGE

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In this paper we show results of Monte Carlo modeling of electrons and heavy particles induced spatially resolved emission intensity and the Doppler profile of H α line in pure H₂ discharge focusing on anisotropy of elastic scattering of heavy particles. For most intense inelastic scattering processes of heavy particles we used simplest assumptions. In particular we present study where transport of H⁺ and fast H particles is modeled by anisotropic scattering. For H⁺, H₂⁺, H₃⁺, fast H and H₂ we modeled scattering at the surface and of the molecules. Electron transport is also modeled by using available differential scattering cross sections. Anode and cathode boundaries are taken into account regarding electrons and heavy particles [4]. In order to achieve consistency with results of other authors we select conditions of simulation appropriate for moderate E/N (E-electric field, N-gas density) that are selected from experimental Townsend discharges in pure H₂.

In this study we used cross sections sets of Phelps [1] for H_3^+ ions transport, while for other particles we used data in Ref. [2]. For H^+ ions transport in this study we used either momentum transfer cross section of Phelps [2] or total cross section of Krstić and Shultz [3] for elastic scattering with differential cross section and for first three vibrational channels [3] of excitation asuming forward scattering. Surface effects to heavy particle transport are accounted for by using reflection coefficients for heavy particles from ref. [2] and cosine angular



Fig.1. H α emission at E/N=350 Td [2]. Thick black dashed line – sum of all contributions; elastic scattering for H⁺ and fast H treated by momentum transfer cross section [1] and isotropic scattering in CM. In charge transfer (CT) collisions with H₂, H⁺ goes forward in CM. Thick (violet) line-squares – sum of all contributions, elastic scattering for (f)H and H⁺ accounted for DCS (ANISO) while CT for H⁺ + H₂ CT was isotropic in CM.

distribution of reflected fast H.

Figure 1. shown excellent agreement with 350 Td spatial profile provided that we: use for H^+ and fast $H - H_2$ anisotropic elastic scattering (total cross section) - including differential cross sections [3] and for $H^+ - H_2$ charge transfer (CT) we use isotropic scatter (cross sections are selected so that the total cross section is the same in both cases) ,all in CM. For the case of isotropic scattering with momentum transfer cross section for fast H and H^+ transport agreement is achieved only in the anode side of discharge. Contribution of fast H, H^+ and electrons for this case is also shown in Fig. 1.

In Figure 2. we show comparison of our MCS results with experiment at 1 kTd (E=95 V/cm, N=0.95 10^{-16} cm⁻³). As in Fig. 1 we obtained higher emission if we use momentum transfer cross sections from [2] with isotropic scattering [thick dashed (black) line]. For H⁺ charge transfer we used forward scattering as in Fig. 1. Excellent agreement with experiment is obtained if we use anisotropic elastic scattering of fast H and H⁺, also with forward scattering for H⁺CT scattering. With long dashed (green) line we show emission if CT collisions of H⁺ with H₂ is treated isotropically. These results clearly shows that not only precise description of electron-H₂ collisions is needed to explain emission close to anode boundary but also how precise scattering description of H + H₂ and H⁺ + H₂ collisions up to 100 eV collision energy is necessary to explain spatially resolved emission in pure H₂ Townsend discharge at moderate E/N. More studies heading in that direction [3,5] are needed.



Fig.2. E/N=1 kTd. Lines have the same meaning as in Fig.1. Additionaly, long dash (green) line represents sum of all contributions where for H^+ and fast H we used DCS (ANISO) and for CT for H^+ on H_2 forward scattering.

References

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