Voltage waveform tailoring in radio frequency plasmas for surface charge neutralization inside etch trenches

Florian Krüger\textsuperscript{1,2,4}, Sebastian Wilczek\textsuperscript{1}, Thomas Mussenbrock\textsuperscript{2} and Julian Schulze\textsuperscript{1,3}

\textsuperscript{1} Department of Electrical Engineering and Information Science, Ruhr-University Bochum, D-44780, Bochum, Germany
\textsuperscript{2} Electrodynamics and Physical Electronics Group, Brandenburg University of Technology Cottbus-Senftenberg, D-03046 Cottbus, Germany
\textsuperscript{3} Department of Physics, West Virginia University, Morgantown, WV 26506, United States of America

E-mail: florian.krueger@rub.de

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Abstract

The etching of sub micrometer high-aspect-ratio (HAR) features into dielectric materials in low pressure radio frequency technological plasmas is limited by the accumulation of positive surface charges inside etch trenches. These are, at least partially, caused by highly energetic positive ions that are accelerated by the sheath electric field to high velocities perpendicular to the wafer. In contrast to these anisotropic ions, thermal electrons typically reach the electrode only during the sheath collapse and cannot penetrate deeply into HAR features to compensate the positive surface charges. This problem causes significant reductions of the etch rate and leads to deformations of the features due to ion deflection, i.e. the aspect ratio is limited. Here, we demonstrate that voltage waveform tailoring can be used to generate electric field reversals adjacent to the wafer during sheath collapse to accelerate electrons towards the electrode to allow them to penetrate deeply into HAR etch features to compensate positive surface charges and to overcome this process limitation. Based on 1D3V particle-in-cell/Monte Carlo collision simulations of a capacitively coupled plasma operated in argon at 1 Pa, we study the effects of changing the shape, peak-to-peak voltage, and harmonics’ frequencies of the driving voltage waveform on this electric field reversal as well as on the electron velocity and angular distribution function at the wafer. We find that the angle of incidence of electrons relative to the surface normal at the wafer can be strongly reduced and the electron velocity perpendicular to the wafer can be significantly increased by choosing the driving voltage waveform in a way that ensures a fast and short sheath collapse. This is caused by the requirement of flux compensation of electrons and ions at the electrode on time average in the presence of a short and steep sheath collapse.

Keywords: plasma etching, electric field reversal, voltage waveform tailoring, capacitively coupled plasma, plasma sheath, plasma, low temperature plasma

1. Introduction

Plasma etching is an integral part of semiconductor integrated circuit processing. Virtually all micro- and nanometer scale electronics rely on the spatially discriminatory treatment of surfaces to generate structures through deposition and removal of material [1]. The generation of sub micrometer high-aspect-ratio (HAR) structures, such as contact holes or trenches, generally...
relies on a high degree of directionality of accelerated ions. Consequently, directional plasma etching is mostly performed at low gas pressures due to the longer mean free paths of particles and at low driving frequencies in combination with high driving voltage amplitude of several thousands of volts (applied capacitively to the wafer) to accelerate ions to high velocities perpendicular to this electrode [1–4].

Etching sub micrometer HAR features into insulating materials such as SiO₂ or materials masked with insulators, e.g. photoresist-masked polysilicon, is sometimes accompanied by charging effects [5], leading to a multitude of undesired consequences. This includes, among others, a reduction of the ion flux at the bottom of the feature [6] or the creation of unwanted profile deformation issues such as notching, microtrenching or twisting [7]. This can, in turn, impair the performance of the affected component. These profiles are not limited to specific material compositions, but are generally best understood for Si and SiO₂. While the respective mechanisms differ in detail, all of them can at least partially be attributed to the disparity in the angular and velocity distribution functions of ions (IADF/IVDF) and electrons (EADF/EVDF) at the wafer [7].

The positive ions are accelerated towards the electrode surface by the potential drop in the plasma sheath. In contrast, the electron transport to the surface is impeded by the sheath electric field. Thus, electrons reach the wafer surface only during the short sheath collapse within each radio frequency (RF) period. Typically, in classical etch reactors, thermal electrons reach the wafer and, thus, in contrast to the ions, cannot penetrate deeply into HAR features. When etching dielectrics, the time averaged local surface fluxes of positive and negative charges must balance in steady state [8]. The ion angular distribution at the wafer is highly anisotropic allowing them to etch HAR structures and to penetrate deep into the etched trenches [1]. Consequently, net charges can accumulate over time on surfaces inside etch features. This generates electric field components perpendicular and parallel to the surface, which can deflect incoming ions, causing the unwanted differential etching [7]. The mentioned mechanisms are schematically depicted in figure 1 for combinations of Si and SiO₂.

The notching phenomenon describes the opening of a groove, the ‘notch’, generally found at the bottom of etched trenches of non-conductive materials or at the interface of a conductive material with an underlying insulator. Their origin has been attributed to electric field induced distortion of ion trajectories, as proposed by Arnold et al [5, 7, 9–11].

Microtrenching refers to the formation of small trench structures, where the underlying silicon substrate has been exposed near the bottom edges, leaving an oxide island in the center. Since the conducting silicon underlayer does not allow positive charge accumulation, ions tend to be further deflected towards the unwanted feature, enhancing the effect [7, 12].

The unilateral deflection of HAR structures, that can be observed during the etching of dielectrics, is called twisting. While its exact cause is still a matter of ongoing research, several contributing mechanisms have been identified. Nobuyuki et al [13] found that mask deformation strongly impacts bottom profile degradation. A link between its occurrence and the angle and velocity distribution of incident electrons and ions has been verified by Kushner et al [14].

Due to the technological relevance, a multitude of remedies for the aforementioned problems have been proposed and investigated:

1. Neutral beam etching [15] aims to reduce surface charges inside etch features by extracting ions from a plasma and neutralizing them (at least partially) before they are used for surface treatment. Due to the fact that neutralization processes such as volume neutralization [16] or grid based methods [17] introduce additional isotropy and reduced particle energies, their applicability for HAR processes is limited. Although the concept of neutral beam etching represents a promising alternative to traditional designs such as inductively and capacitively coupled plasma reactors (ICP and CCP, respectively), it has not yet found widespread industrial application [3].

2. The deposition of conducting carbon [18], fluorocarbon [18] and metal [19] films has been studied and it was found that the additional current paths significantly reduced the presence of bound surface charges. However, because of the introduction of additional processing steps and chemistry, existing, already complex procedures are further complicated and prolonged.

3. Highly directional fluxes of negatively charged particles such as ions or electrons can be utilized to neutralize the positive surface charges. Successful negative ion extraction in relevant process compositions has been demonstrated, by applying a bias voltage in the afterglow phase of pulsed CCP [20] and ICP [21] discharges. Alternatively, Highly directional electron fluxes onto a substrate can be produced in DC-augmented capacitively coupled plasmas (DC-CCPs). By applying a DC-bias voltage at the electrode opposite of the etched substrate, secondary electrons are generated by ions impinging on the DC electrode, producing highly energetic electron beams up to a few keV with small angular spreads. These beams subsequently traverse the bulk region and are able to overcome the opposing sheath potential and enter the HAR structures to neutralize the positive surface charges [14]. This method, however, suffers from the presence of an unwanted DC current and the low fluxes of energetic

![Figure 1. Surface charge effects responsible for notching, trenching and twisting in Si and SiO₂ HAR etch processes.](image-url)
electrons into etch profiles, since secondary electron emission yields are typically low.

The approach proposed and investigated in this work aims to provide an alternative method of negating surface charge effects in a way that it
• utilizes traditional and well understood reactor concepts,
• minimizes interference with process composition and chemistry,
• is not fundamentally limited to certain gas compositions (presence of negative ions),
• is independent of the reactor layout.

The subject of this work is to investigate the use of tailored voltage waveforms (TVW) in order to generate and control electric field reversals at the wafer during the local sheath collapse. Such field reversals lead to the acceleration of a high number of bulk electrons into etch profiles, i.e. they cause the generation of high fluxes of directional electrons with the ability to penetrate deeper into HAR structures to neutralize surface charges inside these trenches.

Electric field reversals are ultimately caused by the requirement of a local balance of positive ion and electron fluxes at dielectric boundary surfaces in electropositive plasmas on time average [1, 8]:

$$\int_{0}^{T_{RF}} (\Gamma_{e}(t) - \Gamma_{i}(t)) \, dt = 0.$$  \hspace{1cm} (1)

Here, $\Gamma_{e}(t)$ and $\Gamma_{i}(t)$ denote the respective time dependent surface wall fluxes of electrons and ions, respectively. $T_{RF}$ is the duration of one RF period. For most of the RF period, electrons are confined to the plasma bulk by the sheath electric field. However, when the sheath collapses, electrons reach the wafer. The number of electrons reaching the electrode during this short period of time must be sufficient to compensate the ion flux on time average. If the electron transport to the wafer is limited, electric field reversals will be generated during sheath collapse to accelerate electrons towards the wafer to ensure that enough electrons reach this boundary surface during sheath collapse to ensure flux compensation on time average. At high pressures, collisions between electrons and heavy particles can limit the electron transport to the electrode by exerting a net drag force on electrons that lowers their mobility [22, 23]. Electric field reversals in single or dual frequency CCPs in high pressure regimes have been observed experimentally in hydrogen [23–27] and neon [23] as well as by simulations in argon [23, 28], helium [23], hydrogen [29] and nitrogen [22]. At lower pressures, the presence of field reversals can be attributed to inertia effects. If the sheath collapses too quickly, electrons cannot follow due to their inertia and electric field reversals must be generated to ensure flux compensation at the electrode on time average [30, 31]. Moreover, a short sheath collapse enhances the reversed electric field, since there is less time per RF period to compensate the ion flux to the electrode by electrons.

While most previous investigations of electric field reversals were limited to a maximum of two frequencies, it can be instructive to examine non-sinusoidal waveforms and their effects on the electron dynamics during the sheath collapse.

Using multiple harmonic frequencies, locked in phase, a wide variety of TVW can be created and applied to a discharge. Operating capacitive RF plasmas at a high number of consecutive harmonics including impedance matching has been demonstrated experimentally [32–34]. In the case of ions, the use of certain TVW was found to provide enormous control of ion energy distributions at the electrodes [35–39].

In this way peaks-waveforms can be created using a fundamental frequency, $f_{0}$, and $N$ subsequent harmonics. The application of such waveforms leads to the electrical generation of a strong negative DC self bias voltage, $\eta$, via the electrical asymmetry effect (EAE) that causes the mean ion energy at the powered electrode to be higher compared to the grounded electrode [37]. Schulze et al. presented a detailed derivation of the EAE [36], in which they found the peaks-waveform to lead to the generation of the maximum DC self bias.

The application of peaks-waveforms is expected to have drastic consequences on the electron dynamics and the generation of electric field reversals during sheath collapse at the powered electrode, too, since it leads to a shorter and faster sheath collapse compared to single frequency discharges. Thus, depending on the exact shape of the waveform and the discharge conditions electrons will not be able to follow the collapsing sheath by diffusion due to their inertia and electric field reversals will be generated. In this work, we employ particle-in-cell/Monte Carlo collision (PIC/MCC) simulations of capacitively coupled RF discharges operated at 1 Pa in argon, to investigate the effects of voltage waveform tailoring (VWT) on the electric field reversal during sheath collapse as well as on the electron angular and velocity distribution function (EADF/EVDF) at the wafer surface by changing the number of driving harmonics, their frequencies, the driving voltage amplitude and the shape of the voltage waveform systematically. We demonstrate that the field reversal, the EADF and the EVDF at the wafer surface can be controlled by VWT in a way that should allow for the acceleration of a high number of bulk electrons deeply into HAR etch profiles to compensate positive surface charges inside these trenches. This corresponds to a proof-of-principle demonstration of a novel technique to avoid this major limitation of process performance in HAR plasma etching of dielectrics.

The paper is structured as follows: In section 2, the used PIC/MCC code is described and the applied voltage waveforms are introduced. In section 3, the results are presented. This section is divided into 4 parts corresponding to the effects of the variation of (i) the number of driving harmonics, (ii) the total voltage amplitude, (iii) the fundamental driving frequency for peaks-waveforms, respectively, and (iv) of the shape of the driving voltage waveform. Finally, conclusions are drawn in section 4.

2. Simulation setup

A geometrically symmetric CCP is studied by means of 1DV3 PIC/MCC simulations. The electrostatic code developed by Mussenbrock has been benchmarked against other PIC/MCC implementations by different authors [40]. Collisions are implemented based on a MCC scheme for an argon background gas. The cross sections for ion-neutral (isotropic and backward
elastic scattering) and electron-neutral (excitation, ionization and elastic) collisions are taken from the JLLA database [41]. The gas pressure, $p$, gas temperature, $T_g$, and the electrode gap, $L_{\text{gap}}$, are kept constant at $p = 1$ Pa, $T_g = 300$ K and $L_{\text{gap}} = 50$ mm, respectively. The electrodes are assumed to be infinite, planar and parallel. The grounded electrode is located at $x = 50$ mm and at the driven electrode at $x = 0$ mm different voltage waveforms, $V(t)$, are applied. The etch process itself is not included in the simulation, i.e. no etch trenches are considered. This is justified by the fact that the plasma does not penetrate into sub micrometer features, since the trench diameter is much smaller than twice the sheath width [42, 43]. Therefore, energy distribution functions of different particle species obtained from our simulations at the electrode surface can be assumed to be good approximations of distribution functions at the plasma-facing orifice of a sub micrometer HAR etch feature. In sections 3.1–3.3, a peaks voltage waveform, $V(t) = V_{\text{peak}}(t)$, is applied, which is constructed by a set of $N$ harmonic frequencies:

$$V(t) = V_{\text{peak}}(t) = V_{\text{tot}} \sum_{k=1}^{N} 2 \cdot \frac{N - k + 1}{N(N + 1)} \cos(2\pi f_0 t + k\pi).$$

(2)

The fundamental frequency is kept constant at $f_0 = 5$ MHz in sections 3.1 and 3.2, while it is varied from 5 to 15 MHz in section 3.3. $k$ is the harmonic order of the frequency and $V_{\text{tot}}$ is the total voltage amplitude. Figure 2(a) shows various peaks-waveforms for different choices of $N$. Increasing $N$ causes a decrease of the peak width and, thus, a shorter and steeper sheath collapse at the driven electrode. In section 3.4, customized voltage waveforms, $V(t) = V_{\text{custom}}(t)$, are used according to:

$$V(t) = V_{\text{custom}}(t) = V_{\text{tot}} \sum_{i=0}^{4} a_i \cos(2\pi f_0 t + k_i \pi).$$

(3)

Here, $k_i$ is the harmonic order and $a_i$ the respective relative harmonic’s amplitude. $k_i$ and $a_i$ are chosen in a way to minimize the duration of the sheath collapse at the powered electrode by choosing $k_0 = 1$, $k_1 = 2$, $k_2 = 10$, $k_3 = 15$, $k_4 = 30$ and $a_i = 0.2$ $\forall$ $i$. The fundamental frequency is set to be $f_0 = 2$ MHz. The corresponding waveform is depicted in figure 2(b).

For every simulation, an equidistant grid is discretized with a grid cell size of $\Delta x = L_{\text{gap}}/N_{\text{cells}}$, where $N_{\text{cells}}$ is the number of grid cells and varies between 250 and 600. The time step is given by $\Delta t = (f_0 N_{\text{stage}})^{-1}$, where $N_{\text{stage}}$ is the number of time steps within the fundamental radio frequency period, $T_{\text{RF}} = 1/f_0$ and changes between 2000 and 15 000. Due to the wide range of resulting plasma densities and due to the variation of the fundamental frequency as well as the number of harmonics, $\Delta x$ and $\Delta t$ are adjusted in order to fulfill the classical stability and accuracy conditions in all cases [44, 45]. All simulations have been performed with $10^3$ super-particles for each species, after convergence is achieved. In order to simplify the study, a constant ion induced secondary electron emission coefficient of $\gamma = 0.1$ is used and no reflection of particles at the electrode is considered (electron sticking of $s = 1$). Recording of diagnostic data is carried out for a set number of RF periods after convergence has been reached. Incident particles are defined as those which, at any given time, leave the predefined simulation boundaries ($0 < x < L_{\text{gap}}$). These particles’ velocity information is saved and compiled into EADF and EVDF histograms.

3. Results

In this section, a wide range of external control parameters (number of harmonics, total voltage amplitude, fundamental frequency, waveform shape) are varied to study their effects on the electron dynamics at the electrode as well as the electric field reversal during the sheath collapse in a capacitive RF plasma operated in argon at 1 Pa by VWT. In sections 3.1–3.3, the peaks-waveform is chosen as the shape of the driving voltage waveform, since it ensures a short and steep sheath collapse at the powered electrode, where the wafer is assumed to be located. In section 3.4, a customized driving voltage waveform is used based on the insights obtained in previous sections to generate an even stronger electric field reversal and even more anisotropic electrons at the wafer surface.

3.1. Peaks-Waveform: variation of the number of harmonics

First, for the peaks-waveform, the number of harmonics is varied from $N = 3$ to $N = 17$ at otherwise constant discharge conditions. For this parameter variation, a fundamental
driving frequency of $f_0 = 5\ MHz$, a gas pressure of 1 Pa and a voltage amplitude of $V_0 = 1000\ V$ are chosen as fixed input parameters. Exemplary waveforms are illustrated in figure 2(a). This plot shows, that the peak width of the voltage waveform, during which the sheath collapses at the powered electrode, and the rise-/fall-time decrease as a function of the number of harmonics, i.e. the local sheath collapse gets shorter and steeper. This is expected to cause a stronger electric field reversal, since electrons can reach the wafer during a shorter period of time to compensate the positive ion flux on time average and they can hardly follow the quick sheath collapse due to their inertia. This, in turn, will influence the electron dynamics at the electrode.

In order to identify the optimal waveform, the EVDF and the EADF at the electrode are investigated in detail. Figure 3 shows the normalized EADF (a) and the normalized EVDF at the electrode surface (b) for a selected number of harmonics averaged over one RF period. The EADF gets more narrow and its maximum is shifted to smaller angles relative to the surface normal by increasing the number of harmonics. For $N = 15$, its maximum is found at $\theta_{\text{max}} \approx 17^\circ$. In parallel, the maximum of the EVDF at the electrode surface is shifted towards higher velocities ($v_{e,n,max} \approx 3.3 \cdot 10^6\ m/s$ at $N = 15$). In classical single frequency discharges, thermal (isotropic) electrons reach the electrode by diffusion during the sheath collapse and arrive at the electrodes at velocities of $v_{e,n} \approx 3 - 5 \cdot 10^5\ m/s$. Thus, these results demonstrate the enormous potential of VWT to accelerate energetic anisotropic electrons into a HAR trench, which requires small values of $\theta$ and high values of $v_{e,n}$.

Figure 4(a) shows the mean angle of electrons impinging at the electrode relative to the surface normal, $\bar{\theta}$, and mean normal electron velocity, $\bar{v}_{e,n}$, at the powered electrode (a) as well as the average electron density, $n_e$, and the DC self bias, $\eta$, (b) as a function of the number of harmonics, $N$, in case of a peaks-waveform and for $p = 1\ Pa$, $f_0 = 5\ MHz$ and $V_{\text{tot}} = 1000\ V$.

Figure 3. Electron angular distribution function (EADF) (a) and electron velocity distribution function (EVDF) (b) at the powered electrode surface in case of a peaks-waveform for different numbers of consecutive harmonics, $N$, and $p = 1\ Pa$, $f_0 = 5\ MHz$ and $V_{\text{tot}} = 1000\ V$.

Figure 4. Mean angle of electron incidence relative to the surface normal, $\bar{\theta}$, and mean normal electron velocity, $\bar{v}_{e,n}$, at the powered electrode (a) as well as the average electron density, $n_e$, and the DC self bias, $\eta$, (b) as a function of the number of harmonics, $N$, in case of a peaks-waveform and for $p = 1\ Pa$, $f_0 = 5\ MHz$ and $V_{\text{tot}} = 1000\ V$. 

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velocity indicates a linear trend and might reach higher velocities at higher harmonics. However, higher harmonics above $N > 17$ are beyond the scope of this study due to numerical and practical limitations.

A linear increase of the average plasma density, $n_e$, (black solid line) and an increase of the absolute value of the DC self-bias voltage (red dashed line), $\eta$, as a function of $N$ are observed (see figure 4(b)). Increasing the number of harmonics of a constant fundamental frequency at fixed total voltage amplitude leads to a more effective electron power gain and, thus, to an enhanced ionization and a higher plasma density [1]. For single frequency discharges this effect has been investigated in the context of $\alpha$-mode heating for a wide variety of plasma regimes, both theoretically [46–49] and experimentally [26, 27, 50–52]. The DC self-bias (red dashed line in figure 4(b)) can be varied between 585 and 730 V by changing the number of harmonics. This is caused by an increase of the difference between the absolute values of the extrema of the driving voltage waveform as a function of $N$ according to the EAE [36].

The origin of the resulting electron distribution functions at the wafer is related to the dynamics of the electric field in the vicinity of the driven electrode during sheath collapse. Spatio-temporal plots of the electric field in this region are shown in figure 5 for different numbers of harmonics, $N$. The sheath collapses at a time of $t_{coll} \approx 95$ ns. Clearly, an electric field reversal is generated during the sheath collapse and its magnitude increases as a function of $N$ up to values of 4000 V m$^{-1}$ for $N = 15$, since the duration of the sheath collapse is decreased and the ion flux to the electrode is enhanced, i.e. more electrons must reach the electrode during sheath collapse to compensate the ion flux on time average. This is the reason for the observed changes of the EADF and the EVDF at the electrode surface as a function of $N$. The ion flux increases as a function of $N$ similarly to the average electron density. At constant driving voltage this also causes the maximum sheath width to decrease as a function of $N$, which can be observed clearly in figure 5. In fact, the exact spatio-temporal dynamics of the electric field are affected by the increase of the plasma density as a function of $N$, which leads to a smaller sheath for a given driving voltage amplitude, and by the increase of the absolute value of the DC self bias as a function of $N$, which leads to an increase of the maximum sheath voltage at the powered electrode in low pressure electropositive discharges [36]. While the increase of the plasma density causes a slower sheath collapse, the increase of the maximum sheath voltage causes a faster sheath collapse. These effects compensate partially. In fact, figure 5 shows that the maximum sheath width decreases as a function of $N$, i.e. the effect of the increased plasma density on the maximum sheath width dominates.

Figure 5 also shows additional oscillations of the electric field at the sheath edge during the phase of sheath expansion. These dynamics are characteristic for multi frequency capacitively coupled plasmas and related to the nonlinearity of such systems, i.e. to the self-excitation of the Plasma Series Resonance [53–56]. These field oscillations contribute to the electron power gain and enhance the ionization. However,
they do not influence the electron dynamics at the electrode directly, since the instantaneous sheath potential (negative electric field in figure 5) is too high for electrons to overcome this potential and reach the electrode.

3.2. Peaks-Waveform: variation of the total voltage amplitude

The time and space resolved electric field near the powered electrode is depicted in figure 8 for different total driving voltages, $V_{\text{tot}}$. With increasing $V_{\text{tot}}$, a significant increase of the electric field reversal can be observed, while the sheath width slightly increases. The absolute value during the electric field reversal for $N = 5$ and $V_{\text{tot}} = 4000$ V is in the range of 3000 V m$^{-1}$ (see colorbar in figure 8). The corresponding EADF and EVDF as well as the electron’s mean angle of incidence and mean velocity are depicted in figures 6 and 7, respectively. In comparison with the variation of the number of harmonics, the case for $N = 15$ and $V_{\text{tot}} = 1000$ V yields a higher absolute value for the electric field which is in the range of 4000 V m$^{-1}$ (see colorbar in figure 5). Consequently, smaller angles of incidence of electrons relative to the surface normal as well as higher electron velocities perpendicular to the surface are obtained by changing the number of harmonics. Therefore, under the discharge conditions studied here, tailoring the voltage waveform by varying the number of consecutive harmonics is more efficient with respect to the electron dynamics than varying the total voltage.

3.3. Peaks-Waveform: variation of the fundamental frequency

In this section, the effect of changing the fundamental driving frequency, $f_0$, on the EADF and the EVDF at the powered electrode are studied. A peaks-waveform constructed based on $N = 5$ consecutive harmonics of $f_0$ is used at 1 Pa in argon. The electrode gap is 50 mm. Decreasing the fundamental frequency at a constant driving voltage amplitude leads to a decrease of the plasma density and, eventually, no plasma can be sustained. Therefore, under the discharge conditions studied here, tailoring the voltage waveform by varying the number of harmonics is more efficient with respect to the electron dynamics than varying the total voltage.
Figure 8. Space and time resolved electric field at the driven electrode for different total voltages $V_{\text{tot}}$: $V_{\text{tot}} = 750$ (top left), $V_{\text{tot}} = 1250$ (top right), $V_{\text{tot}} = 2500$ (bottom left), $V_{\text{tot}} = 4000$ (bottom right), in case of a peaks-waveform and for $p = 1 \text{ Pa}, f_0 = 5 \text{ MHz}$ and $N = 5 \text{ V}$. Only a fraction of the fundamental RF period that includes the local sheath collapse is shown.

Figure 9. Electron angular distribution function (EADF) (a) and electron velocity distribution function (EVDF) (b) at the powered electrode surface in case of a peaks-waveform for different fundamental driving frequencies at $p = 1 \text{ Pa}$ and $N = 5$. The driving voltage amplitude is adjusted to maintain a constant average electron density of $n_e = 1.5 \cdot 10^{15} \text{ m}^{-3}$.

$n_e = 1.5 \cdot 10^{15} \text{ m}^{-3}$. Figure 9 shows the effects of changing the fundamental driving frequency from 15 to 5 MHz on the EADF and the EVDF at the wafer. Decreasing $f_0$, while increasing $V_{\text{tot}}$ to maintain a constant plasma density, leads to the generation of more directed electrons at the electrode surface. Figure 10(a) shows the corresponding decrease of the mean angle of electron incidence at the electrode relative to the surface normal and the increase of the mean normal electron velocity towards lower values of $f_0$. Figure 10(b) shows the change of the total driving voltage amplitude as a function of $f_0$ required to maintain a constant average plasma density as well as the absolute value of the DC self bias as a function of the fundamental driving frequency. $|\eta|$ increases towards lower values of $f_0$, since the driving voltage amplitude is increased. The observed changes of the EADF and the EVDF at the wafer surfaces are caused by a different spatio-temporal dynamics of the electric field reversal for different fundamental driving frequencies (see figure 11). While the
strength of the field reversal is in all cases in the same range (500–1000 V m⁻¹), the region in space and time, where and when a reversed field is generated, is different. Only for \( f_0 = 5 \text{ MHz} \), the region of reversed electric field reaches the electrode. This leads to a continuous acceleration channel for the electrons throughout the sheath region during sheath collapse and, thus, more energetic electrons hit the surface in this scenario. At higher fundamental driving frequencies, the field reversal stops a few mm in front of the electrode and the remaining negative electric field in direct vicinity of the electrode leads to a deceleration of electrons. Consequently, the EADF and EVDF for these frequencies indicate a different shape compared to the \( f_0 = 5 \text{ MHz} \) case. The reason why the field reversal reaches the electrode surface at low driving frequencies is the fact that higher driving voltage are used at lower frequencies. Thus, the voltage drop across the local sheath is enhanced and ions are accelerated to higher velocities inside the collisionless sheath. Flux continuity
remains relatively low, because the customized waveform used. Discharge conditions: argon, 1 Pa, 50 mm electrode gap.

In this section, the effects of the customized voltage waveform are studied. These results indicate that a further reduction of $f_0$ will lead to the generation of even more directed electrons at the wafer. This regime was not studied here due to computational limitations. At lower driving frequencies the duration of the fundamental RF period and, thus, the computational time increase. Simultaneously, the driving voltage must be increased to maintain the plasma. In order to fulfill all stability criteria of PIC/MCC simulations, a smaller time step is required.

The findings obtained for the peaks-waveform show that energetic directed electrons can be generated during the sheath collapse in vicinity to the wafer based on this driving voltage waveform in low pressure RF plasmas via the generation of electric field reversals during the local sheath collapse. Increasing the number of harmonics, $N$, and the total driving voltage amplitude, $V_{\text{tot}}$, as well as decreasing the fundamental driving frequency, $f_0$, were found to enhance this effect.

### 3.4. Customized driving voltage waveform

In this section, the effects of the customized voltage waveform defined by equation (3) on the generation of an electric field reversal during sheath collapse and on the EADF as well as the EVDF at the wafer surface are investigated. In order to minimize the duration of the sheath collapse at the powered electrode, while using only a relatively low number of 5 harmonics, we choose $k_0 = 1$, $k_1 = 2$, $k_2 = 10$, $k_3 = 15$, $k_4 = 30$ and $a_i = 0.2 \quad \forall \ i$ in equation (3) and study the effects of changing the total driving voltage amplitude, $V_{\text{tot}}$, in argon at 1 Pa and 50 mm electrode gap. This corresponds to a superposition of frequencies between 2 and 60 MHz. The goal is to increase the magnitude of the electric field reversal during sheath collapse by minimizing its duration in order to generate more directed electrons at the wafer surface that will propagate deeply into HAR etch features to compensate positive surface charges inside these structures. Clearly, our choice of voltage waveform shape is only one of many possible examples and no systematic optimization has been performed. Such an optimization of the waveform remains a topic for future work. Here, our intention is to demonstrate that tailoring the driving voltage waveform beyond using a peaks-waveform allows to further optimize the generation of energetic directed electrons at the wafer in the frame of a proof-of-principle investigation.

In comparison to the results shown in sections 3.1–3.3, figures 12 and 13 show that using this customized driving voltage waveform allows to generate more energetic directed electrons at the wafer at low driving voltage amplitudes and a low number of harmonics, i.e. the mean normal electron velocity at the powered electrode increases to a maximum of about $4.1 \cdot 10^6$ m·s$^{-1}$ for $V_{\text{tot}} = 1000$ V at a low mean angle of electron incidence at the wafer relative to the surface normal of about 20°. This corresponds to an electron energy of about 50 eV in the direction perpendicular to the wafer. Considering that the electron energy parallel to the wafer is of the order of 1 eV, this corresponds to a very strong anisotropy of electrons. According to figure 13(b) the average plasma density as well as the absolute value of the DC self bias both increase as a function of $V_{\text{tot}}$. However, compared to other (peaks-)driving voltage waveforms (see previous sections), $|\xi|$ remains relatively low, because the customized waveform used here is not optimized to induce a maximum electrical asymmetry.

These effects are caused by an enhanced electric field reversal during the sheath collapse, which is induced by the customized driving voltage waveform by shortening the duration of the sheath collapse at the powered electrode within each period of the fundamental driving frequency. In comparison to the peaks-waveform (see figure 5), figure 14
clearly shows this effect. While the mean angle of electron incidence hardly depends on the total driving voltage amplitude, there is a maximum of the mean normal electron velocity at the wafer for \( V_{\text{tot}} = 1000 \) V.

Figure 14 shows the spatio-temporal dynamics of the electric field at the driven electrode. In all 4 cases two pronounced electric field reversals appear during the sheath collapse at approximately \( t_1 \approx 237 \) ns and \( t_2 \approx 247 \) ns. However, for \( V_{\text{tot}} = 500 \) V and \( V_{\text{tot}} = 1000 \) V the first electric field reversal at \( t_1 \) does not reach the electrode and electrons are decelerated in the remaining negative field region, i.e. the first sheath collapse is incomplete. Only in the second field reversal at \( t_2 \) a continuous acceleration channel is present. Therefore, the EVDF at the electrode shows two peaks for \( V_{\text{tot}} = 500 \) V (at about \( 2.8 \times 10^6 \) m s\(^{-1}\) and at about \( 3.6 \times 10^6 \) m s\(^{-1}\)) and for \( V_{\text{tot}} = 1000 \) V (at about \( 1.3 \times 10^6 \) m s\(^{-1}\) and at about \( 3.4 \times 10^6 \) m s\(^{-1}\)).

Figure 13. Mean angle of electron incidence relative to the surface normal, \( \bar{\theta} \), and mean normal electron velocity \( v_{e,n} \) at the powered electrode (a) as well as the average electron density and the absolute values of the DC self bias (b) as a function of the total driving voltage amplitude, \( V_{\text{tot}} \). The customized waveform specified by equation (13) with \( k_0 = 1, k_1 = 2, k_2 = 10, k_3 = 15, k_4 = 30 \) and \( a_i = 0.2 \) \( \forall \ i \) is used. The fundamental frequency is set to be \( f_0 = 2 \) MHz and 5 non-consecutive harmonics are used. Discharge conditions: argon, 1 Pa, 50 mm electrode gap.

Figure 14. Space and time resolved electric field at the driven electrode for custom waveform with total applied voltages \( V_{\text{tot}} \): \( V_{\text{tot}} = 500 \) (top left), \( V_{\text{tot}} = 1000 \) (top right), \( V_{\text{tot}} = 1500 \) (bottom left), \( V_{\text{tot}} = 2000 \) (bottom right). The fundamental frequency is set to be \( f_0 = 2 \) MHz and 5 non-consecutive harmonics are used. Discharge conditions: argon, 1 Pa, 50 mm electrode gap. Only a fraction of the fundamental RF period that includes the local sheath collapse is shown.
higher voltages ($V_{\text{tot}} = 1500 \text{ V}$ and $V_{\text{tot}} = 2000 \text{ V}$), both field reversals with almost the same structure and magnitude reach the driven electrode, thus, a second peak in the EVDF is not present. If the sheath collapses only once per low frequency period, there is less time for electrons to compensate the ion flux on time average compared to scenarios, where two full sheath collapses occur per low frequency period. Thus, for cases, where the sheath collapses fully only once per low frequency period, a stronger field reversal with a maximum close to the electrode surface is generated. This leads to the generation of more anisotropic and energetic electrons at the wafer. Here, this is the case for 500 and 1000 V. In case of 1000 V, the plasma density and the ion flux are higher. Thus, more electrons must be drawn to the electrode compared to the 500 V scenario. Therefore, the reversed field is higher in this case.

4. Conclusion

The use of TVW to generate and control electric field reversals during the sheath collapse in low pressure capacitive RF plasmas was investigated to assess the potential of this technology to accelerate electrons into sub micrometer HAR etch features to compensate positive surface charges inside these structures. The effects of different driving voltage waveforms on the electron angular and velocity distribution functions (EADF/EVDF) at the wafer surface were studied. It was found that peaks-waveforms lead to the generation of strong electric field reversals and highly energetic directed electrons at the electrode surface, since their presence ensures a short and steep sheath collapse within each period of the fundamental driving frequency. This enhances the electric field reversal, since the ion flux to this electrode must be balanced by electrons on time average and electron transport to the electrode by diffusion is insufficient in the presence of such a short and steep sheath collapse. Increasing the number of consecutive harmonics used to construct the peaks-waveform and the total driving voltage amplitude as well as decreasing the fundamental driving frequency were found to enhance the generation of directed energetic electrons at the electrode surface due to their effects on the reversed electric field during sheath collapse. Finally, a customized driving voltage waveform was designed based on 5 harmonics of a fundamental driving frequency to minimize the duration of the sheath collapse. Such a waveform can be generated and matched with reasonable efforts experimentally. For a fundamental driving frequency of 2 MHz and a total driving voltage amplitude of 1000 V, a high flux of directed electrons at the wafer at mean velocities perpendicular to the electrode of $4.1 \cdot 10^6 \text{ m s}^{-1}$ (approximately 50 eV) could be generated during sheath collapse with small angular spread. These results show that TVWs can be used to control electric field reversal during the sheath collapse in capacitive RF plasmas and to accelerate electrons to high velocity perpendicular to the wafer in close vicinity to its surface. This provides the basis for using this technology to compensate positive surface charges inside HAR etch profiles to avoid various limitations of dielectric plasma etching. In comparison to existing methods, this technology generates a high flux of directed electrons, does not require DC power sources, and can be added to any etching process without modifying the reactor itself.

Clearly, these findings correspond to a proof-of-principle demonstration. More detailed parameter variations are required to optimize this technology. Multi-dimensional simulations that self-consistently include the etch profile and the charge dynamics inside trenches should be performed including lower driving frequencies, higher voltages, and asymmetric reactor designs. Also, experimental tests are required. Finally, the effect should be modeled and the use of TVWs in remote plasma sources should be studied, where the plasma is not generated by the TVW itself, but only the ion and electron distribution functions at the wafer are controlled in this way.

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ORCID iDs

Florian Krüger @ https://orcid.org/0000-0003-2761-905X
Sebastian Wilczek @ https://orcid.org/0000-0003-0583-4613
Thomas Mussenbrock @ https://orcid.org/0000-0001-6445-4990
Julian Schulze @ https://orcid.org/0000-0001-7929-5734

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