Low Pressure Deposition in a High Density Plasma CVD Reactor

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Abstract. High-density plasma chemical vapor deposition (HDP-CVD) reactors are used to provide void-free gap fill of high-quality dielectric films in high aspect ratio device structures in semiconductor processing. The ability to deposit at low pressure is essential for high-quality films and uniform profiles. To investigate issues related to low-pressure deposition and electron/ion/neutral transport property effects, we have used the Hybrid Plasma Equipment Model (HPEM) developed at the University of Illinois at Urbana-Champaign to simulate a 2D reactor geometry. In this study, ion and neutral energy distribution functions obtained from Monte Carlo simulations were used to determine transport coefficients for use in the heavy particle momentum conservation equations. The HDP-CVD reactor considered is an approximation to a hemispherical inductively coupled plasma (ICP) source for 200-mm wafer processing. The gas injection source in these models is a ring near the base of the dome. Model results indicate that the gas precursor uniformity across the pedestal (where a wafer for semiconductor processing would be located) is improved for the low-pressure conditions (i.e. 5 millitorr and below) for a commonly used SiO_2 deposition chemistry (i.e. SiH_4, O_2, and Ar). Additionally, even at pressures considered high and more continuum-like in HDP-CVD applications (i.e. 15 millitorr), there are significant differences in the computational results when the transport properties are not calculated using a Monte Carlo simulation model.

INTRODUCTION

High-density plasma chemical vapor deposition (HDP-CVD) reactors are used to provide void-free gap fill of high-quality dielectric films in high aspect ratio device structures in semiconductor processing. The ability to deposit at low pressure is essential for high-quality films and uniform profiles [1]. There have been numerous publications about the experimental details used in HDP-CVD for semiconductor processing, but there has been little in the way of publication for the modeling of silane-based chemistries in inductively coupled, high-density plasmas for either 2D or 3D geometries. Gochberg and Rault [2] presented DSMC modeling work using a simple approximation to silane deposition chemistry, which assumed that all SiH_x radicals were evenly distributed and deposited in a transport-limited manner on surfaces. Meeks, et. al. [3] proposed a very complex chemistry model with several hundred reaction mechanisms for gas phase and surface reactions. However this work used a 0D (well-stirred approximation) model, and using a chemistry model with several hundred reactions in a 2D/3D model is not considered a reasonable approach. Keiter and Kushner wrote a short note on using a reduced reaction set to model a reactor in 3D [4] using the Hybrid Plasma Equipment Model (HPEM, [5,6,7]), and Kinder, et. al., used HPEM results to study trench filling in HDP-CVD [8].

The HPEM software has undergone numerous improvements since its inception, and is a far more complete and capable code today than it was in the 1990's. One particular improvement that was made recently involved the addition of a module where the ion and neutral transport coefficients are kinetically derived and implemented in fluid equations. The goal here was to improve the accuracy of HPEM at lower pressures where the Knudsen number (λ/L or mean free path divided by a characteristic dimension) is large (i.e. a few tenths or more). This module is called the IMCS (Ion/neutral Monte Carlo Simulation). Vyas [9] and Vyas and Kushner [10,11] used this new capability in application to hollow cathode magnetron sputtering for semiconductor processing. Here, we explore the use of this software improvement in the modeling of HDP-CVD processes. We will compare and contrast the

use of various HPEM software transport modules in a 2D inductively coupled plasma reactor containing a mixture of SiH_4, O_2 and Ar.

MODEL

The geometric model investigated here is seen in Figure 1. It is nominally a non-commercial 200-mm HDP-CVD reactor with a curvilinear shape. The coils around the outside of the curved top of the reactor are evident. Since the 2D version of HPEM used here can only handle Cartesian coordinates, a stair-stepped geometry and mesh were created. The simulated process conditions are 3 kW ICP power at a frequency of 400 kHz, a gas flow of 280 sccm total (the ratio is $Ar/O_2/SiH_4$= 1/6/3), and there was no pedestal bias voltage applied. The gas inlet is a ring near the bottom of the curvilinear part of the reactor, in a manner similar to the geometry used in experiments performed by Tuszewski and Tobin [12], though the location of the pedestal in this work is several inches lower than in the aforementioned experiments. The nominal pressure quoted for each model is the pressure at the pump port at the bottom of the reactor. There is no SiO_2 surface deposition allowed in this model. The gas precursors are simply cracked by the plasma, reacting in the gas phase only, and every species is pumped out of the system.

The chemistry is defined using 20 different species in addition to the 3 neutral precursors (argon ions, argon metastables, neutral, excited and ionized O, 5 species of neutral and ionized SiH_x, 5 species of neutral and ionized H_x, SiH_2O, H_2O, and OH. The model includes 51 gas phase reactions in total, including electron impact reactions.

The simulation used in this work incorporates a newly developed computational technique in which a Monte Carlo simulation for ion and neutral transport (IMCS) is integrated with fluid based transport modules in HPEM. In this model, the ion and neutral velocity distribution functions obtained from the IMCS are used to calculate transport coefficients that are then employed in heavy particle momentum conservation equations.

Within HPEM, solutions were sought using three different variations as described in Table 1. Variation 1 used fully fluid models for electrons and all ions and neutrals. In Variation 2, the electron transport was modeled with a Monte Carlo simulator, and the ions and neutrals were modeled using fully fluid transport properties. In Variation 3, the electron transport was modeled as Monte Carlo and the new IMCS module was used to model the transport properties of the ions and neutrals. We will be concentrating on cases with nominal pressures of 5 and 15 millitorr. Five millitorr and below is a typical operating pressure for HDP-CVD semiconductor processing chambers, and well within the flow regime where non-continuum effects from high Knudsen numbers will be seen.

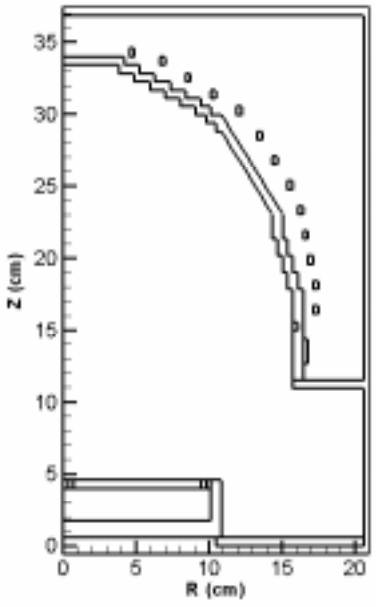


FIGURE 1. ICP reactor geometry.

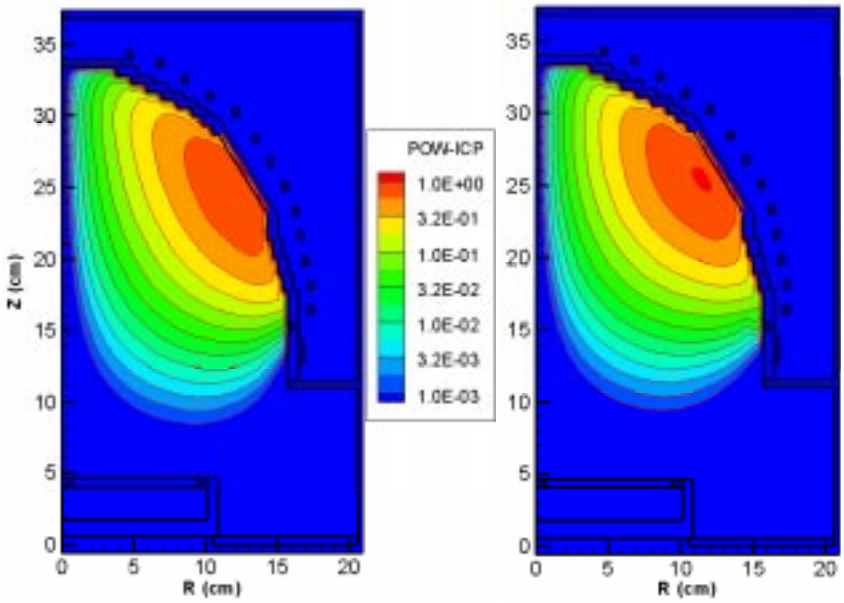


FIGURE 2. Power density (W/cm^3) for the (a) 5 millitorr, and (b) 15 millitorr cases.

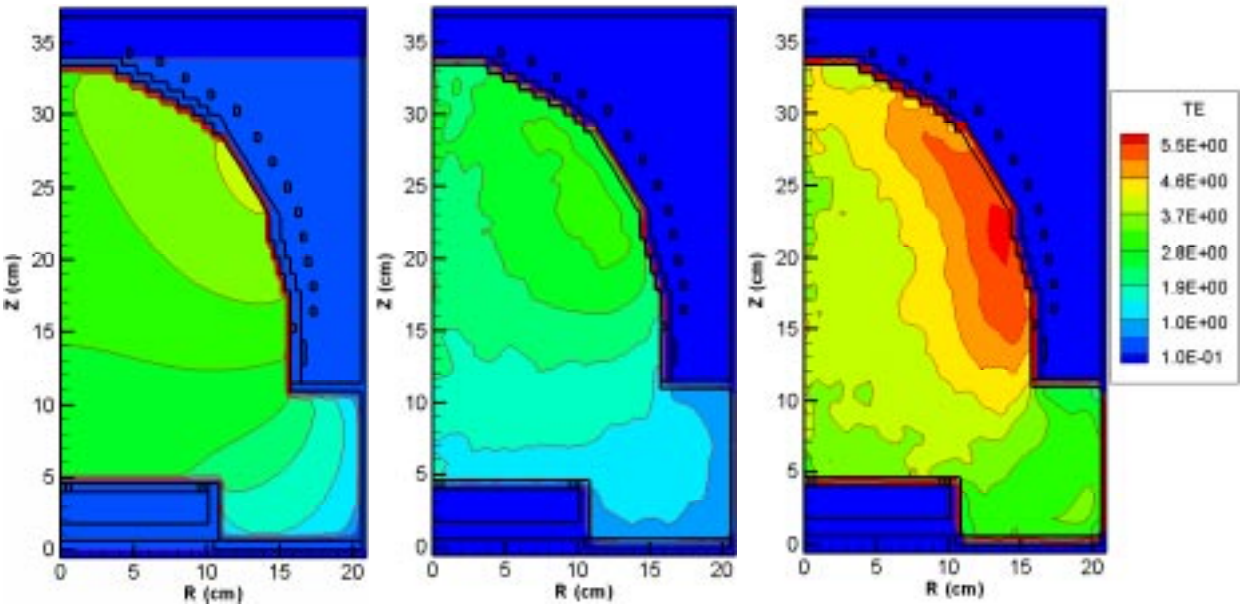
COMPUTATIONAL RESULTS

Results for power density are shown in Figure 2. The power density is largely unchanged in all the model variations for each pressure investigated. There are only small differences in power density over the range of pressures that were examined. Figure 3 shows the electron temperature for the three different 15 millitorr variations that were examined. Clearly, there are differences between the three variations, but the largest change is seen in the 15 millitorr case using Variation 3 (Monte Carlo properties for electrons, ions, and neutrals). The largest electron temperature in the chamber rises (near the coils) by approximately 1.0 eV when using the new IMCS module for calculating transport properties. The electron temperature above the pedestal in the chamber also increases significantly when the IMCS is used when comparing Variations 2 and 3. Figure 4 shows the electron temperature for the 5 millitorr cases. Unfortunately, the IMCS case (Variation 3) would not run correctly and we only see results for Variations 1 and 2. Similar changes are seen between Variations 1 and 2 at the lower pressure, and similar results are expected (i.e. as seen in the 15 millitorr case) once the issue with the IMCS module is cleared up.

Figures 5 and 6 show the SiH_2^+ number density in the chamber for the 15 and 5 millitorr cases, respectively. These contour plots are similar for the other major species number densities in the system, i.e. O_2^+, O^+, H_2^+, O, etc. At the surface if the pedestal, the species number densities are lowest for Variation 2, and are the largest for Variation 1. Variation 1 shows the largest region of high number density of all the cases. Variation 3 shows the largest number densities seen in the regions farthest away from the ICP coils. Similarly significant differences in the plasma potential and electron densities are also seen, but not shown in this paper.

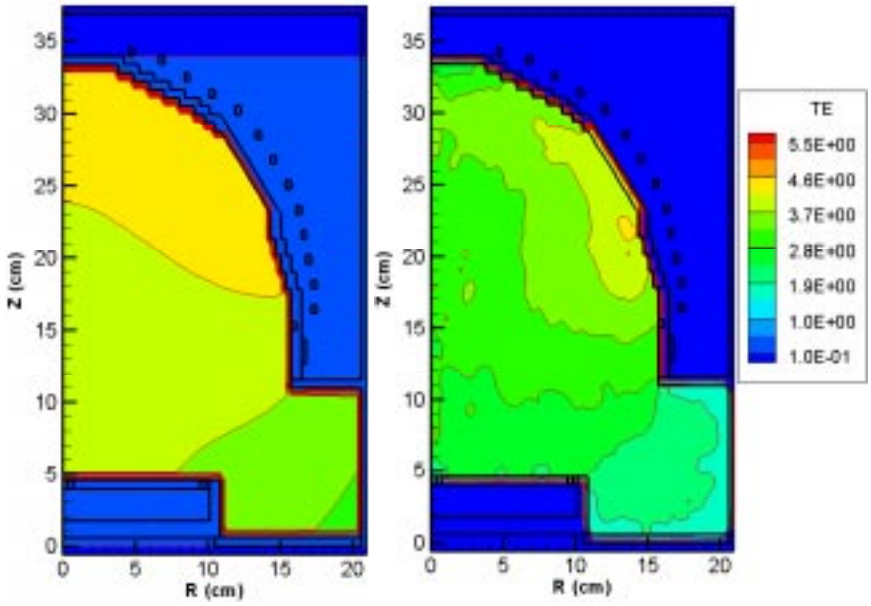
TABLE 1. Description of the various computational models used.

Cases	Electron Treatment	Ion Treatment	Neutral Treatment
Variation 1	Fully fluid model	Fully fluid model	Fully fluid model
Variation 2	Monte Carlo Simulator	Fully fluid model	Fully fluid model
Variation 3	Monte Carlo Simulator	Monte Carlo Simulator	Monte Carlo Simulator



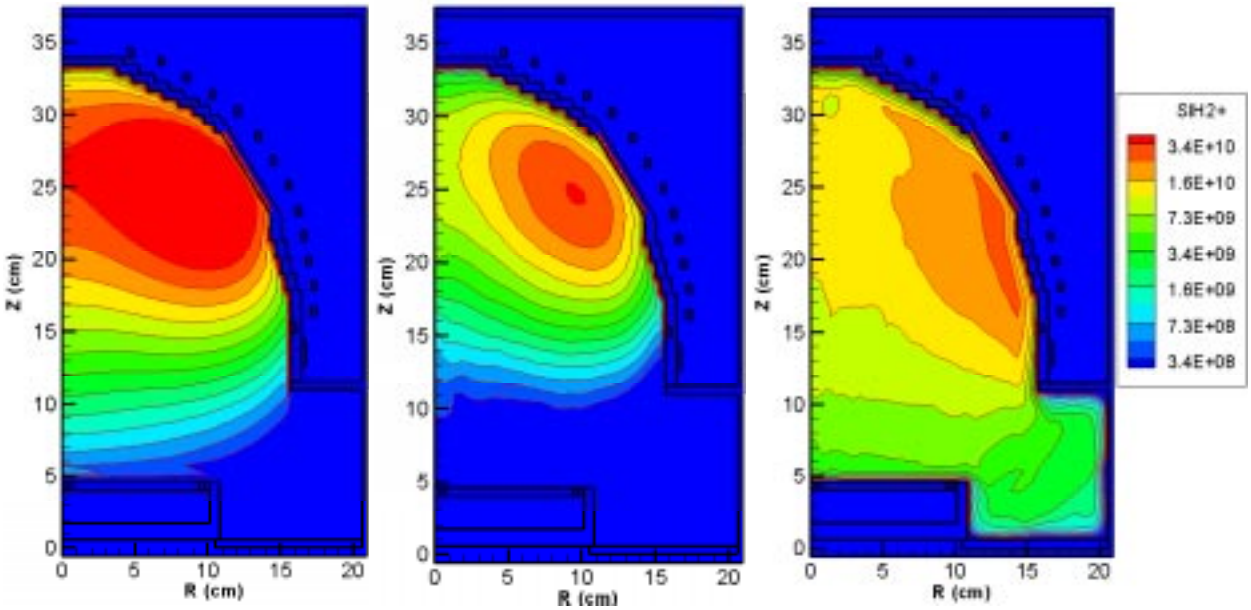
(a) (b) (c)

FIGURE 3. Electron temperatures (eV) at 15 millitorr for (a) Variation 1, (b),Variation 2, and (c) Variation 3.



(a) (b)

FIGURE 4. Electron temperatures (eV) at 5 millitorr for (a) Variation 1 and (b) Variation 2.



(a) (b) (c)

FIGURE 5. SiH_2^+ number density (cm^{-3}) at 15 millitorr for (a) Variation 1, (b) Variation 2, and (c) Variation 3.

Figure 7(a) shows the precursor uniformity for the SiH_2^+ flux at the pedestal. Clearly, as the operating pressure drops in the HDP-CVD chamber, the uniformity of the precursor gas species fluxes gets better. This provides some numerical evidence backing up the experimental claim that HDP-CVD performance improves with reducing pressure. The total ion fluxes for various cases are plotted in Figure 7(b) as a function of radius on the pedestal. At 15 millitorr, the magnitudes of the predicted fluxes are quite different, though Variations 1 and 2 show quite similar uniformities. Variations 1 and 2 at 5 millitorr show much closer flux magnitudes, but the difference in the uniformity is significant.

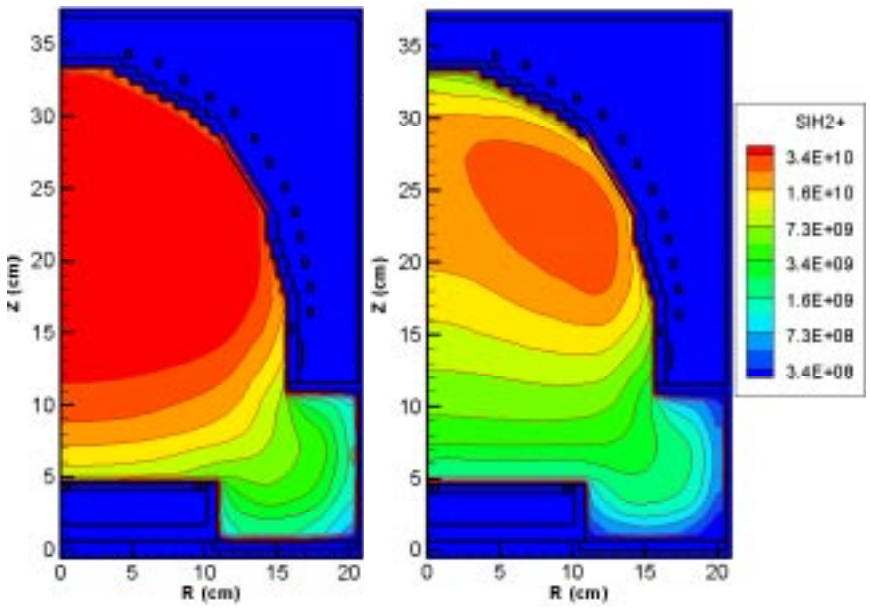


FIGURE 6. SiH_2^+ number density (cm^{-3}) at 5 millitorr for (a) Variation 1 and (b) Variation 2.

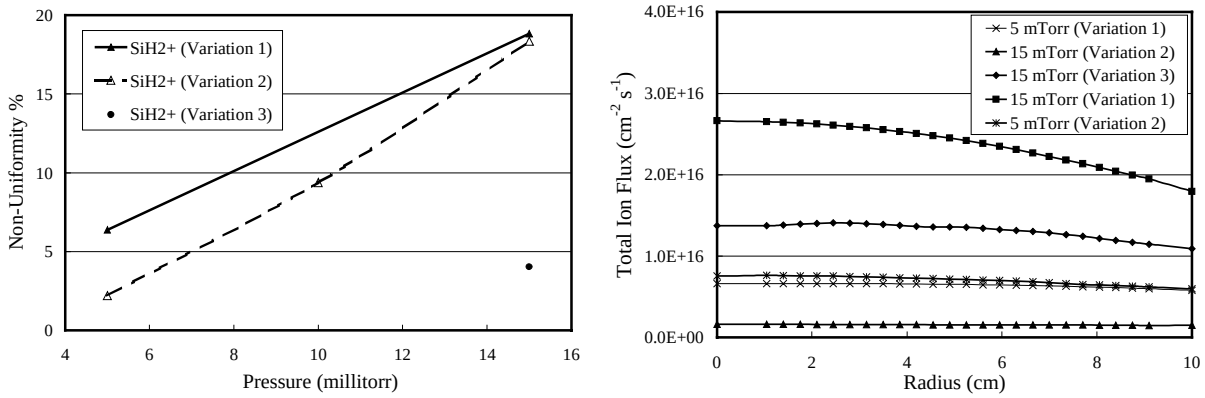


FIGURE 7. (a) SiH_2^+ flux non-uniformity (%) vs. pressure, (b) total ion flux (cm^{-2} s^{-1}) vs. radius on pedestal.

The modeling work presented here shows that there are clear differences in results using the new IMCS transport property module within HPEM. However, without further investigation, it is not clear exactly when this additional computational complexity will be required, or how accurate it is. Comparisons to experiments, both with and without surface deposition should be made. The Tuszewski and Tobin [12] data for a gas mixture of argon, oxygen, and hydrogen at 5 millitorr with 2 kW of RF power at 460 kHz could be used for this. In fact, Kinder [13] has done modeling work for these operating conditions using commercial plasma modeling software. This effort would need to be repeated using HPEM with and without the IMCS. Though the Tuszewski and Tobin data is without surface deposition, the conditions are quite close to HDP-CVD operating conditions and should provide good insight into the accuracy of MPEM with the IMCS.

CONCLUSIONS

High-density plasma CVD is examined computationally to illustrate the need for low pressures in obtaining uniform thin film deposition. We also investigate a new Monte Carlo capability to compute ion and neutral species transport coefficients at low pressures and compare that to results using the previous fully fluid models in the Hybrid Plasma Equipment Model (HPEM) from the University of Illinois at Urbana-Champaign. The three variants examined all showed significant differences amongst themselves at a 15 millitorr operating condition, but differences were much smaller at 5 millitorr.

Model results indicate that the gas precursor uniformity across the pedestal (where a wafer for semiconductor processing would be located) is improved for pressures at 5 millitorr and below for a commonly used SiO_2 deposition chemistry containing SiH_4, O_2, and Ar. Additionally, even at pressures considered high and more continuum-like in HDP-CVD applications (i.e. 15 millitorr), there are significant differences in the results when the transport properties are not calculated using a Monte Carlo simulation model. Unfortunately, results at 5 millitorr using the new Monte Carlo capability did not run correctly. Further work will be required to fully evaluate this new HPEM module in this HDP-CVD application.

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