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Equipment Simulation for Studying the Growth Rate and its Uniformity of Oxide Layers Deposited by Plasma-Enhanced Oxidation

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***Abstract*—We present for the first time an equipment simulation study for a reactor for plasma-enhanced oxidation powered by 10 individually tunable microwave sticks. The simulated dependence of the oxidation rate on the distance between the sticks and the wafer and the simulated across wafer-uniformity well agree with measured data. The presented methodology allows one to study and optimize the process with respect to uniformity and growth rate for instance by adjusting the individual powers of the sticks or the geometrical configuration.**

Keywords—Plasma oxidation; plasma reactor modeling; microwave plasma; oxidation rate uniformity

I. INTRODUCTION

Plasma oxidation allows the growth of silicon oxide layers with a thickness of up to 10 nm at temperatures below 400 °C. It is a rather new process in semiconductor technology. In Fig. 1, a schematic view of the process chamber is shown. The system consists of a specially designed low pressure microwave discharge unit above the substrate in a vacuum-sealed aluminum reactor. The microwave discharge unit (2.45 GHz) consists of an array of antennas which overlay the wafer and the silicon edge guard ring. The microwave power of each antenna is individually controllable in the range between 250 and 1500 W. Each microwave coaxial antenna is encapsulated by a quartz tube and consists of an inner and a partly opened outer coax electrode. The quartz tube is filled with air at atmospheric pressure to suppress plasma between the electrodes and for cooling. At the end of the inner electrode a linear oscillator is working as an ignition unit for the plasma. The microwave coming from the generator is guided between the inner and outer coax electrodes to the ignition oscillator. The propagation of the plasma starts from the ignition oscillator to the specially designed opening of the outer electrode that provides very homogenous plasma in a large process window independent of the working pressure of the process gases.

The wafer support is designed for rotation during the process and the distance between wafer and discharge unit can

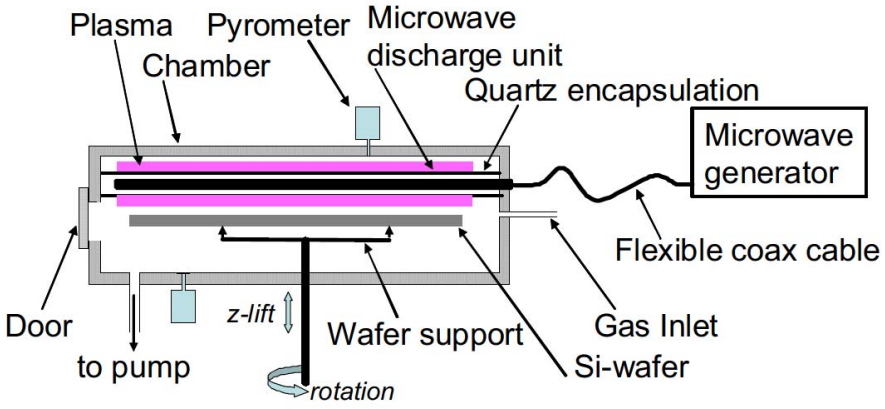

Fig. 1: Schematic process chamber cross section of the plasma oxidation reactor studied in this work.

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be varied by a z-lift. The rotation of the wafer results in a rotationally symmetric power density visible to the wafer.

Simulation provides a means to study the impact of different parameters on the oxidation rate and on the across-wafer uniformity. In this work, we focus on the geometric aspects of the system, that is, the dependence of the oxidation rate on the distance between the wafer and the substrate and on the across-wafer uniformity of the oxidation rate.

II. Simulation Approach

The plasma-enhanced system described above cannot be simulated based on capacitive or inductive power coupling as it is used in conventional plasma reactors. Also approaches for modeling guided microwave power delivery [2] cannot be applied to this system.

It would be computationally very expensive and numerically difficult, if possible at all, to model the plasma formation in the microwave sticks individually by resolving their real geometry in detail. Therefore we use an approach where the power generation is lumped into power-delivering objects (corresponding to the microwave sticks) with homogeneous power density.

The plasma simulator we employ is Q-VT [3] which assumes rotationally symmetric simulation systems. Therefore, in a preprocessing step, the power delivered by the linear plasma sticks of the real system is transferred to the rotationally symmetric distribution as seen from the wafer due to its rotation. For this, we assume that the power density does not vary along the microwave sticks. As result, separate radial areas with different powers are obtained which can be fed into Q-VT [3] as power values for 10 virtual electrodes operated at 2.45 GHz (Fig. 2). It should be noted that these virtual electrodes actually represent 3D toroids (with rectangular cross sections), as the cross sectional view shown in Fig. 2 needs to be rotated to obtain the 3D system represented by the cross sectional view.

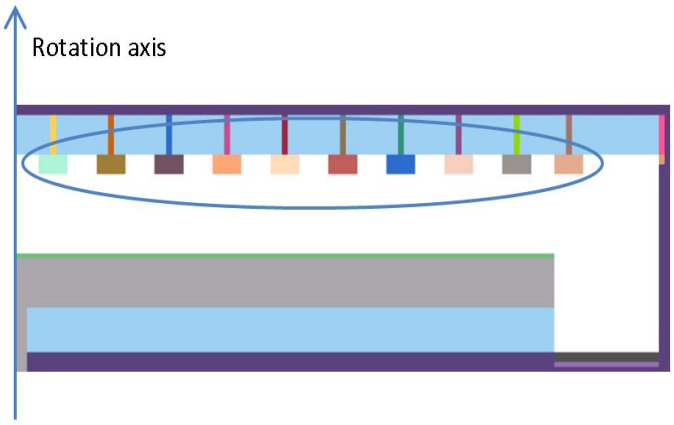

Fig. 2: Simulation setup. The blue ellipse marks the 10 virtual microwave sticks (which are actually toroids) used for the rotationally symmetric simulation model with the rotation axis as denoted. The wafer is represented by the green line on top of the grey region.

The power attributed to the 10 virtual electrodes depends on the individual power values of the real electrodes. Therefore, tuning of the power values of the microwave sticks can be mapped onto the distribution of the powers for the 10 virtual electrodes. As an example, in Table I the powers used for the 10 virtual electrodes for the simulation setup in Fig. 2 are listed. These powers have been calculated for 10 microwave sticks all having the same power. This boundary condition for the microwave sticks has been assumed for all simulations shown in this paper.

Due to the high frequency, the full wave solver of Q-VT has to be employed for the electrical part of the plasma simulation. Various reactions for the interaction of oxygen ions and radicals and electrons are used and the electron kinetics is modeled with the Monte Carlo module [3].

TABLE I
POWERS FOR THE VIRTUAL ELECTRODES FOR THE SIMULATION SETUP SHOWN IN FIG. 2.

Number of virtual electrode (from 1 for the very left and 10 for the very right electrode in the setup in Fig. 2)	**Power assigned to the electrode in the simulation (W)**
1	187
2	467
3	749
4	1032
5	1314
6	1598
7	1729
8	1463
9	998
10	411

III. Results

As an example, Fig. 3 shows the simulated spatial distribution of the O^+ ions for a setup with 10 equally powered microwave sticks for an oxygen plasma at a pressure of 500 mTorr.

In order to investigate the uniformity of the silicon oxide layers, the radial distribution of the rate limiting species is of interest. It has been proposed [4] that the electron concentration determines the oxidation rate. In our simulations we observed that the electron concentration well correlates with the O^+ ion concentration. However, the latter exhibits less noise compared to the electron concentration. Therefore, we used the

concentration of the O^+ ions to study the variations of the oxidation rate for different geometries and across the wafer.

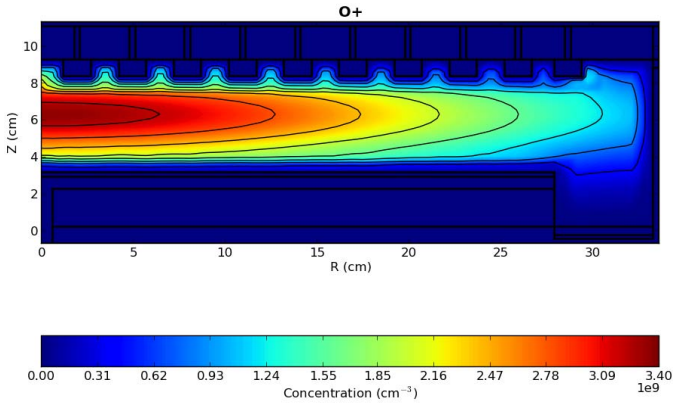

Fig. 3: Simulated spatial distribution of the O+ ion concentration in the reactor. The reactor is assumed to be rotationally symmetric, the rotation axis is at R=0.

In Fig. 4, we compare the simulated average O^+ concentration (relative values) on the wafer to measured oxidation rates (average over the wafer) for different distances between sticks and wafer. The simulation well reproduces the dependence seen in the experiment. It should be noted, that no free parameters have been adjusted in the simulations.

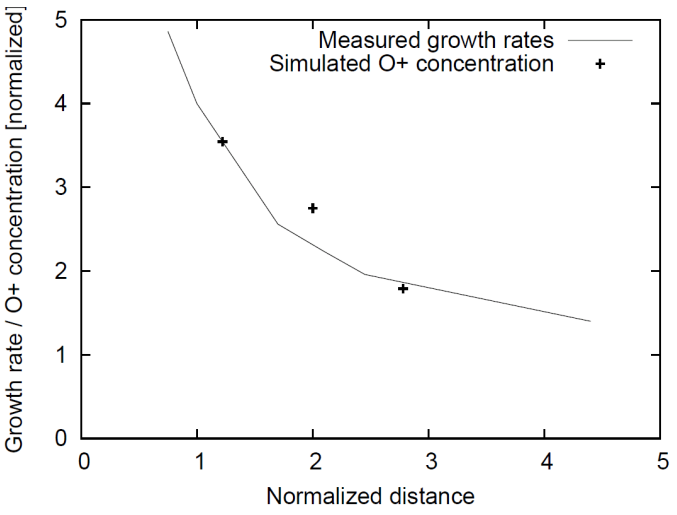

Fig. 4: Comparison between measured data (growth rate) and simulation results (O^+ concentration) with respect to the dependence on the distance between sticks and wafer. The simulation shown in Fig. 3 is the one for the normalized distance of 2.78.

Fig. 5 shows a comparison of the simulated across-wafer profiles of the concentration of the O^+ ions and the measured growth rate (relative values). We carried out the comparison for the three distances between the wafer and the substrate shown in Fig. 4 for the simulated data. In Fig. 5 (a), (b), and (c) we show the comparisons for normalized distances of 2.78, 2.0, and 1.22, respectively.

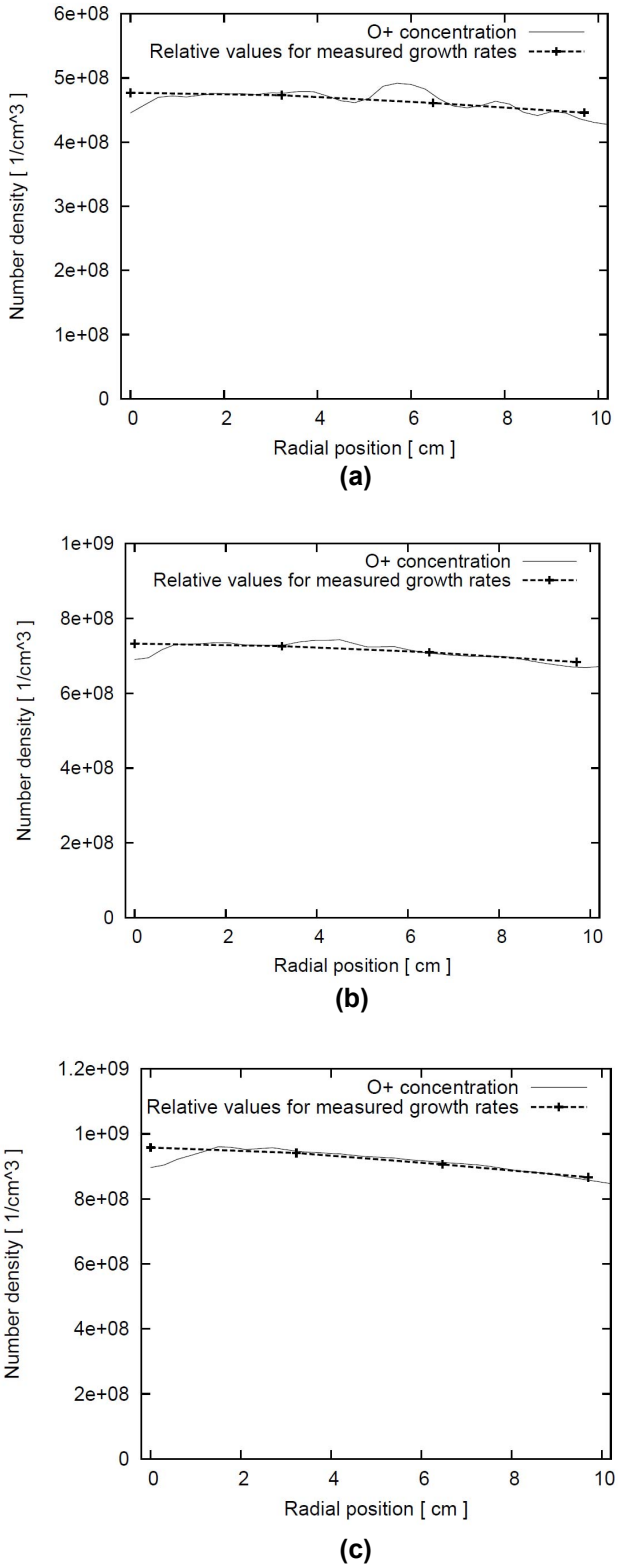

Fig. 5: Across-wafer profile of the O^+ concentration for the simulations shown in Fig. 4 compared to relative values r_{rel} (see text) of the measured growth rate. (a), (b), and (c) correspond to normalized distances of 2.78, 2.0, and 1.22, respectively. Please note that the growth rate values have been evaluated only at the radial positions denoted by the symbols thus not resolving finer radial patterns.

To allow a direct comparison of the growth rates to the O^+ concentrations, we introduce the "relative growth rate" r_{rel} as

$$r_{rel} = r / r_{av} \cdot c_{av} \quad (1)$$

where r is the growth rate, r_{av} is the growth rate averaged over the wafer, and c_{av} is the O^+ concentration averaged over the wafer.

Good agreement between the simulated variations of the O^+ flux and the measured variations of the oxidation rate is observed. The non-uniformity increases with decreasing normalized distance. The relative non-uniformity (here defined as *total-range* variation) is 6.5 %, 7 %, and 10 % for relative distances of 2.78, 2.0, and 1.22, respectively. The simulations well predict the trend seen in the experiment. The decrease of the simulated O^+ concentration towards the radial position of 0 cm is supposed to be at least partially artificial; a refined analysis is currently ongoing.

IV. Conclusions

We have introduced and demonstrated a concept which allows one to model a reactor for plasma-enhanced oxidation based on a microwave plasma generated by individually tunable sticks. To this end, we have implemented a methodology which allows us to map the power of the plasma generating sticks onto simulation objects which are part of a setup for the plasma simulation tool Q-VT.

We validated the simulation by comparing measured growth rates to the concentration of the O^+ ions and their variations. We observed that the simulated dependence of the oxidation rate on the distance between the sticks and the wafer and the simulated across wafer-uniformity well agree with measured data.

Using the presented simulation flow, it is possible to adjust the powers of the sticks or the geometry in order to study and optimize the layer thickness uniformity.

Acknowledgment

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