Evolution of Charged Particle Densities After Laser-Induced Photodetachment in a Strongly Electronegative RF Discharge

M. Yan, A. Bogaerts, and R. Gijbels

Abstract—**The temporal and spatial evolutions of charged particle densities after laser induced photodetachment in a SiH_4/H_2 RF discharge have been modeled by a particle-in-cell/Monte Carlo (PIC/MC) method. Two dips in the evolution of the electron density and the positive ion density, which are observed by experiments in the literature, are explained. The images indicate that the two dips occur at different moments in time.**

Index Terms—**Electromagnetive RF discharge, laser-induced photodetachment, particle-in-cell/Monte Carlo modeling.**

LASER-INDUCED photodetachment is used to obtain the negative ion density in electronegative discharges from the measured density of the detached electrons (e.g., [1] and the references therein). Since the evolution of the charged particle densities is coupled through the electric field generated by the net space charge, the behavior of one species strongly influences the behavior of the others. The evolution of the electron, negative ion, and positive ion density, simultaneously in time and in space are illustrated in this paper.

A kinetic particle-in-cell/Monte Carlo (PIC/MC) model [2] is used to simulate the relaxation process after photodetachment in a SiH_4–H_2 (1:9) discharge. This study serves as an example to qualitatively demonstrate the characteristics of the relaxation process after photodetachment in strongly electronegative discharges. Therefore, only electrons (e^-), positive ions (SiH_3^+, H_2^+) and negative ions (SiH_3^-) and some of their reactions, are taken into account [2]. It should be realized that certain potentially important reactions, such as $H_2^+ + H_2 \rightarrow H_3^+ + H$; $H_2^+ + H \rightarrow H^+ + H_2$; and $SiH_3^- + H \rightarrow SiH_2^- + H_2$, are not taken into account in the present model. For a really comprehensive model, it would probably be necessary to include them. However, the present paper does not focus on the chemical reactions, but it outlines the general tendencies in the behavior of electrons, positive, and negative ions after laser-induced photodetachment. The discharge parameters are an applied RF frequency of 13.56 MHz, an applied voltage of 200 V, and a gas pressure of 400 mtorr. The initial conditions and assumptions for the simulations are the following: The only laser induced reaction considered is photodetachment, $SiH_3^- + h\nu \rightarrow SiH_3 + e^-$. The electron affinity of SiH_3 is 1.4 eV [3], [4]. The laser is fired at the beginning of an RF cycle and the pulse duration is neglected. All the detached electrons have an energy of 0.2 eV.

Manuscript received June 25, 2001; revised November 7, 2001.

The authors are with the Department of Chemistry, University of Antwerp, Wilrijk-Antwerp B-2610, Belgium (e-mail: bogaerts@uia.ua.ac.be).

Publisher Item Identifier S 0093-3813(02)03355-6.

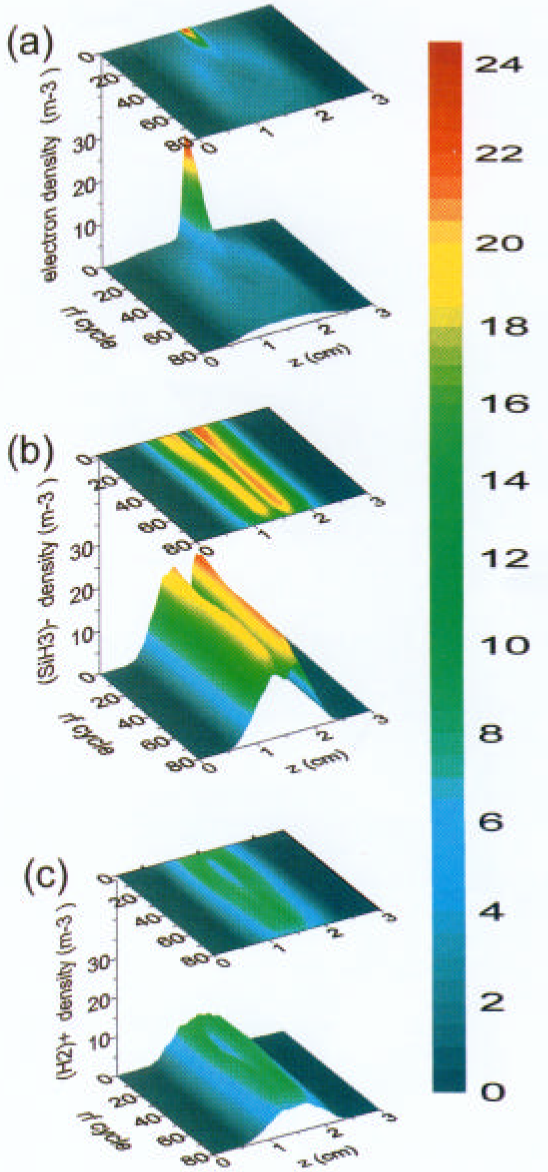

Fig. 1. Temporal and spatial evolution of the charged particle densities (10^{15} m^{-3}) after photodetachment: (a) electron density; (b) SiH_3^- ion density; and (c) H_2^+ ion density.

The negative ion density (SiH_3^-) in the laser impact region drops 100% due to the photodetachment and the same number of elec-

0093-3813/02$17.00 © 2002 IEEE

trons is released at exactly the same position. The positive ion density does not change during the laser pulse. The process is considered to be one-dimensional (1-D). The laser beam is assumed to be infinite in the directions parallel to the electrodes. The gap between the two electrodes is 3 cm and the laser is focussed at the middle of the discharge with a 2-mm width.

The temporal and spatial evolution of electron, negative ion (SiH_3^-) and positive ion (H_2^+) densities after photodetachment are shown in Fig. 1(a)–(c) (combined surface and contour images). It can be seen that after "0" RF cycles (just after photodetachment), as assumed, the electron density at the laser impact region [Fig. 1(a)] shows a dramatic jump corresponding to the dip of the negative ion density [Fig. 1(b)], whereas the H_2^+ density [Fig. 1(c)] remains unchanged. Note that the SiH_3^+ density is not shown here because it changes less as a function of time than the H_2^+ density due to its heavier mass. The absolute value of its density is, however, such that the overall charge neutrality is preserved [3], [4].

During the first 30 RF cycles, as appears from Fig. 1(a), the local (i.e., at the laser impact region) e^- density drops quickly and almost recovers to its original value, whereas the dip in the SiH_3^- density profile is relatively slowly filled up. The local H_2^+ density decreases rather strongly, shown as a dip after 20 RF cycles in Fig. 1(c). The relaxation process of the charged particle densities can be understood as follows: The electrons have a large mobility and, hence, the smoothing of the e^- density is faster than that of the SiH_3^- density. As a result, a charge separation and, hence, an electric field is created at the edge of the laser impact region [3], [4]. This field lowers the e^- flux and accelerates the smoothening of the SiH_3^- density. Simultaneously, it also forces the positive ions to move in the same direction as the electrons, which results in the dip. This dip has also been observed in experiments [5].

After 30 RF cycles, the gradient of the e^- density at the laser impact region becomes small. The electric field becomes weak and eventually it changes sign. This change of sign in the field results from the fact that the diffusion flux of the negative ions becomes stronger than that of the electrons. This field forces the positive ions to follow the negative ions and it also increases the flux of electrons toward the presheaths. As a result, the e^- density at the laser impact region after about 40 RF cycles shows a local minimum (indicated by the dark region in Fig. 1(a).

After 40 RF cycles, the ion densities recover more slowly, because the rearrangement of the ion density profiles after the strong perturbation by photodetachment is more or less finished. The recovery of ion densities mainly depends on the small net increment between the production and the loss, hence it will take a very long time [3].

In conclusion, from the images of the temporal and spatial evolution of the charged particle densities after photodetachment in SiH_4/H_2 discharges, it can be seen that the electrons, positive, and negative ions all influence the recovery process and are multirelated. In the experiment result [5], the dips in the electron and positive ion density appear to occur at the same time for a H_2 discharge. The images obtained from the simulation clearly show that the two dips can in general occur at different moments in time, because of the different mechanisms responsible for these dips.

References

[1] M. Bacal, "Plasma diagnostics in negative ion sources," *Plasma Sources Sci. Technol.*, vol. 2, no. 2, pp. 190–197 , 1993.

[2] M. Yan and W. J. Goedheer, "Particle-in-cell/Monte Carlo simulation of radio frequency SiH_4/H_2 discharges," *IEEE Trans. Plasma Sci.*, vol. 27, pp. 1399–1405, Oct. 1999.

[3] M. Yan, A. Bogaerts, R. Gijbels, and W. Goedheer, "Kinetic modeling of relaxation phenomena after photodetachment in a RF electronegative SiH_4 discharge," *Phys. Rev. E*, vol. 63, no. 026405, pp. 1–9, 2001.

[4] ——, "Local and fast relaxation phenomena after laser induced photodetachment in a strongly electronegative RF discharge," *Phys. Rev. E*, vol. 65, no. 016408, pp. 1–9, 2001.

[5] P. Devynck, J. Auvray, M. Bacal, P. Berlemont, J. Bruneteau, R. Leroy, and R. A. Stern, "Photodetachment technique for measuring H^- velocities in a hydrogen plasma," *Rev. Sci. Instrum.*, vol. 60, no. 9, pp. 2873–2878, 1989.