Stochastic Approach in Approximation of the Transient Plasma Sheath Behavior in FEM

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Abstract: Recently, the advanced plasma tools have been using very high frequency power sources (>100 MHz) and their combination to excite plasma utilized in semiconductor technology. This approach is evoking the regimes that are less understood and currently a subject to many studies and experimental investigations. The paper describes quasi-stochastic approach applied for sheath properties and used in dual frequency ($f_1 >> f_2$) capacitively coupled plasma transient simulations. The initial phase of these modeling activities and investigations shown a good numerical stability of a computational scheme. The validation of a proposed numerical model and its equivalence to full transient solution are discussed.

Keywords: plasma simulation, capacitively coupled plasma, stochastic approach.

1. Introduction

The advanced plasma tools have been using very high frequency power sources (≥ 100 MHz) or combination of RF and DC supplies applied to specific hardware components. The reason for this is to take more advanced control over the plasma processes and their performance at the wafer surface in semiconductor technology.

Recently, the capacitively coupled plasma (CCP) reactors have employed dual-frequency (DF) power delivery or even more sophisticated techniques to control the energy and density of the ions and radicals at the wafer surface. This approach is evoking the regimes that are less understood and currently a subject to many theoretical studies[1] and experimental investigations. The technical innovation and more complex chemistry process development for fine tuned semiconductor manufacturing tools and processes are challenged not only by design and/or material changes but also by a fundamental understanding and response of the plasma under the impact of the combination of multiple RF power sources, such as skin effects, standing wave effects, local vs. non-local plasma heating effects, etc.

Use of the modeling and numerical simulation plays an important role in development of plasma equipment and related etch processes in plasmas. Specifically, FEM plasma fluid modeling is attractive and practical alternative to a full kinetic theory treatment of the plasma. It can provide both computational economy and physical insight. Besides the FEM approach, there are numerous models on the plasma starting from PIC simulation towards a pure fluid or hybrid fluid-kinetic models and, generally, they work well for particular tasks in bulk plasmas.[2] The plasma boundary - sheath - behavior is described either by analytical models (accuracy may impacted by proper assumptions) or particle-in-cell (PIC) models (time consuming approach). When looking for transient plasma solutions, on two or more different time scales, both methods are getting computationally very time consuming. Paper is introducing a quasi-stochastic approach used for DF transient plasma simulations ($f_1 >> f_2$). In Section 2 we will describe the generic configuration and conditions of the DF CCP reactor (Sec. 2.1), briefly refer to a single frequency (SF) sheath model (Sec. 2.2) and implemented plasma bulk model (Sec. 2.3). The use of the Multiphysics COMSOL is reviewed in Sec. 2.4. The principles and implementation of the stochastic approach are discussed in Sec. 3. The results on a validation of the proposed numerical model and its equivalence to full transient solution are discussed in Section 4.

2. Model Description

2.1 Reactor Configuration

The typical CCP etching reactor is illustrated in Figure 1. The plasma is formed by an excitation of the reactive gases under pressure in range from tens to hundreds mTorr, and plasma itself is enclosed within metallic reactor. In certain portion of the chamber, the internal surfaces are formed either of metallic or dielectric materials. Specifically, we considered quartz in this study and metal is considered to be a perfect conductor (PEC). The silicon wafer is placed on the RF powered metallic pedestal. Typical frequency range of the power supply is from several MHz to over 100 MHz. Moreover in RF plasma processing, the self-bias on dielectric substrates may be developed.[3]

Principally, between plasma and internal surfaces there is so-called “plasma sheath” which is always formed at the plasma boundary, and its properties are usually considered as ones for vacuum. However, in numerical model exploring ~100 MHz excitation range the geometrical atributes of the sheath and wall material properties adjacent to sheath have to be considered consistently.

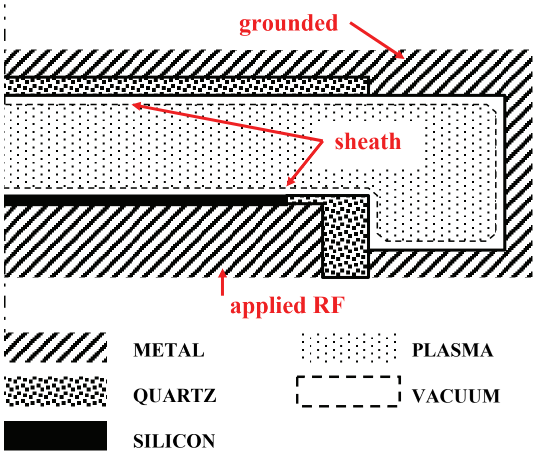

Figure 1. Scheme of generic CCP etching reactor.

2.2 Single Frequency Sheath Model

In this particular study an intermediate version of the model on CCP reactor prepared under COMSOL Multiphysics environment was explored and, currently, it is undergoing a continued development. Code is based on modeling the electromagnetic effects in CCP described recently by Lee et al., in Ref.[4] For more details we refer readers to above cited reference. Briefly, reciting from the published paper, this model couples Maxwell equations, fluid plasma equations and a sheath model with stochastic heating effects when power is deposited from a single-frequency RF source. In such model, the sheath thickness is formally considered to be constant and its actual physical properties are mimicking by use of a variable sheath dielectric constant while computational convenience of not moving plasma-sheath interface (computational grid) is retained [*ibid*].

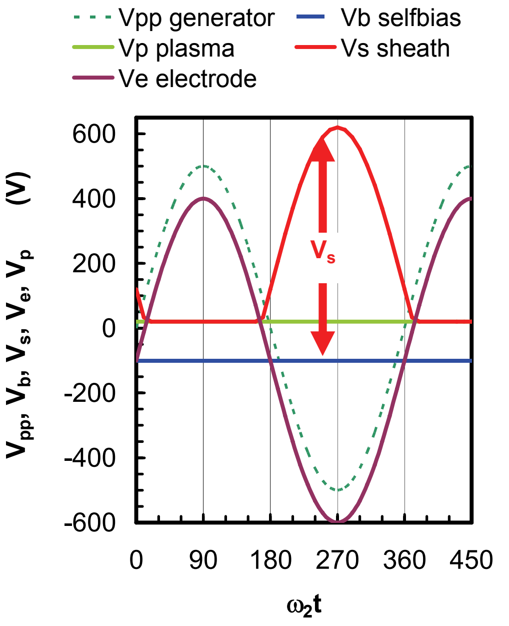

Figure 2. The model considered a sinusoidal signal shape from the RF generator (V_{pp}), the selfbias (V_b), imposed a RF electrode (V_e), a plasma potential (V_p), and sheath voltage (V_s).

We have accommodated a phenomenological model to our configuration and conditions. The RF power may be applied to upper or lower electrode, UEL or LEL, respectively. We investigated LEL connected to the RF power (f_1=100 MHz). The initial simulations showed that model provides results in qualitative agreement with experimental data at various operational conditions.[5] Now, the second frequency was applied. This was done through a transient model at 2 MHz cycle, which was implemented through the sheath properties. Figure 2 illustrates the signal shape at the sheath (V_s) at the second frequency (f_2) assuming the negative selfbias potential at the wafer holder (V_b) and superimposed RF amplitude from generator (V_{pp}). The potential difference between RF electrode (V_e) and plasma potential (V_p) is constituting the actual sheath voltage (V_s). We have to notice that the interprettation of the sheath voltage is largely simplified here, and more sophisticated description from literature should be used in further development. Though simplified approach, but fair enough to understand the code performance. Our other reasons to proceed in this manner were to avoid ambiguity due to the potential convergence issues, better focus on core model development and its numerical testing.

2.3 Plasma Fluid Model

Plasma generation and transport was computed by ambipolar-drift diffusion approach[6] considering a transient mass balance equation for *"i"* type of the ions in a form

$$\frac{\partial n_i}{\partial t} + \nabla\left(-D_a \nabla n_i + n_i \vec{u}\right) = R_i \tag{1}$$

where symbol D_a stands for an ambipolar diffusion coefficient. Equation (1) shows more generic formulation designated for presence of the multiple ions in plasma, however, we applied it for Ar^+ ions only, thus index *"i"*=1. To advance with model development, we also stripped-off Navier-Stokes module components in Eq. (1) - to free computational resources. Gas flow impact was not investigated in this work, but formally model accommodates to this component and it will be subject to the next level simulation tasks.

In generic form, the neutrals in plasma will comply with mass balance Eqs. (2) with considering a generation/recombination total reaction rate, Eq. (3), of species n_k with cross-sections for individual generation and recombination rates due to the collisions with electrons, σ_{jk} and σ_{kj}, respectively; the rate constants for forward (R_{jkl}) and backward (R_{kjl}) reactions due to the collisions with species n_k or n_j, that is

$$\nabla\left(-D_k \nabla n_k + n_k \vec{u}\right) = R_k \tag{2}$$

where $k =$ all neutral species,

$$\begin{aligned} R_k = n_e \sum_j n_j \left\langle \sigma_{jk} v_e \right\rangle + \sum_{j,l} R_{jkl} n_j n_l - \\ - n_e n_k \sum_j \left\langle \sigma_{kj} v_e \right\rangle - n_k \sum_{j,l} R_{kjl} n_l \end{aligned} \tag{3}$$

Symbol v_e is electron velocity and D_k is diffusion coefficient of *"k"-th* particle. Again, the incompressible Navier-Stokes single gas transport (stationary case) with velocity $\vec{u}(r,z)$ is formally assumed but currently not used in a computation. Using a single inert gas (argon) as working medium has simplified also the reaction terms in Eq. (3).

The electron (T_e) temperature computation considered the energy conservation equation in a form

$$\begin{aligned} \frac{\partial}{\partial t}\left(\frac{3}{2} n_e T_e\right) + \nabla\left(\frac{5}{2} T_e \Gamma_e - k \nabla T_e\right) = \\ = Q_{abs} - e\Gamma_e E_a - \frac{3m}{M} v_m n_e T_e - \sum_i V_i v_i n_e \end{aligned} \tag{4}$$

where E_a is an ambipolar electric field, Γ_e - electron flux, v_i - the collision frequency of *"i"*-th reaction and V_i is its threshold, e - elementary charge, m - electron mass, M - total mass of two particles in elastic collision, c_p, ρ and k are gas heat capacity, density and thermal conductivity of the gas mixture, respectively.

Further assumptions made in model were: (1) an assumption that Bohm flux is entering a thin sheath, thus it is determined by the electron density (n_e) and the electron temperature (T_e); (2) the neglection of a sputtering and (3) the secondary electron emission by ions. The incorporation of these effects will be essential in refined model version and it is under consideration.

2.4 Use of COMSOL Multiphysics

On formal side, the model was built in COMSOL Multiphysics environment in 2D geometry with an axial symmetry. Further, it is utilizing: (1) TM Waves Module for 100 MHz wave propagation into a plasma, (2) and (3) Convection and Diffusion Modules (one for plasma fluid the another for neutral species), and (4) Convection and Conduction Module to account the electron energy balance. We sustained a gas flow module inactive during computation. Because our goal was to clarify the applicability of the new method and algorithm in numerical terms, and to avoid complex chemistry ambiguity during its validation by experiments, we choose the simplest case – an inert argon gas as medium for plasma generation.

At the computation start, typically, the initial conditions for most concentrations variables were set to much lower values then expected solution (about $\times 10^{-6}$) or to zero. The coupled model scheme was repeatedly computed using the instantly updated data on all involved variables and parameters from instant solution which served as initial data for the next cycle until the convergence was achieved.

3. Stochastic Formulation of Sheath

Computation on 100 MHz and 2 MHz timescale corresponds to cycle times 10 ns and 500 ns, respectively. The time step at short scale is even shorter (<1 ns). Our initial procedure was a sequential computation of the plasma distributions at various phases of the 2nd applied frequency. For instance, at the phase steps set to 10° this represents up to 36 cases to complete 2 MHz cycle, which in the real time and 64 bit PC with 16 GB internal memory still took considerable CPU time to accomplish (about 1 to 4 hours per single phase converging computation). Thus DF transient model took significant computational time to provide converged solution over 500 ns cycle. Thus in our development, we had to search for different approach – a much faster model. This was accomplished by an introduction a "stochastic equivalence approach" for sheath domain to sustain fast computation cycles and still generate results that correspond to dual-frequency plasma behavior. In other words, this approach formulates the "*transient PDE simulation*" into a computationally significantly reduced task - "*stochastic or quasi-stochastic PDE simulation*" (see, Figure 3).

That means in a numerical model, the transient characteristic – here it is a time-dependent variable $\Psi(x,z,t)$ in point $P\{x,z\}$ within domain $D^2\{x,z\}$ - is transformed into the spatial characteristics with a probability function $\Theta \equiv \Theta[\Psi(x,z)]$ defined in the identical point. In this way, the time variable is excluded from consideration in a transient model, and a random assignment of the values of $\Psi(x,z)$ from interval $\left\langle \Psi^{min}(x,z); \Psi^{max}(x,z) \right\rangle$ in each point $P\{x,z\}$ in domain $D^2\{x,z\}$ will reconstruct a probability distribution function $\Theta \equiv \Theta[\Psi(x,z)]$.

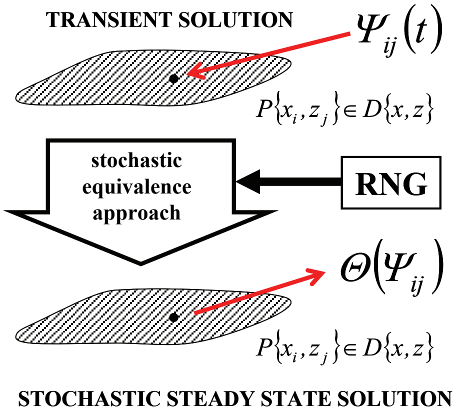

Figure 3. The principal scheme of the stochastic equivalence approach implementation (*RNG* - Random Number Generator).

The method of random assignment and grid resolution will determine the accuracy and propriety of such approach and should be confirmed numerically and by experimental observations. Currently, in described model, the actual "sheath-plasma" interface properties are not absolutely random but given by harmonic function derived for plasma sheath (Figure 2) from RF waveform at fundamental harmonic 2 MHz (quasi-stochastic noise). Suggested approach formally emulates the interface properties that could be observed in real plasma by probing the "plasma-sheath interface" properties randomly in times that are larger than period of the second frequency. The "infinitively small" spatial periods (about 0.1mm << grid dimensions << sheath or plasma dimensions) are then used to specify quasi-stochastic properties of such plasma sheath. Obviously, the output may be sensitive to meshing resolution in sheath domain, thus, the proposed transient-to-spatial conversion algorithms were tested on mesh sensitivity and showed consistent results for spatial period << grid dimensions.

4. Results and Discussion

4.1 Transient Model

Using described above model for CCP at primary excitation by frequency f_1=100 MHz, we computed the transient plasma distributions over the various phases of the low frequency cycle (f_2=2 MHz,), and it is shown in Figure 4. From this result it is immediately seen that second frequency excitation will have an impact on plasma distribution due to the variation of the plasma distribution over the RF cycle. The time-average plasma density over 2 MHz cycle is depicted in Fig. 4 by rectangle symbol.

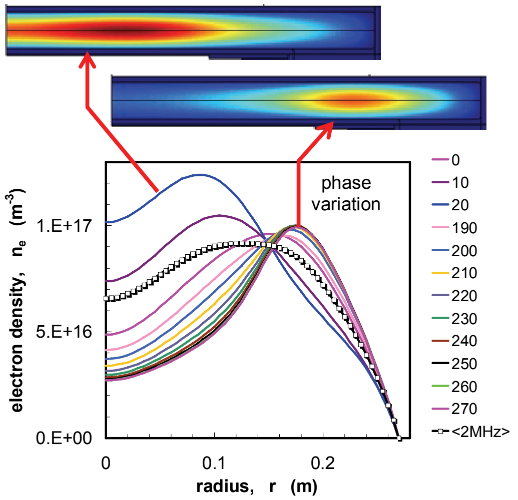

Figure 4. The plasma density radial distributions solved for 100 MHz during the over-imposed transient solution at the secondary frequency of 2 MHz. Argon pressure was 100 mTorr. The solutions are showed only for selected phases due to a specific signal shape at 2 MHz.

4.2 Stochastic Model

This initial effort – a time consuming transient solution (part of these results were shown in Figure 4) - has been compared with results obtained by new "stochastic" approach. Figure 5 shows radial plasma density across the wafer calculated both from transient and stochastic solutions at argon pressure 10 and 100 mTorr. From these simulations the reasonable agreement can be observed, specially at reduced pressure, and it has found confirmation by the experimental results as well, in Ref.[5a]

The next steps in this investigation were numerical and experimental validation at conditions with respect to the wider process window parameters. Further simulations are still undergoing currently, and due to the scope and limitations of this paper only several examples are presented to reader.

a) For instance, we processed a wider data set obtained from described above model and it was related to plasma profile development over the wide range of the explored pressures (Figure 6). The observation, that low pressure CCP (100 MHz) is center-peaked, but with increase of the pressure the maximum is moving off-center, this is well confirmed from other experimental studies and modeling investigations[5].

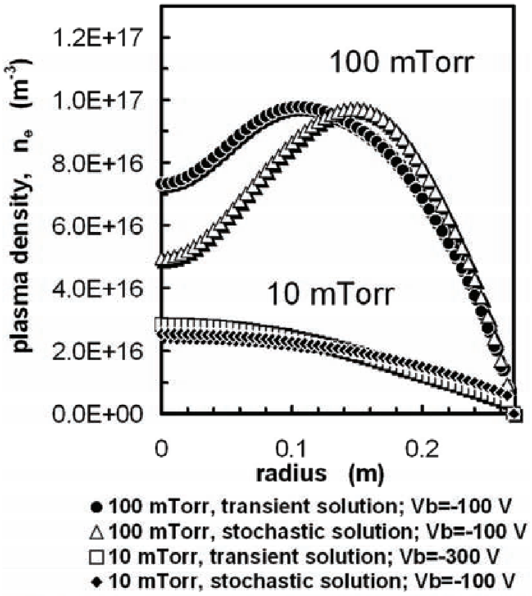

Figure 5. Radial distributions of the plasma calculated by transient and stochastic approach. Operating pressure 100 mTorr, the base 1st frequency f_1=100 MHz at V_{pp}=500 V, the 2nd frequency f_2=2 MHz at V_{pp}=500 V and V_{bias}=-100 V.

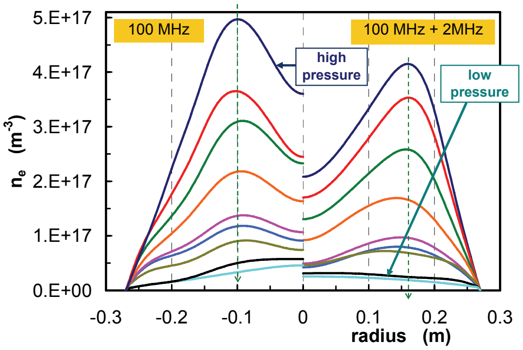

Figure 6. Radial distributions of the plasma at various pressures (10 mTorr to 500 mTorr) calculated by stochastic approach without (left) and with (right) applied dual freaquency. The 1st frequency f_1=100 MHz at P_{RF}=100 W, the 2nd frequency f_2=2 MHz at V_{pp}=500 V and V_{bias}=-100 V.

The described stochastic DF CCP model provided the interesting results when applied the second frequency (2 MHz) at investigated conditions. For instance, it indicated that maximum is more off-set and absolute plasma density is reduced. Such variation will have direct impact on the process uniformity which is important in technology performance.

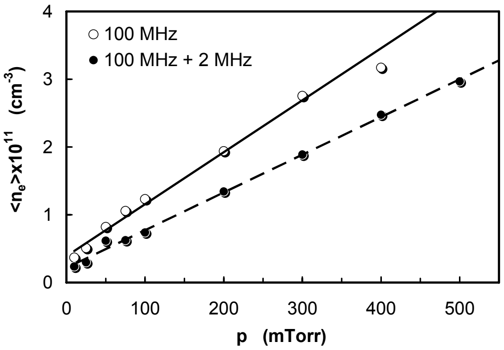

Figure 7. Average plasma density (over wafer radius) vs argon pressure in the case of single frequency (100 MHz) and dual frequency (2 MHz) power excitation. The other process parameters were kept constant.

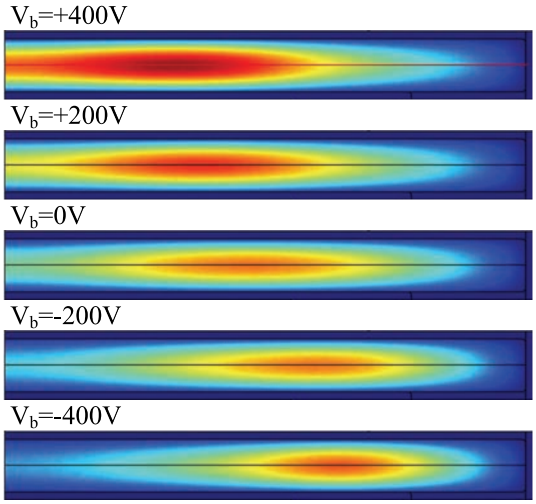

Figure 8. Radial distributions of the plasma at various selfbias potential at the wafer electrode at 100 mTorr other parameters were kept constant. DF CCP stochastic approach: f_1=100 MHz at P_{RF}=1000 W, f_2=2 MHz at V_{pp}=500 V and V_{bias}=-100 V.

b) The impact of the pressure in SF and DF CCP is shown in Figure 7, showing the influence of the 2nd frequency on the plasma density (radial profiles were influenced, too). The reduction of the bulk plasma density could be interpreted by increased ion flux towards the wafer surface due to the larger sheath voltage. At the same generation rate (RF power at 100 MHz is kept constant) the loss at wafer is increased. We neglected here the 2 MHz power delivery into the bulk plasma, assuming it is a fraction from high frequency heating of the plasma.

c) One more example on parametric study – the radial distributions of the plasma at various self-bias potential (formally sustained at the wafer electrode) were investigated at 100 mTorr, other parameters were kept constant. Under these conditions the DF CCP stochastic approach revealed that process uniformity will be effected due to the shift of the maximum plasma density outwardly at more negative bias potential (Figure 8).

Though, we do not pretend to discuss above given results within this paper, but we can conclude these and many other results were achieved and illustrate the advantage of the use of the stochastic approach in DF CCP with significant savings in computational time resources.

4. Conclusions

Nevertheless, the heuristic approach apparent at the initial phase of these modeling activities, we can conclude that analysis and numerical testing showed that numerical stability of a new computational scheme is not different from SF model, and, more important, computationally the DF cases are solved within by order shorter times than complete transient case. The comparison to available literature data and ongoing experimental validation confirmed also qualitative agreement of the stochastic method. The validation by experimental data is still undergoing and will be presented in future works. Next systematic investigations should be focused on completeness and optimization of the new method. For instance, the answers related to the limitation of such method are unknown. The specific knowledge of stochastic PDEs would be of a great value for further investigations. Furthermore, a methodology has to be developed to extract useful information and characteristics from the solution obtained by stochastic approach that would be otherwise easily available from transient solution. In future developments, the intention is to consider more accurate extension of the RF sheath theory[6], cleared of some specific limitations in this investigations, and fully implement described above model for DF CCP.[7] Finally, we are concluding that stochastic method has a potential and it is suitable for further analysis of DF CCP reactor design and plasma properties.

8. References

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