Rapid two-dimensional self-consistent simulation of inductively coupled plasma and comparison with experimental data

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A methodology has been developed to achieve rapid two-dimensional self-consistent simulation of plasma transport and reaction in an inductively coupled source of arbitrary geometry and with arbitrary plasma and surface chemistries. In this modular finite element fluid simulation the reactor was divided into bulk plasma and sheath. The bulk plasma was assumed quasineutral and the electrons were assumed to be in Boltzmann equilibrium. Separate modules computed the power deposition into the plasma, electron temperature, charged species densities, and neutral species densities. Simulation results agreed favorably with available experimental data, taken in a chlorine plasma in a Gaseous Electronics Conference reference cell, without using any adjustable parameters. Rapid convergence makes the simulation tool especially attractive for technology computer-aided design (TCAD) applications. © *1996 American Institute of Physics.* [S0003-6951(96)00818-2]

High plasma density ($>10^{17}$ m^{-3}) sources show great promise for meeting the demands of gigascale integrated circuits.[1] Inductively coupled plasma (ICP) sources are particularly promising due to simplicity of their design.

Modeling and simulation can provide insight into the spatiotemporal plasma flow, and can aid in the design of new plasma sources.[2] Two-dimensional (2D) models[3–9] are particularly useful for design purposes since the etch or deposition uniformity along the wafer can be predicted as the reactor operating conditions vary. Most of the 2D ICP simulations reported so far are based fully[3–6] or partly[7–9] on the continuum or ''fluid'' approximation. Recent comparisons of fluid with kinetic particle in cell simulations of radio frequency (rf) plasmas[10] have shown that the fluid approximation provides surprisingly reasonable results even down to pressures at which this approximation would be considered highly suspect.

To be used as a technology computer-aided design (TCAD) tool, a computer simulation must be accurate, user friendly and able to execute rapidly on a desktop computer. These features allow one to conduct parametric investigations easily to study the effect of different reactor designs and operating conditions on the plasma etch or deposition characteristics. In this spirit, Paranjpe developed a rapid time-independent 2D ICP simulation, based on ambipolar diffusion.[5] The author also made the local field approximation, expressing the ionization rate as a function of the local azimuthal electric field. This assumption is not expected to hold at the low operating pressures of interest at which the electron energy relaxation length exceeds the reactor dimensions.[11] Kortschagen *et al.* used the so-called nonlocal electron kinetics approach to simplify the Boltzmann equation for the electron distribution function.[12] Both Paranjpe and Kortschagen *et al.* simulated an argon plasma (no plasma chemistry) in a simple rectangular geometry. A rapid 2D simulation of a capacitively coupled reactor was also reported recently by Brinkmann *et al.*[13] The authors also separated the bulk plasma from the sheath and made the assumption of quasineutrality in the bulk. A similar approach was followed by Meyyappan and Govindan in their 1D simulation of an electron cyclotron resonance plasma.[14]

In this letter we report on a rapid 2D self-consistent ICP finite element simulation using the fluid approximation. The simulation was validated by comparing predictions of spatially averaged and spatially resolved plasma properties with experimental data taken in a Gaseous Electronics Conference Inductively Coupled Plasma (GEC-ICP) cell.[15]

The present model employs a ''modular'' approach and it is a simplification of that reported earlier.[3] The power deposited into the plasma was calculated by an electromagnetics (EM) module. Results reported below used the EM module of Jeager and Berry[16] although similar results were obtained with the University of Houston EM module used previously.[3] The power deposition was used in an electron energy module to determine the electron temperature and the rate coefficients of electron-impact reactions. These were in turn used as source terms in separate modules describing neutral and charged species transport. By iterating among the modules, a self-consistent solution was obtained. This modular approach is in essence an ''equation splitting'' strategy that is used to overcome the disparate time scales associated with electron (<1 ns) and heavy species (10 s of μs for ions and perhaps 100 s of ms or longer for neutrals) transport and chemistry. Furthermore, the bandwidth of the matrices resulting after spatial discretization is reduced greatly by implementing a smaller number of equations per module.

The present model differs from the previous one[3] in the following:

(1) The plasma reactor was divided into bulk plasma and sheath. This way, the extreme spatial stiffness associated with the thin (100 s of μ) sheaths was avoided. The sheath can be described by a semianalytical model developed by Riley.[17] The details of the sheath model are not important for

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the present simulation because (a) capacitive coupling from the coil is not considered, (b) an unbiased substrate is used, and (c) the focus of this letter is the bulk plasma, and comparisons with data are made for species densities in the bulk plasma.

(2) Instead of solving Poisson's equation, quasineutrality was assumed to prevail in the bulk plasma. This is an excellent approximation for the bulk since the Debye length is exceedingly small compared to the reactor dimensions. Of course, Poisson's equation has to be solved in the sheath. In the present model, the positive and negative ion densities were solved using the corresponding particle balance equations, and the electron density was calculated through the electroneutrality constraint.

(3) The electrons were assumed to be in Boltzmann equilibrium, implying that the electric field force almost balances the electron pressure force in the momentum balance equation. This assumption was verified by using the results of the full simulation.[3] The space charge field was then calculated through the electron pressure gradient $\mathbf{E} = \Delta(kT_e n_e)/(q n_e)$, where k, T_e, n_e, and q are the Boltzmann constant, electron temperature, electron density, and charge, respectively.

Boundary conditions were imposed essentially at the reactor wall assuming a very thin sheath. The sheath was, therefore, handled as a discontinuity of the potential at the wall. The positive ion flux out of the plasma was set equal to the local density times the local Bohm velocity. The negative ion density was set equal to zero, and the gradient of the electron temperature was set equal to zero along the walls.

Implementing the above simplifications resulted in a dramatic reduction in the CPU time required to achieve a converged solution. For the full chlorine chemistry[3] and full 2D GEC-ICP geometry[15] implemented herein, convergence was obtained after ~1 h of CPU on a 125 MHz Hewlett-Packard workstation. After a converged solution has been obtained, further simulations at nearby operating points can be even faster. This makes the simulation particularly attractive for TCAD applications. Significantly, the simulation results are in quantitative agreement with laboratory data. Details of the numerical procedure and grid resolution effects on accuracy will be presented elsewhere.

Base case conditions for this simulation were: pressure 20 mTorr, coil excitation frequency 13.56 MHz, plasma power 180 W, flow rate 20 sccm of pure chlorine, no substrate electrode bias, and no wafer present (no etching). The base case conditions were used unless noted otherwise. The chlorine chemistry was identical to that used previously[3] except that no etching was allowed to compare with the GEC-ICP data taken without a silicon wafer present. The wall recombination probability of Cl atoms was fixed at 0.1 on all surfaces, a value used before the experimental data were known.

Power was found to be deposited in a toroidal shape, peaking near the middle turn of the five turn coil (see Fig. 1 for location of coils). The azimuthal electric field which sustains the plasma decayed over a distance of ~1 cm (skin depth) under these conditions.

The density profile of the dominant ion (Cl^+) is shown in Fig. 1 (left-hand side). The Cl^+ ions peak on axis, despite

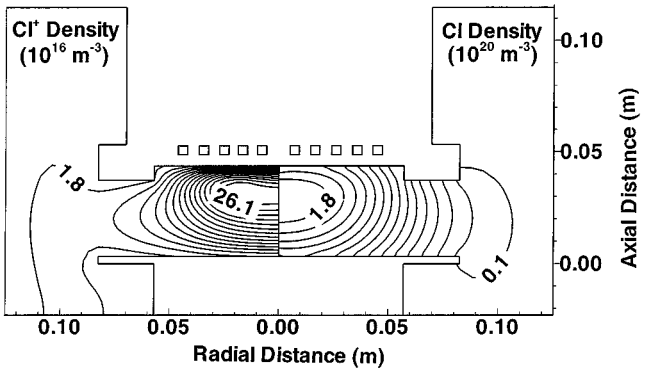

FIG. 1. Cl^+ ion (left-hand side) and Cl atom (right-hand side) number density distributions for 20 sccm, 180 W, 20 mTorr chlorine plasma sustained by an inductively coupled source in a Gaseous Electronics Conference cell geometry. A cross section of the planar coil is also shown.

the fact that the ion production rate had a peak off axis. The plasma is very well confined despite the low operating pressure. The peak Cl^+ ion density is nearly 3×10^{17} m^{-3}. The ion density drops by an order of magnitude beyond a radial distance of ~0.06 m. These results are similar to those obtained by Ventzek *et al.*[8] in the GEC-ICP geometry in pure argon and in an argon–chlorine mixture.

The atomic chlorine number density is shown in Fig. 1 (right-hand side). The flow is quite diffusive due to the very low gas flow rate (20 sccm). The Cl atom density is highest near the reactor center and shows a smooth radial decay towards the surrounding chamber. The molecular chlorine number density distribution was ''complementary'' to that of Fig. 1 (right-hand side). Molecular chlorine was depleted in the main body of the plasma but reformed by wall recombination reactions further downstream.

The calculated line-integrated electron densities as a function of power (solid line) are compared with experimental data (solid squares) taken by microwave interferometry[15] in Fig. 2. The agreement is thought to be good, considering that no rate coefficients were adjusted in the simulation. The electron density increases linearly with power, as expected

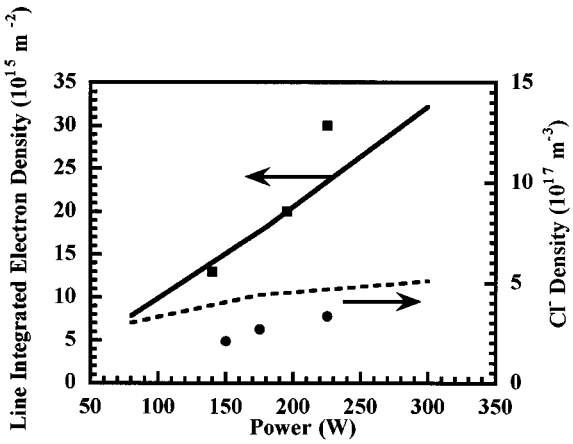

FIG. 2. Comparison between simulation results (lines) and experimental data (points) for a 20 mTorr chlorine plasma. Left-hand side axis: line-integrated electron density through the reactor midplane; solid squares are data from Ref. 15. Right-hand side axis: negative ion density at the reactor center; solid circles are data from Ref. 18.

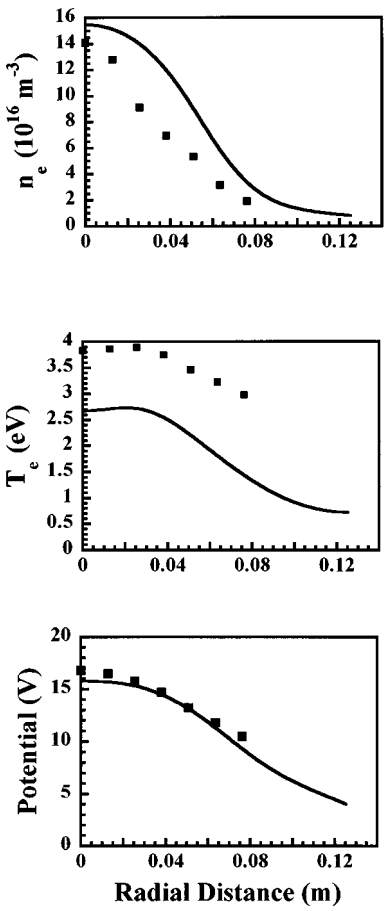

FIG. 3. Comparison between simulation results (lines) and experimental data (points, Refs. 15 and 18) of spatially resolved electron density (top), electron temperature (middle), and plasma potential (bottom) in a chlorine plasma. Conditions: 180 W and 20 mTorr.

for a system for which most of the power input by the rf coil is consumed for plasma production. Predictions of negative ion density at the reactor center as a function of power (dashed line) are compared with preliminary experimental data (solid circles)[18] also in Fig. 2. The agreement is within a factor of two, which is thought to be good considering that the negative ion densities were inferred from laser photodetachment data, and are expected to be accurate to within a factor of two, due to uncertainties in the photodetachment cross section.[18] A comparison between the predicted (lines) and measured (points)[15] radial profiles of electron density, electron ''temperature,'' and plasma potential are shown in Fig. 3. The radial profiles were measured by using a Langmuir probe. Again, the agreement between simulation and experiment is very good. The width of the electron density profile (Fig. 3, top) is rather small, suggesting a well-confined plasma. The predicted electron temperatures (Fig. 3, middle) are ~50% lower than the measured values, possibly due to the assumption of the Maxwellian electron energy distribution function used in the simulation. Also, it is well known that the errors in the electron temperature measurement using Langmuir probes can be substantial.[19] Figure 3 (middle) shows that the electron temperature gradients are rather small due to the high thermal conductivity of the electron gas at the low operating pressure. Finally, the predicted plasma potentials match the data quite well (Fig. 3, bottom). Overall, the agreement between simulation and experimental data is remarkable considering that no adjustable parameters were used. Good agreement was also obtained with data in argon discharges; detailed comparisons will be reported elsewhere.

In summary, a methodology has been developed which allows for a rapid self-consistent simulation of two-dimensional inductively coupled plasma reactors of arbitrary geometry and with arbitrary plasma and surface chemistries. The experimentally validated model is significant for TCAD applications which require rapid evaluation of reactor performance for screening alternative designs or different chemistries.

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