Applications of Plasma Modeling for Semiconductor Industry

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Abstract

Plasma processing plays a significant role in semiconductor devices technology. Development of new plasma systems, such as high-density plasma reactors, required development of plasma theory to understand a whole process mechanism and to be able to explain and to predict processing results. A most important task in this way is to establish interconnections between input process parameters (working gas, pressure, flow rate, input power density) and a various plasma subsystems (electron gas, volume and heterogeneous gas chemistry, transport), which are closely connected one with other. It will allow select optimal ways for processes optimization.

Key words: Plasma processing, high-density plasma, plasma modeling.

Introduction

Plasma processing of semiconductor materials is one of the main parts in microelectronic devices technology. Plasma processes are characterized by sufficient advantages in comparison with a traditionally used last 20 years thermal or wet methods due to a lot of factors. Among these factors are high resolution, selectivity and anisotropy in plasma etching processes; fine, uniform and controllable structure of plasma coatings; and ability to supply low substrate temperatures together with the achieving high processing rates.

In our days, development of plasma technology in semiconductor industry follow by the way of development of new plasma systems, which should combine the advantages of "old" systems and should be free from theirs disadvantages. High-density plasma (HDP) reactors have additional progressive features in comparison with traditional systems due to the ability to provide the process with independent control of ion energy and ion flux to substrate surface. Additionally, in HDP reactors high processing rates can be obtained without ion-induced damaging.

In this paper we shall discuss a relationships between plasma theory and practical applications and the abilities of plasma modeling. We shall attract dominant attention on the basic structure of plasma model, on the comparison of various modeling methods and on the practical applications of modeling results.

Basic concepts

Term "plasma" was first applied by Langmuir in 1928. Nevertheless, a first investigations of electrical discharge were started more than 100 years earlier by W.Gilbert, B.Franklin and E.G. von Kleist. Significant progress in development of physics of gas discharge was made during 19th century by H.Davy and M.Faraday. At that period basic terminology and concepts of plasma physics were developed.

From the physical point of view plasma is environment, which contains both neutral and charged particles and satisfy to the requirements of *quasi-neutrality* and a *spatial charge separation.* First requirement means that for a whole plasma volume we should obtain an equal volume densities of positive and negative charged particles: $n_- + n_e = n_+$. Second requirement is connected with a correlation $L >> r_D$, where L – typical linear size of plasma area, r_D – Debae shielding distance. There are a lot of systems, which satisfy to both requirements, but only a very limited number of them are used in a semiconductor technology.

In further discussion we shall attract the attention only on low-temperature plasmas, which are formed by electrical discharge in gas under the pressure lower than atmospheric.

Plasma industrial applications

Variety of tasks, solved using low-temperature plasma is connected with multi-channel interaction between plasma and solid state surface. Plasma environment contains both charged (ions, electrons) and neutral (free atoms and radicals) particles, which are supply a variety of interaction mechanisms. Generally, it is possible to select three groups processes, which are depends on plasma-forming gas and surface nature:

1. Removing of the material from the solid state surface;
2. Deposition of the material on the surface;
3. Surface modification.

First, plasma may play a role only an environment supporting a transport of the particles. Second, plasma may be a source of the particles. Third, plasma may play a role of energy source and catalyst. And forth, plasma may combine two or more roles mentioned above. A simplest classification of plasma processes according to the main application purposes is shown in fig.1.

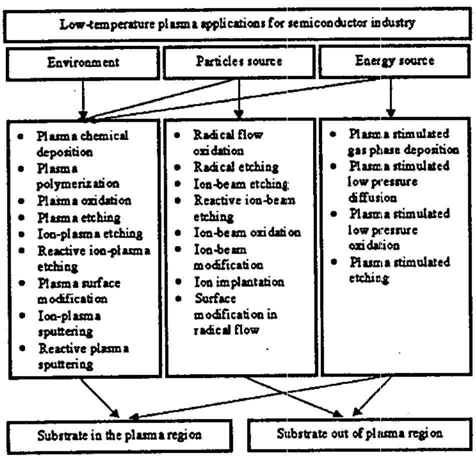

Fig1. Classification of plasma processes according to a dominant plasma role.

Plasma modeling: concepts and approaches

Last 10 years in plasma processing area we have a situation, when a practical applications of majority of processes are significantly overtake a level of plasma theory development. That is why, for a process optimization engineers very often use a method of "blind search", which is based only on empirical investigations and results. This method is characterized by three sufficient disadvantages. First, it requires a lot of time. Second, it does not guarantee positive result. And third, in the case of success the results can't be directly transferred to another system, which is similar but not the same.

Term "plasma modeling" is very wide and assumes at least two meanings:

- theoretical calculations of plasma and process parameters, which can't be obtained by experiments.
- global description of plasma system aimed to connect input parameters of process with a final effect.

Therefore, development of plasma theory and thus plasma modeling methods is able to bring a sufficient contribution to technology. The main reason of such conclusion is that qualitative model is able to describe global interconnections between various sublevels of plasma system. Necessity of plasma modeling is also caused by the fact that plasma diagnostics method has either limited abilities or not able to supply appropriate accuracy. That is why a combination of experimental and modeling methods is a powerful tool for plasma investigations.

From the general point of view, plasma modeling may be realized in direct or self-consistent modes. Direct modeling includes step-by-step procedure and requires as input parameters a lot of plasma diagnostics results as well as process conditions (gas pressure and flow rate, power density and plasma excitation frequency). Self-consistent mode requires as input parameters only process conditions, while diagnostics data are used only as model optimization criteria. Nevertheless, there are list of input parameters, which are required for all modes of plasma modeling:

- Cross section of electron impact processes;
- Reduced electric field strength - E/n_0;
- Reduced frequency - ω/n_0
- Magnetic field strength

These parameters directly determine characteristics of energy transfer from electromagnetic field to electron gas and from electron gas to "heavy" particles. Moreover, these parameters are used as a "similarity criteria" to adapt a model for the system of various geometry and power density.

As for model output parameters, theirs number is determined by the "dimension" of model. "Dimension" is a specific term, which characterize model abilities for description of spatial and time effects in plasma system. First and simplest level is "zero-dimensional" (0D) model, which allow to obtain mean volume densities of neutral and charged particles and theirs fluxes to the surface. 1D model gives information about radial distribution of particles in reactor chamber. 2D model takes into account radial and axial distributions while a 3D model adds to these features time-dependent effects. Unfortunately high-dimensional models are so complicated that require a CPU time, which comparable with or even more than "blind search" duration.

Model structure

For any plasma model development, the task of primary importance is to establish intercoupling connections between an external process and equipment parameters, internal plasma characteristics and final process effect. A simplest scheme of such connections is shown in fig.2.

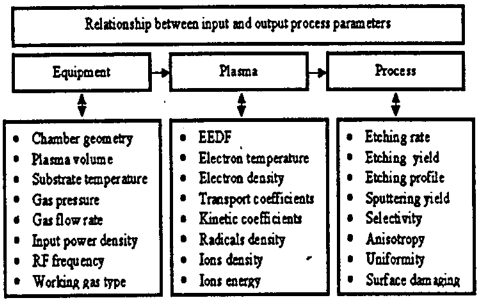

Fig.2 Scheme illustrated the relationships between input and output process parameters.

It is evidently clear that the final etching effect, including all process parameters mentioned in fig.2, is formed under the simultaneous action of the fluxes of various kinds of active species and plasma irradiation. These fluxes are qualitatively determined by internal plasma parameters, which are connected with input parameters (power, pressure, flow rate, reactor geometry), but depends on the large number of physical and chemical processes, both volume and heterogeneous. The best way for the analysis of internal plasma characteristics is to "divide" them to several coupled subsystems, which include processes described by a similar physical or chemical content. Such approach allow to select at least four subsystems:

- Subsystem of electron gas;
- Subsystem of charged particles;
- Subsystem of neutral particles;
- Subsystem of heterogeneous chemistry.

A simplest scheme illustrated connections between various subsystems is shown on fig.3.

It is very important to attract the attention on direct connection between heterogeneous chemistry and electron gas characteristics and this is especially important for etching systems description. The reason is that highly volatile reaction products may change content of gas phase and thus the basic characteristics of all subsystems.

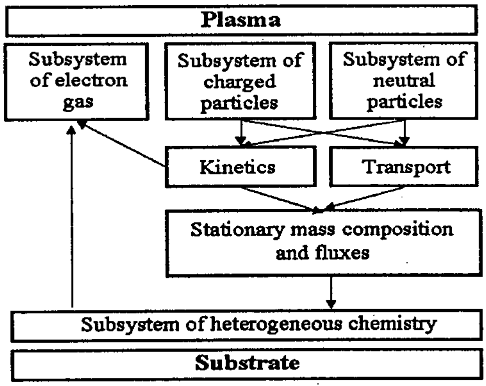

Fig.3. Scheme illustrated connections between various subsystems in plasma.

<u>a) Subsystem of electron gas</u>

Subsystem of electron gas usually is based on the Boltzmann kinetic equation (as a form of energy conservation law for plasma electrons) and power balance equation. This subsystem describes a combination of physical processes such as transition of energy from electromagnetic field to electrons and energy dissipation during the collisions of electrons with "heavy" particles. In simplest form, Boltzmann and power balance equations may be written as:

$$\frac{d}{d\varepsilon}\left[\left(\beta+\frac{kT}{e}\gamma\right)\frac{df(\varepsilon)}{d\varepsilon}\right]+\frac{d}{d\varepsilon}[\gamma f(\varepsilon)]+S_{un}=0 \quad (1)$$

$$W=\frac{P}{V_p}=W_{el}+W_{un}+W_{ion} \quad (2)$$

where ε – electron energy, $f(\varepsilon)$ – EEDF, β and γ - parameters determined by nature of working gas, input power density and discharge excitation method, S_{un} –

integral of unelastic collisions, W_{el}, W_{un} and W_{ion} – power densities used up for elastic processes, unelastic processes and for acceleration of secondary electrons produced by ionization. First summand in left-hand side in equation (1) represents the energy transferred to the electrons from electromagnetic field, second summand takes into account electron energy loss in elastic collisions and last summand represents energy loss in unelastic collisions.

As output parameters, this subsystem gives us electron energy distribution function (EEDF), electron temperature, transport coefficients (diffusion coefficient and mobility) and rate coefficients of electron impact processes.

Simplest models exclude Boltzmann equation from electron gas subsystem assuming Maxwellian or Dryvestainian EEDF. Note, that in real case EEDF always occupies an intermediate position.

b) Subsystems of particles kinetics and transport

Second and third subsystems are based on the kinetic schemes of charged and neutral particles formation and decay including chemical processes and transport effects. Kinetic scheme for a simple diatomic gas may include more than 30 reactions, such as:

- electron impact processes;
- volume recombination;
- heterogeneous recombination;
- ion-neutral and neutral-neutral interactions;

These reactions form complicated consequent and parallel chains. That is why this subsystem is very sensitive to accuracy of input parameters. Basic equations for each kind of charged (3) or neutral (4) particles may be written as:

$$\frac{d}{dx}\left(-D\frac{dn_c}{dx}+n_c\mu_c E\right)=R_F-R_D \qquad (3)$$

$$n_n D\left[\left(\frac{1}{L}\ln\frac{n_n}{n_0}\right)^2-\frac{Q}{LD}\ln\frac{n_n}{n_0}\right]=R_F-R_D \qquad (4)$$

where n_c and n_n – volume densities of neutral and charged particles, n_0 – total density of neutral particles, D – diffusion coefficient, Q – gas flow rate, μ- mobility, E – electric field strength, R_F and R_D – total rates of particles formation and decay. As input data these subsystems required a kinetic coefficients of volume and heterogeneous recombination of neutral and charged particles while output parameters are volume densities and fluxes.

c) Subsystem of heterogeneous chemistry

Forth subsystem is especially important for etching processes modeling and includes description of adsorption-desorption equilibrium (taking into account both spontaneous and stimulated mechanisms) and a surface chemistry analysis from the point of view of active centers theory. This theory assumes a surface as a combination of active centers, which are able to join chemically active species from gas phase. The etching rate determines by the relative fraction of free active centers θ while other active centers in amount of $(1-\theta)$ may be occupied by reaction products as well as by chemically inert particles. As input parameters this subsystem requires:

- Flux of chemically active species;
- Flux of chemically inert species;
- Reaction probability
- Flux and energy of ions;
- Flux of UV irradiation;
- Substrate temperature

First three values allow to estimate total rate of active centers decay while last three parameters determine the rate of active centers cleaning due to both spontaneous (thermal) and activated desorption.

A simultaneous mathematical description and solution of all subsystems allow to create general model of etching process which is directly connects an input process parameters with a final effect of treatment. One of the main advantages of such a model is the ability to predict the change of process characteristics after the changing of input parameters, working gas or plasma excitation method.

Conclusion

Plasma processes play dominant role in semiconductor technology. Improvement and development of new plasma systems, such as high-density plasma reactors, required a development of plasma theory and plasma modeling methods to understand connections between process parameters and final process result.