Plasma Ionization in Low-Pressure Radio-Frequency Discharges—Part II: Particle-in-Cell Simulation

A. Meige, D. O'Connell, T. Gans, and R. W. Boswell

***Abstract*—Plasma ionization in the low-pressure operation regime ($<$ 5 Pa) of RF capacitively coupled plasmas (CCPs) is governed by a complex interplay of various mechanisms, such as field reversal, sheath expansion, and wave–particle interactions. In a previous paper, it was shown that experimental observations in a hydrogen CCP operated at 13.56 MHz are qualitatively well described in a 1-D symmetrical particle-in-cell (PIC) simulation. In this paper, a spherical asymmetrical PIC simulation that is closer to the conditions of the highly asymmetrical experimental device is used to simulate a low-pressure neon CCP operated at 2 MHz. The results show a similar behavior, with pronounced ionization through field reversal, sheath expansion, and wave–particle interactions, and can be exploited for more accurate quantitative comparisons with experimental observations.**

***Index Terms*—Capacitively coupled plasma (CCP), field reversal, heating, particle-in-cell (PIC) simulation, RF, wave particle interaction.**

UNDERSTANDING ionization mechanisms and plasma sustainment in low-pressure RF capacitively coupled plasmas (CCPs) is crucial in improving performances and further developing technological applications of such plasmas. The recent advance in optical diagnostics [1] made it possible to show that a complex interplay of ionization through field reversal, sheath expansion, and, in particular, wave–particle interactions plays a fundamental role in sustaining such discharges ([2] and references therein). In this paper, the authors compared their experimental results with the results of a particle-in-cell (PIC) simulation developed by Vender and Boswell [3]. The results predicted by the simulation 15 years earlier turned out to be in good qualitative agreement with the new experimental results. However, the simulation represents a symmetrical system with an RF sheath on both sides, so it was not clear to what extent the observed ionization mechanisms were not due to the mutual interaction of the two sheaths. In this paper, we simulate a highly asymmetrical CCP with a lower excitation frequency (2 MHz) and another for a noble gas (neon), and we show that the observed ionization mechanisms are qualitatively similar. The new asymmetrical simulation of a neon plasma excited with lower RF frequency allows a more accurate and simpler comparison with experimental observations (in particular, with the new experiment results depicted in Part I of this paper).

Manuscript received November 30, 2007; revised January 27, 2008.

A. Meige is with the Laboratoire de Physique et Technologie des Plasmas, Ecole Polytechnique, 91128 Palaiseau, France (e-mail: meige@lptp.polytechnique.fr).

D. O'Connell is with the Center for Plasma Science and Technology, Ruhr University, 44801 Bochum, Germany.

T. Gans is with the Centre for Plasma Physics, Queen's University, BT7 1NN Belfast, U.K.

R. W. Boswell is with the Space Plasma Power and Propulsion Group, Research School of Physical Sciences and Engineering, Australian National University, Canberra, ACT 0200, Australia.

Color versions of one or more of the figures in this paper are available online at http://ieeexplore.ieee.org.

Digital Object Identifier 10.1109/TPS.2008.926833

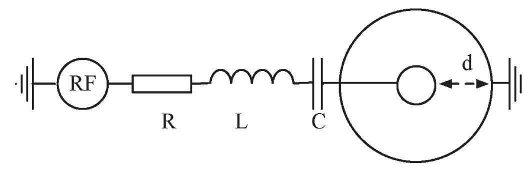

Fig. 1. Schematic of the spherical simulation.

The 1D3V simulation that we have developed is based on the well-known PIC scheme [4], [5]. As shown in Fig. 1, the system modeled by the simulation consists of two concentric spherical electrodes, which are separated by a distance d in which the plasma is formed, and an external circuit. Such a geometry was chosen to fit the experimental system that we wish to simulate (a gaseous electronic conference cell without counter electrode, resulting in a very asymmetric system with a significant RF sheath at the RF electrode and a much smaller sheath at the grounded wall [2]). The RF voltage is applied onto the inner electrode (which is also referred to as *live electrode or left electrode* in the following), whereas the outer electrode serves as a reference and its potential is set to zero. The PIC simulations includes an external *RLC* circuit [6], and the results shown in this paper were obtained for $R = L = 0$ and $C = 1$ nF, allowing a self-bias of the discharge [7]. Electron-neutral collisions are treated by a usual Monte Carlo module [8] and with the use of the experimental cross sections of neon compiled by Pitchford *et al.* [9]. In the following, only ionizing collisions were considered.

The results presented in the following are for a 1-m-long system represented by 350 cells. The surface ratio between the outer and inner electrode is 10. Simulations were run for 5 ms, with a time step of 0.8 ns. Up to 10^5 macroparticles per species were used. The "pressure (i.e., the neutral density used to calculate the ionization frequency)" is $P = 2$ Pa. The mass of ions is that of neon. The RF voltage is 500 V, and the RF frequency is 2 MHz. The maximum plasma density reached in the bulk is slightly below 1.5×10^{13} m^{-3}.

Because of the large asymmetry of the system that the circuit capacitor charges up, the live electrode develops a large dc offset (known as self-bias voltage), and the excursion of the bulk voltage is therefore much smaller than that in the symmetrical case. This results in a large RF sheath at the live electrode

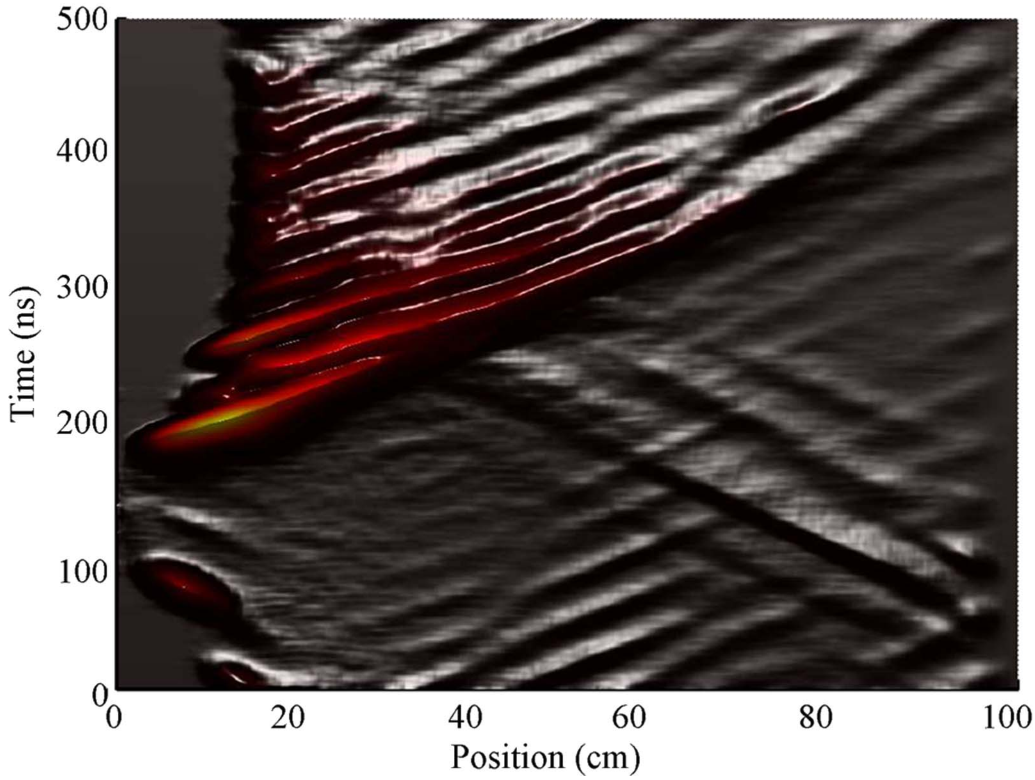

Fig. 2. Spatiotemporal ionization source term (brighter colors (yellow) indicate higher ionization source term).

and almost no sheath at the grounded electrode. Fig. 2 shows the spatiotemporal ionization source term during an RF cycle (averaged over 8000 RF cycles) self-consistently calculated by the simulation; brighter colors (yellow) indicate regions with a higher ionization source term. This graph is somewhat related to the power absorbed by the electrons, except that sole electrons with an energy above the ionization energy threshold are visible. Several regions of phase space are noticeable. When the RF sheath collapses, the excess of negative charges in the plasma resulting from the constant flux of positive ions to the electrodes creates an electric field (with a field reversal different from that observed in electronegative plasmas [10]) that is large enough to accelerate bulk electrons toward the live electrode, creating the peak in the ionization source term visible between 20 and 100 ns in the sheath region (between 0 and 20 cm). As the RF sheath expands again, electrons in its vicinity are accelerated back into the plasma with a kinetic energy of above 25 eV, creating another peak in the ionization source term whose maximum is slightly before 200 ns at around 10 cm from the electrode. The secondary ionization waves are observed after 220 ns and are detailed in [2]. They essentially result from an electron two-stream instability between the bulk electrons and the electrons accelerated by the moving sheath. Finally, the ionization waves that are observed to propagate from the smaller right sheath toward the plasma bulk between 0 and 250 ns result from the fast electrons coming from the left-hand side of the system that are reflected by the right sheath.

A full 1D3V spherical PIC simulation was used to simulate an asymmetric RF CCP run at 2 MHz in neon. Ionization through field reversal, sheath expansion, and wave–particle interactions was observed for low-pressure conditions, and it was shown that these ionization mechanisms are local phenomena and not related to a possible interaction between the two RF sheaths existing on both sides of a symmetrical system, as was used in the simulation depicted in [2]. Future work will focus on more quantitative comparisons of simulation results and experimental observations.

REFERENCES

[1] T. Gans, J. Schulze, D. O'Connell, U. Czarnetzki, R. Faulkner, A. R. Ellingboe, and M. M. Turner, "Frequency coupling in dual frequency capacitively coupled radio-frequency plasmas," *Appl. Phys. Lett.*, vol. 89, no. 26, pp. 261 502-1–261 502-3, Dec. 2006.

[2] D. O'Connell, T. Gans, D. Vender, U. Czarnetzki, and R. Boswell, "Plasma ionization through wave-particle interaction in a capacitively coupled radio-frequency discharge," *Phys. Plasmas*, vol. 14, no. 3, p. 034 505, Mar. 2007.

[3] D. Vender and R. W. Boswell, "Electron-sheath interaction in capacitive radio-frequency plasmas," *J. Vac. Sci. Technol. A, Vac. Surf. Films*, vol. 10, no. 4, pp. 1331–1338, Jul. 1992.

[4] R. W. Hockney and J. W. Eastwood, *Computer Simulation Using Particles*. Bristol, PA: IOP, 1988.

[5] C. K. Birdsall and A. B. Langdon, *Plasma Physics via Computer Simulation*. Bristol, PA: IOP, 1991.

[6] J. P. Verboncoeur, M. V. Alves, V. Vahedi, and C. K. Birdsall, "Simultaneous potential and circuit solution for 1D bounded plasma particle simulation codes," *J. Comput. Phys.*, vol. 104, no. 2, pp. 321–328, Feb. 1993.

[7] H. B. Smith, C. Charles, R. W. Boswell, and H. Kuwahara, "Bias formation in a pulsed radiofrequency argon discharge," *J. Appl. Phys.*, vol. 82, no. 2, pp. 561–565, Jul. 1997.

[8] V. Vahedi and M. Surendra, "A Monte Carlo collision model for the particle-in-cell method: Applications to argon and oxygen discharges," *Comput. Phys. Commun.*, vol. 87, no. 1, pp. 179–198, May 1995.

[9] L. C. Pitchford, J. P. Boeuf, and W. L. Morgan, *The Siglo Data Base, CPAT and Kinema Software*. [Online]. Available: http://www.siglo-kinema.com

[10] R. A. Gottscho, "Glow-discharge sheath electric fields: Negative-ion, power, and frequency effects," *Phys. Rev. A, Gen. Phys.*, vol. 36, no. 5, pp. 2233–2242, Sep. 1987.