Modeling Remote H_2 Plasma in Semiconductor Processing Tool

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Abstract: The H_2 plasma is typically used in semiconductor industry for materials processing, surface preparation and cleaning of the silicon wafers and thin films. In this contribution we have explored a potential and capabilities of the COMSOL Multiphysics sw for modeling the H_2 remote plasma. The developed 2D/3D plasma fluid model is described by the set of the species and energy balance equations in generic semiconductor tool chamber with remote Inductively Coupled Plasma (ICP) source. Background H_2 gas flow is described by incompressible Navier-Stokes equations for low speed isothermal flow. To understand the H_2 plasma composition in actual geometry and the distribution of the individual components, the multiple diffusion and convection application modes were used to solve the system of the coupled equations. Boundary conditions indicated importance of the material properties for the H radical distribution. The electrostatics mode for electric potential distribution was involved into coupling scheme to satisfy a plasma quasi-neutrality condition, and to couple $\vec{E}$ field to an ambipolar diffusion coefficient (model in "drift-diffusion" driven transport approximation). The fast hydrogen atoms and molecules are generated in plasma through charge exchange collision mechanism. The influence of the technological parameters and used materials has been investigated by simulation. The simulation cases were tested also using 64-bit PC (8 GB memory).

Keywords: plasma fluid model, hydrogen chemistry, plasma reactor.

1. Introduction

Semiconductor wafer processing involves many various processes: the physical and chemical methods of preparation and processing materials and thin films, typically in complex plasma environment, the reacting gas/flow mixtures, in many circumstances including heat transfer conditions, the chemical and energetic interaction of species with surfaces, the involvement of the static or RF electromagnetic fields and their coupling to the processing media. Moreover, such complex multiphysics and chemistry engineering occur within the large dimensional scale, ranging from 1 m down to 10^{-9} m and uniformity requirements are below several percent within the silicon wafer (∅300 mm).

In past design of manufacturing equipment & processes depended mostly on the empirical methods due to the rapid pace of innovation and incomplete understanding of the fundamental physical and chemical phenomena in the technological processes. The university models were well developed but user interface was strongly personalized, and industry used only simple geometry models or analytical approach models. Today the use of trial-and-error methods is more expensive and time-consuming.

Computational modeling provides better understanding of the manufacturing processes, supplements the conventional experimental techniques and significantly reduces overall development time and cost. In industrial equipment/technologically-oriented company the major reasons for effective and accurate modeling are to make R&D budget efficient and to reduce the design cycle and make new tool/process product-worthy (an accurate up-to-date material's properties database, the SW at reasonable cost, highly flexible and productive). Further, to find a shortcut to optimize process development, and to provide more precise and applicable modeling data, which are close to technology's people, the outputs are expressed by technologically conventional parameters.

2. Remote Hydrogen Plasma Cleaning

The H_2 plasma is typically used in semiconductor industry for materials processing, surface preparation and cleaning of the silicon wafers and thin films. It is an important component of the process integration, the metalization performance enhancement, and yield optimization. The standard off-situ methods for semiconductor surface cleaning are wet or ultraviolet (UV)-ozone based procedures.[1] However, the technologies based on the clustered tool approach require in-situ surface preparation process. One method of *Si* surface preparation under UV conditions is an UV flash of the substrate at a temperature greater than 1000 °C. Alternatively, the combination of a wet chemical treatment and UHV annealing to temperatures of 850 °C can be used to obtain atomically clean surfaces[2] cleaning. An ion bombardment cleaning at low energy or sputter etch back cleaning techniques are used as well as, the problem is the induced crystal structure disorder and the ion incorporation. While high temperature annealing may remove some aspects of the disorder and the impurities, the defects usually remain. The suppression of some of these effects can be expected when using hydrogen ions instead of noble gas ions.[3-5] For instance, a good quality low damage GaAs surface cleaning was achieved using atomic hydrogen generated by thermal dissociation of H_2 molecules around 130 Pa pressure range. A predictive reactor model for *H*-radical distribution is a perequisition for tool design and development.

3. Plasma Reactor Model

Plasma processes in semiconductor reactor include phenomena on many different scales (complex multiphysics and chemistry occur within large dimensional scale). A need of the hierarchy of the models is evident to investigate the technological processes at the wafer surface in correlation to the reactor design and process parameters, see Fig. 1.

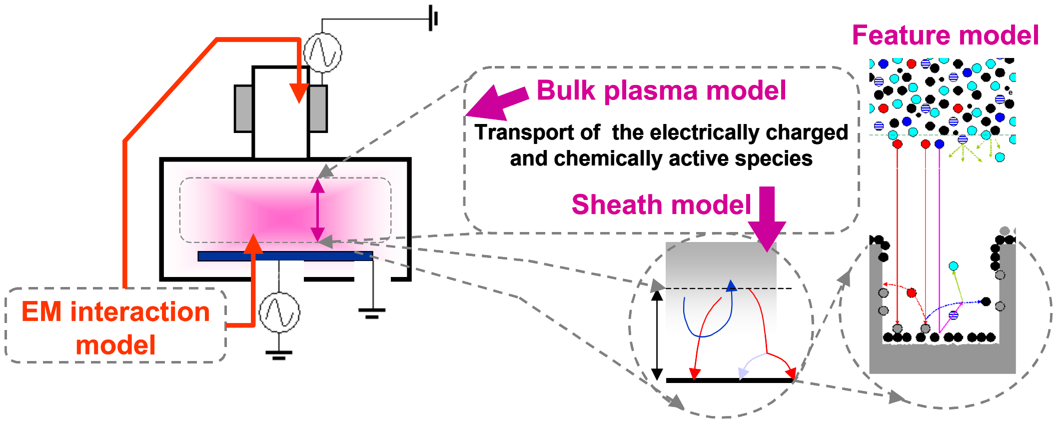

Figure 1. The plasma processing is characteristic by multiscale and multiphysics modeling.

As a baseline reactor we considered a generic cylindrical chamber with radius *R* and height *L*, with remote Inductively Coupled Plasma (ICP) source at the top. Gas flow is directed through the chamber of the ICP source, then as downstream plasma through the processing chamber and pumped out. The actual structure of the ICP source does not impact the distribution and composition above the wafer, which are determined primarily by transport and generation or loss collisions in bulk plasma. Thus the generation of the electron-ion pairs by ICP source was simplified and estimated as

$$G(P_{RF}) = \frac{P_{RF} f_{ICP}(x,y,z)}{V_{ICP} N_A \sum_i E_{inelastic}(i)} \qquad (1)$$

where $G(P_{RF})$ is in [mol cm^{-3} s^{-1}], $E_{inelastic}$ is the energy per inelastic collision of type "*i*", and $P_{RF} = const$ is applied ICP RF power. The function $f_{ICP}(x,y,z)$ is a simplified geometry function of the heating ICP zone, that is determined by a coil geometry, excitation frequency, ω_{RF}, and plasma conductivity, σ_p, skin depth is

$$d_s = \sqrt{2/(\omega_{RF}\mu_0\sigma_{plasma})} \qquad (2)$$

$$\sigma_p = e^2 n_e/(m_e \nu_{e-n}) \qquad (3)$$

where μ_0 - permeability of free space, e - elementary charge, n_e - electron density, m_e -

electron mass and ν_{e-n} - electron-neutral collision rate. An accurate solution will require coupling the electromagnetic fields self-consistently with a plasma properties, expressing the RF power density, p_{RF}, by using variable σ_p, thus

$$p_{RF} = (1/2)\times\sqrt{\omega_{RF}\mu_0/(2\sigma_p)}\times\left|(\hat{n}\times\vec{H})\right|^2 \quad (4)$$

where $\hat{n}$ is a unit vector normal to plasma surface.

3.1 Plasma Model

The actual 2D/3D plasma fluid model was described by the set of the species and energy balance equations (chcd). Thus, the stationary continuity equation for electrons has been used as it follows

$$\partial n_e/\partial t = 0 = -\vec{\nabla}\vec{\Gamma}_e + S_e \quad (5)$$

where electron flux in "drift-diffusion" transport approximation is given by relationship

$$\vec{\Gamma}_e = -D_e\vec{\nabla}n_e + \mu_e(\vec{\nabla}V)n_e \quad (6)$$

and S_e is an electron generation/loss term.

The electrostatics mode (emes) for electric potential distribution (reactor size is <<1/4 wavelength) in Poisson equation form

$$\Delta V = -(e/\varepsilon_0)\times\left(\sum_{+,-} z_i n_i - n_e\right) \quad (6)$$

was involved into coupling scheme to satisfy a plasma quasi-neutrality condition, and to couple the $\vec{E}$ field to an ambipolar diffusion coefficient. Here, $z_i = \pm 1$ for positive and negative♣ ions, and $i = H^+, H_2^+, H_3^+$.

The mass balance equations (chcd) for all positive positive ions H^+, H_2^+, and H_3^+ have generic form

$$-\vec{\nabla}\vec{\Gamma}_i + S_i = 0 \quad (7)$$

with fluxes

$$\vec{\Gamma}_i = -D_i\vec{\nabla}n_i + z_i\mu_i n_i E_{eff} \quad (8)$$

and S_i is ion generation/loss term. A local flux balance of the charged species $\sum \Gamma_i = \Gamma_e$ is maintained by effective electric field E_{eff}. As the first approximation we simplified this approach by expressing the ion flux in a form $\vec{\Gamma}_i = -D_{amb}\vec{\nabla}n_i$, where, D_{amb}, ambipolar diffusion coefficient is coupled with electron temperature by Einstein relationship $D_{amb} \cong D_i(1 + T_e/T_i)$. Here, D_i is diffusion coefficient of the ions, T_e, T_i - electron and ion temperature, respectively.

Continuity equations for the neutrals are as follows ($n = H, H_2, H^i, H_2^{i,j,k}$)

$$-\vec{\nabla}\left(-D_n\vec{\nabla}n_n\right) + \langle S_n\rangle = 0 \quad (9)$$

with average $\langle S_n\rangle$ generation/loss terms.Formal assumption for plasma heating was included into the model through a heat transfer application mode (htgh) that is a total neutral gas energy balance is described by equation

$$0 = -\vec{\nabla}\left(-k_{gas}\vec{\nabla}T_{gas}\right) + Q_n \quad (10)$$

where Q_n is homogenous gas heating source term, k_{gas} - thermal conductivity. More accurate thermal non-equilibrium model has been currently under development to account for multiple temperature distributions for individual species – such are H, H_2, H^+, H_2^+, H_3^+, and negative ions H^- (including fast H and H_2 "beam" temperatures).

At the plasma-walls interface we assumed infinitively thin sheath and considered following boundary conditions:

$$\vec{j}_{H_k^+}\Big|_{boundary} = n_{H_k^+}\vec{u}_{B(H_k^+)} \ (k=1,2,3) \quad (11)$$

$$j_e\Big|_{boundary} = \sum_{k=1,2,3} j_{H_k^+}\Big|_{sheath} \quad (12)$$

$$j_H\Big|_{boundary} = -\frac{1}{4}\gamma_{rec}^{wall} n_H v_{th(H)} + \\ + \left(1-\gamma_{rec}^{wall}\right)\sum_{k=1,3} j_{H_k^+}\Big|_{boundary} \quad (13)$$

$$j_{H_2}\Big|_{boundary} = \frac{1}{2}\gamma_{rec}^{wall} j_H\Big|_{boundary} + \quad (14)$$

$$+\frac{1}{2}\gamma_{rec}^{wall}\sum_{k=1,3} j_{H_k^+}\Big|_{boundary} + \sum_{k=2,3} j_{H_k^+}\Big|_{boundary}$$

♣ the model does not consider the negative ions where $u_{B(H_k^+)} = \sqrt{k_B T_e / m_{H_k^+}}$ is Bohm velocity for individual ions and γ_{rec}^{wall} is recombination probability at walls.

3.2 Hydrogen Chemistry

In no case, there is intention of this paper to describe a complete H_2 chemistry under plasma conditions. The principal reason of this work has been to perform feasibility study on plasma reactor simulation utilizing Multiphysics coupling capabilities. Primarily, we accounted only for the electron impact collisions in investigated model and the major species such are H, H_2, H^+, H_2^+, H_3^+. As a matter of fact, the accurate description of the chemistry has been reported as the main issue for reliable modeling of hydrogen containing plasmas.[6] For example, the fast hydrogen atoms and molecules may be generated in plasma through charge exchange collision mechanism. As the major source of the H radicals it is considered to be H_3^+ ion. More extensive work has to be done in the future. The scale of current investigation in this work is summarized in Table 1.

Table 1: The species and chemistry used in actual model. Model accounts for charged species H^+, H_2^+, H_3^+, balanced with electrons, and neutral species H and H_2.

SPECIES	COLLISIONS	TRANSPORT
Following species were considered in model: H_2 H_2^+ electrons H H_3^+ H^+	**Considered 15 collisions in model. There are possible 51 collisions in total based on literature review.**	Convective directional flux from the inlet orifice and diffusion motion in reactor space.
Species neglected in this version: H^- $H_2^*(j)$ $H_2^*(n_1)$ fast H $H_2^*(v)$ $H_2^*(n_2)$ fast H_2 H^* metastable $H_2^*(n_3)$	Accounting for excitational energy transfer (species on the left) will increase and sustain higher hydrogen dissociation level within the reactor.	

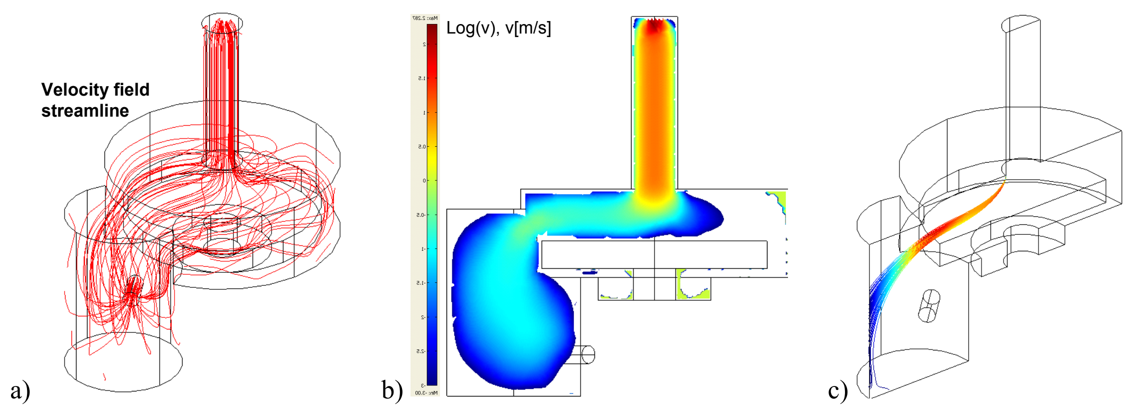

Figure 2. Gas flow study in hydrogen remote plasma reactor: (a) streamlines in full 3D model; (b) The gas flow velocity distribution, and (c) Tracking of the light particles originated in ICP source location.

4. Simulation Results and Discussion

Background H_2 gas flow was described by incompressible Navier-Stokes equations (chns) for low speed isothermal flow. The full 3D gas flow model was simulated considering asymmetric pumping outlet. Characteristic gas flow streamlines are shown in Fig. 2-a. The gas velocity distribution is also illustrated in baseline reactor in Fig. 2-b, indicating the highest velocity flow within the ICP source. The ICP source zone is possible source of contamination due to large RF power applied to the coil (several kW), it may be a source of the particles due to the extensive thermal load on the ceramic walls. We have found the particle's tracing tool as a practical instrumentation in analysis of the contamination particles concentration and their localization.

Involvement of the additional convection and diffusion application modes for individual species inside the plasma reactor allowed us to determine their distributions within the ICP zone. However, the computing increased significantly and instead of the full 3D model we had to run reduced geometry – half or even quarter size, axially symmetric 3D models, to reduce computational duration.

The ICP discharge at 60 Pa is well localized within the ICP source. The Fig. 3 shows species distributions in ICP remote quartz tube. Under investigated conditions the H_2^+ has significantly larger population than H_3^+ or H^+. Various researchers observed similar results also experimentally, and the branching ratio of 0.93 is typically for the H_2^+ (0.07 for H^+).

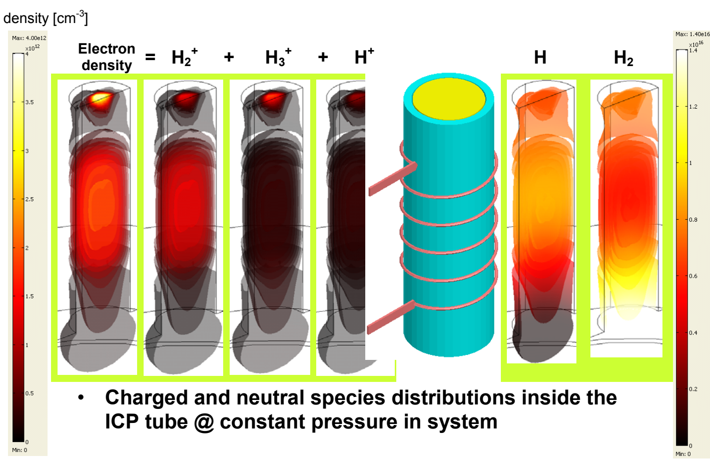

Figure 3. The concentration isosurfaces for the various species in the zone of the ICP source.

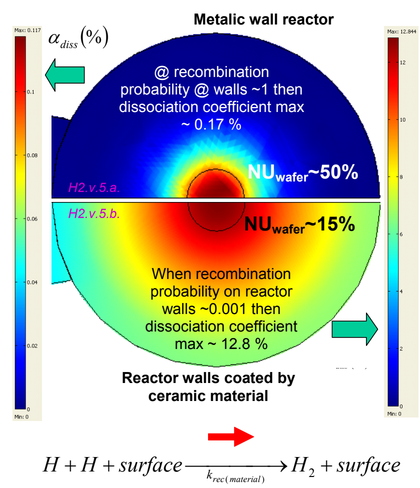

Figure 4. The *H* radical distribution at the wafer surface.

The hydrogen radicals created within ICP source are recombining at the reactor walls and in dependence on the surface properties their population is reduced. The dissociation coefficient within ICP source was up to 70 %. However, the recombination probability of the *H*-radicals on the metallic surface is 1000-times higher than on the ceramic ones, thus the radicals are expected to be diminished significantly in metallic walls reactor.

This is obvious from the next Fig. 4, which illustrates the *H* radical distribution at the wafer surface in two different reactors. The metallic reactor generated very low hydrogen dissociation ratio (<1%) and extremely low radial uniformity ~50 %. The application of the quartz covered interior of the vacuum chamber improved dissociation to ~13 % and nonuniformity dropped to 15 %. It is evident that quartz coating of the interior is important for sustaining high processing rate and its uniformity. On the other hand the H_3^+ ions have had relatively longer lifetime than other H_2^+ and H^+ (see Fig. 5) and were expanding into the reactor volume. Due to the high population of the H_3^+ ions and their dissociation and/or recombination, they represent the major channel of the generation and sustaining *H* radicals in reactor.

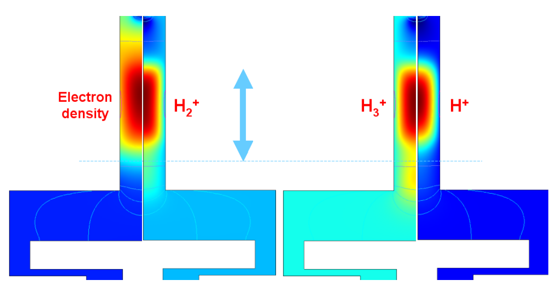

Figure 5. The *H* radical distribution at the wafer surface.

In the simulation flow we explored multiple showerhead variation with intention to optimize the radical density at the wafer surface. The Fig. 6 shows uniformity achieved with specific showerhead included in the model. The optimization of the chamber geometry with novel showerhead design allowed improving nonuniformity down to 4 % (with edge exclusion). Solution has achieved comparable process rates to the initial baseline rate. To compensate for 4 % nonuniformity, only ~9% overtime has been required to complete whole wafer surface.

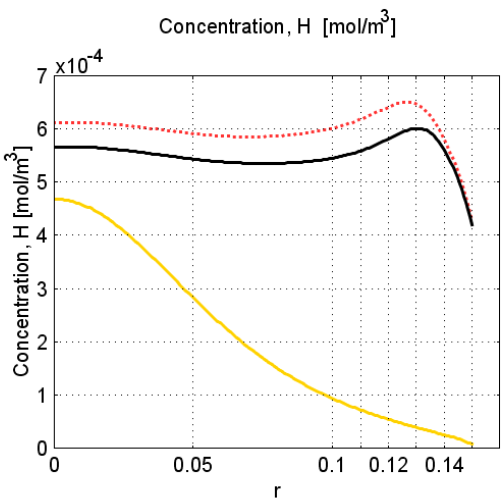

Figure 6. The impact of the optimization of the chamber geometry with novel showerhead design allowed improving nonuniformity down to 4 % with edge exclusion.

Initial results in this work were obtained by simulation using 32 bit PC. Not optimized fully model, large 3D geometry, and complex chemistry did not allowed to explore the potential and capabilities of the sw package in full extend. The 3D model had to be reduced into 2D in axial symmetry to achieve converging solutions in reasonable times. Since, the geometrical features in this model are in the range from ~ 1 mm to ∅60 cm, and there is plan to set full 3D model including electromagnetic coupling to account for an actual geometry of the ICP antenna, to include the majority of the most important hydrogen chemistry, and consideration of the surface reaction at the wafer, currently, a continuing work has been done with simulation at the more powerful PC (64 bit Windows) offering 8 GB memory. The Reaction Engineering Lab will be explored to compare performance with previous model setup.

5. Conclusions

The modeling approach and experience with COMSOL Multiphysics modeling to assist in an equipment design and process development has been shared in this work. The 2D/3D plasma fluid model was developed for application in hydrogen remote plasma cleaning within the BEOL processing of the silicon wafers. The model was described by the set of the species and energy balance equations in generic semiconductor tool chamber with remote Inductively Coupled Plasma (ICP) source. Background H_2 gas flow was described by incompressible Navier-Stokes equations for low speed isothermal flow. The multiple diffusion and convection application modes were used to solve the system of the coupled equations with appropriate boundary conditions. The electrostatics mode for electric potential distribution was involved into coupling scheme to satisfy a plasma quasi-neutrality condition, and to couple $\vec{E}$ field to an ambipolar diffusion coefficient (model in "drift-diffusion" driven transport approximation).

6. References

1. W. Kern, *Handbook of Silicon Wafer Cleaning Technology: Science, Technology and Applications*, Noyes, Park Ridge, NJ (1993)
2. D. B. Fenner, D. K. Biegelsen, and R. D. Bringans, *J. Appl. Phys.* **66**, 419 (1989)
3. K. Miyake, *Jpn. J. Appl. Phys.* **28**, 2376 (1989).
4. H. Yamada, *J. Appl. Phys.* **65**, 775 (1989)
5. T. Koui.I. Suemune, A. Kishimoto, K. Hamaoka,and M. Yamanishi, *Jpn. J. Appl. Phys.* **30**, 3203 (1991)
6. B. Kalache, W. Morscheidt, K. Hassouni, T. Novikova, and P. Roca i Cabarrocas, *Proceedings of the 15th International Symposium on Plasma Chemistry* p. 3201, (2001)