Simulation Images from a Low-Pressure Chlorine Plasma Reactor Using DSMC

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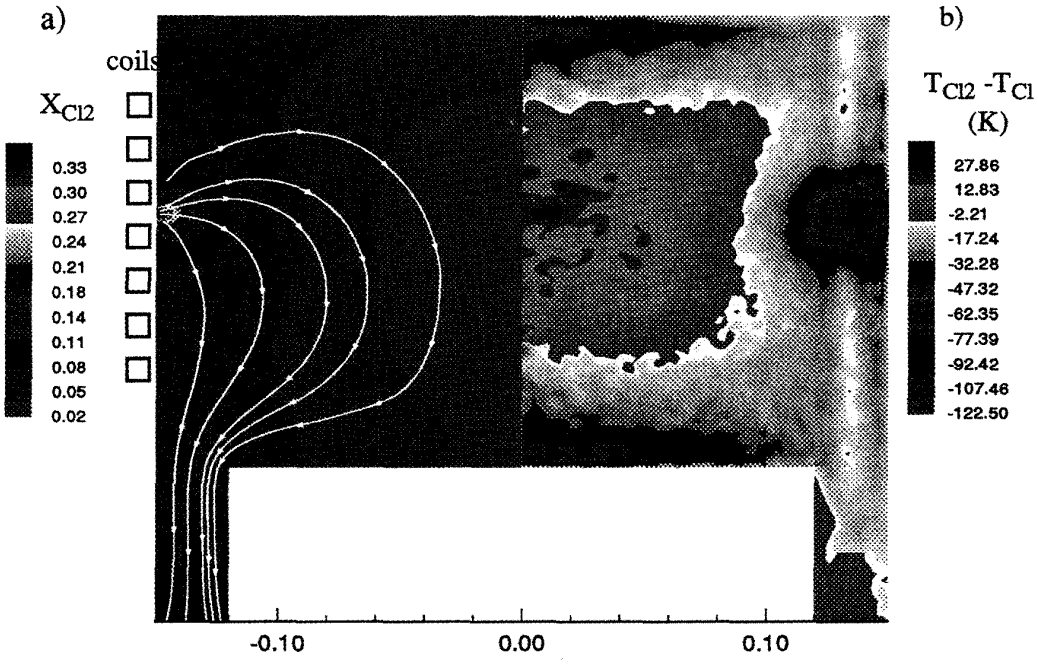

Fig. 1. (a) Cl_2 molefraction with velocity streamlines and (b) spacial variation between T_{Cl2} and T_{Cl} at 10 mtorr for a chlorine plasma reactor with side coils.

Abstract— **Modeling of high-density chemically reacting plasmas at low pressures (<10 mtorr) is of interest to the microelectronics industry for improving tool and process designs. High-density plasma simulations were performed using a fluids code to predict electron behavior, coupled to a Direct Simulation Monte Carlo (DSMC) program for neutral and ion transport. Images presented are for a chlorine plasma simulation at 10 mtorr and include the temperature difference between neutral species, depicting the nonthermal equilibrium nature of the plasma, and angular and energy distributions of ions and neutrals to the wafer surface.**

RESULTS presented are for simulations of polysilicon etch using pure chlorine at 10 mtorr in a plasma reactor with an inductively coupled source. Traditional numerical simulation tools employ a fluid approximation for the transport of the neutral and ion species; this assumption begins to breakdown at this pressure (10 mtorr), where the mean-free path is on the order of the wafer dimension. This problem was overcome by using Direct Simulation Monte Carlo (DSMC) particle simulation method for the neutral and ion transport; a fluid model was used to supply electrostatic fields, electron impact rates, and electron densities. The fluids code solved Maxwell's equations to calculate power deposition into the discharge, and the self-consistent electrostatic fields were computed from the Poisson's equation [1]. Due to the computationally intense nature of DSMC, simulations were performed on a 1024-node nCUBE-2 massively parallel computer.

Species modeled were the feed gas, pure Cl_2, reactants Cl_2^+, Cl, Cl^+, Cl^-, and the etchant $SiCl_2$. The gas phase mechanism included six electron impact reactions, charge exchange reactions, and ion–ion recombination reactions. Surface recombination of Cl to form Cl_2 had a probability of 0.0082, and Cl atoms etched the silicon to form $SiCl_2$ with probability of 0.1. Details of the chemical reactions and the power deposition profile are described in [2]. The highly dissociative nature of the Cl_2 plasma is shown in Fig. 1(a). Fig. 1(b) displays the nonthermal equilibrium nature of the plasma, temperature differences between Cl_2 and Cl were predicted to range from −40 to 125 K. The main

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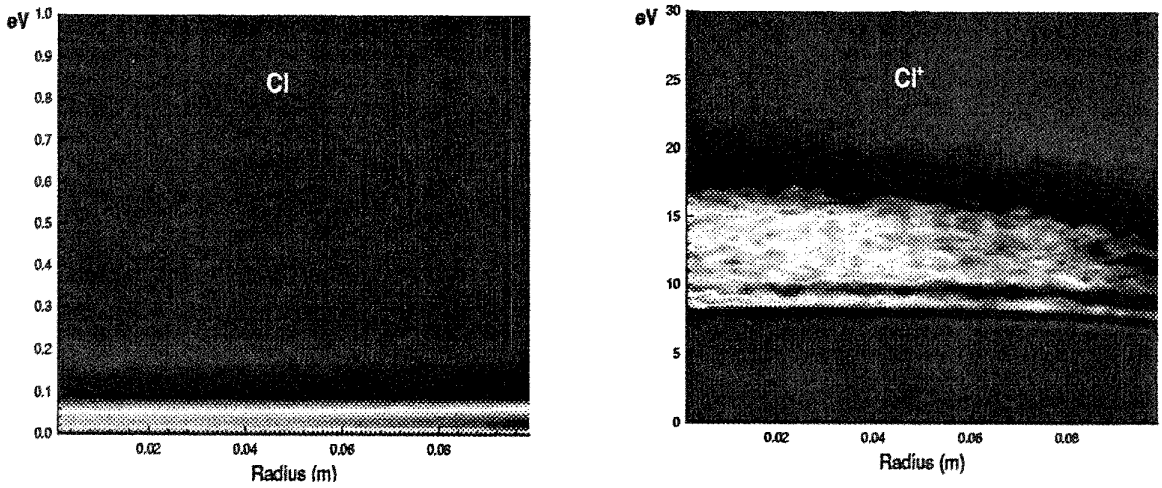

Fig. 2. Incident energy distributions for Cl and Cl^+ across the wafer.

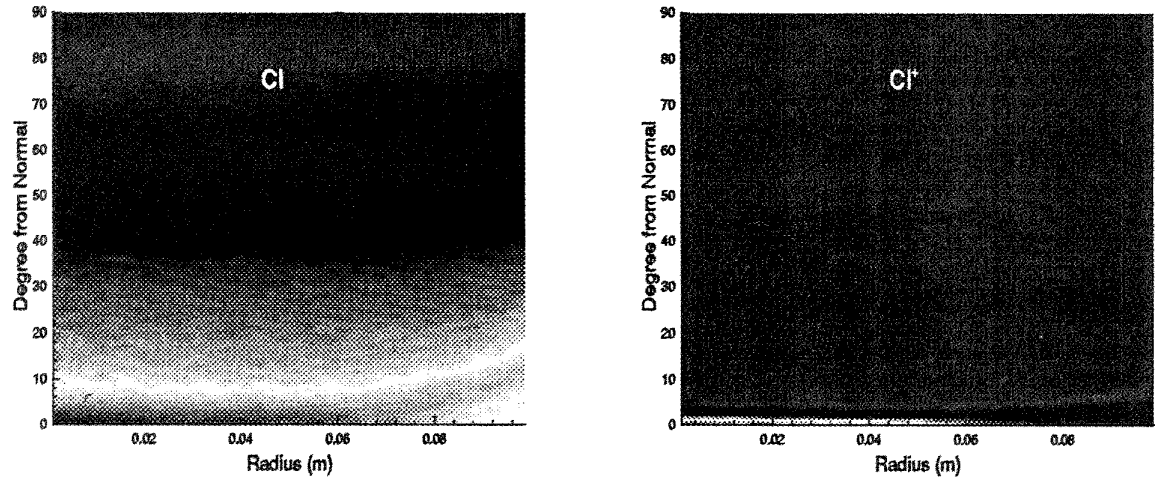

Fig. 3. Incident angular distributions for Cl and Cl^+ across the wafer.

mechanism for gas heating is by collisions with energetic ions in charge exchange reactions and ion–ion recombination reactions. The incident energy and angular distributions on the wafer are natural outputs from a particle-based simulation; these distributions are shown in Figs. 2 and 3 [3], [4]. The Cl atoms incident on the wafer are largely thermalized while the Cl^+ ions are accelerated to an energy similar to that of the sheath potential (~13 V). Angular distributions display the directionality of the Cl^+ as compared to that of Cl. It is interesting to note the change in energy and angular distributions for both the neutrals and the ions at the edge of the wafer. The edge of the wafer is exposed to an excess concentration of Cl, leading to increased charge exchange reactions, consequently the energy of the neutrals increased and the energy of the ions decreased. These distributions can provide a detailed boundary condition for a profile simulation code.

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