Process control in low pressure capacitive radio frequency plasmas based on kinetic simulations

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Capacitively couple radio-frequency plasma (CCP) sources with relatively simple reactor designs and the ability to generate a high density of active particles such as electrons, ions, and radicals with controllable energies, have irreplaceable applications in microscopic-scale surface modifications. These include plasma-enhanced chemical vapor deposition (PECVD) and plasma etching, both of which are fundamental processes in semiconductor manufacturing [1,2].

The development of the microelectronics industry is closely linked to advances in semiconductor processing equipment, which in turn heavily depend on improvements in plasma source technology. According to Moore's law, the number of transistors on a microchip doubles approximately every two years. To support this trend, the continuous increase in wafer size and the simultaneous decrease in feature dimensions demand precise plasma control in both etching and deposition processes. In etching, energetic ion bombardment and high fluxes of selected reactive neutral radicals are essential to achieve nanometer-wide vertical trenches with high aspect ratios (HAR). In deposition, however, ions with relatively low but controllable energies are required to prevent surface damage. Plasma uniformity is critical in both processes to ensure high-quality results over large areas. In general, the flux–energy distribution functions of electrons, ions, and active neutral species (radicals) play a decisive role in determining process outcomes through their interactions with material surfaces. Achieving ultimate control over these distributions requires a comprehensive scientific understanding of plasma operation mechanisms under commercially relevant conditions.

Motivated by this, process control in low-pressure CCPs based on voltage waveform tailoring [3-6], electrode surface customization [7,8], and applying an external magnetic field [9] was investigated using one-dimensional (1D) and two-dimensional (2D) particle-in-cell/Monte Carlo collision (PIC/MCC) simulations. Detailed results and discussions of these investigations can be found in the author's doctoral dissertation [10]. This paper focuses on one of these control concepts: plasma uniformity control through electrode structure customization [7]. In this work, the electron heating dynamics inside a single trench structure and the potential of embedding multiple trenches into the counter (grounded) electrode to enhance plasma uniformity is investigated based on 2d3v (two dimensional in space and three dimensional in velocity space) GPU accelerated PIC/MCC simulations code.

As shown in figure 1(a), simulations are first performed for a CCP reactor with a ring shaped trench at the powered electrode. The simulation results show that the plasma density above the trench is significantly enhanced compared to the case where a planar powered electrode is used.

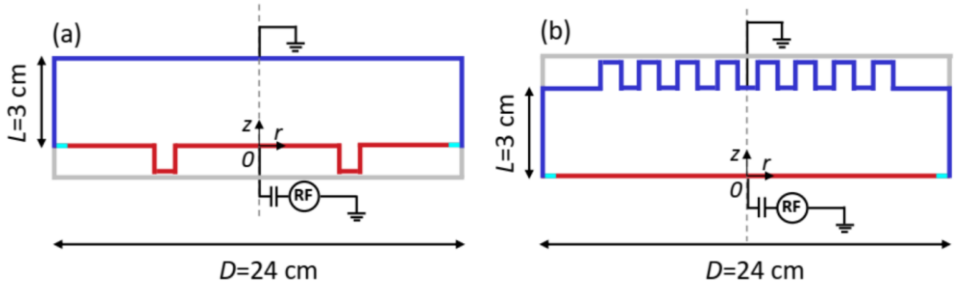

Figure 1 Reactor geometries investigated: planar grounded electrode and structured powered electrode including a single ring-shaped rectangular trench (a), and planar powered electrode and structured grounded electrode including multiple trenches (b). The powered and grounded electrodes are indicated by the red and dark blue lines, respectively. The light blue segments represent a dielectric spacer in between the powered and grounded electrodes [7].

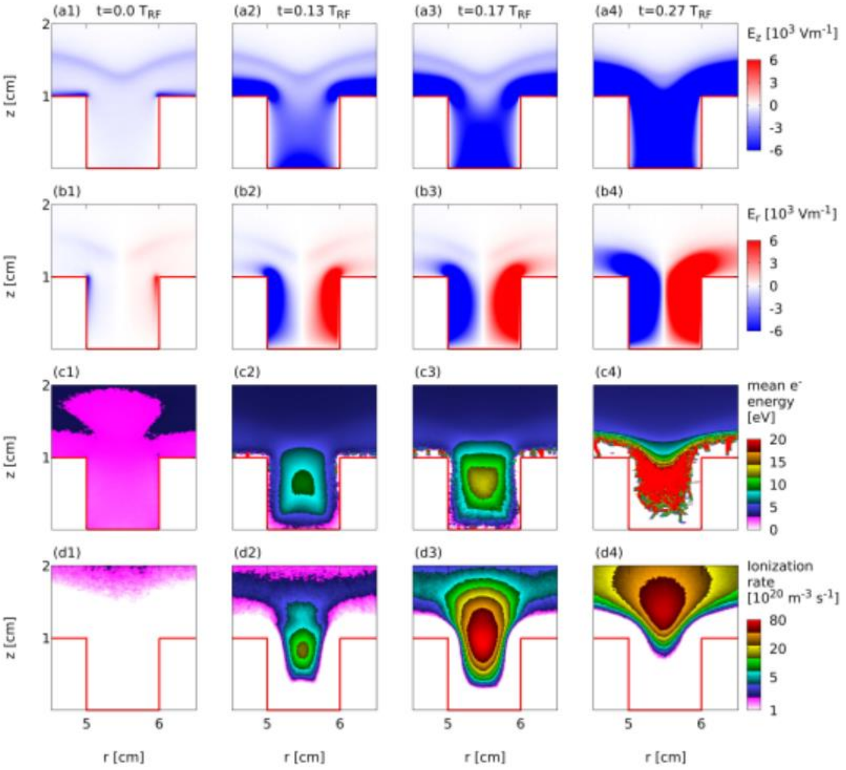

Figure 2: 2D spatial distributions of the electric field in the axial direction E_z (a1) - (a4), the electric field in the radial direction E_r (b1) - (b4), the mean electron energy (c1) - (c4), and the ionization rate (d1) - (d4) near the trench at four different times during the sheath expansion phase at the powered electrode within one RF period. Discharge conditions: Ar gas, p = 10 Pa, f = 13.56 MHz, V_0 = 300 V, L = 3 cm, 24 cm electrode diameter [7].

The physics behind this effect can be understood based on figure 2, which gives the spatial distributions of the electric field in the axial and radial directions, the mean electron energy, and the ionization rate in the vicinity of the trench and during the sheath expansion. At $t/T_{\rm rf} = 0$, the sheath is fully collapsed, which allows the electrons to penetrate into the trench. While it starts to expand, an electric field is built up in the trench in both the axial and radial directions. The electrons are accelerated in the electric field, which enhances the mean electron energy and leads to an ionization peak inside the trench. This effect is enhanced with the further expansion of the sheath until the sheath is fully expanded and most of the electrons are kicked out of the trench by the sheath, as shown in the last column in figure 2. At this point, a strong ionization peak is formed at the orifice of the trench. The strong ionization inside and above the trench finally enhances the local plasma density.

By tracing the trajectory of an exemplary electron inside the trench during the local sheath expansion, a bounce resonance movement of the electron between the sheaths at the vertical trench sidewalls is revealed, while the time evolution of the electron energy indicates a gradual increase during this process. This happens, because the sidewall sheaths are expanding simultaneously and the electron is accelerated by the sheaths continuously due to the bounce resonance heating. These computational observations agree with experimental findings of Schmidt et al. [11] and explain these measurements.

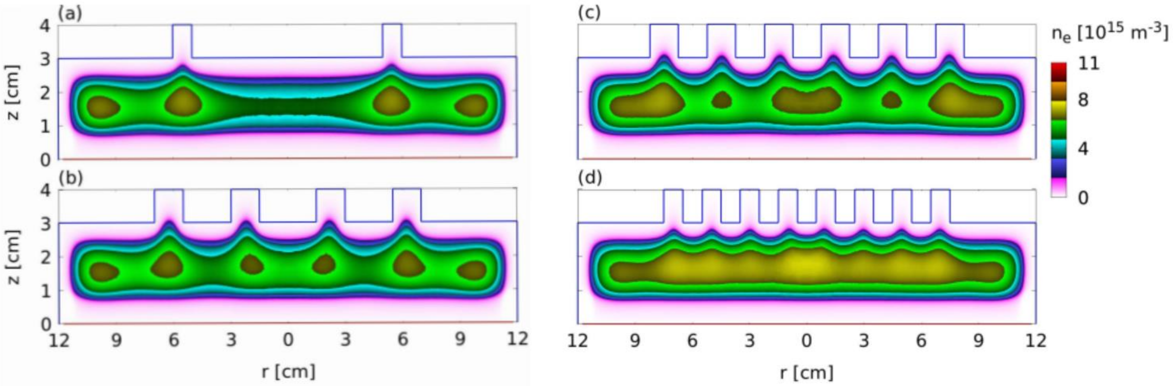

Figure 3: 2D spatial distributions of the time-averaged electron density for a reactor with ring-shaped trench(es) at the grounded electrode: one trench (w = 1 cm, d = 1cm, where w and d are the trench width and trench depth, respectively) at r = 5.5 cm (a); two trenches (w = 1.5 cm, d = 1 cm) at r = 2.25 cm and r = 6.25 cm (b); three trenches (w = 1.5 cm, d = 1 cm) at r = 1.5 cm, r = 4.5 cm, and r = 7.5 cm (c), and four trenches (w = 1 cm, d = 1 cm) at r = 1 cm, r = 3 cm, r = 5 cm, and r = 7 cm (d). The other discharge conditions are the same as in figure 2 [7].

Since this “trench effect” is expected to help improve the plasma uniformity above the wafer, which is typically placed at a planar powered electrode, multiple ring-shaped trenches are positioned at the counter grounded electrode, as shown in figure 1(b). It is found that at the discharge conditions studied here, plasma density peaks are formed near the sidewall, since the superposed sheaths at the reactor corners enhance the electron heating near the edges, which is known as the electrostatic edge effect. The trenches are, therefore, set at relatively small radial positions at the grounded electrode. The number of the trenches is gradually increased to find the best plasma uniformity. As shown in figure 3, electron density peaks are always formed below the trenches due to the locally enhanced electron power absorption and ionization rates and the magnitudes of the peaks are comparable to the density near the sidewall. In the presence of four ring-shaped trenches, the plasma uniformity is fairly good. In this way the relative nonuniformity ($n_{\max}/n_{\min} - 1$, where $n_{\max}$ and $n_{\min}$ are the maximum and minimum electron densities in the bulk region at z = 1 cm, respectively) is reduced from 43% (no trench case) to 6% (four trenches case).

These results show that at the relatively low pressures studied here, the plasma uniformity near the wafer can be improved significantly by embedding trenches into the grounded electrode. Although different reactor configurations might be used in commercial CCPs, the plasma nonuniformities caused by edge effects or electromagnetic skin/standing wave effects in such reactors are also expected to be reduced by adjusting the number and dimensions of such trenches.

The studies presented in this paper as well as in the dissertation of the author [10] are expected to provide a better understanding of the discharge mechanisms of CCPs operated under process relevant conditions and act as a knowledge basis for optimizing their engineering applications in industry.

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