Direct Simulation Monte Carlo (DSMC) of Rarefied Gas Flow During Etching of Large Diameter (300-mm) Wafers

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Abstract— **Strong density gradients of a gas species can be sustained even at very low pressures when the reaction probability of that species is high. Under these conditions, inlet gas arrangements are very important to reaction uniformity.**

AS microelectronic devices are scaled down to enhance functionality and speed, wafer size increases to accommodate the larger dice and improve throughput. For example, the wafer diameter is projected to increase from the current 200 to 300 mm by the year 2001 [1]. Uniform deposition and etching of thin films over these large diameter wafers is of major concern to the microelectronics industry. Also, flat panel display and solar conversion technologies require uniform processing over large area substrates. Computer simulation can provide valuable insight concerning the physicochemical processes occurring in the reactor and can be used as a guide to new reactor designs that deliver uniform etching or deposition.

As the reactor operating pressure is lowered, collisions of gas species with the reactor walls become increasingly dominant. Direct Simulation Monte Carlo (DSMC) is ideally suited for such problems of rarefied gas dynamics. A brief introduction to DSMC is given in [2]; details can be found in [3]. In this paper, we report results of a two-dimensional (2-D) DSMC simulation of etching a large diameter wafer.

An outline of the reactor under consideration is shown in Fig. 1 (top). The axisymmetric reactor has a diameter of 0.4 m and a height of 0.05 m. The wafer (0.3-m diameter) sits flush with the bottom wall of the reactor with the wafer axis being identical to the reactor axis. A mixture of 70% Cl_2 and 30% Ar by volume is fed through three concentric rings at radial locations of 0.01, 0.07, and 0.13 m. The total gas flow rate is 70 sccm, and it is distributed proportionately to the ring radius. This inlet arrangement is a 2-D model of more complicated designs normally used in practice which consist of individual gas jets. The reactor is pumped symmetrically around the outer periphery; the pump region is not shown in Fig. 1 (top).

One of the goals of this study was to examine the effect of reactor geometry and inlet feed design on the etching uniformity across the 300-mm wafer. To obtain the worst case scenario, molecular chlorine was assumed to etch the aluminum covered wafer with a surface reaction probability of 100%, i.e., the etch rate is completely governed by the rate of transport of etchant to the wafer surface. Thus the overall reaction was represented by $Al + 3/2\ Cl_2 \rightarrow AlCl_3$. No gas phase reactions or plasma effects were considered.

The reactor was divided into 4625 cells with the cells clustered around the gas inlet jets and near the wafer surface. Five-hundred thousand computational particles were followed for 250 000 time steps, each of 10^{-6}-s duration. Each simulation lasted ~12 h on a 1024-node nCUBE-2 massively parallel supercomputer. The gas entered under choked flow conditions. The reactor walls were at a temperature of 300 K, except for the wafer which was maintained at 350 K. All images were generated using the commercial software package Tecplot®.

Fig. 1 (top) shows the pressure distribution in the reactor. The nominal pressure is 0.133 Pa (1 mtorr); the pressure in the inlet jets is of course much higher. Even when the jet inlet region is excluded, however, significant pressure gradients are still observed across the reactor. These gradients became worse as the flow rate was increased. A local maximum in pressure is observed on the wafer, directly under the jets.

The density distribution of molecular chlorine is shown in Fig. 1 (middle). Strong density gradients are sustained over distances much smaller than the mfp. This is because the chlorine density has to drop from the feed value to almost zero near the wafer surface where chlorine reacts with 100% probability. Under the present conditions, the gas mfp is ~5 cm (excluding regions in the immediate vicinity of the inlet ports), comparable to the reactor height. Thus, chlorine molecules do not suffer enough collisions to equilibrate with the gas. In fact, many of the entering chlorine molecules may strike the wafer (and react there) before they have a chance to suffer any collision. The jet action of the feed is seen to penetrate considerably into the reactor under these low pressure conditions. A small fraction of chlorine escapes with the exhaust gas. Fig. 1 (bottom) shows the density distribution of the reaction product, aluminum trichloride. Of course, the product density is highest near the wafer and lowest near the inlet jets. Significant nonuniformity of the product distribution is observed despite the very low pressure. The etch rate distribution (not shown) exhibited local maxima near the radial locations corresponding to the inlet jets. As the flow rate was increased, the etch rate maxima became stronger. When the gas was distributed uniformly across a 15-cm diameter "porous wall" inlet (essentially no jet action), etching was more uniform.

Density differences across the reactor of up to 50% were observed for argon, despite the fact that argon is chemically "inert." This is because of the pressure drop in the system and because the flow of argon is coupled to that of the reactive species. This result brings about a word of caution: One should be careful when using argon as an actinometer gas to monitor the spatially resolved density of a radical. The commonly used assumption that argon density is uniform may not be valid.

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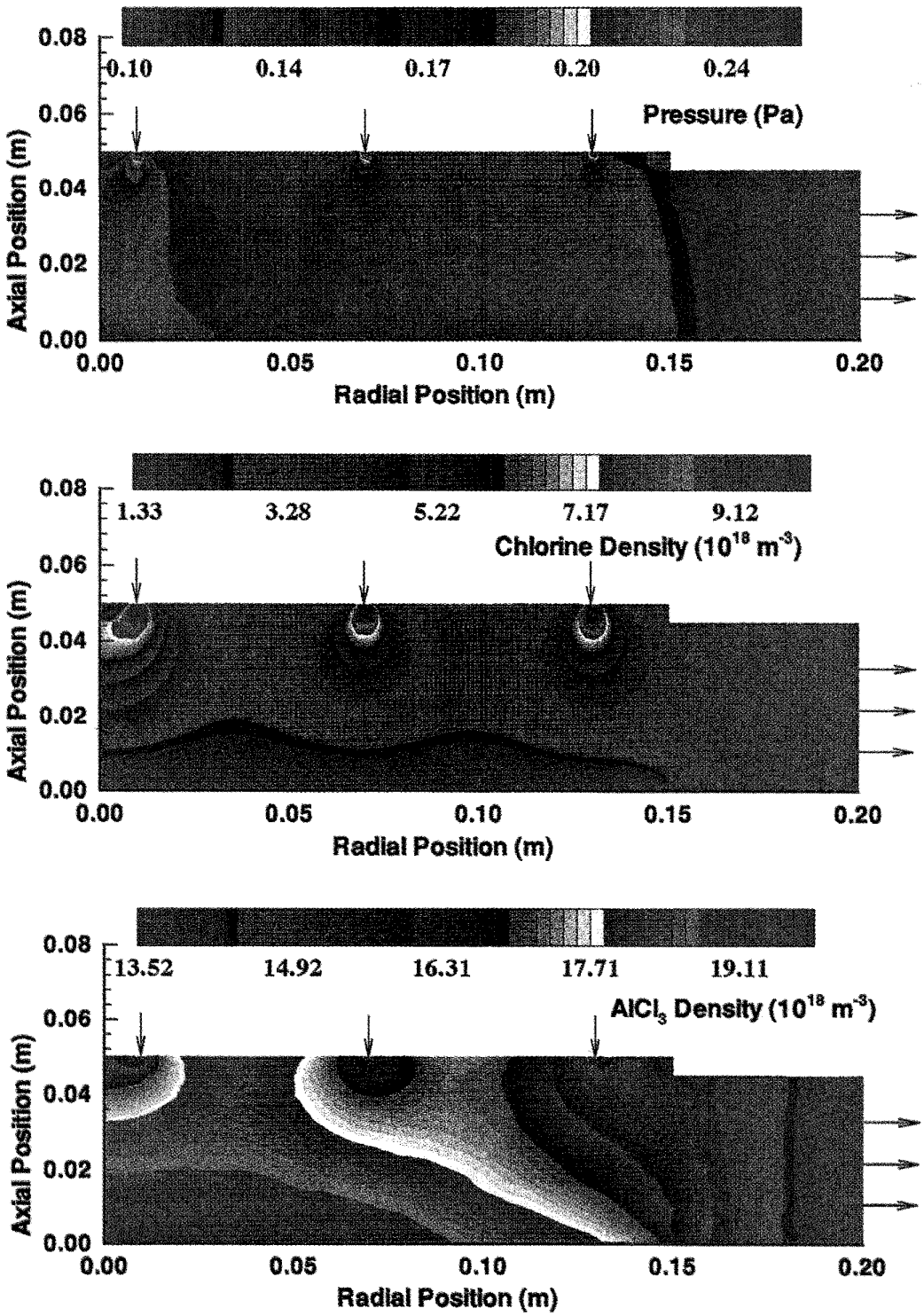

Fig. 1. Top: pressure distribution. Middle: molecular chlorine etchant density distribution. Bottom: aluminum trichloride product density distribution.

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