Metallic contamination in hydrogen plasma immersion ion implantation of silicon

Paul K. Chu, a) Ricky K. Y. Fu, Xuchu Zeng, and Dixon T. K. Kwok
Department of Physics & Materials Science, City University of Hong Kong, 83 Tat Chee Avenue, Kowloon, Hong Kong

(Received 27 March 2001; accepted for publication 23 July 2001)

In plasma immersion ion implantation (PIII), ions bombard all surfaces inside the PIII vacuum chamber, especially the negatively pulsed biased sample stage and to a lesser extent the interior of the vacuum chamber. As a result, contaminants sputtered from these exposed surfaces can be reinjected into or adsorb on the silicon wafer. Using particle-in-cell theoretical simulation, we determine the relative ion doses incident on the top, side, and bottom surfaces of three typical sample chuck configurations: (i) a bare conducting stage with the entire sample platen and high-voltage feedthrough/supporting rod exposed and under a high voltage, (ii) a stage with only the sample platen exposed to the plasma but the high-voltage feedthrough protected by an insulating quartz shroud, and (iii) a bare stage with a silicon extension or guard ring to reduce the number of ions bombarding the side and bottom of the sample platen. Our simulation results reveal that the ratio of the incident dose impacting the top of the sample platen to that impacting the side and bottom of the sample stage can be improved to 49% using a guard ring. To corroborate our theoretical results, we experimentally determine the amounts of metallic contaminants on 100 mm silicon wafers implanted using a bare chuck and with a 150 mm silicon wafer inserted between the 100 mm wafer and sample stage to imitate the guard ring. We also discuss the effectiveness of a replaceable all-silicon liner inside the vacuum chamber to address the second source of contamination, that from the interior wall of the vacuum chamber. Our results indicate a significant improvement when an all-silicon liner and silicon guard ring are used simultaneously. © 2001 American Institute of Physics. [DOI: 10.1063/1.1404422]

I. INTRODUCTION

Silicon-on-insulator (SOI) introduces many advantages over bulk silicon substrates such as the elimination or mitigation of latch up, alpha-particle soft errors, short-channel effects, source/drain punch through, and hot carriers.1,2 There are several methods to produce SOI substrates and hydrogen plasma immersion ion implantation (PIII) coupled with wafer bonding and ion cut3–5 has been demonstrated to be an effective and economical means. The biggest advantage of PIII compared to conventional beam-line ion implantation is its high throughput as the implantation time does not depend on the wafer dimensions and also because of the high ion flux ($>10^{15}$ cm$^{-2}$ s$^{-1}$).6–9 The absence of an ion filtering mechanism reduces the cost and footprint of a PIII instrument, but all ion species, including contaminants that are sputtered or etched from exposed surfaces including the inner wall of the vacuum chamber and sample stage, are co-implanted into the silicon wafers. Although the sputtering yield of hydrogen is relatively small, the dose required in the ion-cut process is quite high (between $5 \times 10^{16}$ and $1 \times 10^{17}$ cm$^{-2}$). In addition, there exist heavier ionized atmospheric contaminants such as C, N, and O in the plasma because PIII equipment is typically not designed for ultrahigh vacuum operation.10 These atmospheric ions including oxygen, nitrogen, carbon, and water can cause significant sputtering of the exposed surfaces. The interior wall of the vacuum chamber is another source of contamination but can be shielded by a liner made of silicon.11 On the other hand, it is difficult to cover the sample stage entirely with a silicon-compatible material on account of the stringent requirements for high electrical conductance, high voltage operation, in situ monitoring devices, as well as a sample cooling mechanism.9 A sample chuck made of a more conventional material such as stainless steel is easier to machine12,13 but introduces metallic impurities into the plasma. These contaminants may decrease the SOI yields and also introduce detrimental effects such as leakage current in devices fabricated in the materials.

In this study, we theoretically and experimentally investigate the contamination issues in hydrogen PIII. Using particle-in-cell (PIC) modeling, we simulate the relative ion doses impacting the top and other surfaces of the sample chuck assembly. The ions impacting the top of the sample chuck are the “good” ones because they go directly into the silicon wafer provided the wafer covers the entire sample platen, but those impinging into the other areas of the sample chuck can lead to sputtered particles. If the sample chuck or stage is made of stainless steel, transition metals can be released which can be reintroduced into the silicon wafer as contaminants. The number of particles sputtered from each region is proportional to the relative ion dose, and so it is important to understand the relationship between the relative

---

a)Author to whom correspondence should be addressed; electronic mail: paul.chu@cityu.edu.hk
ion doses impacting the top, side, and bottom of the sample stage and the processing parameters. We theoretically investigate three practical sample stage configurations: (i) a bare conducting sample chuck with an exposed high-voltage feedthrough, (ii) a conducting sample chuck with the high-voltage feedthrough/supporting rod shielded by a quartz (insulating) shroud, and (iii) a bare conducting sample chuck with a silicon guard ring to reduce the number of ions impacting the side and bottom of the sample chuck. We derive the evolution of the ion dose ratio for different accelerating voltages as well as pulse durations. To verify the theoretical results, hydrogen PIII experiments are conducted under configurations (i) and (iii). Total-reflection x-ray fluorescence (TXRF) and secondary ion mass spectrometry (SIMS) are employed to determine the amount of metallic contaminants on the implanted silicon wafers. We also discuss the role of a replaceable all-silicon liner inside the vacuum chamber with respect to contamination control.

II. THEORETICAL SIMULATION

The potential, ion density distribution, and incident ion doses at various locations of the sample platen are theoretically investigated. Three sample chuck configurations are considered here (Fig. 1): (a) wafer chuck with all areas exposed to the plasma; (b) wafer chuck with the high-voltage feedthrough/supporting rod shielded by a quartz tube; and (c) 100 mm wafer holder covered by a 150 mm silicon wafer on which another 100 mm silicon wafer is placed to imitate the situation with a 25 mm guard-ring extension.

Owing to the complexity of the plasma, two assumptions are made in our PIC modeling. First, the ions are assumed to be noncollisional and cold. Second, they acquire directed motion only by the electric field. The electrons are assumed to be in thermal equilibrium, and so the electron density \( n_e \) is given by Boltzmann’s relationship

\[
 n_e = n_0 \exp \left( \frac{e \phi}{kT_e} \right),
\]

where \( n_0 \) is the initial ion density, \( k \) is the Boltzmann constant, and \( T_e \) is the electron temperature. The simulation region displayed in Fig. 1 is evenly divided into finite grids of the same area. Initially, particles are evenly distributed among them except in the region adjacent to the wafer holder and supporting rod. The initial values of the potential, density, radial velocity, longitudinal velocity, position, and electric field are first entered into each grid. The pulse duration is divided into a series of time steps, and in each time step, Poisson’s equation is solved to determine the particle motion and redistributed ion density. Poisson’s equation relates the potential \( \phi \) to the electron density \( n_e \) and ion density \( n_i \) as follows:

\[
 \nabla^2 \phi = -\frac{e}{\varepsilon_0} (n_i - n_e),
\]

where \( \varepsilon_0 \) is the permittivity in free space and \( e \) is the electron charge. The ion motion is governed by Newton’s equations of motion

\[
 F = Ma, \tag{3}
\]

\[
 \mathbf{V}(f) = \mathbf{V}(I) + at, \tag{4}
\]

\[
 \Delta \mathbf{d} = \mathbf{V}(I) + \frac{1}{2}at^2, \tag{5}
\]

where \( F \) is the force applied on the particle and given by

\[
 F = -q \nabla \phi, \tag{6}
\]

where \( q \) is the charge of the particle, \( M \) is the mass of the particle, \( a \) is the acceleration, \( \mathbf{V}(f) \) and \( \mathbf{V}(I) \) are the final and initial velocity, and \( \Delta \mathbf{d} \) is the distance traversed by the particle in time \( t \).

Due to the cylindrical symmetry of the three configurations, these equations can be rewritten in cylindrical coordinates

\[
 \frac{\partial^2 \phi}{\partial r^2} + \frac{1}{r} \frac{\partial \phi}{\partial r} + \frac{\partial^2 \phi}{\partial z^2} = -\frac{e}{\varepsilon_0} \left( n_i - n_0 \exp \left( \frac{e \phi}{kT_e} \right) \right), \tag{7}
\]

\[
 \mathbf{V}_r(f) = \mathbf{V}_r(I) - \frac{q}{M} \frac{\partial \phi}{\partial r} t, \tag{8a}
\]

\[
 \mathbf{V}_z(f) = \mathbf{V}_z(I) - \frac{q}{M} \frac{\partial \phi}{\partial z} t, \tag{8b}
\]

\[
 \Delta r = \mathbf{V}_r(I) t - \frac{1}{2} \frac{q}{M} \frac{\partial \phi}{\partial r} r^2, \tag{9a}
\]

\[
 \Delta z = \mathbf{V}_z(I) t - \frac{1}{2} \frac{q}{M} \frac{\partial \phi}{\partial z} r^2. \tag{9b}
\]

FIG. 1. Schematic diagram of the three PIII configurations, the right half being the simulation region: (a) Plain wafer holder. (b) Supporting rod/high-voltage feedthrough shielded by a grounded quartz tube. (c) A 100 mm wafer holder covered by a 150 mm silicon wafer to imitate a silicon guard ring.
To approximate the potential, we use the centered difference approach,\(^{19}\) and
\[
\frac{\partial^2 \phi}{\partial r^2} \approx \frac{\phi_{i+1,j} - 2 \phi_{i,j} + \phi_{i-1,j}}{(dr)^2},
\]
\[
\frac{\partial^2 \phi}{\partial z^2} \approx \frac{\phi_{i,j+1} - 2 \phi_{i,j} + \phi_{i,j-1}}{(dz)^2},
\]
\[
\frac{\partial \phi}{\partial r} = \frac{\phi_{i+1,j} - \phi_{i-1,j}}{2dr}, \quad \frac{\partial \phi}{\partial z} = \frac{\phi_{i,j+1} - \phi_{i,j-1}}{2dz}. \quad (10)
\]
The potential along the surface to the chuck is represented in the centered difference relationship, Eq. \(\sim\).

The potential \(\phi\) at the feedthrough is exposed but the wafer holder is covered. The ions will impact the quartz shroud. In the third configuration, the supporting rod are totally exposed to the plasma. In the second configuration, the dimensions of our semiconductor PIII machine.\(^{20}\) The simulation parameters are: grid spacing \(h = \text{wafer radius}/10\) and time step \(\Delta t = (h/10) \times (1/\omega_{pe})\) where \(\omega_{pe}\) is ion plasma frequency. Initially, 100 particles are uniformly placed in each cell. In the first configuration, the whole wafer stage and supporting rod are totally exposed to the plasma. In the second configuration, the supporting rod is totally shielded by a quartz tube which is assumed to have a negligible thickness and has a zero surface potential at all times. In this case, no ions will impact the quartz shroud. In the third configuration, the feedthrough is exposed but the wafer holder is covered by a 150-mm-diam conducting wafer with a negligible thickness.

III. EXPERIMENT

Silicon wafers 100 mm in diameter were implanted at below 150°C using our semiconductor PIII instrument.\(^{20}\) The hydrogen dose was approximately \(5 \times 10^{16} \text{ atoms/cm}^2\) as calculated from the SIMS results. The implantation conditions were: 0.4 mTorr hydrogen pressure, 20 kV pulse bias, 30 \(\mu\)s pulse duration, and 100 Hz pulsing frequency.

To assess the effectiveness of a liner shielding the interior of the vacuum chamber, one wafer was implanted with an Al liner in place. The second wafer was implanted using
our replaceable silicon liner. The silicon liner consists of a stainless steel cage that fits inside the vacuum chamber. Silicon wafers were cut to different sizes to line the interior of the cage and held on by quartz pins, similar to putting tiles on the wall. Individual silicon wafers can be replaced if damaged or contaminated. The third wafer was implanted with a 150 mm silicon wafer inserted between the sample chuck and itself to imitate a silicon guard ring. The sample description is summarized in Table I. The silicon liner is expected to reduce Al contamination while the guard ring should block stainless steel contamination sputtered from the side and bottom of the sample chuck in the third configuration. However, it should be noted that since our aluminum liner has been used extensively before these experiments, it contains metallic contaminants from prior experiments, and our results should be evaluated with this in mind.

TXRF analysis was performed to measure the amount of surface metals on the implanted wafers. TXRF uses a glancing x-ray beam to excite fluorescence of elements in the top 5–10 nm. The energy-dispersive detector of TXRF detects elements heavier than sulfur in a 1 cm² area. Two spots were analyzed on each sample: center and 1 cm from the edge. To measure the light elements such as B and Al, secondary ion mass spectrometry (SIMS) was utilized. In addition, since some of the sputtered contaminants may be reimplanted into the silicon wafer to some depth, TXRF does not convey the full story and SIMS is used to measure Fe deeper than 5 nm. Oxygen ion bombardment was employed to determine the B, Al, and Fe depth profiles, whereas cesium ion bombardment SIMS was utilized to disclose the H, C, O, and N in-depth distributions and doses in the samples. The latter information

<table>
<thead>
<tr>
<th>Sample</th>
<th>PIII conditions</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Al liner</td>
</tr>
<tr>
<td>2</td>
<td>Si liner</td>
</tr>
<tr>
<td>3</td>
<td>Si liner and 150 mm Si guard ring</td>
</tr>
</tbody>
</table>

FIG. 2. Normalized temporal potential contour lines showing the change in the applied electric field about the sample stage at −20 kV biased voltage for a pulse duration of 4 µs: (a) 100 mm bare stage, (b) 150 mm bare stage, (c) 100 mm shielded stage, (d) 150 mm shielded stage, and (e) 100 mm stage with 150 mm guard ring (25 mm radial extension).
is important because, even though these atmospheric ions only constitute a few percent of the total ion current (primarily hydrogen), their sputtering yield is much higher and they contribute significantly to sputtered metallic contaminants.

IV. RESULTS AND DISCUSSION

PIC simulation is conducted in a cylindrical symmetry and only half of the chamber needs to be included in the process. We simulate cases in which \( -20 \) or \( -40 \) kV with a pulse duration of 30 \( \mu s \) is applied to the sample stage. Figure 2 illustrates the temporal evolution of the potential contour lines for the three configurations shown in Fig. 1 at a bias voltage of \( -20 \) kV. At the initial state (rise time) of the pulse, the contour of the sheath is quite similar to the shape of the stage. As time elapses, the sheath expands at different speeds in different regions and gradually loses its conformal shape, finally evolving into a sphere-like or disk-like shape and reaching the chamber wall. As shown in Figs. 2(a) and 2(b) (bare sample stage), the edge of the electron sheath has already hit the chamber wall. When the ions cross the sheath, the strong electric field between the stage and the chamber wall pushes them towards the stage. Under the influence of the quartz tube and the covering wafer, the expansion of the potential contour lines is more restricted as illustrated in Figs. 2(c)–2(e). As the supporting rod is totally shielded and has a zero potential, no ions will be accelerated towards and impinge into it. With a 150 mm silicon wafer covering the 100 mm sample stage, the incident ions from the top of the chuck will not impact the edge of the chuck because they are blocked by the extension or guard ring.

The temporal evolution of the ion density is exhibited in Fig. 3. When the implantation duration is long, a zero ion density contour line is observed. The ions begin to exhaust from the supporting rod and gradually extend in both cases (i) and (ii) whereas in case (iii), the ions exhaust from the corner between the chuck and the supporting rod. Consequently, more and more ions will be exhausted in the lower part of the chamber and lesser ions will impact the edge and
bottom of chuck as well as the supporting rod as the ions will not be refilled during the duration of the pulse. Hence, the top of the sample stage receives a higher relative dose.

The plots of the incident dose ratio—number of ions impacting the top surface of the sample platen to that impacting the side and bottom of the sample stage (including the high-voltage feedthrough in the case of the bare chuck—versus the implantation time during each voltage pulse are exhibited in Fig. 4. A higher incident dose ratio is observed on the top surface at ~40 kV. It is because the expansion speed of the ion sheath is faster at a higher voltage due to the following relationship:

\[
\frac{ds}{dt} = \frac{4}{9} \frac{\varepsilon_0}{n_i} \sqrt{\frac{2 V_a}{q m s^2}},
\]

where \(\varepsilon_0\) is the permittivity of free space, \(n_i\) is the ion density, \(q\) is electron charge, \(m\) is the mass of the ion, \(V_a\) is the potential applied to the stage, and \(s\) is the location of the sheath edge relative to the stage. As the ion sheath area relative to the exposed area of the top surface of the chuck changes as the ion sheath gradually expands, more ions are collected at the top surface to the chuck. It is also the main reason for the increase in the incident dose ratio as time elapses in all three cases. Initially, the exposed area ratios are 14.66% and 19.17% for the 100 and 150 mm bare sample chuck, respectively, whereas they are 34.65% and 38.60% for the shielded chuck. This is because no ions impact the supporting rod/high-voltage feedthrough in the latter case. For the sample chuck with a guard ring, the exposed area ratio is 19.17%. During an individual pulse, the incident dose ratio at the top surface of the bare chuck is about 25%–40% depending on the implantation time. These ratios reach about 35%–41% and 40%–49% for the shielded stage and the stage with the guard ring, respectively. The dose ratio is higher in case (iii) than in case (i). The extension or guard ring in configuration (iii) blocks ions from impacting the edge of the chuck, and so a higher effective dose on the silicon wafer surface results. Consequently, the guard ring reduces the amount of contaminants sputtered from the edge and bottom of the stage. Though not simulated, it is reasonable to assume that the guard ring also blocks such sputtered contaminants from reaching the top of the sample stage. It should be noted that even though the use of a quartz shroud such as the one described in configuration (ii) eliminates sputtering of the supporting rod as well as reduces the ion current and subsequently the load of the power modulator, it is sometimes not preferred in hydrogen PIII experiments. It has been shown that an insulating shroud perturbs the electric field and ion motion, thereby causing lateral variation in the ion implant dose across the wafer.\(^2\) Hence, in spite of some of the attractive features, configuration (ii) must be

---

**FIG. 4.** Ratio of incident dose impacting the top of chuck or wafer to that impacting the other parts of the stage under ~20 and ~40 kV biased treatment: (a) bare chuck, (b) chuck with shielded feedthrough, and (c) stage with guard ring.

**TABLE II.** TXRF results (in units of \(10^{10}\) atoms/cm\(^2\)).

<table>
<thead>
<tr>
<th></th>
<th>S</th>
<th>Cl</th>
<th>K</th>
<th>Ca</th>
<th>Ti</th>
<th>Cr</th>
<th>Mn</th>
<th>Fe</th>
<th>Ni</th>
<th>Cu</th>
<th>Zn</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sample 1</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Center</td>
<td>1500</td>
<td>4700</td>
<td>2700</td>
<td>3800</td>
<td>1100</td>
<td>200</td>
<td>80</td>
<td>1600</td>
<td>100</td>
<td>200</td>
<td>200</td>
</tr>
<tr>
<td>Edge</td>
<td>1200</td>
<td>3100</td>
<td>1200</td>
<td>7600</td>
<td>400</td>
<td>200</td>
<td>60</td>
<td>1700</td>
<td>50</td>
<td>100</td>
<td>300</td>
</tr>
<tr>
<td>Sample 2</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Center</td>
<td>1000</td>
<td>1300</td>
<td>&lt;20</td>
<td>50</td>
<td>&lt;5</td>
<td>&lt;3</td>
<td>10</td>
<td>200</td>
<td>2</td>
<td>1</td>
<td>40</td>
</tr>
<tr>
<td>Edge</td>
<td>1000</td>
<td>2000</td>
<td>40</td>
<td>200</td>
<td>&lt;5</td>
<td>70</td>
<td>20</td>
<td>500</td>
<td>40</td>
<td>&lt;1</td>
<td>50</td>
</tr>
<tr>
<td>Sample 3</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Center</td>
<td>400</td>
<td>300</td>
<td>&lt;20</td>
<td>200</td>
<td>&lt;5</td>
<td>&lt;3</td>
<td>2</td>
<td>40</td>
<td>1</td>
<td>&lt;1</td>
<td>7</td>
</tr>
<tr>
<td>Edge</td>
<td>900</td>
<td>300</td>
<td>&lt;20</td>
<td>200</td>
<td>&lt;5</td>
<td>&lt;3</td>
<td>&lt;1</td>
<td>20</td>
<td>1</td>
<td>&lt;1</td>
<td>6</td>
</tr>
</tbody>
</table>
used with caution. All in all, with regard to contamination control, configuration (iii) is the most practical and effective one if an all-silicon chuck cannot be made. Therefore, we have only conducted experiments to compare the differences between configurations (i) and (iii), and the results will be discussed in the next section.

Table II shows the TXRF results acquired from two spots on each of the wafers described in Table I: center and 1 cm from the edge. The TXRF data show that the dirtiest sample is 1 that was implanted using the Al liner without a guard ring. In comparison, the silicon wafer implanted using the silicon liner and silicon guard ring (sample 3) has the least amount of transition metals on the surface. Comparing samples 1 and 2, the silicon liner shows an appreciable effect, but as aforementioned, it should be noted that our Al liner has been contaminated by metals sputtered from the stainless steel stage in prior experiments.

To measure the light elements such as B and Al as well as implanted Fe, oxygen bombardment SIMS was used, and the results are exhibited in Table III. Since there is a SIMS artifact in the near surface region, integrated dose calculation is performed only from 5 nm from the surface for Fe or 10 nm from the surface for B and Al. That is to say, the SIMS results complement the TXRF results. The amounts of implanted hydrogen, carbon, nitrogen, and oxygen are determined by cesium ion bombardment SIMS (Table IV). There is a slight difference in the calculated hydrogen doses in sample 1 versus the other two samples. The combined C, O, and N doses in the three samples also display a similar trend, about a factor of 2 between sample 1 and samples 2 and 3. This may be due to the silicon liner changing the characteristics of the plasma. Even after normalizing the TXRF results by multiplying the metal concentrations observed on samples 2 and 3 by two, there is still a big difference between samples 1 and 3. The improvement in the surface metal concentration using the silicon liner and guard ring is very significant. It should also be mentioned that C, O, and N are implanted and not adsorbed, as demonstrated by their Gaussian-like shape in the SIMS profiles.

## V. CONCLUSION

Using theoretical simulation, we investigate the dose ratios impacting the top, side, and bottom surfaces of three sample chuck configurations. Knowing the relative incident dose on the top of the chuck provides an effective way to control and adjust the operating conditions to minimize sputtered contaminants from the side and bottom of the sample stage. Our model shows that the incident dose ratio at the top surface of the chuck can reach 49% if a guard ring is used. Experimentally, we observe significant improvement with regard to transition metal contamination using an all-silicon liner for the interior of the vacuum chamber and a silicon guard ring on the sample stage. These components are mechanically easy to implement in PIII and other plasma equipment. Our SIMS results also show that Fe, C, N, and O not only adsorb onto the silicon surface but also are implanted into the silicon wafers.

## ACKNOWLEDGMENTS

The work described in this article was jointly supported by grants from the Hong Kong Research Grants Council (CERG No. 9040412 or CityU No. 1003/99E and No. 9040498 or CityU No. 1032/00E) as well City University of Hong Kong (SRG No. 7001028).

## REFERENCES

11. US patent No. 6,120,660.