Equivalent electric circuit model of accurate ion energy control with tailored waveform biasing

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Equivalent electric circuit model of accurate ion energy control with tailored waveform biasing

Qihao Yu (余骑浩)1,∗, Erik Lemmen1, Bas Vermulst1,∗, Adriaan J M Mackus2, Wilhelmus M M (Erwin) Kessels2 and Korneel Wijnands1

1 Department of Electrical Engineering, Eindhoven University of Technology, PO Box 513, The Netherlands
2 Department of Applied Physics, Eindhoven University of Technology, PO Box 513, The Netherlands

E-mail: q.yu@tue.nl and b.j.d.vermulst@tue.nl

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Abstract

For atomic scale plasma processing involving precise, (an)isotropic and selective etching and deposition, it is required to precisely control the energy of the plasma ions. Tailored waveforms have been employed to bias the substrate table to accurately control this ion energy. Recent research has shown that switched-mode power converters can be used to generate this kind of waveform, with the benefit of increased energy efficiency and flexibility compared to the traditionally used linear amplifiers. In this article, an improved equivalent electric circuit model of the plasma reactor is proposed to allow simulation and bias waveform optimization. The equivalent electric circuit is analysed for different process phases, including the charge, discharge, and post-discharge phase. The proposed model is suitable for electric circuit simulation and can be used for predicting the electric waveforms and ion energy distributions. Plasma parameters are required as input for the model, thus an empirical parameter identification method based on the electrical measurements of the bias voltage and output current waveforms is introduced. Since these electrical measurements do not interact with the plasma process, the proposed parameter identification method is nonintrusive. Experiments have been carried out, which demonstrate that the proposed model and parameter identification method provide the expected accuracy.

Keywords: atomic layer etching, atomic layer deposition, equivalent electric circuit, ion energy distribution, switched-mode power converter, tailored waveform biasing

(Some figures may appear in colour only in the online journal)

1. Introduction

Plasma processing is crucial in semiconductor manufacturing, such as plasma etching and deposition to fabricate nanodevices. With the size of integrated circuits (ICs) continuing to shrink, atomic scale processing, including atomic layer etching (ALE) and atomic layer deposition (ALD), turns to be vital since these methods can offer high selectivity, precise thickness control and 3D processing of the materials [1]. Taking plasma ALE for example, the thickness of the etched material is precisely controlled by the use of the self-limiting reactions. During such an ALE process, the substrate surface is typically first exposed to the reactive species to weaken the binding energy between the surface and bulk atoms of the substrate [2]. The goal of this step is to modify the surface so that the surface atoms can be removed without affecting the underlying material [3]. After that, energetic plasma ions bombard...
the modified substrate surface [4]. The ions should carry sufficient energy such that they can break the weakened bonds and knock out the surface atoms. Meanwhile, the energy of the ions should not exceed the threshold for etching the underlying bulk material. Therefore, the ion energy distribution (IED) should fall into a narrow window to achieve such etch selectivity. Under some circumstances, this energy window can be as narrow as 10 eV such as the plasma ALE of Ge by using Cl₂ plasma for surface modification [5].

Figure 1 shows a schematic representation of a typical inductively coupled plasma (ICP) reactor often employed for ALE. It shows the common case that the substrate is smaller than the table, for which part of the table is also exposed to the plasma. As shown in figure 1, gas is infused from the top, and the plasma is ignited and sustained in the chamber by an external radio-frequency (RF) power source through a matching network unit. The pressure in the chamber is kept low. This reduces the particle collisions in the plasma sheath near the substrate surface, allowing for ion bombardment. To do so, often, a power converter is connected to the table, which generates a negative voltage on the substrate surface. As a result, the ions in the bulk plasma are accelerated towards the table, and bombard the substrate surface to remove the target material. Moreover, the normal direction of ion bombardment to the substrate surface enables anisotropic etching.

Ion energy can be controlled by biasing the substrate surface voltage with a power converter. A narrow IED calls for a quasi-constant substrate surface voltage potential. For a conductive substrate, the ion energy can be controlled by a dc bias voltage. However, for a dielectric substrate, there is an equivalent substrate capacitance [6]. The bombarding ions are accumulated on the substrate surface, thus the voltage potential of the substrate surface increases, known as the charging effect, leading to a broad IED.

Different techniques have been studied targeting a narrow IED for the dielectric substrates. In traditional single-frequency capacitively coupled plasmas (CCPs), a single power source is used to control the ion density, ion flux, ion energy and other plasma properties, which can easily lead to plasma nonuniformity [7, 8] and makes it hard to accurately control the ion energy independently of ion flux [9]. Dual-frequency CCPs were therefore proposed [10, 11]. It uses a high-frequency RF source to mainly control ion flux and an RF source of lower frequency to control ion energy separately. It offers a better plasma uniformity over large surface areas compared to the single-frequency CCPs [12]. However, the coupling effect of the two RF sources can cause issues such as substrate damage or reduced etching rate [13]. A better decoupled control of ion flux and ion energy in dual-frequency CCPs can be obtained by controlling the phase shift between two fixed-frequency RF sources utilizing the electrical asymmetry effect, as done in [14–17]. Moreover, other voltage waveform tailoring techniques, such as using a low-frequency square waveform with high-frequency harmonics [18, 19], have also been developed for CCPs.

Compared to CCPs, ICPs enjoy the benefit of higher plasma density. ICPs are the focus of this article. In such ICP, the RF power is inductively coupled to the plasma across a dielectric window, which yields a low plasma floating potential of typically 20 to 40 V with respect to the substrate and enables better decoupled control of ion flux and ion energy [9]. Different biasing techniques for ICPs have been studied [20–22], including RF biasing [23–25], pulse-shaped biasing [26–28], and tailored waveform biasing [29–33], the voltage waveforms of which are shown in figures 2(a)–(c), respectively. The negative parts of all the three biasing waveforms are used to create a negative voltage potential on the substrate surface to enhance ion energy. The bombarding ions are charging the substrate capacitance during this time. Therefore, to prevent over-voltage on the substrate, a short positive voltage is applied to attract the electrons and reset the voltage potential periodically, i.e. discharging the substrate.

The RF biasing creates a sinusoidal voltage potential on the substrate surface, thus generating a broad and bimodal IED as depicted in figure 3 [34, 35], which is not preferred in atomic scale processing. Although increasing the RF biasing frequency helps narrowing the IED, it is limited by the ion mass and it is much less effective for light ions such as hydrogen. Furthermore, a sufficiently large biasing frequency makes the RF wavelength comparable to the substrate dimension, and this can cause severe nonuniformities [23].
pulse-shaped biasing could deliver a narrow single-peak IED as depicted figure 3 under specific conditions, specially for a dielectric substrate with large capacitance. However, the IED is heavily distorted if the substrate capacitance is small, since a small substrate capacitance leads to a large voltage potential rise due to the charging effect, thus resulting in a broad IED [30]. Although increasing pulse-shaped biasing frequency can reduce this charging effect as well, similar drawbacks occur as for increasing the RF biasing frequency. Compared to the pulse-shaped biasing, tailored waveform biasing uses a negative voltage slope to compensate the charging effect. The voltage slope rate should be well tuned, the value of which is determined by the properties of the substrate and the ion flux. Under this circumstance, the voltage potential of the substrate bottom is linearly decreasing, thus the substrate surface potential remains quasi-constant. Tailored waveform biasing requires a significantly reduced repetition frequency compared to the RF biasing and pulse-shaped biasing. The capability of accurate ion energy control makes tailored waveform biasing well-suited for the highly-selective atomic scale processing.

Traditionally, the tailored waveform is generated by class-A linear amplifiers, which are typically energy inefficient. In addition, a tuned matching network is necessary in order to match the impedance of the linear amplifier and the plasma reactor [25]. Recently, switched-mode power converters (SMPCs) have been applied to generate the tailored waveform, which have a significantly higher energy efficiency compared to the linear amplifier [36]. It also advantageously omits the matching network since the converter operates in a quasi-dc mode. The bias waveform can be actively and flexibly tailored by this converter, with controllable pulse magnitude and voltage slope rate. The SMPC brings huge convenience and flexibility to the tailored waveform biasing. However, for electrical engineers, an equivalent electric circuit (EEC) model of the reactor is needed to conduct circuit simulations and optimize the electrical design. For plasma physicists, it is also desired to combine the simulation of the bias converter and the plasma reactor to predict the IED and optimize the bias waveform. A complete EEC model of the reactor enables this combined simulation on the circuit level, which tremendously reduces the computation time compared to a traditional plasma simulation method like particle-in-cell (PIC).

Although some reactor models have been derived in previous research, most of them are used for RF biasing [9, 25, 32, 37–39] or are a steady-state simplification of tailored waveform biasing [36, 40, 41]. These models cannot be directly used for transient analysis in tailored waveform biasing because the discharge process is not accurately included. In [42], a modified model is proposed, which emulates the discharge process by a virtual sheath reset circuit. While this modified model can roughly represent the charge and discharge processes, and thus can be used for electric circuit simulation, it significantly increases the complexity of the circuit. In this article, an improved EEC model is introduced with detailed analysis of the transient response during the charge, discharge, and post-discharge phase.

Parameters of the EEC model, including the values of the capacitors and currents, are required in order to fulfill circuit simulation and IED prediction. Typically these parameters are derived from plasma physics theory. However, the derived parameters can be variant and nonlinear, which unnecessarly increases the complexity of the model [25]. Furthermore, the determination of some parameters demands intrusive measurements of plasma properties, such as measuring the ion density with a Langmuir probe [43]. In this research, a parameter identification method is introduced, which linearizes the electric parameters in the model within the operating range. The method is fully based on nonintrusive electrical measurements, being the voltage and current waveforms on the power converter side.

With the proposed model and the parameter identification method, a plasma reactor can be simulated in a typical circuit simulation software, such as SPICE or MATLAB/Simulink. Both the electric waveforms and the IEDs are predicted with the simulation model by applying the same bias voltage waveforms as applied to the plasma reactor. In this article, the predicted waveforms and IEDs are compared to the experimental measurements obtained from a plasma reactor for verification.

The structure of this paper is as follows: first, the EEC models, including the traditional model and the improved model are derived in section 2, followed by the parameter identification method in section 3. Next, the experimental validation is carried out and discussed in section 4. Finally, section 5 concludes the paper.

2. Reactor model

2.1. Traditional EEC model of the plasma reactor

In a typical ICP reactor, the bulk plasma is confronted with two major surfaces, which are the grounded reactor wall and the substrate table that can be biased. The area of the reactor wall is larger than that of the table. Therefore, the plasma reactor can be simplified as an asymmetrical parallel plate system as depicted in figure 4(a). In most cases, a dielectric substrate is
used, as presented by the grey area in the figure. The traditional EEC model focuses on RF biasing as described in [9, 25, 32, 37–39], which can be generalized by the EEC model shown in figure 4(b). In this model, two sheaths are formed between the plasma and reactor wall, and the plasma and substrate, respectively. Each sheath is modelled by a constant current source, a sheath capacitor and a diode in parallel. The current sources account for the equivalent currents generated by bombarding ions. The dielectric substrate is modelled by a capacitor $C_{\text{sub}}$. The bombarding ions enter the sheath with an initial unbalance between the inflow and outflow current. After reaching the steady-state, the net current flowing through the blocking capacitor is zero in each repetition period and the voltage over the blocking capacitor can be considered constant [44]. It should be noted that $u_{\text{sub}}$ here can be seen as the bias voltage after the blocking capacitor. Therefore, it can be described by

$$\Delta E_i = e V_{\text{rf}} \left( \frac{1}{C_{\text{sh0}}} - \frac{1}{C_{\text{ch1}}} \right) \left( \frac{1}{C_{\text{sub}}} \right).$$

This results in a bimodal IED as shown in figure 3. In practice, ion transition in the sheath takes time. Therefore, the extra energy ions obtain in the sheath is the average of $e u_{\text{ch1}}(t)$ over the ion transit time. This effect can reduce the width of IED.

The traditional EEC model is able to explain the RF biasing while it cannot directly be used for the tailored waveform biasing. In the tailored waveform biasing, bombarding ions are accumulated on the substrate surface and charging $C_{\text{sub}}$ when a negative voltage slope is applied to the table, as depicted in figure 2(c). $C_{\text{sh0}}$ should be periodically discharged by a positive voltage pulse to avoid over voltage. During the positive voltage pulse, fast-moving electrons are attracted, thereby discharging the capacitors rapidly. However, in the traditional EEC model, the capacitors can only be discharged through the current sources $I_0$ and $I_1$. The ion current is significantly smaller than the electron current, resulting in a slow discharge process in this model. Furthermore, the discharge electron current decays exponentially as depicted in [30], which cannot be realized by the constant current sources.

Besides, after the positive discharge voltage, denoted by $V_d$ in this article, is applied and the circuit reaches its steady-state,
the voltage of $C_{\text{sub}}$ should be fully discharged to zero. The voltage potential of the substrate surface should be $V_d$. Consequently, the substrate surface has a higher voltage potential compared to the grounded reactor wall. The plasma potential $u_p$ is determined by the surface with a higher voltage potential [45] as

$$u_p = V_d + V_p. \quad (7)$$

Here $V_p$ is the floating potential of the plasma. The voltage of $C_{\text{sh1}}$ should represent the voltage over this sheath, thus it is close to zero since the floating potential $V_p$ is typically small [9]. However, due to the capacitive voltage divider formed by $C_{\text{sh1}}$, $C_{\text{sh1}}$ and $C_{\text{sub}}$ as shown in figure 4(b), the capacitors cannot be completely discharged when $u_{\text{out}} = V_d$ according to Kirchhoff’s voltage law. Instead, voltage drops over $C_{\text{sub}}$ and $C_{\text{sh1}}$ remain positive, the magnitudes of which are determined by $V_d$. As a result, the steady-state obtained in the traditional model deviates from the practice. Therefore, a different EEC is required to model tailored waveform biasing.

### 2.2. Proposed improved EEC model of the plasma reactor

An improved EEC model is proposed as depicted in figure 5. An extra sheath is formed between the exposed part of the table (as depicted by the gridded part in figure 1) with the plasma. This extra sheath is seldom discussed in previous research but it is essential, especially for the existence of the diode $D_2$. The diode $D_2$ provides an extra path during discharge so that $C_{\text{sh1}}$ and $C_{\text{sub}}$ can be fully discharged when the positive discharge voltage $V_d$ is applied and $D_2$ is conducting. Since the reactor is always grounded and the sheath between plasma and the reactor wall is not of interest, this sheath is omitted for simplicity. Meanwhile, a resistor $R_p$ is used to represent the bulk plasma and provide a fast RC discharge path, which is exponentially decaying. Besides, there exist parasitic capacitors between the table and the reactor wall, the substrate and the reactor wall, as also shown in figure 1. Those capacitors are modelled as a lumped table capacitor $C_t$, $L_s$ is the stray inductance in the power converter and the table connection.

The modelled process can be divided into three individual phases as shown in figure 6, i.e. the charge phase, the discharge phase, and the post-discharge phase. The part of the tailored waveform when the table is negatively biased is defined as the charge phase since the ions are accumulating on the substrate surface and charging the substrate capacitor during this time. When a positive voltage $V_d$ is applied to the table, the capacitors are discharged within a short time, which is defined by the discharge phase. After the capacitors are fully discharged, the positive voltage can be held for a short time, which is defined by the post-discharge phase. Each phase is analysed in detail in this section. The waveform of $u_t$ is the so-called tailored waveform. The target of the SMPC is to generate a voltage waveform $u_{\text{out}}$ in order to obtain the desired $u_t$.

#### 2.2.1. Charge phase

The ion energy is required to remain in a specific narrow window for processing with high selectivity. Therefore, $u_{\text{sh1}}$ is desired to be a negative constant value. Since ions are accumulated and charging the substrate, this phase is designated as charge phase. From the EEC model, $u_{\text{sh1}}$ is determined by

$$C_{\text{sub}} \frac{d}{dt} (u_{\text{sh1}} - u_t) = I_{i1} + C_{\text{sh1}} \frac{d}{dt} (u_p - u_{\text{sh1}}) \quad (8)$$

During charging when the reactor table is negatively biased, the grounded reactor wall has a higher voltage potential than the table. The plasma potential is determined by the surface with the higher voltage potential [45]. Therefore, in practice, the plasma has a positive potential $V_p$ with respect to ground. Since this voltage is relatively small compared to the bias voltage, it is omitted here for simplicity. In the model, the plasma potential $u_p$ is determined by

$$u_p = R_p i_p = -R_p (I_{i1} + I_{i2} + i_{\text{sh1}} + i_{\text{sh2}}), \quad (9)$$

which yields a negative value during the charge phase. Therefore, $R_p$ should be sufficiently small during this phase, so that $u_p \approx 0$. $I_{i1}$ is causing charge accumulation on $C_{\text{sub}}$ and should be compensated. As a result, a constant $u_{\text{sh1}}$ requires a voltage slope on $u_t$ defined by

$$\frac{d u_t}{dt} = -\frac{I_{i1}}{C_{\text{sub}}}. \quad (10)$$
In other words, $u_t$ should linearly decrease with a slope rate of $-I_1/C_{\text{sub}}$ to exactly compensate the ion charge accumulation effect for a constant ion energy [26]. Assuming the duration of the voltage slope is $T_{\text{slope}}$ (as annotated in figure 6), the magnitude of the voltage change $\Delta V$ during the charge phase is given by

$$\Delta V = \frac{du_t}{dt} T_{\text{slope}} = -\frac{I_1}{C_{\text{sub}}} T_{\text{slope}}.$$  \hspace{1cm} (11)

Contrastingly, for pulsed-shape biasing as depicted in figure 2, the charge effect is not compensated and the substrate surface could rise by $|\Delta V|$ during the charge phase. A small $C_{\text{sub}}$ or a large charging time (low repetition frequency) could lead to large voltage rise and a broad IED.

In this article, the condition that (10) is achieved is defined as the optimal operating point. Consequently, the EEC model in figure 5 can be simplified as shown in figure 7(a) during the charge phase.

2.2.2. Discharge phase. Because $C_{\text{sub}}$ is continuously charging during the charge phase, it is required to discharge it periodically to avoid over-voltage on the substrate. By applying a positive voltage pulse to the table, both the substrate and table sheath are restructured and reformed. The capacitor $C_{\text{sh1}}, C_{\text{sh2}}$ and $C_{\text{sub}}$ are discharged by attracting the electrons instantly, which is realized by RC discharge through resistor $R_p$ in the circuit model.

First, $u_{c_{\text{sh1}}}$ is positive, thus diode $D_1$ is blocking. $C_{\text{sub}}$ is discharging through $C_{\text{sh1}}$. The equivalent circuit representing the moment when $C_{\text{sh1}}$ is not fully discharged is shown in figure 7(b).

After $C_{\text{sh1}}$ is fully discharged, $u_{C_{\text{sh1}}}$ turns to zero and $D_1$ is conducting, $C_{\text{sub}}$ is discharging through $D_1$. The ion current $I_{1i}$ is completely flowing through $D_1$. The equivalent circuit representing the moment after $C_{\text{sh1}}$ is fully discharged is shown in figure 7(c). Since $C_{\text{sub}}$ and $C_{\text{sh2}}$ are in parallel, both capacitors should be fully discharged at the same time.

The RC discharge process represents the sheath collapsing. The discharge current in the loop is decaying exponentially. Normally this process happens in a short time up to hundreds of nanoseconds [30].

2.2.3. Post-discharge phase. After $C_{\text{sh2}}$ and $C_{\text{sub}}$ are fully discharged, the voltages over $C_{\text{sh1}}, C_{\text{sh2}}$ and $C_{\text{sub}}$ become zero and $D_2$ is conducting. The plasma potential $u_p$ is then clamped to the discharge voltage $V_d$ in this case. The ion current $I_{12}$ is completely flowing through $D_2$. The equivalent circuit at this moment is shown in figure 7(d).

The post-discharge phase is preferred to be short such that the ion energy is well defined during the most of the duration of the waveform, thereby increasing the throughput. On the other hand, the post-discharge phase is a degree of freedom to adjust the bias waveform repetition period. The time duration of the charge phase $T_{\text{slope}}$ is rather fixed because $\Delta V$ is limited by the output capacity of the power converter. The time duration of the discharge phase is determined by the plasma properties and the operating condition, thus it cannot be controlled. By controlling the duration of the post-discharge phase, the bias waveform repetition period (and the frequency) can be flexibly tailored. The total time duration of the discharge phase and the post-discharge phase is denoted by $T_{\text{pulse}}$ as shown in figure 6.

After the post-discharge phase is finished, a negative voltage pulse should be applied to the table to restart the charge phase. The magnitude of this voltage pulse determines the ion energy. Assuming $u_t$ changes from discharge $V_d$ to a negative start voltage $V_s$, it must be stressed that before $u_t$ turns negative, $D_2$ is conducting and the voltages over $C_{\text{sh1}}, C_{\text{sh2}}$ and $C_{\text{sub}}$ are clamped to zero. Only after $u_t$ is below zero, $D_2$ is blocking and the equivalent circuit turns from figures 7(d) to (a) again by rapidly recharging $C_{\text{sh1}}, C_{\text{sh2}}$ and $C_{\text{sub}}$ through $R_p$. It should be noted that this recharging process also takes time comparable to the discharge phase. However, since its equivalent circuit is the same as the charge phase, it is not separately classified for brevity. Due to the capacitive voltage divider formed by $C_{\text{sh1}}$ and $C_{\text{sub}}$, $u_{\text{sh1}}$ obtains an initial value at the beginning of the charge phase governed by

$$u_{\text{sh1}} = \frac{C_{\text{sub}}}{C_{\text{sub}} + C_{\text{sh1}}} V_s.$$  \hspace{1cm} (12)

Since $C_{\text{sub}}$ is typically much larger than $C_{\text{sh1}}$, $u_{\text{sh1}}$ can be approximate by $V_s$.

3. Parameter identification

In order to conduct circuit simulation, the parameters of the EEC model should be accurately identified. In this section, a parameter identification method is introduced, which is fully based on the nonintrusive electrical measurements. Specifically, only the waveforms of $u_{\text{out}}$ and $i_{\text{out}}$ are required. In practice, the sheath capacitance $C_{\text{sh1}}$ and $C_{\text{sh2}}$, the ion current $I_{1i}$ and $I_{12}$ are nonlinear and voltage dependent. If and only if the optimal operating point is achieved, $u_{\text{sh1}}$ and $C_{\text{sh1}}$ can remain constant during the charge phase [25]. In this work, these parameters are assumed to be constant around the optimal operating point for simplicity. In addition, $C_{\text{sub}}$ is assumed to be constant since the processing depth of the substrate is negligible compared to its height. $C_1$ can also be assumed to be constant since the area and distance of each surface remain basically unchanged.

During the charge phase as depicted in figure 7(a), the reactor system with the converter can be generalized by

$$i_{\text{out}} = \left( \frac{C_{\text{sh1}} C_{\text{sub}}}{C_{\text{sh1}} + C_{\text{sub}}} + C_{\text{sh2}} + C_I \right) \frac{du_t}{dt} \cdot \frac{C_{\text{sub}}}{C_{\text{sub}} + C_{\text{sh1}}} I_{1i} - I_{12}.$$  \hspace{1cm} (13)

By varying the voltage slope $\frac{du_t}{dt}$, the output current $i_{\text{out}}$ changes accordingly. With a fixed $\frac{du_t}{dt}$, $i_{\text{out}}$ can be treated as constant during the charge phase. $u_t$ can then be approximated by $u_{\text{out}}$ despite the presence of $L_n$. Normally, the value of $C_{\text{sh2}}$ and $I_{12}$ are relatively small so they are assumed to be zero in this section. Therefore, a simplified description of the system is given by

$$i_{\text{out}} = \left( \frac{C_{\text{sh1}} C_{\text{sub}}}{C_{\text{sh1}} + C_{\text{sub}}} + C_I \right) u_{\text{out}} - \frac{C_{\text{sub}}}{C_{\text{sub}} + C_{\text{sh1}}} I_{1i},$$  \hspace{1cm} (14)
where $\dot{u}_{out} = \frac{du_{out}}{dt}$. The effective capacitance $C_{eff}$ and effective current $I_{eff}$ can be defined by

$$C_{eff} = \frac{C_{sub}}{C_{sh1} + C_{sub} + C_t}$$

and

$$I_{eff} = -\frac{C_{sub}}{C_{sub} + C_{sh1}}I_{i1} = \left(\frac{C_{sh1}}{C_{sh1} + C_{sub}} - 1\right)I_{i1}.$$  

(15)  

(16)

Note that both $C_{eff}$ and $I_{eff}$ are variant at different operating points and they are dependent of $u_{out}$. In the identification procedure, a set of different output voltage slopes $\dot{u}_{out,x}$ ($x = 1, 2, 3, \ldots, n$) with a sufficiently small step size should be applied, and the resultant output current $i_{out,x}$ ($x = 1, 2, 3, \ldots, n$) during the charge phase should be measured. As a result, the value of $C_{eff}$ and $I_{eff}$ at the corresponding $\dot{u}_{out}$ can be approximated by

$$C_{eff,x} = \frac{i_{out,x+1} - i_{out,x}}{\dot{u}_{out,x+1} - \dot{u}_{out,x}}$$

and

$$I_{eff,x} = \frac{i_{out,x}i_{out,x+1} - i_{out,x+1}i_{out,x}}{\dot{u}_{out,x+1} - \dot{u}_{out,x}}.$$  

(17)  

(18)

If $\dot{u}_{out,x}$ ($x = 1, 2, 3, \ldots, n$) covers a sufficiently large range, the optimal operating point can be found. Assuming the optimal operating point is found at $x = k$, $\dot{u}_{out,k}$ should be equal to $-I_{i1}C_{sh1}^{-1}$ according to (10). Under this circumstance, $u_{sh1}$ is constant and there is no current flowing through the modelled sheath capacitor $C_{sh1}$. $C_{sh1}$ can be omitted in the circuit depicted in figure 7(a). Consequently, the system can be equivalently simplified as

$$i_{out} = C_t\dot{u}_{out} - I_{i1}.$$  

(19)

This simplification can also be derived by substituting $\dot{u}_{out} = -I_{i1}C_{sub}^{-1}$ in to (14), because essentially (19) is a special point of the generalized system depicted by (14). Since

$$C_t \leq C_{eff} = \frac{C_{sub}}{C_{sh1} + C_{sh1} + C_t}$$

and

$$-I_{i1} \leq I_{eff} = -\frac{C_{sub}}{C_{sh1} + C_t}I_{i1}$$

always stand, the value of $C_t$ and $I_{i1}$ can be obtained by finding the minimum effective capacitance and current as

$$C_t = \min(C_{eff,x}) = C_{eff,k}$$

and

$$I_{i1} = \min(I_{eff,x}) = -I_{eff,k},$$

(20)  

(21)  

(22)  

(23)

respectively. It should be pointed out that $I_{i1}$ can also be calculated from (19) after finding $C_t$. While theoretically the minimum of the effective capacitance and current should be achieved at the same $\dot{u}_{out}$, both methods should give the same result.

The above analysis utilizes the special format of the proposed circuit model at the optimal operating point to calculate the exact value of $C_t$ and $I_{i1}$. The benefit of this method is that the value of $C_{sh1}$ and $C_{sub}$ are not required, meaning the method is immune of the nonlinear $C_{sh1}$ effect. Therefore, the identification of $C_t$ and $I_{i1}$ are expected to be accurate. Nonetheless, the value of $C_{sh1}$ has to be linearised and assumed to be constant within the covered range of $\dot{u}_{out,x}$ ($x = 1, 2, 3, \ldots, n$). Defining a constant equivalent capacitance and current by

$$C_{eq} = \frac{C_{sh1}C_{sub}}{C_{sh1} + C_{sub} + C_t}$$

and

$$I_{eq} = \frac{C_{sub}}{C_{sub} + C_{sh1}}I_{i1},$$

(24)  

(25)

(14) can be rewritten as

$$i_{out} = C_{eq}\dot{u}_{out} - I_{eq}.$$  

(26)
A linear regression can be determined within the operating range, which is able to find the value of $C_{eq}$ and $I_{eq}$ by least squares method by minimizing the function

$$f(C_{eq}, I_{eq}) = \sum_{i=1}^{n} (C_{eq}I_{\text{out,i}} - I_{eq}I_{\text{out,i}})^2. \quad (27)$$

Based on the practical measurements, typically $C_{\text{sub}}$ (typically of nanofarad magnitude) is much larger than the sheath capacitance (typically of sub-nanofarad magnitude), (24) can be further approximated by

$$C_{eq} \approx C_{sh1} + C_{t}. \quad (28)$$

As a result, linearised $C_{sh1}$ can be calculated by

$$C_{sh1} = C_{eq} - C_{t}. \quad (29)$$

$C_{\text{sub}}$ can be further solved from (25), yielding to

$$C_{\text{sub}} = \frac{C_{sh1}I_{eq}}{I_{11} - I_{eq}}. \quad (30)$$

Up to now, the parameters essential for the charge phase have been completely extracted. On the other hand, during the discharge phase, there is a resonance in transient response with a frequency of $f_{i}$ in the loop. This resonance comes from the LC network formed by the plasma reactor and the stray inductance $L_{s}$. The value of $L_{s}$ can be determined by

$$L_{s} = \frac{1}{4\pi^2 f_{i}^2 (C_{t} + C_{\text{sub}})} \quad (31)$$

when the optimal operating point is achieved.

During the discharge phase, capacitor $C_{sh1}$, $C_{sh2}$ and $C_{\text{sub}}$ should be discharged within hundreds of nanoseconds through resistor $R_{p}$. Therefore, during this phase $R_{p}$ can be approximated by

$$R_{p} = \frac{\tau}{C_{\text{sub}}}, \quad (32)$$

where $\tau$ is the time constant of the RC circuit. Based on the RC discharge circuit, it takes about $2.3\tau$ to discharge the capacitor voltage to 10% of the initial value. Since the sheath collapsing and reforming takes up to hundreds of nanoseconds, a typical value of $\tau$ can be tens of nanoseconds.

During the post-discharge phase, the output current is determined by

$$i_{\text{out}} = \frac{V_{d}}{R_{p}}. \quad (33)$$

Since the net output current of the converter should be balanced due to the blocking capacitor, and the net current through all the capacitors are zero due to the periodic capacitor voltages, the output current during the post-discharge phase should be governed by

$$i_{\text{out}} = \frac{T_{\text{slope}}}{T_{\text{pulse}}} I_{12}. \quad (34)$$

As a result, the plasma resistor $R_{p}$ can be obtained by

$$R_{p} = \frac{T_{\text{pulse}} T_{\text{slope}}}{T_{\text{prof}} I_{12}}. \quad (35)$$

4. Experimental verification

4.1. Experimental setup

To verify the proposed EEC model and the parameter identification method, experiments were conducted with an Oxford Instruments FlexAL plasma reactor as shown in figure 8(a), which is a tool for ALD but can also be used for ALE. The RF bias generator was uninstalled and a dedicated SMPC was used to deliver the required tailored waveforms. The SMPC was coupled with the reactor table with a blocking capacitor of 2 $\mu$F. The details of the SMPC are provided in [36, 46]. An argon plasma was created with an ICP source through an automatic matching network. The plasma source can deliver up to 600 W power at 13.56 MHz. It contains a three-turn water-cooled copper coil around a cylindrical 65 mm Al$_2$O$_3$ ceramic plasma tube. The distance between the substrate and the plasma source is in the order of 25 cm. The pressure inside the reactor was kept at 2.2 mTorr. More details of the plasma reactor can be found in [47]. Four-inch and eight-inch silicon wafers with 400 nm silicon dioxide were used as the dielectric substrates.

The process of the experimental verification is depicted in figure 9. First, bias voltage waveforms with different voltage slopes were applied to the plasma reactor with a wafer on the table. The output voltage waveforms were measured with a differential voltage probe. The output currents of the power converter were measured with the current sensor. Second, the applied bias voltage waveforms and the measured output current waveforms are used for parameter identification as explained in section 3. The identified parameters are then substituted back to the EEC model for circuit simulation. The simulation was conducted in MATLAB/Simulink with SimScape toolbox.

The model used for simulation is depicted in figure 10. Compared to the EEC model depicted in figure 5, $I_{12}$ and $C_{sh2}$ are neglected as explained in section 3. An ideal switch $S$ and resistor $R_{pd}$ are added. The status of the switch is controlled...
The ions enter the sheath with an initial energy $eV_p$, where the floating potential $V_p$ is typically 20 to 40 V [9]. The ions obtain extra energy in the sheath, the value of which is determined by the instantaneous voltage of $u_{Cb1}$. In practice, since the ions have a finite transit time $\tau_i$ in the sheath, they do not respond to instantaneous $u_{Cb1}$. Instead, the ions respond to the averaged $u_{Cb1}$ within $\tau_i$ [43]. This results in a damped effect and can be represented by a transfer function in $s$ domain as

$$H_{\text{damp}}(s) = \frac{1}{\tau_i s + 1}.$$  \hspace{1cm} (36)

The transit time can be approximated by the inverse of the ion plasma density frequency $\omega_i$ as

$$\omega_i = \frac{\sqrt{\epsilon_0 n_{is}}}{\rho_i \lambda_i},$$  \hspace{1cm} (37)

where $n_{is}$ is the ion density at the boundary of the sheath, $\epsilon_0$ is the vacuum permittivity and $m_i$ is the ion mass [43]. In this work, an estimated ion density $n_{is} = 1 \times 10^{15}$ m$^{-3}$ is used [25] and $m_i = 40$ amu.

Furthermore, the ion energy can be affected by the collisions in the sheath, which broadens the IED [30, 48]. In practice, measurement with RFEA can also broaden the IED due to the scattering of ions on the RFEA’s grids [30, 43]. These broadening effects is equivalent to a normally distributed noise defined by

$$f(E_i) = \frac{1}{\sigma \sqrt{2\pi}} \exp \left[ -\frac{1}{2} \left( \frac{E_i - \mu}{\sigma} \right)^2 \right],$$  \hspace{1cm} (38)

where $\mu$ is the mean of the noise and $\sigma$ is the standard deviation of the noise. In this article, $\mu$ is assumed to be zero and a typical variance $\sigma^2 = 10e^2V^2$ is adopted [43].

The simulation can generate a discrete time series $\{t[1], t[2], \ldots, t[m]\}$ and the corresponding energy series $\{E_1[1], E_1[2], \ldots, E_1[m]\}$, where $m$ is the total number of simulated moments within one repetition period and $E_1[j](j = 1, 2, 3, \ldots, m)$ is the energy of the ions arriving at the substrate surface at time $t[j]$. If the ion flux is assumed to be constant over the period, then the normalized ion flux $P(E)$ can be approximated by

$$P(E) = \frac{1}{T} \sum_{1 \leq j < m; E_1[j] < E + \Delta E} t[j + 1] - t[j],$$  \hspace{1cm} (39)

where $T$ is the repetition period and $\Delta E$ is the resolution of the IED measurement. Consequently, the IED can be predicted based on this circuit simulation. In order to verify the accuracy of the prediction, IEDs were measured with a commercial gridded retarding field energy analyser (RFEA) from Impedans Ltd. with a resolution $\Delta E = 1$ V as comparison. The RFEA was placed on the top of the substrate, as shown in figure 8(b). It should be noted that RFEA measurement is intrusive and can disturb the EEC model. Therefore, the electric waveform measurement experiment, the RFEA was removed.

4.2. Parameter identification

Figure 11 shows the measured electric waveforms, including the output bias voltage and output current waveforms for the four-inch wafer with 200 W ICP power. The applied bias voltage waveforms have a repetition frequency of 100 kHz. The time percentage of the charge phase is 90% and the time percentage of the discharge phase and post-discharge phase add...
The discharge voltage $V_d$ is fixed at 50 V and the negative voltage applied to restart the charge phase $V_s$ is fixed at $-100$ V. Therefore, at the optimal operating point, the average ion energy is expected to be approximately 100 eV. The voltage slope rate is controllable and ranges from approximately 0 to $-16.7 \times 10^4$ V s$^{-1}$ in this experiment. Consequently, the peak-to-peak voltage of the bias waveforms is determined by the slope rate and ranges from 150 to 300 V. As can be seen, the output current is quasi-constant in the charge phase. When applying a different voltage slope $i_{\text{out}}$, a different dc output current $i_{\text{out}}$ is obtained. As analysed in section 3, the dataset of the voltage slope $i_{\text{out}}$ and dc current $i_{\text{out}}$ can be used for identifying $C_i$ and $I_i$.

The measured dataset of the effective capacitance and current is shown in figure 12(a). As can be seen, $C_{\text{eff}}$ and $I_{\text{eff}}$ share a similar trend with the varying $i_{\text{out}}$. The reason is that they have the same coefficient of $C_{\text{sh1}}(C_{\text{sh1}}+C_{\text{sub}})^{-1}$, according to (15) and (16). Theoretically, $C_{\text{eff}}$ and $I_{\text{eff}}$ should reach the minimum value at the same $i_{\text{out}}$. However, $C_{\text{eff}}$ reaches its minimum when $i_{\text{out}} = -5.586 \times 10^4$ V s$^{-1}$ as denoted by the red pentagon in figure 12(a), while $I_{\text{eff}}$ just reaches its local minimum. When $i_{\text{out}}$ becomes more negative, $I_{\text{eff}}$ has a trend towards more negative value than the local minimum. This deviation is because the ion current $I_{i_1}$ is not constant as assumed in the previous analysis. Instead, $I_{i_1}$ increases when $i_{\text{out}}$ becomes more negative, i.e. the voltage drop on the substrate sheath increases. To keep the model simple and functional within the reasonable slope rate range, the effective current is selected at the same operating point where the minimum effective capacitance is obtained. As a result, $C_i = C_{\text{eff,min}} = 2.22 \text{ nF}$ and $I_i = -I_{\text{eff,min}} \approx 0.01265 \text{ A}$.

Figure 12(b) shows the measured output current at different output voltage slopes and its linear regression. The resultant linearized equivalent capacitance and current are $C_{\text{eq}} = 2.66 \text{ nF}$ and $I_{\text{eq}} = 0.0111 \text{ A}$, respectively. $C_{\text{sh1}}$ and $C_{\text{sub}}$ can be solved by (29) and (30), giving $C_{\text{sh1}} = 0.435 \text{ nF}$ and $C_{\text{sub}} = 3.09 \text{ nF}$.

The resonance in the waveform is measured to be of $f_i = 14 \text{ MHz}$. The stray inductance $L_s$ can then be determined by (31) and is 25 nH. In addition, an equivalent series-resistance $R_i$ is present in the loop, which is 1.5 $\Omega$. Apart from these, selecting $\tau = 50$ ns as introduced in section 3, $R_p$ can be calculated by (32) and is 17.6 $\Omega$. The value of $R_p$ should be sufficiently large since $I_2$ is neglected as explained in section 3. In this case, $R_p = 6000 \Omega$ is sufficient. The value of $R_p$ affects $i_{\text{out}}$ during the post-discharge phase, which is not of interest. Therefore, it is not required to be very accurate. In short, all the parameters are identified and summarized in table 1.

4.3. Electric waveform and ion energy distribution prediction

By substituting the identified parameters back to the EEC model and applying the same bias voltage waveforms to it for circuit simulation, the electric waveforms can be predicted. Figure 13 shows the predicted waveforms at the optimal operating point from the circuit simulation based on the EEC model. Both the sheath surface potential $V_{\text{sh1}}$ and the ion energy $E_i$ are quasi-constant during the charge phase. The
Figure 13. The predicted electric waveforms from the circuit simulation based on the EEC model. The measured and predicted $i_{\text{out}}$ are almost overlapping.

Figure 14. A zoomed-in view around the discharge phase of the predicted electric waveforms from the circuit simulation based on the EEC model.

Figure 15. The IED prediction from the waveform of $E_i$.

waveform of $u_{C_{\text{sh1}}}$ and $u_{C_{\text{sub}}}$ cannot be measured with this experimental setup but the predicted results are in line with the measured results demonstrated in [30]. Figure 14 shows a zoomed-in view around the discharge phase of the waveforms. As can be seen from figures 13 and 14, the predicted $i_{\text{out}}$ matches the measured $i_{\text{out}}$ generally in transient behaviour, magnitude and resonant frequency.

Additionally, the IED can be predicted based on the predicted waveform of $E_i$ according to (39), as shown in figure 15. Similarly, by applying the same bias voltage waveform to both the simulation model and the plasma reactor with an RFEA presented, the predicted and measured normalized IED can be compared. Figure 16 shows comparisons of the predicted and measured results for different voltage slopes. The predicted results can generally represent the trend of the measured ones. Furthermore, the full width at-half-maximum (FWHM) and the average energy at different voltage slope rates from both the simulations and measurements are compared, as shown in figure 17. On the one hand, the predicted IEDs accurately find the optimal slope rate which leads to the minimum FWHM. On the other hand, the predicted average values of the ion energy are within 10 eV difference compared to the measurements. It should be noted that the IED can only be measured with RFEA, which is interactive with the plasma processing and IEDs. The IED in the case without RFEA is inherently different from that with RFEA. This might contribute to the deviation of the comparison.

4.4. Discussion

The same experiments were also carried out for the eight-inch wafer and at different ICP powers. The resultant identified parameters are shown in table 2. As can be seen from the table, $C_i$ is uniform and around 2.3 nF for different wafers with different ICP powers, which makes sense because both the area of and the distance between the table and reactor wall remain unchanged. The extracted $C_{\text{sub}}$ is of several nanofarads for both applied wafers. However, the extracted $C_{\text{sub}}$ of the same wafer is expected to be the same with different ICP powers while they deviate in the results. The reason is that $C_{\text{sub}}$ is calculated based on multiple extracted parameters, including $C_{\text{sh1}}$, $I_{\text{eq}}$ and $I_{i1}$, according to (30). Since inaccuracy occurs when identifying each parameter, it will be accumulated on $C_{\text{sub}}$, i.e. the identification of $C_{\text{sub}}$ is more sensitive.

The identified values of $C_{\text{sh1}}$ are around 0.4 nF for different wafers with different ICP powers. Furthermore, the current $I_{i1}$ has a positive correlation with the ICP power. It is interesting to note that even the eight-inch wafer is four times the area of the four-inch wafer, the value of their $C_{\text{sh1}}$ and $I_{i1}$ are still similar when employing the same ICP power. This similarity is due to the neglection of the $C_{\text{sh2}}$ and $I_{i2}$. In (24), the
Figure 16. Comparison of the predicted and measured normalized IED for the four-inch wafer with 200 W ICP power at voltage slope rate of (a) $0.056 \times 10^4$ V s$^{-1}$, (b) $-3.023 \times 10^{-6}$ V s$^{-1}$, (c) $-5.722 \times 10^6$ V s$^{-1}$, (d) $-6.753 \times 10^6$ V s$^{-1}$, (e) $-7.983 \times 10^6$ V s$^{-1}$, and (f) $-9.982 \times 10^6$ V s$^{-1}$.

Figure 17. Comparison of the predicted and measured FWHM and average energy for the four-inch wafer with 200 W ICP power at different voltage slope rates.

Table 2. The identified parameters of the plasma reactor with different wafers at different ICP powers.

| Wafer        | ICP power (W) | Four-inch | Eight-inch |
|--------------|--------------|-----------|------------|
|              | 200          | 600       | 200        | 600       |
| $C_t$ (nF)   | 2.22         | 2.36      | 2.31       | 2.34      |
| $C_{sub}$ (nF) | 3.09         | 4.35      | 2.84       | 3.65      |
| $C_{sh1}$ (nF) | 0.435        | 0.386     | 0.409      | 0.402     |
| $I_i1$ (mA)  | 12.65        | 15.26     | 11.99      | 15.24     |

The equivalent capacitance $C_{eq}$ is defined and in (27), its value is obtained by linear regression, as shown in figure 12(b). This value is obtained based on the simplified system described by (19) which neglects $C_{sh2}$ and $I_{i2}$ in the real system as described by (14). In other words, the real definition of $C_{eq}$ is

$$C_{eq} = \frac{C_{sh1}C_{sub}}{C_{sh1} + C_{sub}} + C_{sh2} + C_t \approx C_{sh1} + C_{sh2} + C_t. \quad (40)$$

As a result, the previously identified $C_{sh1}$ is actually the sum of real $C_{sh1} + C_{sh2}$. Similarly, the previously identified $I_i1$ is actually the sum of real $I_{i1} + I_{i2}$ according to (21). Because the total exposed area (equal to the total area of the solid part and the gridded part of the table as depicted in figure 1) is constant, both the sum of the sheath capacitance and ion current should roughly maintain similar values even when a different wafer is used. This effect also evidences that there is an extraneous sheath between the plasma and the exposed part of the table.

To summarize, in this section, the parameters of the EEC model are identified based on the experimental measurements. The EEC model is simulated by using the identified parameters. Both the predicted electric waveforms and IEDs align well with the measured results. The same experiments were conducted for two different wafers with different ICP powers while similar results were obtained, demonstrating the wide application scope of the proposed method. The possible reasons for the deviation between the simulations and measurements are also analysed.

5. Conclusion

The equivalent electric circuit (EEC) model of the plasma reactor is essential for circuit simulation and bias waveform optimization in atomic scale processing with tailored waveform biasing. Traditional EEC models are typically used for RF biasing and not suitable for tailored waveform biasing, mainly because the capacitors in the circuit cannot be rapidly and completely discharged during the discharge phase. In this article, an improved EEC model of the plasma reactor is introduced. The improved EEC model simplifies the plasma by a resistor...
thus providing a fast discharge path for the capacitors. Meanwhile, it adds another sheath between the bulk plasma and the exposed part of the reactor table, being the table sheath, so that all the capacitors can be fully discharged to zero voltage. In tailored waveform biasing, there are three different processing phases including the charge phase, the discharge phase, and the post-discharge phase. The proposed model is analysed in details during all of these phases.

Additionally, a parameter identification method is proposed to fulfil the simulation of the EEC model on the circuit level. It is fully based on electrical measurements, using only the waveforms of output voltage and current. Both waveforms can be easily measured and the measurements are nonintrusive to the process. The identification method linearizes all the components, including the sheath capacitors and currents. With the proposed EEC model and parameter identification method, the electric waveforms and IEDs can be predicted by circuit simulation. Experiments have been conducted for verification. The alignment between the predictions and measurements underlines the correctness and accuracy of the proposed EEC model and parameter identification.

This research bridges the gap between plasma processing and bias power converter design. It gives an electrically equivalent description of the plasma reactor and provides more insight into the process from the electrical engineering’s perspective. Accordingly, the EEC can be used to design and optimize the SMPC for electrical engineers, thus significantly improving the process efficiency. Meanwhile, a well-designed bias converter also enhances tailored waveform biasing in the future. Moreover, it poses a new way for plasma parameter identification, with which linearized plasma parameters, such as sheath capacitance and ion current, can be obtained nonintrusively. Additionally, the IEDs can be predicted with circuit simulation, which can be a supplement and substitute to the traditional plasma simulation method like PIC, enjoying the advantage of considerably reduced computation time. This model might also be used for bias waveform optimization and IED tailoring.

The proposed model is expected to be compatible with other bias waveforms like RF biasing and pulse-shaped biasing but requires further experimental validation. For the future research, it is recommended to improve the accuracy of the parameter identification by taking nonzero $C_{\text{sh}2}$ and $I_{\text{I2}}$ into consideration.

**Data availability statement**

The data generated and/or analysed during the current study are not publicly available for legal/ethical reasons but are available from the corresponding author on reasonable request.

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**ORCID iDs**

Qihao Yu (余 骐 浩) [https://orcid.org/0000-0001-5318-434X](https://orcid.org/0000-0001-5318-434X)

Erik Lemmen [https://orcid.org/0000-0002-4471-1352](https://orcid.org/0000-0002-4471-1352)

Bas Vermulst [https://orcid.org/0000-0001-9019-6147](https://orcid.org/0000-0001-9019-6147)

Adriaan J M Mackus [https://orcid.org/0000-0001-6944-9867](https://orcid.org/0000-0001-6944-9867)

Wilhelmm M M (Erwin) Kessels [https://orcid.org/0000-0002-7630-8226](https://orcid.org/0000-0002-7630-8226)

Korneel Wijnands [https://orcid.org/0000-0003-3302-1599](https://orcid.org/0000-0003-3302-1599)

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