Kinetic simulation of a nanosecond-pulsed hydrogen microdischarge

Z. Donkó,1,a) J. Schulze,1,2 S. Müller,2 and U. Czarnetzki2

1Research Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, P.O Box 49, H-1525 Budapest, Hungary
2Institute for Plasma and Atomic Physics, Ruhr-University Bochum, Universitätsstrasse 150, 44780 Bochum, Germany

(Received 8 April 2011; accepted 31 May 2011; published online 21 June 2011)

The electron dynamics in a nanosecond-pulsed microdischarge in high pressure hydrogen gas is investigated space and time resolved by particle-in-cell simulations. The discharge is driven by a 10 ns voltage pulse with a peak of 1.3 kV followed by an approximately constant voltage of 300 V during 150 ns. The time resolved current, electric field, electron density, and spatio-temporal excitation rates are compared to experimental and modeling results under identical discharge conditions. Via this synergistic approach, the development of the discharge and the different phases of distinct electron dynamics are identified and understood. © 2011 American Institute of Physics. [doi:10.1063/1.3601486]

Atmospheric pressure microdischarges can be used for medical and plasma surface processing applications avoiding the necessity of expensive and large vacuum systems. Thus, the physics of these discharges has attracted increasing attention during the past years. Several types of electrode configurations have been developed and a wide variety of phenomena (e.g., self-pulsing and mode transitions) have been studied.1–3 Despite the small size of these devices, state-of-the-art diagnostics methods have been applied to reveal details of discharge operation.4–11 In microdischarges excited by nanosecond pulses, transient electron dynamics takes place on a nano- or subnanosecond time scale. In combination with the small discharge dimensions, this makes numerical and experimental investigations particularly challenging. While a number of experimental investigations of such plasma sources have already been performed,6–10 we are not aware of any detailed kinetic simulation studies.

Here, we present such numerical investigations and compare our results to previous experimental and modeling results. We study the dynamics of a plane-parallel discharge excited by a high voltage (HV) nanosecond pulse with a peak of ~1.3 kV, in molecular hydrogen gas. The electrode gap is L=1.2 mm and the gas pressure is 230 mbar. Previous experimental studies on this system using various diagnostics10 have revealed a complex spatial and temporal dynamics of different parameters, such as the optical emission, electric field, current, and electron density. The present letter intends to provide insight into these observations via numerical simulations.

The simulation code is based on the Particle-in-Cell method complemented with a Monte Carlo treatment of collision processes (PIC/MCC). The cross sections for e+H2 collisions are taken from Ref. 12, with the exception of the elastic momentum transfer collision, for which we use data from Ref. 13. The processes include rotational, vibrational, and electronic excitations, as well as ionization. The ion kinetics is treated in a simplified way: upon ionization, the H3+ ions created are assumed to be immediately converted to H2+ ions. This is justified by the large cross section14,15 of this process. For H3+ ions – the only ionic species considered – two reaction processes: elastic and proton transfer collisions are taken into account.14,15 All collisions take place between the traced particles and H2, dissociation of the gas (i.e., the presence of atomic hydrogen) is neglected.

An (ion-induced) secondary emission coefficient of γ=0.13 and an electron reflection coefficient of R=0.2 are assumed at the electrodes. The gas temperature is set to 300 K. The simulation starts with seeding N0 superparticles (equal number for electrons and ions) into the gap, which represent the charged particles remaining from a previous pulse. Due to the high pressure diffusion is slow and recombination between electrons and H2+ is the dominant loss channel between the repetitive discharge pulses.16 This mechanism results in a flat density profile; correspondingly we use a uniform spatial distribution of the seeded species. We use an initial density n0=5.25×1010 cm−3, which results in a good agreement between the calculated and measured values of the discharge current during the quasi-dc part following the HV pulse. The voltage waveform applied to the cathode is taken from the experimental recording.10

Figure 1(a) shows the applied voltage waveform. The voltage peak centered around 26 ns has a width of about 8 ns. Beyond the HV peak (at t≈40 ns) the voltage settles around 300 V and decays subsequently later (not shown). Further panels of Fig. 1 display simulation results for the dynamics of the discharge current and its constituents at the cathode [Fig. 1(b)], the electric field in the discharge center [Fig. 1(c)], and the electron density [Fig. 1(d)] in the center. These data, as well as the spectrally integrated and spectrally resolved light emission patterns (excitation rates) are compared next with the respective experimental results.10 Figure 2(a) shows the total electron impact excitation rate (excluding rotational and vibrational excitation), panels (b) and (c), respectively, show the electron impact excitation rates of the Fulcher α (σ 3Πg→a 1Σg−) band (having a threshold energy εth=14.0 eV) and the Balmer alpha (Hα) transition (resulting from dissociative excitation, εth =16.6 eV). Figures 2(d)–2(f) show the corresponding experimental observations.10

---

a)Electronic mail: donko@mail.kfki.hu.
At the beginning of the voltage pulse (10 ns < t < 23 ns), there is only little space charge inside the gap, the electric field in the discharge center follows the driving voltage [Fig. 1(c)], and the reduced electric field is spatially homogeneous (Fig. 3). During this time, “residual” electrons are accelerated toward the anode causing a weak excitation maximum around 20 ns [feature “I” in Fig. 2(a)]. This feature clearly shows up both in the simulation and experimental data for the Fulcher band, but the electron energy is not high enough to excite the Fulcher band and in the case of Hα we find a significant difference, i.e., the ratio is higher for Hα. This can be explained by the higher electric field in the cathode region, compared to the positive column, and consequent higher electron energy (Hα excitation is more sensitive to highly energetic electrons). The simulations clearly reproduce this behavior. Due to a drop in the voltage around 32 ns and its subsequent increase to a quasi-dc level the excitation rate rapidly drops and later grows to a lower level, re-establishing the classical glow discharge structure (“IV” + “V” and a weak anode glow “VI”). As a marked difference, light emission in the experiment is observed even beyond 45 ns in that region (Fig. 3) does not allow significant electron impact excitation. This feature is believed to be caused by recombination radiation — not included in the simulation. Note that the experimentally observed light emission of Hα is very weak in this region.

The electron density, $n_e$, from the simulation agrees well with the value determined from measurements of the electric field and the discharge current using the following relation based on the assumption, that the total current is the sum of electron conduction and displacement current (ions are effectively immobile)

$$n_e(t) = \frac{1}{e E(t)} \left[ \frac{I(t)}{A} - \frac{e_0}{A} \frac{\partial E}{\partial t} \right].$$

Here, $A$ is the electrode area and we take the electron mobility $\nu_e$ to be $0.27$ $m^2 V^{-1} s^{-1}$ at 27 $Td$, which corresponds to the bulk $|E|/n$ in the quasi-dc phase. (The value of $\nu_e$ does not change significantly over the $|E|/n$ range of interest.) Following a rapid rise the electron density in the bulk settles at 1.1 $\times 10^{12}$ $cm^{-3}$ [see Fig. 1(d)]. Regarding the ion density in the quasi-dc sheath, we find a value of 1–1.4 $\times 10^{12}$ $cm^{-3}$, which is in good agreement with the experimental value of 1.3 $\times 10^{12}$ $cm^{-3}$.

In summary, we studied the dynamics of a nanosecond-pulsed hydrogen microdischarge at nearly atmospheric pressure, space and time resolved, by PIC/MCC simulations and

![FIG. 1. (Color online) Temporal evolution of the (a) driving voltage; (b) conduction, displacement, total and corrected total current at the cathode (simulation) as well as the total measured current; (c) electric field in the discharge center; (d) electron density in the center from the simulation and calculated according to Eq. (1) using experimental input data.](image-url)
compared our results to measurements under identical discharge conditions. The simulations revealed different phases of the electron dynamics providing a detailed understanding of these transient phenomena.

This work is funded by the Hungarian Fund for Scientific Research (Grant No. OTKA K77653), the RUB Research Department Plasma, the Alexander von Humboldt foundation, and DFG (FOR 1123).

FIG. 2. (Color online) Calculated spatio-temporal distributions of the excitation rate (given in units of \(10^{18}\) cm\(^{-3}\) s\(^{-1}\)): (a) total rate (excluding rotational and vibrational excitation), (b) Fulcher \(\alpha\) band, and (c) \(H_\alpha\) line. Plots (d)–(f) show the corresponding experimentally observed light emission intensity (given in arbitrary units).

FIG. 3. (Color online) Spatio-temporal distribution of \(|E|/n\), in Td.

---