A technique for implementing complex boundary configurations in industrial plasma modelling and simulation

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Declaration

I hereby certify that this material, which I now submit for assessment on the programme of study leading to the award of Master of Science is entirely my own work, that I have exercised reasonable care to ensure that the work is original, and does not to the best of my knowledge breach any law of copyright, and has not been taken from the work of others save and to the extent that such work has been cited and acknowledged within the text of my work.

> Taghreed Abu Shamaleh, July 2010 ID No.: 51150221

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I would like to express my deepest gratitude to every single person who has been part of my rich and colourful experience as a postgraduate student at DCU.

Through the ups and downs, and even though my hexa-thon-isc course of study has not came to the expected –and muchly anticipatedend, the richness that has been bestowed on me, my outlook to science, physics, and life, has exceeded even my wildest dreams. This can never be overlooked as it changed me for the best, and widly opened new and exciting frontiers toward knowledge that I have never imagined.

The future is unknown, but as always, I am welling to embrace my bliss.

Taghreed Abu Shamaleh Dublin July 2010

Abstract

The use of plasma as an industrial tool has become the norm within the surface treatment industry. However; our understanding of the plasma surface interactions is still within the R&D phase.

What can be done experimentally is limited due to the electromagnetic properties of plasma and the intrusive nature of the methods available for experimentalists. Incorporating complex boundaries (reactor walls/treated surfaces/external circuitry) in computerized simulation is a sought after goal in the battle of understanding industrial plasma peculiarities.

A flexible-easily configurable- modus operandi has been devised to implement the effects of complex boundaries within the vicinity of an electromagnetically active system. The technique is based on the spatial conversion of the system into dynamic electromagnetically timevariable elements, then using circuit/Maxwellian approach to obtain and analyze time snapshots of the spatial voltage distribution across the system. The technique has been benchmarked using simplified case studies/models that can be theoretically analyzed, and has been found to be both robust and reliable.

We used this technique to analyze a plasma system within the vicinity of complex boundaries. The plasma itself has been implemented within the simulation using two different theoretical approaches, further demonstrating the flexibility of the technique.

The end result of this study yield in two folds: the potential distribution along adjustable boundary layers, with a special interest in what is commonly known as a triple junction configuration. And the impact of the used plasma model on the results.

We conclude with a discussion of the results, and future planned work.

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Outline

In an age where everything is geared toward unification, it's a bit of a disappointment to see that the trend within plasma physics research is heading toward the opposite direction.

You will notice that the general feel throughout this study is to explore the possible venues of unification and reconciliations between the various theoretical treatments used in the study of plasma systems. However, we find it quiet important to state that our prime goal will be the investigation of the effects of complex boundaries within the vicinity of plasma system.

A technique will be devised to implement the effects of complex boundaries within the vicinity of plasma system. The algorithm will be based on the spatial discretization, and the use of circuit/maxwillian approach to integrate the discretised system within a common numerical treatment. Eventually ending up with the spatial voltage distribution across the system, and most importantly, along the composition of the boundaries.

Our starting point is that the theoretical treatment of a plasma reactor can be divided into a study of (linked) sub-systems without losing track of the way they influence each other (Kaganovish 2002, Poiunto 1986). We follow by a proposed elaboration and systemization of circuit theory. A method that has been initially used in plasma modelling in the early 40s, became fairly popular during the 60s and 70s, and is still actively in use among experimentalist within the field...

A rigorous and flexible computational approach based on the fusion between electromagnetic theory and nodal analysis has been formulated to systemize the conversion of the spatial continuum into a discrete circuit equivalence, and then computerize the process of analysing such system no matter how finely meticulous the conversion process is.

The developed algorithm has been carefully devised to enable it to be easily interface-able into more complicated treatments. The method has been tested using simplified case study/models, and has been proven to give an excellent accuracy compared to theory. The physical assumption used in developing the mathematics behind the technique provides an excellent way to extend the treatment to include the effect of the external circuitry within any simulation of any form. It can also offer a convenient link between theory and experiment. This will definitely lead to a better interpretation and interaction between experimental measurement and simulation.

In chapter one, we outline the relation between the concepts of field theory and circuit theory, the limitations, and how to properly link between the both of them. We emphasize the fact that both theories contain the same concepts and can present the same picture but from a different point of view. We then discuss why we think circuit theory sometimes has an advantage, and can contribute to a better understanding of any (classical) system under study.

A literature review will be presented in chapter two to demonstrate the different approaches (and levels of complexities) used to implement and take advantage of the ideas accessible via circuit theory by various researchers, and for various purposes. Many of the concepts used in the development of this study were scattered through these papers.

In chapter three, we introduce the concept of triple junction configuration (TJC), a highly common configuration structure in plasma reactors. Using the previously developed method, we integrate a TJC into a plasma system model. The introduction of the plasma has been made as flexible as possible to enable the testing of various plasma representations; including two semi-theoretical representations each included a different plasma sheath treatment.

We present Results showing the voltage and field distributions for the various parts along the triple junction boundaries in chapter four. The effect of the dielectric resistively on the way the plasma perceives the ground through will also be investigated.

Although there are some differences between what we get from various the theories, the general trend shows that the higher the resistivity of the dielectric layer is, the more capable it will be of screening the details of the electrical non - homogeneity behind it from being "sensed" by the plasma.

As this proves the necessity to take the electrical non – homogeneity of boundaries into consideration if a homogeneous particle bombardment is critical (as in case of the reactor walls), it also

indicates the ability to locally alter the ion bombardment energy via carefully tuning the non-homogeneousness of the configuration behind the dielectric (as in the case of chip etch for example).

The profile of the voltage distribution along the dielectric surfaces indicates that the existence of the metallic bridge causes irregularities in the profile, hence a possibility of current flow along the dielectric surface, and the existence of surface charging process. All of which might be related to the wall ceramic cracking phenomenon observed in plasma reactors under working stress. The reason behind this conclusion is that the ceramic cracking phenomenon shows bifurcation behavior [miller (1989), (1994), Chalmers et al (1995)], indicating that an accumulating process is involved.

The results indicate that the range of irregularity in the voltage distribution along the dielectric surface depends on the resistance of the dielectric.

We conclude that factors of the external environment of a plasma reactor have the potentials for being used as a way to tune the plasma processing operations. It also shows the tendencies to generate an unusual stress that can in the long run lead toward undesirable effects when not accounted for - under operation conditions.

While the work in this thesis proposes the possibility and introduces the principles on which this issue can be tackled. Further work has to be done before this can be utilized on a more efficient way.

The relation between field theory and circuit theory

Introduction

With the increasing demand for an in depth understanding of the various processes involved in material processing, plasma physics has attracted a continuously growing interest within both academia and industry. Plasma material processing is a highly popular environment for material properties alteration processes, and an essential pillar in the microchip industry.

The understanding of what really happens (both macroscopically and microscopically) at plasma boundaries under various conditions is one of the essential targets to be achieved. It will enable more control and predictability over the end result of the processing operation.

Much effort has been and is being devoted to the treatment of plasma boundaries when the plasma is facing an electrically non homogeneous border [see for example Kim et. Al. (2004) and (2004]. Under operation conditions, complex boundaries within the vicinity of plasma processing cell are the rule not the exception. For that reason, developing a simple to apply , robust technique to deal with such complexity should provided a huge advantage toward the development of better and more efficient processing techniques .

Circuit theory has been extensively used in the past to tackle various problems in plasma physics. Literature review shows the

various approaches of that usage. But before presenting these approaches, or proceed into presenting the work we have done, it worth spending some time clarifying the origin of circuit theory.

Maxwell equations, field theory

Tackling electromagnetic phenomena from a macroscopic point of view is one of the most common practices within the field of plasma physics. Such approach is completely justified when the system's dimensions are much bigger than atomic dimension, and charge magnitudes are larger than atomic charges. By doing so, we are allowed to ignore the granular structure of matter and charge.

The usual electromagnetic field equations are expressed in terms of six quantities. These are:

E the electric intensity (volts per meter)

H the magnetic intensity (amperes per meter)

D the electric flux density (coulomb per square meter)

B the magnetic flux density (Weber per square meter)

J the electric current density (amperes per square meter)

ρ The electric charge density (coulombs per cubic meter)

Whenever the above quantities are well behaved, they obey the differential form of Maxwell's equations:

$$\vec{\nabla} \times \vec{E} = -\frac{\partial B}{\partial t}$$
$$\vec{\nabla} \cdot \vec{B} = 0$$
$$\vec{\nabla} \times \vec{H} = -\frac{\partial \vec{D}}{\partial t} + \vec{J}$$
$$\vec{\nabla} \cdot \vec{D} = \rho$$
[1-1]

These equations include the information contained in the equation of continuity:

$$\vec{\nabla} \cdot \vec{J} = -\frac{\partial \rho}{\partial t}$$
[1-2]

Which is nothing but another form of the conservation of charge law.

For each of equations in 1 - 1, there is a corresponding integral form:

$$\oint \vec{E} . d\vec{l} = -\frac{d}{dt} \iint \vec{B} . d\vec{s}$$

$$\oint \vec{B} . d\vec{s} = 0$$

$$\int \vec{H} . d\vec{l} = \frac{d}{dt} \iint \vec{D} . d\vec{s} + \iint \vec{J} . d\vec{s}$$

$$\oint \vec{D} . d\vec{s} = \iiint \rho \ d\tau$$

And of course, the integral form of the equation of continuity (eq. 1-2) is:

$$\oint \vec{J}.d\vec{s} = -\frac{d}{dt} \iiint \rho \, \mathrm{d}\tau$$
[1-4-b]

The equations in 1 - 4 (a and b) are actually more general as they do not require the various quantities to be well behaved. This is in fact very important feature in relation to this study. The quantities described above are what are commonly referred to as field quantities.

Field quantities vers. Circuit quantities

For each field quantity there is an associated circuit (or integral) quantity. These circuit quantities are:

V the voltage (volt)

I the electrical current (amperes)

Q the electric charge (coulomb)

 φ the magnetic flux (weber)

 ϕ^e the electric flux (coulombs)

U the magneto - motive force (amperes)

The explicit relationship between the field quantities and the circuit quantities can be summarized using the following equations :

 $v = \int \vec{E} . d\vec{l} \qquad \qquad \phi = \iint \vec{B} . d\vec{s}$ $i = \iint \vec{J} . d\vec{s} \qquad \qquad \phi^e = \iint \vec{D} . d\vec{s} \qquad \qquad [1-5]$ $q = \iiint \rho \ d\tau \qquad \qquad u = \int \vec{H} . d\vec{l}$

Linking between field theory and circuit theory

Equations 1 - 1 to 1 - 4 contain only field quantities, hence called field equations. While equations 1 - 5 contain circuit quantities and

hence called circuit equations. However; equation 1 - 4 (the differential form of Maxwell equations) can be writer in a mixed form as follow:

$$\oint \vec{E} \cdot d\vec{l} = -\frac{d\varphi}{dt}$$

$$\oint \vec{B} \cdot d\vec{s} = 0$$

$$\int \vec{H} \cdot d\vec{l} = \frac{d\varphi^e}{dt} + i$$

$$\oint \vec{D} \cdot d\vec{s} = q$$

$$[1-6]$$

And for the continuity equation:

$$\oint \vec{J}.d\vec{s} = -\frac{dq}{dt}$$
[1-7]

An alternative way of writing equations 1 - 6 and 1 - 7 is by the use of the notation of summation " Σ ". The summation symbol is set to denote the summation of a quantity over a closed contour as a replacement of the line-integral quantity, or the summation of a quantity over the closed surface as a replacement for the surface - integral quantities.

Accordingly; equation 1 - 6 will become:

$$\sum v = -\frac{d\varphi}{dt}$$

$$\sum \varphi = 0$$

$$\sum u = \frac{d\varphi^{e}}{dt} + i$$

$$\sum \varphi^{e} = q$$
[1-8]

And finally, the circuit form of eq 1 - 7 is:

$$\sum i = -\frac{dq}{dt}$$
[1-9]

Note that the first equation in the 1 - 8 set is the generalized form of Kirchoff's voltage law, while equation 1 - 9 is the generalized form of Kirchoff's current law.

In addition to Kirchoff's laws, circuit theory uses a number of "element laws".

Ohm's law for resistors, namely:

$$v = Ri$$
[1-10]

Which is a special case of the constitutive relationship:

$$\vec{j} = \sigma \vec{E}$$
 [1-11]

Also...

The equation for capacitors,

$$q = Cv$$
 [1-12]

expresses the same concept as:

$$\vec{D} = \varepsilon \vec{E}$$
 [1-14]

We can also get the following from the equation of continuity:

$$i = \frac{dq}{dt}$$
[1-14]

Hence the capacitor equation can be re-written as:

$$i = C \frac{dv}{dt}$$
[1-15]

In addition, the equation of inductors:

 $\varphi = Li$ [1-16]

Expresses the same concept as:

$$\vec{B} = \mu \vec{H}$$
[1-17]

From the first Maxwell equation we have:

$$v = \frac{d\varphi}{dt}$$
 [1-18]

So the inductor equation can also be written as:

[1-11]

$$v = L \frac{di}{dt}$$

Summary

The brief discussion presented in this chapter was an introduction to the notion that many mathematical forms exist and can be used to describe a single physical concept, system, or phenomenon. An understanding of the insight behind each mathematical vision, its extensions, and it limitations, enable us to link between those various forms in a correct way. That is specifically of high importance for the purpose of this study.

Through the few previous pages, we laid the background by which a field based description of a plasma system (whether through theory or simulation) can be inter-faced with a circuit theory based simulation. This will be of great value when dealing with a fairly non homogenous system (as in the case under study) or when you plan to implement the reactor external circuitry effect within a field based simulation for a more rigorous results .

The presented concepts should also be thoroughly considered when comparing experimental results (a circuit theory based description of the plasma) with theory or simulation (usually a field based description).

Circuit theory as used in plasma physics

Introduction

Plasma is the term we use to identify a fourth state of matter [Chen (1984)]. Being ionized; it's basically a composition of positive and negative charges. While it's common that negative charges are carried by electrons, and positive charges are carried by ions, this is not always the case [Fitzpatrick (2008)]. For the purpose of this study, we are limiting our treatment to such a condition.

In addition to the electric nature of plasma as a medium, plasma is also a composition of particles of various masses. The difference in the inertial properties of these particles would also mean differences in response time, and hence differences in the dynamic behaviour caused by the exerted field generated forces. This specific property is what leads to one of the most fascinating aspects related to plasma electrodynamics; the formation of the plasma sheath along boundaries [Chen (1984), Lieberman (1995)].

Recent years witnessed an increasing trend in using plasma in material processing. Be it etching, deposition, or surface properties alterations, the entire surface treatment process takes place specifically in the plasma sheath. Most common plasma diagnostics are intrusive in nature, which means that whatever we learn about the plasma is

delivered to us via its sheath region. Also, let's not forget that the Plasma itself is contained in a reactor vessel.

Visually speaking, the sheath region is easily distinguished from the bulk plasma by being dark in comparison. Electrically speaking, in an ideally isolated classical plasma, because of the free charges tendencies to distribute themselves to maintain the highest level of mechanical stability, one wouldn't expect big macroscopic electrical perturbations in the plasma bulk. The existence of solid boundaries within the vicinity of a plasma medium disturbs this equilibrium. Because of that, what applies to the bulk wouldn't necessarily apply to the sheath regions.

The sheath is always negatively biased with respect to the bulk. Because of this, ions entering the sheath will undergo an acceleration as they head toward the surrounding surfaces.

In the absence of collisions, one would expect the ions leaving the glow to reach the bombarded surface with energy equal to the bias voltage. Due to collisions, lons inertia, and their tendency to respond to the time averaged RF field, lons arrive at the surface with an energy distribution. The energy distribution is highly affected (among many various parameters) by the magnitude and the wave form of the time varying potential across the sheath.

The ability to determine the ion bombardment energy distribution (IED) means the ability to determine the degree of anisotropy in which the plasma processing operation occurs. It also gives an indication to

the possibility of the occurrence of the ion impact induced damage to surfaces.

An accurate presentation of the ion bombardment energy distribution should include a model that is able to predict the wave forms across the plasma sheath.

In an effort to predict these wave forms, researchers have used various combinations of circuit elements for modelling the plasma sheath in their equivalent circuit models of plasma reactors.

Literature review

The earliest citation of the use of circuit theory in plasma physics was published in German by Schneider (1954). It took nearly a decade for the concept to be deployed and re-used again in a paper written by Butler and Kino (1964). It is been observed that the application of RF voltage to any of the several electrode configuration around the outside of the plasma discharge tube causes a constriction of the luminous portion of the plasma away from the inner walls. Butler and Kino explained it as an RF rectification effect that leads to the formation of a thick sheath . A theory based on circuit theory principles was devised to describe this observation, and a suggestion (based on the theory they proposed) has been made to use these observations as an external diagnostic probe technique .

Gould (1964) used a circuit theory approach to clarify the observed differences in the measured electron density obtained by the resonance probes, and that obtained by Langmuir probes. It has been suggested that the difference can be attributed to neglecting the capacitive nature of the sheath. Mayer (1964)

In his paper, Gould presents the physical basis underlying this theory, and an attempt to derive an expression for the sheath capacitance.

In the 1970s, a series of papers were published - based on the work done on plasma sputter system - by the plasma research group at IBM [see for example : Koenig et. al. (1070) Logan (1970) (1974)]. In their published work, the IBM group set some guidelines on how circuit theory can be used to relate experimental measurement to the physical quantities of interest. Circuit theory for them was a link between the taken measurements and the theory that can be devised to describe the system's behaviour, and sometimes a way to explain the behaviour itself.

Koenig and Maissel [K &M (1970)] suggested an RF impedance network to model RF sputtering system. The purpose was to qualitatively study the voltage distribution in their system. The sheath in the model was represented with a capacitor and a diode in parallel. The capacitor is to present the fact that the RF sheath (to a first approximation) has a capacitive behaviour. While the diode mimics the electrons behaviour during that small fraction of RF cycle in which the

electrons are allowed to reach the surface to balance the relatively small (nearly) continual ion current.

Keller and Pennebaker (1979) continued to develop Koenig and Maissel's model, expanded upon the concepts presented in their paper. The main goal was to obtain an understanding of the factors that control ion bombardment. A more generalized form of K & M's model was presented : The proposed model is devised to give both qualitative and quantitative characterization of the electrical properties of RF sputtering systems . Their model was also applicable to the various types of sputter systems (namely : tuned substrate , driven substrate , and controlled area region of electrodes "CARE " sputtering systems.

Horwitz (1984) tried to model a sputtering systems as well. The model he used was similar to the one used by K & M's . However, Horwitz made some modification to the sheath representation within the network model. A resistor has been added to the sheath equivalent circuitry, and a comparison between two extreme cases has been carried out by adding an inductive component to one of them.

Horowitz was basically concerned with the relative ion bombardment energy ratio at the electrodes in a simple RF system. This factor is of great importance as it determines what the sputter system is used for. It is also of high significance as far as the process of contamination in the reactor is concerned. The ion energies have been calculated from the electrical properties of the system .

Another prospective of using circuit theory is that presented by Ilić (1981). Ilić's aim was to demonstrate a technique that can be used for easy and an non-invasive monitoring of the impedance of the plasma. A procedure has been developed to measure the required parasitic circuit components of the matching network at the operating frequency. Once determined, the complex plasma impedance can be used to deduce the plasma electron density, and electron-neutral collision frequency. The deduction procedure is based on a circuit model of the electrical loading effects of the bulk plasma.

Zarowin (1984), with a focus on the chemistry in the process, started by establishing the relation between the etch isotropity factor, etch rate and the ion energy. A link was then established between the electric field of the sheath and the gas pressure to the ion transport directionality (measured by the etch isotropity factor). He then linked the electric field (controlling the ion transport) with the RF current density and frequency of the excitation. Zarowin was able to do that via a proposed discharge equivalent circuit that contain a representation of both the displacement current and the conducting one. In his paper; Zarowin differentiated between the case of high RF and low RF through the nature of the expected current currier in both cases.

A special notice is to be taken of the work of Metze et al (1986). Metze et. al. proposed an equivalent circuit model for the representation of a planar RF reactor. The main emphasis was on the incorporation of the physical properties of the plasma sheath adjacent

to the electrodes. The sheath in the model they proposed was (for the first time!) a time varying capacitor and current source. Metze et. al. Proposed circuit components with high non linear dependency on the potential across the sheath. The model was devised to evaluate the effect of the non-linear sheath properties and system asymmetricity on the resulting voltage waveforms, and the developed DC voltage biases across the plasma sheath.

Metze et. al. (1986) indicated that a similar approach can be used to extend the analysis presented in their paper to include other parameters of interest (for example : the effect of reactor walls etc..). The effect of these parameters on the electrical properties of the reactor (specifically the sheath) can be investigated by adding suitable corresponding circuit elements to the equivalent electric circuit discussed.

In their attempt to conduct a study on the affect of the external circuit on the performance of RF plasma processing reactor, Rauf and Kushner (1998) capitalized upon the idea proposed by Metze et al, with some adjustments.

The assumptions used in the derivation of the non - linear link between the physical sheath and the equivalent circuit components, as used by Metze et. al. are applicable only to the case in which the excitation frequency is less than the ion plasma frequency, i.e. when both the electrons and the ions are expected to response instantaneously to the applied voltage. Hence; Metze's approach can't be adopted for high RF frequencies without alteration.

The required adjustment is to adopt a theoretical link (a sheath model) that is valid within the frequency limit of interest (i.e. for the case when the excitation frequency is bigger than the ion frequency and less than the electors frequency). For that purpose one can either adopt a Riley's approach (1995) (1996), or incorporate Lieberman's sheath (1988) instead.

Rauf et. al. (1998) decided on using the generalized Riley sheath model in their work to establish the required link. Because of the difference between the plasma and the circuit time scales, a straight forward simulation of the plasma and the external circuitry - togather - was impractical. A logical alternative is to establish a link between two separate simulations. The hybrid plasma equipment model (HPEM), a field theory ,two dimensional plasma fluid simulation approach, is used to simulate the plasma. The results of that simulation is then used to construct a simple circuit representation of the plasma reactor including the sheath impedances. The generated circuitry is being fed periodically to a circuit model connecting the plasma with the external circuit . Voltages (DC, fundamental and harmonics) and currents at all electrode and reactor surfaces are computed , and then fed back to the plasma simulation as boundary conditions.

Case specifics

All of the previously mentioned works and models dealt with perfectly grounded plasma. In this study, we are more interested in modelling plasma in a poorly grounded system

In real time processing machines, dealing with a poorly grounded plasma is the standard. Boundaries of plasma in a reactor are almost always a distribution of layers of various materials with various dielectric properties and conductivities. That's what drew our attention to triple junction configuration. [see fig. (2-1)]

The triple junction configuration is a system composed of a distribution of vacuum, metal, and dielectric. This configuration can be part of devices in many industrial applications. Plasma material processing industry is no exception.

The scheme is of great importance to high voltage applications as it has been observed that this combination of media – under certain conditions – can facilitate surface discharge process [for a review of the subject see for example Miller (1989) and (1994). See also Chalmers et. al. (1995)]. Experiments conducted by members of the high voltage material science community show a significant reduction of the voltage required for a surface discharge to occur. Another interesting observation is that the threshold for surface discharge to occur using an AC voltage is much less than that in the case of a DC voltage. This threshold decreases with increasing the frequency of the applied voltage.

Numerous studies have been conducted in relation to this issue from the material science point of view. Yet, this would be – to the author's knowledge – the first study to tackle the problem with the



The configuration of a triple junction configuration

existence of the plasma as an active media, not as a product of the discharge.

Several simulation experiments have been conducted by the author as part of the benchmarking process of the algorithm and the code. The discrepancy between a non-active media composite (results can actually be easily obtained analytically [Aidala (1980)], and an active one, as in this thesis, shows that the existence of an active medium like the plasma as part of the geometry does make significant difference on the results, specifically on the voltage surface distribution. This may be an indication that the formulation of the plasma can somehow contribute to that anomalous behaviour observed in such configuration.

The main focus in this thesis is on the changes in the voltage distribution along the surface facing plasma, and the evolution of this voltage distribution as we change the electrical properties of the dielectric region. However, we believe that this work is capable of shading some light upon these unexplained observations connected to TJC. Such endeavour will be saved for future work.
Modelling roadmap

Introduction

In the previous chapter, we saw examples of how circuit theory has been utilized to tackle various issues in plasma physics, specifically in relation to plasma material processing. A thorough read through literature enables us to identify the various approaches used.

Circuit theory can be employed to identify intrinsic plasma properties when integrated as part of an overall theory set to make sense out of the usual experimental measurements. The plasma is looked at as an unknown element, a black box if you will- within a well known circuit that can be investigated and analysed via external measurements. The external circuitry that is attached to the plasma is usually carefully devised to provide the minimum amount of interference possible with the plasma while conducting the investigation process. After identifying the external electrical properties of the circuitry, and based on a certain model relating the external electrical quantities (voltage, capacitance, inductance . . . etc) to the internal use this knowledge to deduce further information about the plasma system under study [for details on the issue, see for example: Hutchinson (2002), Lieberman (1995)].

The circuit approach can also be employed in analytical investigations. The main idea here is the reverse of the previous in

which circuit approach is used to simplify the analysis ending up – eventually - with measurable electrical properties of the system [Metze et . al . 1985]. The way by which this is implemented depends on the theoretical model adopted. In such a case the limitation of the theory should be stated and taken into consideration [Rauf et. al . 1998].

No matter how simple or complex the interface between the plasma and circuit theory is, the end result will be a system that can be treated using network analysis techniques.

The analysis procedure of an electro-magnetically active network composed of various components can vary between the very simple (analytically solvable) [Horowitz(1984), Ilić(1981)]) to the fairly complicated that needs a whole new algorithm developed by its own [Rauf et . al . (1998)].

The implementation done in this work is completely independent. The work presented here starts with an attempt to put a unified simple algorithm for dealing with circuit theory within the world of plasma physics, regardless of the purpose or end use of it. The algorithm was tested individually and has been proved to be accurate.

We introduce a way to implement the effect of wall dielectric cover as an extension of the external electrical circuitry. It provides a convenient way to couple reactor wall and external circuitry at the same time within any theoretical model of a plasma (whether this model is based on a simulation (PIC, fluid, etc.), a pure analytical treatment, or a mixture of both.

The implementation of circuit theory modelling

It's important to keep in mind the following: This part is specifically devised to treat a triple junction configuration within the vicinity of capacitive plasma. The analysis should include a plasma model of some sort.

For the coming segment, and as far as the network analysis part is concerned, the plasma model internals are masked, reproduced as a circuit equivalent, and are in contact with a system of irregular media distribution with varied electrical characteristics.

Keeping that in mind, we propose the following:

- Any spatial distribution of media that have different electrical characteristics and subjected to an electrical stress can be specially divided into elements [Aidala (1980), Rauf (1998)].
- Each element can be converted into an electrical component. This will eventually convert the special distribution into an electrical network.
- The nature and the values of an element of that network should depend on the electrical characteristics of the media which that element represents. Specifically; the dielectric constant and resistively (and anything else which a proper physical presentation of each medium would require) [Aidala (1980)].

- Once the system is properly converted, it is possible to treat the system using the same techniques used for electrical network analysis.
- The method we adopt is based on the application of the circuit theory, specifically the kirchoff's law (a suitable form of the law) accompanied by the method of nodal analysis.

By reaching this point, It is essential that we should be able to:

- Incorporate non-linear components that reflect the adopted plasma model temporal behaviour (implementing some sort of an adaptation to accommodate time varying impedance components)
- Be able to instantaneously track the transient behaviour at any special point of that system.

With such demands; a frequency domain analysis is not an option, the solution has be in the time domain . And hence, any solution should include:

A proper application of kirchoff's law (see chapter one, eqs. [1-8] and [1-9]) with regard to the relationship between the different nodes in the network which produces a system of linked ordinary differential equations with n independent variables (where n is the number of the nodes in a network).

 Solving the system of equations by converting the resulting ODEs into a suitable mathematical form that facilitates a computerized numerical treatment.

Mathematical treatment of the network model

Suppose we have n independent variables that are unknown, but somehow we know how these variables interact with each other. If we are able to write down n number of equations relating these variables together then we should be in position to find the values of these variable by solving the interdependent system of equations they construct.

Assume we have the node "i" that has a possibility to be linked to n number of nodes within an electrical network . We define the following matrices with elements of the following characteristics:

$$C[i, j] = \begin{bmatrix} -c_{ij} & \text{if } i = j \\ -c_{ij} & \text{if } i \neq j : i \text{ and } j \text{ linked} \\ 0 & \text{if } i \neq j : i \text{ and } j \text{ not linked} \end{bmatrix}$$

Where $c_{ij}\,$ is any capacitor linking i node to a j node or to a voltage source .

$$R[i, j] = \begin{bmatrix} \sum_{j=1}^{n} -\frac{1}{r_{ij}} & \text{if } i = j \\ \frac{1}{r_{ij}} & \text{if } i \neq j : i \text{ and } j \text{ linked} \\ 0 & \text{if } i \neq j : i \text{ and } j \text{ not linked} \end{bmatrix}$$
(3-2)

Where \boldsymbol{r}_{ij} a resistance connecting the nodes i and j .

$$\frac{de}{dt}[i] = \begin{bmatrix} c_{ik} \frac{de}{dt_{k}} & \text{i node is connected to } e_{k} \text{ via } c_{ik} \\ 0 & \text{i node not connected to} \\ 0 & \text{a source via capacitor} \end{bmatrix}$$
[3-4]

And finally :

$$e[i] = \begin{bmatrix} \frac{e_k}{r_{ik}} & \text{i node is connected to } e_k \text{ via } r_{ik} \\ 0 & \text{i node not connected to} \\ a \text{ source via risistor} \end{bmatrix} [3-4]$$

Using the previous definitions, the system of differential equations can be represented as follow:

$$c[n][n] * \frac{dv}{dt}[n] + r[n][n] * v[n] = \frac{de}{dt}[n] + e[n]$$
[3-5]

These generalized forms are set basically to describe a network composed of combinations of resistances, capacitors and voltage sources. The approach is so flexible that we can include inductance, current sources, or any kind of electrical components - be it static or with an inherited non - linearity of any nature - if deemed necessary. This will enable us to reflect a faithful overall representation of the system's physical behaviour.

So in other words, the values of any of those elements can be a variable (i.e. can be functions of time, voltage, or any independent variable of interest). Hence, non linear elements can be implemented within this network approach, even if the values of these elements need a different computational code or procedure to be evaluated.

The detailed contents of these matrices depend on the topology of the network under investigation, which is dramatically influenced by the adopted model for representing the plasma . For that, we are going to use two well known analytical plasma models.

In what follows we present an outlined review of the elements of each of the used plasma models, before we proceed to present the results generated from each case. We then follow with a discussion of the significance of the similarities and the differences in the results.

RF analytical plasma

It is near impossible to cover all the articles written in relation to the theory of RF plasma modelling. Needless to say that such an attempt is basically beyond the scope of this study. However, one of the core issues that any plasma analytical model tries to address is the plasma sheath behaviour [Killer et.al. (1979), Lieberman(1988), Pointu (1986), Kaganovich (2002), Riley (1995) and (1996)].

The RF sheath in particular draws special attention due its substantial importance to plasma material processing. Within the wealth of attempts that have been carried out to deal with the issue, there was a special emphasis on the applied frequency. Tackling the case when the applied frequency is less than the ion cyclotron frequency (the low RF frequency limit) is a straightforward task. This is attributed to the fact that the plasma components (ions and electrons) response instantaneously to the temporal voltage variation under such conditions.

When the frequency of the applied voltage approaches or exceeded the ion cyclotron frequency (the high RF frequency limit), the ions - because of their relatively large inertia - start to show an increasing delay in the response to the instantaneous variation of voltage, compared to the electron's instant response. Electrons do not start to show such a delay in response until the microwave frequency limit is reached. In fact, ions' delay in response due to inertia is the source of most of the complications and the enforced approximations that we see in the theories tackling the RF plasma sheath in the high frequency limit.

Now; for the frequency of 13.56 MHz, we need a theory dealing with the upper limit case. Most of the related previous works offer a fusion between theory and numerical modelling [see for example Edelberg (1999), Dai (2002), Biehler (1989)]. For our circuit model we need an expression of the sheath impedance as a function of the voltage across it. Lieberman's work is considered to be one of the few that offer a completely analytical solution. We investigate the possibilities of using two analytical RF sheath models, namely the homogeneous model and the non-homogeneous model.

The adopted approach in these models is that the state of the discharge is specified once a complete set of control parameters is given. The remaining plasma and circuit parameters are then specified as functions of the control parameters [Lieberman (1994)]. Control parameters include a factor depending on RF source (I_{rf} or V_{rf}), the applied frequency ω , the density, and the dimension of the system under consideration.

In his book, Lieberman outlines two approaches (models) for dealing with RF sheath: the homogeneous model, and the nonhomogenous model. Nearly the same assumptions have being used for both models. The difference starts with the assumption made with regard to the ion density behaviour in the sheath. In the homogeneous model, Lieberman assumes the ions with a uniform constant density everywhere in the sheath region. This assumption simplifies the treatment as it disposes of the necessity to consider the mathematical complications imposed by including ion dynamics. The instantaneous sheath thickness variations under such assumption surprisingly takes the simple form of a matrix sheath like structure, with the sheath thickness becoming a function of the square root of the voltage difference across the sheath. Accordingly, the capacitance of the sheath will take the following form:

$$C(\Delta V) = \frac{C_0}{\Delta V} \frac{1}{2}$$
[3-6]

With C_0 a constant depending on the control parameters of the system under consideration [Lieberman (1994)].

In the non-homogeneous model -as the name indicates- the main difference is that ion density in the sheath is considered to be inhomogeneous. Consequently, the time averaged ion dynamics have to be included. Lieberman's non-homogeneous theory does not offer a straightforward expression linking the instantaneous sheath thickness to the instantaneous voltage across the sheath. Instead, it offers two

separate expressions for $V(\phi)$, the voltage across the sheath , and $x(\phi)$, the sheath thickness, both as functions of the phase [Lieberman (1988)]:

$$\frac{x(\phi)}{S_0} = (1 - \cos\phi) + \frac{H}{8} \left[\frac{3}{2} \sin\phi + \frac{11}{18} \sin 3\phi - 3\phi \cos\phi - \frac{1}{3} \phi \cos 3\phi \right]$$
[3-7]

$$V(\phi) = \frac{\pi H}{4} T_e \left[4\cos\phi + \cos 2\phi + 3 + H \left(\frac{15}{16}\pi + \frac{5}{3}\pi\cos\phi - \frac{1}{3}\phi\cos 2\phi + \frac{1}{48}\phi\cos 4\phi - \frac{5}{18}\sin 2\phi - \frac{25}{576}\sin 4\phi \right) \right]$$
[3-8]

With H and S_0 , depending on the control parameters as follow:

$$H = \frac{\tilde{J}_0^2}{\pi \varepsilon_0 T_e e \omega^2 n_0}$$
[3-9]

$$s_0 = \frac{\tilde{J}_0}{e\omega n_0}$$
[3-10]

With J_0 being the amplitude of electrical current density function, ω the radian frequency, e the unsigned electron charge, T_e the electron temperature and n_0 the plasma density for the system under investigation.

Those are the expressions that we will be using to deduce the variation of the sheath thickness as a function of the applied voltage.

The network analysis code structure

When using a plasma model, the code starts by identifying the initial boundary conditions at the edge of the plasma. In an analytical model, the plasma bulk itself is considered to be an equipotential media. The profile of the sheath is then calculated depending on the given plasma parameters using either a suitable sheath model. Based on the obtained data from the previous stage, the sheath impedance profile is then constructed and integrated into the network describing the rest of the unchanging profile of the triple junction [Fig. 3-1].

The constructed network model now describes the entire system's spatial distribution of the electrical characteristics of the media - plus the boundary conditions - at that specific time .

From this point on, the treatment will be the same regardless of what plasma model is in use: The generated scheme of the network is translated into its equivalent system of equations using the methods and concepts developed in the section about the mathematical treatment of networks. The problem now is reduced into solving that



Triple junction configuration, nodal network representation

system of equations for the values of the voltages at each node, which values will be with respect to the ground.

There are various numerical methods that can be used to solve these set of equations. The method adopted in this work is a computational translation of the purely analytical method of Back-Substitution, an analytical matrix based method used in solving sets of n equations with n independent unknowns [for details see for example Watkins (2010)]. The algorithm –and subsequently the code- has been developed independently by the author, which has been made easily possible by the matrix pattern generated from the aforementioned nodal analysis. Taking such a short cut reduces the unavoidable margin of computational error attributed to approximated numerical methods [Press et. al. (2002)].

The values of the node voltages can then be used to calculate a variety of circuit and field related parameters - at that specific time - using the concepts developed in chapter one.

In the analytical modelling approach, The value of the voltage across the spatial sheath is then calculated and used to re-consider the sheath spatial profile and hence the sheath impedance profile. This will be followed with an update of the boundary conditions and the network.

The whole cycle is then repeated all over again. Such scheme enables us to track the transient behaviour of the system.

The calculation presented here will considered two distinct sheath models, the matrix like RF sheath (a Lieberman homogenous sheath [Lieberman (1994)]) and a Child Langmuir like RF sheath (Lieberman non homogenous sheath [Lieberman (1994) and (1988)]).

Another focus point in this study is the effect of the electrical properties of the dielectric facing the plasma on the results. It is of great interest to us to see how the plasma sees the ground through both a perfect dielectric (high resistivity) and a lossy dielectric (low resistivity). In both cases the value of the dielectric constant is kept the same.

Results, discussion, and conclusions

Introduction

The number of results produced by this study is large, and multi layered in nature. Because of that, and before we proceed with presenting them, we find it fit to start by talking about our main focus. We hope that once viewed, it can assist in delivering the coherent insight we are trying to convey.

Focus

In this study we are going to focus on the following:

- The Variation of parameters (voltages and electric field components) as a function of time and space.
- The dependency of the time spatial variation of parameters on the Sheath model used.
- The dependency of the time spatial variation of parameters on the dielectric resistance as the dielectric constant stayed fixed.

Model wise, the voltage values are linked to the nodes, and the concept of nodes is linked to the concept of space. This is how we establish the link between the voltage and the location in order to be able to formulate a clear idea about the voltage distribution along a certain surface or across specific media.

Through this link, we can calculate the field components in two dimensions (along the x or the y axis) , which is what has been done for the sheath region .

Spatially speaking you can see two sub-foci :

- Voltage with respect to the ground for :
 - The upper surface of the dielectric (the plasma ground)
 - The lower surface of the dielectric
- The voltage difference of the following sub-divisions of the system:
 - o The sheath region
 - o The dielectric
 - The vacuum plus the metallic region

For the sheath models focus we have two sub-foci:

- The homogeneous (matrix like) sheath
- The non-homogenous sheath

And finally, for the Electrical characteristics as they change with the dielectric resistivity focus, we have two sub-foci:

- High resistivity dielectric.
- Low resistivity dielectric.



Spatial focus one: voltage distribution along the upper surface of the dielectric surface, with respect to ground

Fig 4 - 1















Fig 4 - 5

Voltage distribution at dielectric upper surface with respect to ground Lieberman/non-homogenous theory (N.H.T) sheath, Lossy dielectric (low resistivity)



Spatial focus two: voltage distribution along the lower surface of the dielectric, with respect to ground

Fig 4 - 6



Fig 4 - 7











Fig 4 - 10

Voltage distribution at dielectric lower surface with respect to ground. Lieberman/non-homogenous theory (N.H.T), Lossy dielectric (low resistivity)



Spatial focus three: voltage dif across the sheath

Fig 4 - 11



Voltage dif across the sheath. Matrix/homogenous theory (H.T), perfect insulating dielectric (high resistivity)

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Fig 4 - 12







Voltage dif across the sheath Matrix/homogenous theory (H.T), lossy dielectric (low resistivity)

Fig 4 - 14



Voltage dif across the sheath Lieberman/non-homogenous theory (N.H.T), lossy dielectric (low resistivity)

Fig 4 - 15



Fig 4 - 16



Fig 4 - 17










Spatial focus six: voltage dif Parallel to the upper surface of the dielectric

Fig 4 - 20











Voltage dif Parallel to the upper surface of the dielectric Lieberman/non-homogenous theory (N.H.T), lossy dielectric (low resistivity)

Fig 4 - 24

















Spatial focus seven: voltage dif across the dielectric surface

Fig 4 - 29



Voltage dif across the dielectric surface Matrix/homogenous theory (H.T), perfect insulating dielectric (high resistivity)



Voltage dif across the dielectric surface Lieberman/non-homogenous theory (N.H.T), perfect insulating dielectric (high resistivity)

Fig 4 - 31



Voltage dif across the dielectric surface Matrix/homogenous theory (H.T), lossy dielectric (low resistivity)



Voltage dif across the dielectric surface Lieberman/non-homogenous theory (N.H.T), lossy dielectric (low resistivity)



Electric field across dielectric surface Matrix/homogenous theory (H.T), perfect insulating dielectric (high resistivity)











Electric field across dielectric surface Lieberman/non-homogenous theory (N.H.T), lossy dielectric (low resistivity)

Fig 4 - 37

Conclusions and discussion

In the previous section, we presented a study of the electrical characterisation of a system of irregular special distribution of media using the concepts developed in chapters one, two, and three. A high density, low pressure, steady state plasma is theoretically incorporated within the analysis via a suitable sheath impedance model based on th Lieberman sheath model (both homogeneous and non homogeneous).

The adopted analysis is based on the concepts of circuit theory (reviewed in chapter one). We showed that circuit theory provides a similar description of the studied system as that offered by the field theory but from a different prospective. We showed that, when properly used, circuit theory can provide a convenient substitute to the field theory. To emphasize that specific point of view, the results shown are a mixture of both.

Results: plasma focus

The analysis carried out for the purpose of this report on a triple junction configuration exposed to the plasma, predicts an observable spatial surface voltage variation along the boundary facing the plasma, which depends on the electrical characteristics of the boundary. This variation has considerable effects on both the electron and ion hitting the surface.

Due to its inertia and the high frequency of the voltage variation across the sheath, ions flux (current) toward the surface is expected to

be nearly constant with time (it only response to the time average of the voltage variation). However, electrons flux (current) has the capacity to vary instantaneously in response to the voltage variation, producing a regular pattern in the time variation of current function.

As the voltage varies across the surface, both ions and electrons will have different spatial variation in their fluxes (currents) along the surface of the dielectric.

Results: boundary media distribution focus

The overall review of the results clearly indicates the establishment of three distinguished regions (see Fig [4-38]), the one facing the vacuum, the one facing the metallic bridge, and a transition area between them. This reflects faithfully the non-homogeneity of the triple junction configuration that is part of the studied system.

The results show the impact of the non-homogenous distribution of conductivities in the backing boundary of the dielectric facing the plasma on the voltage surface distribution. Further investigation (not included in this study) showed that the only effect of the alteration in the conductivity distribution (i.e. shifting the metal/vacuum boundary) is generating a shift in the position of the transition area in the voltage surface distribution. The code - in its current capacity – has enabled us to further investigate the effect of geometrical alteration of the system.

region 1 conductor transition plasma sheath region bulk plasma dielectric region 2 vacuum

The configuration of a triple junction configuration : distigueshed regions.

Results: plasma sheath model focus

Observable difference can be noticed between the results of the sheath homogeneous theory (H.T.) and the sheath non-homogeneous theory (N.H.T.). This comes as no surprise recalling the differences between the assumptions upon which each theory has been built, as described in the previous chapter.

Figures [4-2] to [4-5] show the voltage along the dielectric surface (facing the plasma) with respect to the ground, as illustrated in figure [4-1]. In other words; this is how the plasma perceives the ground through the non-homogeneous media distributions.

H.T. results, shown in figures [4-2] and [4-4], does not reflect a huge difference between the high and the low dielectric resistivity conditions, indicating a considerable screening of the media's non-homogeneity behind the dielectric layer. Nevertheless, unlike the case of high dielectric resistivity (figure [4-2]), one can clearly see a slight (but noticeable) indentation for the low dielectric resistivity case (figure [4-4]).

With the N.H.T plasma (figures [4-3] and [4-5]), the perturbation increases, and expands in space, as the dielectric resistivity goes lower.

Regardless, with both theories, results shows that the media nonhomogeneity screening effect increases as we increase the dielectric resistivity.

As far as the other side of the dielectric is concerned (figure [4-6]) both plasma theories yield nearly the same behaviour (see figures [4-7] and [4-8]) with high resistivities. A gap between the two theories rises and begins to increase as the dielectric resistivity decreases (figures [4-9] and [4-10])

N.H.T predicts higher voltage differences (field variation) a cross the sheath in comparison with H.T., with both giving higher values for the low dielectric case than the higher dielectric resistivity case.(figures [4-12] to [4-19]).

Results: dielectric surface focus

Looking at the voltage difference (and the perpendicular electric field component) across the dielectric surface (figure [4-29]), there wasn't much of a surprise there. Results (figures [4-30]-[4-37]) show two distinctive regions, a typical capacitive behaviour which is sheath model independent, and is solely influenced by its geometry, and the dielectric media distribution and properties inside.

Considering the voltage variation along the dielectric surface (figure[4-20]), a peak is noticed through the surface distribution of the voltage difference (figures [4-25] [4-28]) and the surface field component (figures [4-20] to [4-24]). This peak is localized around the region facing the metal/vacuum media transition surface. The non-homogeneity in the distribution starts with a transient behaviour. The shape, the magnitude, and the temporal progression nature of this

peak has been found to be highly influenced by the dielectric's resistivity.

A similar behaviour to that described earlier (for the voltage difference (field) across the sheath) has been observed when the variation of the voltage difference (field) parallel to the dielectric surface was investigated. This specific point has been explored further due to its relevance to surface discharge phenomenon. The results can be summarized in figure [4-39].

Figure [4-39] shows the variation of the maximum field amplitude value as a function of the logarithm of the dielectric resistivity. The detailed behaviour resulting from H.T. and N.H.T. was a great surprise, especially when compared to the static sheath case. There is a qualitative agreement (to a limit!) between the prediction of H.T. and N.H.T. Yet quantitatively speaking there is a considerable discrepancy, which was not surprising at all. The significances behind these results are in need for further investigation .

Such results are, in my opinion, the most important aspect deduced from this research. The figure clearly emphasizes the existence of an electrical stress in the transitional region. It also shows a dependency on the dielectric's resistivity.

Consequently, it would be of great interest to peruse this further by investigating the consequences of such dependency in detail, as a focus point for future works.



The variation of the parallel field maximum value across the upper dielectric surface as a function of the logarithm of the dielectric resistivity

The results - so far - do not show the long-term effects of these observations on the system, however, they do show the existence of a periodic abnormal stress that might have serious consequences as far as the plasma reactor is concerned. Further studies are needed to clarify this point.

Calculations show that these observations are highly dependent on the electrical properties of the boundary dielectric. The surface voltage variation (and consequently, field and electron current) becomes highly significant with the reduction of the dielectric resistivity.

An interesting consequence to these result is that even before knowing the exact mechanism behind it, the plasma processing operation can be manipulated/controlled via a proper and careful choice of the electrical properties of the boundary material(s) and it's spatial distribution. It also confirms that the existence of a spatially varying electrical media distribution in the vicinity of the plasma should not be ignored. Especially under extended operation conditions.

Finally, it was evident that the behaviour of the parameters under investigation was dramatically dependant on the adopted sheath model. This provides an opportunity for an experimental investigation of the various aspects related to this work, to find out which theory gives a better description for what happens in reality. But most importantly, test and further guide the adopted assumptions, theories, and the approximations used throughout this study, for the benefit of future work.

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