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Capacitive electrical asymmetry effect in an inductively coupled plasma reactor

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Abstract

The electrical asymmetry effect is realized by applying multiple frequency power sources (13.56 MHz and 27.12 MHz) to a capacitively biased substrate electrode in a specific inductively coupled plasma reactor. On the one hand, by adjusting the phase angle θ between the multiple frequency power sources, an almost linear self-bias develops on the substrate electrode, and consequently the ion energy can be well modulated, while the ion flux stays constant within a large range of θ . On the other hand, the plasma density and ion flux can be significantly modulated by tuning the inductive power supply, while only inducing a small change in the self-bias. Independent control of self-bias/ion energy and ion flux can thus be realized in this specific inductively coupled plasma reactor.

Keywords: electrical asymmetry effect, inductively coupled plasma, self-bias

1. Introduction

Inductively and capacitively coupled plasma (ICP and CPP) processing is commonly used in many nanofabrication applications in the semiconductor industry, such as plasma etching, thin film deposition, and sputtering [1, 2]. ICPs are generally characterized by high electron densities and high ion flux, due to the more effective electron heating by the inductive power, which is strongly desired for a given process, as it determines the processing throughput. However, the ion bombarding energy on the substrate surface, which is of great significance to the specific surface processing, is normally quite low with maximum energy at around 20 eV [3], due to the absence of high-voltage sheaths at the substrate electrode. The high-voltage sheaths are typical in CCP, and the averaged sheath voltage drop is normally close to half of the biased radio frequency (RF) voltage [1] at low pressure, i.e., in the order of 100 V. In contrast, the averaged low sheath voltage drop in ICP is around 15 V [1, 3].

A concept of hybrid discharge of ICPs with capacitively biased substrates was proposed to simultaneously control plasma density and ion bombarding energy [4-7]. The idea is that the ICP power controls the plasma density and ion flux, and the capacitively biased RF power (i.e. CCP power) controls the sheath potential drop and consequently the ion energy. However, strong coupling effects between the ICP power and CCP power are reported, which significantly limit this hybrid concept. Lee et al. [8, 9] and Sobolewski et al. [5] observed that the ion flux decreases when raising the bias power applied on the substrate at high ICP powers, while the ion flux does seem independent of the bias power at low ICP powers. Furthermore, Schulze et al. [10] found that sheath heating caused by the substrate bias power (CCP power) affects the electron dynamics and can further enhance the plasma density, whereas the ICP power affects the sheath voltage waveform at the substrate and consequently the ion energy distribution. Therefore, independent modulation of plasma density and ion bombarding energy is very difficult to achieve in hybrid CCP-ICP reactors.

The electrical asymmetry effect (EAE), operated at multiple consecutive harmonics or a tailored waveform, like Gaussian type, sawtooth type, peaks/valleys type, is attracting considerable interest for the separate control of ion flux and ion energy distribution on the substrate [11-21]. By applying an asymmetric voltage waveform, the plasma properties can be significantly tuned. Heil et al. firstly proposed the concept of EAE [11]. They pointed out that by applying a fundamental frequency f and its even harmonic, the discharge symmetry can be changed by tuning the phase shift between the driving harmonics. Meanwhile, an almost linear dc self-bias will develop on the substrate electrode, which can further be used to control the ion energy, while maintaining an almost constant ion flux. We demonstrated that the radial plasma density homogeneity can also be modulated by tuning the phase shift [17]. The EAE was also observed by Johnson et al. when applying a tailored waveform in the shape of 'troughs' [18]. They found that a dramatic shift in the dc bias potential could be induced when simply inverting the voltage waveform, and the growth of thin silicon films can be switched between amorphous and nanocrystalline modes, because of the abrupt change in the ion bombardment energy at the substrate. Furthermore, Lafleur et al. presented an opposite control mechanism in the EAE, i.e. the ion flux can be modulated while keeping an almost constant average ion energy, by using positive Gaussian type pulses [19]. The ion flux (and plasma density) rapidly increases as the pulse width decreases. Hence it is clear that the EAE is an effective technique to separately tune the ion flux and energy on the substrate. However, to our knowledge, all the previous investigations about the EAE are focused on CCPs, and there are no investigations realized EAE in an ICP reactor.

Zaka-ul-Islam et al. made an attempt to investigate the effect of phase shift between ICP and substrate bias CCP frequencies, which are an exact multiple of each other, in an ICP reactor with a small discharge gap of 4.2 cm [22]. They demonstrated that CCP power coupled with the capacitive contribution of the ICP coil, which affects the plasma heating. The heating mechanism can be further modulated by the phase shift. Furthermore, Ahr et al. also observed the coupling effect between inductive and capacitive power sources at the same frequency, but adjustable phase, in an RF biased ICP, at a small discharge gap of 5 cm [23]. They pointed out that the coupling effect significantly influences the plasma density, and consequently substantially reduces the power threshold for the E- to H-mode transition. The coupling effect is strongly dependent on the adjustable phase. Although both studies did not observe any modulation of the self-bias, the coupling effect on the plasma density would greatly limit the independent modulation of the ion flux and ion bombarding energy.

Besides, the approach of non-sinusoidal bias waveform, which is referred to as arbitrary substrate voltage waveform, is attracting growing interest [3, 24-27]. It has been demonstrated that a much narrower ion energy distribution can be achieved by applying an arbitrary waveform, consisting of a short voltage spike in combination with a slow ramp [24]. By this technique, the average ion energy can be tuned to a value between the threshold energies of two materials, and further control the selectivity of plasma processing, which is very important for semiconductor manufacturing. Furthermore, Agarwal et al. proved that such kind of arbitrary waveform technique can be employed to discriminate between the threshold energies during the passivation and etch steps, and further realize the self-limiting plasma atomic layer etching within the same chamber and gas mixture [3]. By making use of a programmable waveform generator, Patterson et al. experimentally introduced an iterative approach using feedback control in the frequency domain to produce arbitrary waveform shapes at the substrate. This iterative experimental system has not only been able to produce a

1
2
3 waveform shape for a narrow ion energy distribution, but also has been able to produce a
4 waveform shape for two groups of ions centered at two different energies [26]. Such
5 investigations were mostly performed at lower frequencies (normally below 2 MHz), as the
6 concept is based on ions being able to follow the sheath voltage waveform. Although the
7 influence of arbitrary waveform on the ion flux has not been investigated, we suspect that the
8 great modulation in the shape of ion energy distribution will induce certain variations in the
9 ion flux, which can be deduced in some degree from the ion energy distributions in Ref. [25].
10
11

12 In this paper, we propose a new technique, which allows combining the hybrid concept of ICP
13 with capacitively biased substrate and the EAE in a specific ICP reactor. By employing two
14 RF biased power sources on the same substrate electrode in an ICP reactor with specific
15 geometry, the plasma density can be well regulated by the ICP power, while the capacitive
16 electrical asymmetry is realized in the large diffusion chamber. We will prove that both the
17 modulation of plasma density/ion flux with small change in self-bias, and the modulation of
18 self-bias/ion energy with small change in plasma density/ion flux, can be achieved to a great
19 extent in this discharge configuration.
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22

23 2. Computational Model

24
25 The ICP geometry used in this work has a similar design as the A601E system, which is
26 widely applied for plasma processing [28-30]. A 2D half cross section of this reactor is
27 presented in figure 1. A mixture of C_4F_8 and SF_6 gas with a total gas flow rate of 120 sccm,
28 which is widely used for plasma etching [28-30], is injected from the top through the nozzle.
29 The gas pressure is fixed at 2 Pa. The plasma is sustained by a multi-turn coil (with 5 turns)
30 surrounding the 20 cm diameter tube, powered by an RF power supply at 13.56 MHz, which
31 generates a continuous RF magnetic field along the z-axis of the tube. Underneath the tube is
32 the diffusion chamber, with 200 mm height, which allows the reactive plasma species to
33 diffuse and homogenize, and finally reach the substrate electrode, which is independently
34 biased by an RF power supply. This RF driving voltage waveform consists of a fundamental
35 frequency component and its second harmonic, and is given by equation (1), where $f =$
36 13.56MHz is the fundamental frequency, $V_0 = 150V$ is the voltage amplitude, and θ is the
37 phase shift between the two harmonics.
38
39
40

$$41 \quad V_{rf} = V_0 [\sin(2\pi ft + \theta) + \sin(4\pi ft)] \quad (1)$$

42
43 In the model, this RF voltage is directly applied to the substrate electrode without the need of
44 any matching system. However, in experiments, the two frequencies are normally matched
45 individually, and more details can be found in Ref. [31]. The ICP power is at the same phase
46 with the fundamental frequency of the RF substrate bias.
47
48

49 In the geometry, only the inner wall of the tube and the substrate is insulating, all the other
50 parts are conducting, and the outside walls of the whole reactor and the top electrode of the
51 diffusion chamber are all grounded. The dc self-bias on the substrate will be calculated self-
52 consistently.
53
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55 The diffusion chamber is half open and half closed with a total diameter around 420 mm,
56 while the substrate electrode has a diameter of 300 mm. The concept here is that ICP power
57 tunes the plasma density in the large diffusion chamber, and the EAE can be capacitively
58 realized between the top and bottom electrodes of the diffusion chamber. In this way, the
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plasma density can be controlled by the ICP power, and the self-bias on the substrate electrode can be independently modulated by the EAE.

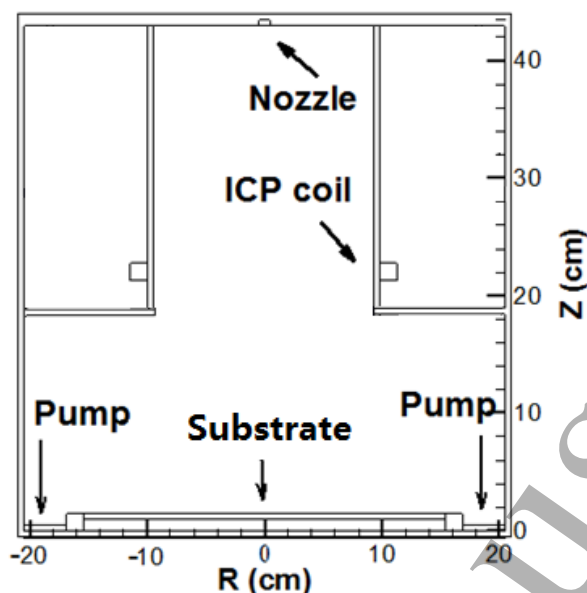


Figure 1. 2D schematic diagram of the ICP reactor, consisting of a source tube and a diffusion chamber. Only the inner wall of the tube and the substrate (including the chuck) is insulating, all the other parts are conducting.

We applied the hybrid plasma equipment model (HPEM), developed by Kushner and coworkers [32, 33], to describe the plasma behavior and the plasma-surface interactions. HPEM is a two-dimensional hybrid Monte Carlo (MC) - fluid model. The MC method is mainly used to describe the electron characteristics, while the fluid model is used to calculate the behavior of the other plasma species. The model consists of three main modules, i.e., (i) an electromagnetics module (EMM), an electron energy transport module (EETM), and a fluid kinetics module (FKM). The EMM is used to calculate the electromagnetic fields by solving Maxwell's equations. These fields are then used as input for the EETM to determine the electron properties. Subsequently, the output results are transferred to the FKM, which treats the ions and neutral species. More detailed explanations of the model can be found in reference [32].

Besides the above three modules, we also applied the Plasma Chemistry Monte Carlo Module (PCMCM) in HPEM, which calculates the energy and angular distributions of ions and neutrals striking the substrate. The PCMCM launches pseudoparticles representing ions and neutrals, based on the electron impact source functions and the time dependent electromagnetic fields. Using a Monte Carlo simulation, the PCMCM tracks the trajectories of the ions and neutrals while capturing their gas phase collisions using the same reaction mechanism as in the HPEM. The energy and angle of pseudoparticles are collected statistically, as they strike specified locations on the substrate, to produce the energy and angular distributions.

An overview of the different plasma species included in the model is presented in Table 1. The gas phase chemistry reaction set between the C_4F_8 and SF_6 based plasma species (including molecules, radicals and ions, as well as the electron impact reactions), is summarized in our previous work [34], and is not repeated here. This chemistry reaction set

has been validated by comparison with experiments, and good agreement was reached between the simulation results and the experimental data in Ref. [34].

Concerning the collisions of plasma species with the reactor walls and substrate, we defined a simplified reaction set, i.e. each species will reflect from the walls and substrate as its neutral ground state counterpart except for electrons, who will be lost permanently at the walls, and removed from the simulations. The F atoms will recombine to F_2 at the walls and substrate with a probability of 20% [35].

Table 1. List of the species included in the model.

Neutral species: SF_6 , SF_5 , SF_4 , SF_3 , SF_2 , SF , S , F , F_2 , F^* , SiF_4 , C_4F_8 , C_4F_7 , C_3F_7 , C_3F_6 , C_3F_5 ,

C_2F_4 , C_2F_3 , CF_4 , CF_3 , CF_2 , CF , C

Charged species: SF_5^+ , SF_4^+ , SF_3^+ , SF_2^+ , SF^+ , S^+ , F^+ , F_2^+ , $C_4F_7^+$, $C_3F_7^+$, $C_3F_6^+$, $C_3F_5^+$, $C_2F_4^+$,

$C_2F_3^+$, CF_3^+ , CF_2^+ , CF^+ , C^+ , electrons

3. Results and discussion

3.1 Self-bias induced by the EAE

Figure 2 shows the time-averaged dc self-bias voltages as a function of phase shift θ , for different ICP powers, i.e. 300W, 800W, and 1500W. The self-bias varies almost linearly with θ at a fixed ICP power. This trend is consistent with the EAE results in CCP [11-17], which implies that a capacitive electrical asymmetry is realized in this ICP reactor. In addition, the self-bias trend lines are almost parallel to each other at the three ICP powers, just with a small downward shift when increasing the ICP power, i.e. the self-bias magnitude becomes higher at larger ICP power. This is because the electron density will be enhanced at larger ICP power (see further), which will induce a relatively high electron flux to the bottom substrate, and thus, a higher self-bias will be developed to balance the electron flux and positive ion flux. The small shift of the self-bias at different ICP power also indicates that the ICP power supply does not greatly affect the capacitive EAE.

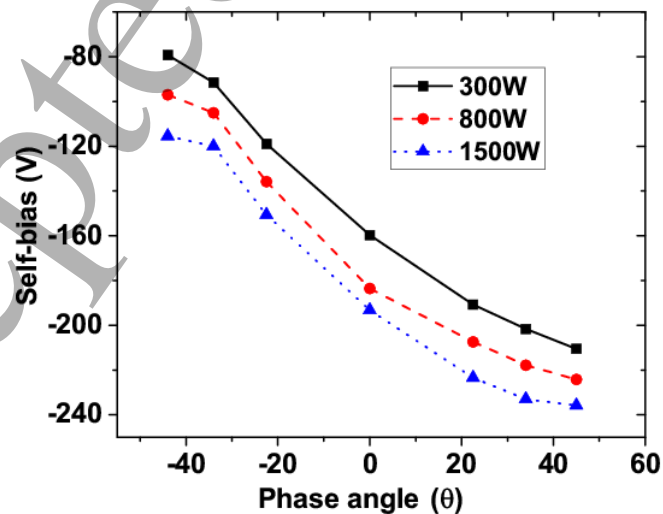


Figure 2. Self-bias at the RF biased substrate electrode as a function of phase shift θ , for different ICP power.

3.2 Ion flux and energy distributions

In figure 3 we plot the fluxes of the most important ions (i.e., $C_2F_4^+$ and SF_5^+) to examine the modulation of the phase shift and ICP power on the ion fluxes. We can see that the fluxes significantly increase upon raising ICP power, especially when raising the power from 800W to 1500W, where the fluxes almost double. Indeed, the electromagnetic field caused by the inductive power will irradiate broader at higher power, yielding more effective heating. Furthermore, the ion fluxes only vary within $\pm 20\%$ for different θ at a fixed ICP power, especially in the range from -25° to 45° .

Thus we can conclude that when raising the ICP power, the ion fluxes can be significantly modulated, while the self-bias only changes slightly at a fixed θ . Vice versa, when changing θ , the self-bias can be greatly tuned, while the ion fluxes only fluctuate slightly at a fixed ICP power supply.

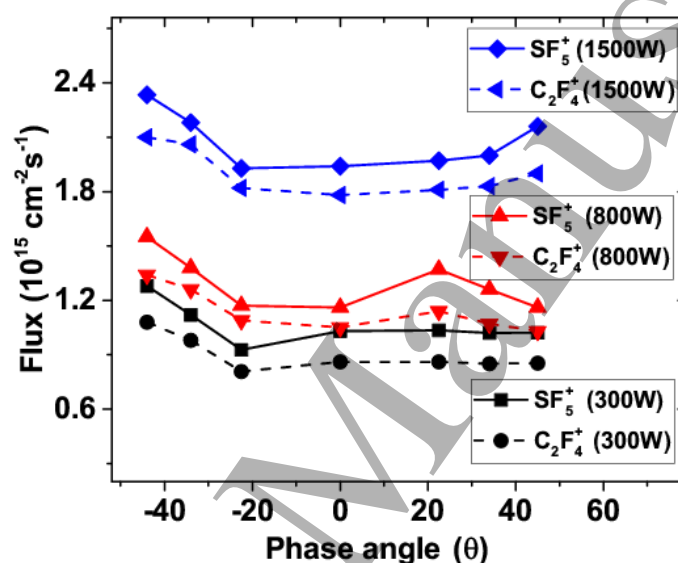


Figure 3. Surface averaged fluxes of SF_5^+ and $C_2F_4^+$ towards the substrate electrode, as a function of phase shift θ , for different ICP power.

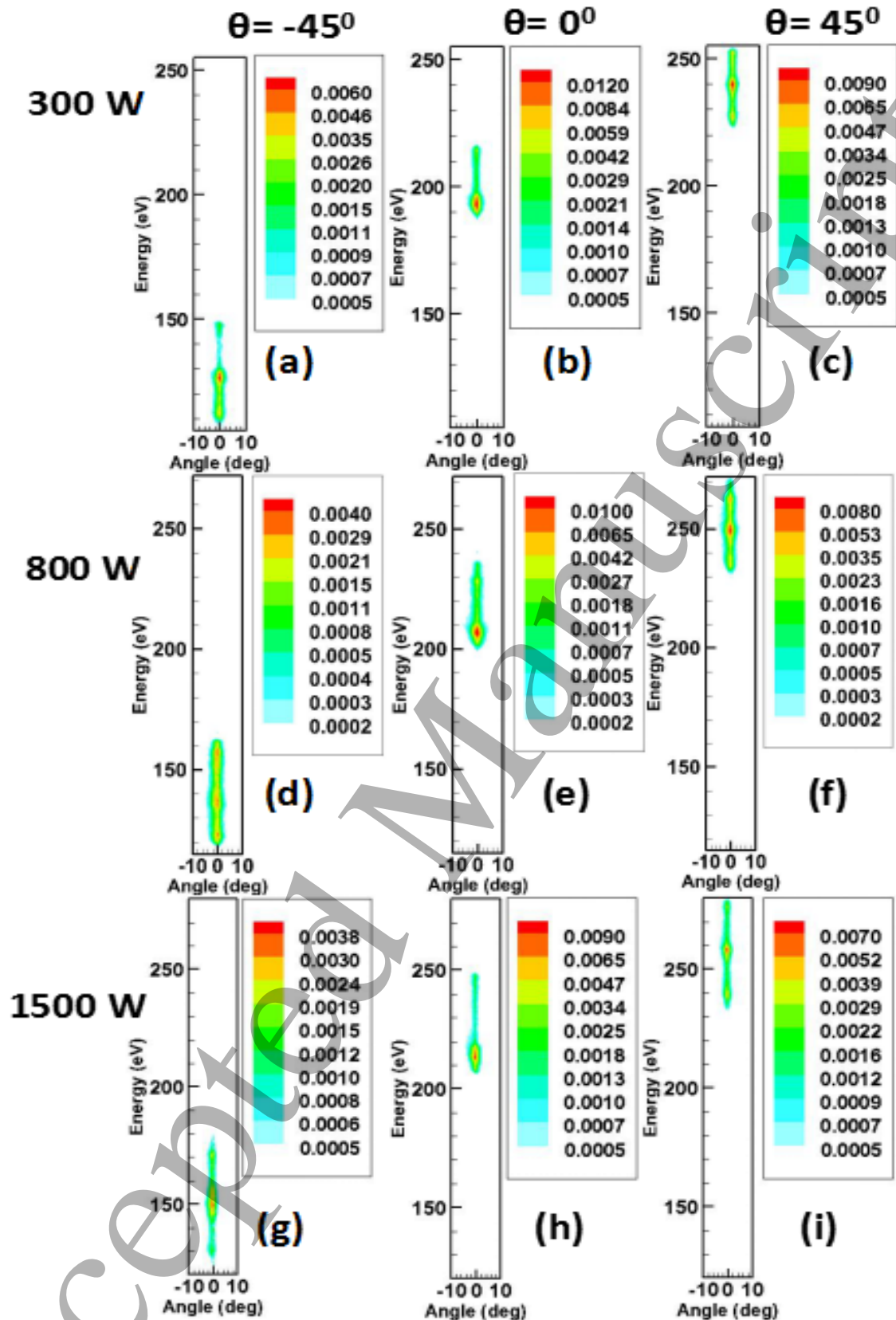


Figure 4. Normalized ion energy and angular distributions of SF_5^+ on the substrate electrode, as a function of phase shift θ , i.e. -45° (a,d,g), 0° (b,e,h), 45° (c,f, i), for different ICP power supply, i.e. 300W (a-c), 800W (d-f) and 1500W (g-i).

To better understand the modulation of the EAE on the ion properties, we further examine the time averaged ion energy and angular distributions of SF_5^+ ions bombarding the substrate in figure 4. The maximum ion energy can be well modulated for all ICP powers (especially at 300 W, the modulation is by a factor of about two), i.e. the ion energy distributions are all moved to larger values as increasing the θ from -45° to 45° , which corresponds to the variation of self-bias in figure 2. Furthermore, one can note that there are three energy peaks in the ion energy distributions at both $\theta = -45^\circ$ and $\theta = 45^\circ$ (more obvious at 800 W), which is consistent with the results in CCP in Ref. [12]. Note that there is 45° phase delay for the sine voltage waveform used in this work, compared to the cosine voltage waveform used in Ref. [12], which was proven in Ref. [17]. This again implies that a capacitive electrical asymmetry is realized in this ICP reactor. Thus, together with figure 3, the independent control of the ion fluxes and ion energy in this type of ICP configuration has been demonstrated. The changes in the ion energy distribution profiles are caused by the variations in the voltage waveform at different θ [12].

Unlike the narrowed spread of ion energy in arbitrary waveform technique [3, 24], the spread of ion energy only slightly changes with the phase shift θ in the EAE, which limits the improvement of selectivity of plasma processing, but the independent control of the ion fluxes and ion energy is also a very important parameter for semiconductor manufacturing.

3.3 Electron distribution profiles

Finally, figure 5 illustrates the influence of the EAE on the electron density profiles. The maximum densities always appear near the coil, resulting from the strong electromagnetic fields. Furthermore, both the maximum values and the profile area increase, due to the stronger and broader electromagnetic field, when raising the ICP power for the same θ . This is also the reason for the significant increase in ion fluxes shown in figure 3. In addition, when fixing the ICP power, the density profiles only change slightly with θ from 0° to 45° , which corresponds to the small fluctuation in the ion fluxes shown in figure 3. However, the density profiles at -45° are much different, with an obvious enhancement near the RF biased substrate electrode. This is because the self-bias is very small at -45° (see figure 2), and the plasma bulk is closer to the substrate electrode. Since the top electrode of the diffusion chamber is half open at the center, the capacitive heating in the diffusion chamber will be more effective when the bulk is close to the bottom substrate electrode. Thus, the small self-bias at -45° induces an enhanced plasma density, which also explains the higher fluxes at -45° in figure 3.

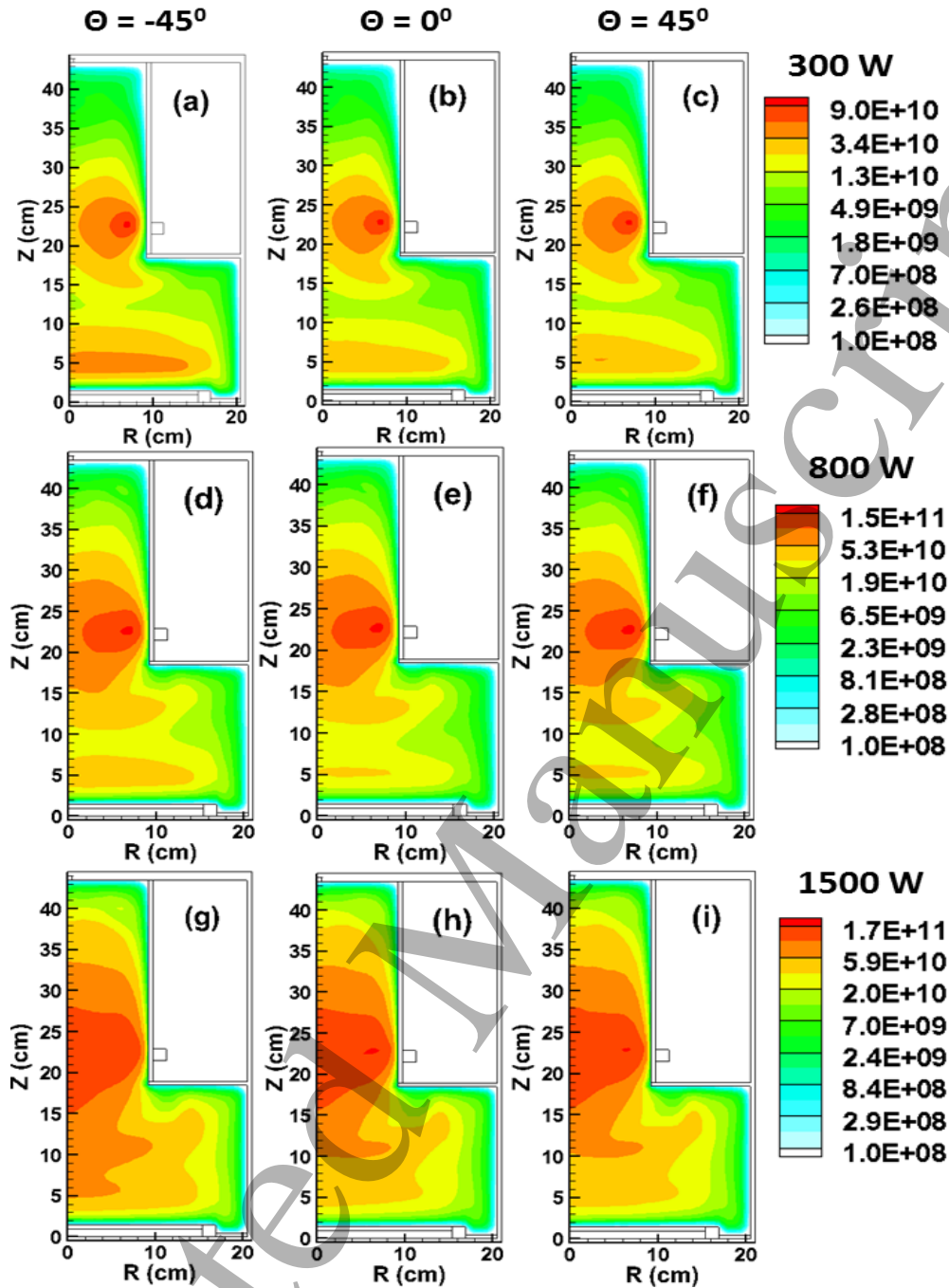


Figure 5. Electron density profiles as a function of phase shift θ , i.e. -45° (a,d,g), 0° (b,e,h), 45° (c,f,i), for different ICP power supply, i.e. 300W (a-c), 800W (d-f) and 1500W (g-i).

4. Conclusions

In conclusion, we propose here a new discharge configuration, which allows exploiting for the first time the EAE in an ICP reactor. By applying a dual frequency driving voltage with fundamental frequency and its even harmonic at the bottom RF biased electrode, the EAE is achieved between the bottom electrode and the half-open top electrode of the diffusion chamber. The plasma properties can further be modulated by tuning the phase shift θ between the harmonics. In particular, we demonstrate that the dc self-bias is approximately a linear function of θ , and consequently the maximum ion energy can be well modulated, while the

ion fluxes stay rather constant within a large range of θ for a fixed ICP power. Furthermore, the ion fluxes vary significantly with raising ICP power, while there is only a small change in the self-bias at fixed θ . Therefore, both independent modulation of the self-bias (and consequently the ion energy) and control of the ion fluxes can be realized via the EAE in this ICP discharge configuration.

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