Monte Carlo simulation and experimental study of stopping power of lithography resist and its application in development of a CMOS/EE process

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Abstract

Implantation of P and B into a Novolac-based positive photoresist is simulated and experimentally studied. The implants are in range: 430-580keV for P, and 180-250keV for B. These implants may be used as isolation field-implants in high-voltage (HV) part of a submicron CMOS/EE process. The purpose of the study is to determine the minimum resist thickness needed to stop the implants, while allowing minimal resist opening line-CD for the isolation doping of HV circuit part. Accurate stopping-power data are not available for Novolac-based resists in the literature. The general literature data are rather scattered, and suggest too thick resist. Thick resist cannot be applied in our process due to a limited aspect ratio of the opening line.

In this study, we determine experimentally the dose fraction that penetrates through the resist into the Si-bulk. On the other side, numerical Monte-Carlo (MC) simulation of the implantation into this resist type is carried out. Critical parameters in the MC simulation are resist-layer specific density after the bake, and the compound (bond-core) correction. The resist density is measured precisely on the wafer. The compound correction is tuned by comparison between the MC simulation results and the measured penetrated dose fraction. The penetrated dose is measured on a short-loop with implantation into the stack resist/SiO₂/Si-wafer, by using surface-charge analyzer SCA 2500.

Minimum resist thickness for the required (but not larger) process margin is applied on a full-flow lot in a deep-submicron CMOS/EE process. A split with a fine variation in the resist thickness confirms very accurate calibration of the MC simulation.
Outline:

- Problem: determination of the minimum resist thickness for minimum CD line-opening in the resist. On the other hand, this resist should stop fully the high-energy P and B implants used as narrow isolation implants in high-voltage EE part.
  Minimum process complexity is required: solution with soft mask is preferred over the hard mask.

- Resist stopping capability is measured in experiment with a short-loop.

- Numerical Monte Carlo simulation of the implantation into the resist is carried out, with calibration (MC simulation of implantation into the resist compound with program SRIM; final resist density as input, compound correction as results)

- Results of the implemented conditions on the full-process flow are shown.

- Conclusion

Problem:

Minimum resist thickness is required for minimum opening line-CD in the resist, while high-energy implants should be stopped fully in the resist.
Minimum process complexity.

- High resist aspect ratio of the problem:
  0.35-0.40µm opening line-CD for isolation in HV part limits resist thickness to around 1.1µm.
  The use of an over-designed resist thickness (according to general tables and reference books) of 1.5-2.0µm is not possible in our process due to a small CD required.

- Thicker resist => larger line opening of the isolation implant in HV part
  => larger cell-to-cell distance in $E^2$ cell array => larger area size of memory block

- Need to stop relatively high E implants: P 430-580keV
  B 180-250keV.

- For this purpose, specially selected resists with increased stopping capability may be applied. However, the use of these resists only for the field implants in a particular process is excluded due to FAB operation logistic. In production, the intention is to use a limited number of resist tracks for various process steps in different technologies.

- No additional process steps for the mask, like hard masks, are allowed.

- Data are inconsistent and spread for the required resist thickness in the literature.

Goal: Determination of the minimum resist thickness that stops the implants fully.
Experimental determination of the resist stopping capability

The experiment is carried out on a short-loop flow, and verified on full-process lots.

Short-loop:
- wafer of the same type as the implant (N type of 6.0Ωcm for implantation of P and P type of 20Ωcm for implantation of B)
- oxidation of HV oxide of 15nm (1st HV oxide step in the real process)
- resist spin and bake, with the conditions like in the real process (splits on different resist thickness)
- implantation (split for different energy of P or B)
- standard resist removal, etc..
- implanted species activation: grow of the final HV oxide of 30nm (2nd HV oxide step) and LV Nwell drive, like in the real process
- forming-gas anneal (425°C, 10% hydrogen)

Measurement and data analysis:
1) Measurement of average doping concentration $N_b$ in the wafer close to the oxide/silicon interface by using surface charge analyzer SCA-2500
   (SCA-2500 utilizes optically induced CV; average $N_b$ in depleted region is measured at inversion onset from the depletion-region width).
2) Monte-Carlo simulation of the implantation into stack “resist/oxide/silicon”, with the thickness and energy like on the processed wafers.
3) Simulation of the doping profile in the bulk for the thermal drive condition like in the short-loop. The “as-implanted” profile from MC simulation is used as input.
   (Note that for small penetrated doses the implanted profile in the bulk is shallower than the depletion region width. Therefore, numerical simulation is necessary for the determination of the depletion-region width and the corresponding equivalent average doping concentration.)
4) MC simulation step 2) and calculation step 3) are repeated until the calculated average doping level in depletion region at inversion-onset corresponds to the value measured in step 1) by using SCA. The compound correction (bond and core approach) is the parameter changed in MC simulation.

The penetrated dose fraction and the corresponding compound correction are determined for each set of resist thickness and implantation energy by using procedure 1) – 4).

The results of calibrated MC simulation and the short-loop are confirmed on a full-flow of a CMOS/EE process.
**Experimental results**

Positive Novolac-based/DNQ resist: OiR38 (Arch Chemicals) is studied.

Using surface-charge analyzer **SCA-2500** we measured the following average doping concentration within the depletion layer width (in inversion) in silicon bulk on the short-loop wafers:

Pattern: 1 – centre, 2 – left, 3 – bottom (wafer flat), 4 – right, 5 – top

<table>
<thead>
<tr>
<th>Energy</th>
<th>resist thickness</th>
<th>wafer</th>
<th>doping concentration [cm(^{-3})] across pattern</th>
<th>Penetration into the bulk</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>p</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>580keV</td>
<td>1.10µm</td>
<td>wf.2</td>
<td>7.7e16 1.0e17 9.8e16 8.6e16 9.0e16</td>
<td>large</td>
</tr>
<tr>
<td></td>
<td>1.40µm</td>
<td>wf.7</td>
<td>6.0e14 5.1e14 5.0e14 5.1e14 5.3e14</td>
<td>no</td>
</tr>
<tr>
<td></td>
<td>1.40µm</td>
<td>wf.25</td>
<td>6.2e14 5.5e14 5.5e14 5.5e14 5.8e14</td>
<td>no</td>
</tr>
<tr>
<td></td>
<td>1.50µm</td>
<td>wf.3</td>
<td>6.4e14 5.6e14 5.7e14 5.6e14 5.8e14</td>
<td>no</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>p</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>520keV</td>
<td>1.00µm</td>
<td>wf.1</td>
<td>7.5e16 8.5e16 1.0e17 8.4e16 8.7e16</td>
<td>large</td>
</tr>
<tr>
<td></td>
<td>1.10µm</td>
<td>wf.9</td>
<td>9.4e14 1.0e15 9.1e14 9.3e14 1.0e15</td>
<td>medium, 0.7%</td>
</tr>
<tr>
<td></td>
<td>1.40µm</td>
<td>wf.14</td>
<td>5.2e14 5.6e14 5.7e14 5.7e14 5.7e14</td>
<td>no</td>
</tr>
<tr>
<td></td>
<td>1.40µm</td>
<td>wf.24</td>
<td>6.3e14 5.5e14 5.6e14 5.5e14 5.6e14</td>
<td>no</td>
</tr>
<tr>
<td></td>
<td>1.50µm</td>
<td>wf.10</td>
<td>6.2e14 5.7e14 5.5e14 5.6e14 5.7e14</td>
<td>no</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>p</strong></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>460keV</td>
<td>1.00µm</td>
<td>wf.17</td>
<td>7.5e14 7.2e14 7.5e14 7.8e14 8.2e14</td>
<td>small, 0.4%</td>
</tr>
<tr>
<td></td>
<td>1.10µm</td>
<td>wf.23</td>
<td>5.5e14 5.1e14 5.0e14 5.1e14 5.2e14</td>
<td>no</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>no</td>
<td></td>
<td>1.50µm</td>
<td>5.3e14 4.9e14 4.9e14 4.8e14 5.0e14</td>
<td>--</td>
</tr>
</tbody>
</table>

Phosphorus dose: 1.0x10\(^{13}\)cm\(^{-2}\)

The SCA-2500 is calibrated by using an undoped test wafer with carrier concentration determined by means of a calibrated four-probe spreading resistance system.
Determination of the penetrated dose fraction

Modelling applied:

1. Profiles of the implantation into the stack “resist/oxide (15nm)/Si-bulk” are simulated by using MC method (program SRIM).
2. Diffusion as in the short-loop (2\textsuperscript{nd} HV oxide step) is simulated, staring from implanted profile (1) as input.
3. Equivalent $V_{th}$, depletion region width in inversion $x_b$ and effective (uniform) bulk doping concentration $N_b$ are calculated on the basis of the final non-uniform bulk profile in (2). For this task MINIMOS 6 simulation is performed.
   Note that the bulk profile is non-uniform, but we have calculated an equivalent doping level on average that will follow as result of the SCA 2500 measurement procedure.
4. MC simulation in (1) is repeated until the calculated $N_b$ becomes equal to the results of the SCA 2500 measurements.

Procedure (1) – (4) has provided the following resulting table:

<table>
<thead>
<tr>
<th>$N_b$ measured by SCA 2500</th>
<th>9.8x10\textsuperscript{16} cm\textsuperscript{-2}</th>
<th>9.0x10\textsuperscript{16} cm\textsuperscript{-2}</th>
<th>9.5x10\textsuperscript{14} cm\textsuperscript{-2}</th>
<th>7.5x10\textsuperscript{14} cm\textsuperscript{-2}</th>
<th>5.0x10\textsuperscript{14} cm\textsuperscript{-2}</th>
</tr>
</thead>
<tbody>
<tr>
<td>$x_b$</td>
<td>108nm</td>
<td>113nm</td>
<td>1.1\mu m</td>
<td>1.24\mu m</td>
<td>1.52\mu m</td>
</tr>
<tr>
<td>equiv. $V_{th}$</td>
<td>-737.5mV</td>
<td>-704.2mV</td>
<td>+29.3mV</td>
<td>+40.7mV</td>
<td>+58mV</td>
</tr>
<tr>
<td>Implant condition</td>
<td>P 580keV into 1.10\mu m resist</td>
<td>P 520keV into 1.00\mu m resist</td>
<td>P 520keV into 1.10\mu m resist</td>
<td>P 460keV into 1.00\mu m resist</td>
<td>no implant</td>
</tr>
<tr>
<td>fitted penetrated dose</td>
<td>1.078x10\textsuperscript{12} cm\textsuperscript{-2}</td>
<td>1.025x10\textsuperscript{12} cm\textsuperscript{-2}</td>
<td>2.86x10\textsuperscript{10} cm\textsuperscript{-2}</td>
<td>1.70x10\textsuperscript{10} cm\textsuperscript{-2}</td>
<td>0.0</td>
</tr>
<tr>
<td>dose fraction of P 1.0x10\textsuperscript{13} cm\textsuperscript{-2}</td>
<td>10.78%</td>
<td>10.25%</td>
<td>0.29%</td>
<td>0.17%</td>
<td>0.0%</td>
</tr>
</tbody>
</table>

Numerical simulation with model tuning

Modelling study of the implantation includes the following steps:

1. Measurement of the final resist specific density after the bake (before implantation).
3. Tuning of the compound correction.

The following chemical constitution is assumed for OiR38 resist:

34 % of H
51 % of C
4 % of N
9 % of O
2 % of S.
This chemical composition equals to that of “Photoresist Siemens” in SRIM compound database, and according to OiR38 manufacturer (Arch Chemicals) it resembles also the actual composition of OiR38.

Please note that a Novolac-based photoresist consists of:
- Novolac resin base (chain of C₈H₅OH), with composition C 53.3%, H 40% and O 6.7%, and
- DQN as PAC, with structure C₁₀H₅N₂O₂SR, where R group is typically OH, OCl or SO₃Cl.

OiR38 consists of around 69% Novolac and 31% DQN.

According to our knowledge, no compound correction has been reported for this organic substance in SRIM and in the literature yet (correction coeff. = 1.0).

The resist density after the bake on the wafer is measured using microgram balance (the use of 25 wafers at the same time reduces error). The real deposited resist surface on the wafer is calculated taking into account the wafer flat (notch) and the ring excluded at the wafer edge. The results are:
- resist weight deposited per wafer after the bake 22.8mg
- resist surface 165.75cm², resist thickness 1.150µm
- It follows resist specific density of 1.20g/cm³

**Results of Monte Carlo simulation by using program SRIM**

A large set of simulations is performed with different implant energy, resist thickness and compound correction (compound corr.). Some of results are displayed in the following figures.

Implantation is simulated into the following stack: resist/15nm-oxide/Si-bulk. Incident angle 0°. Resist density equals 1.20g/cm³.

P 430keV, resist 1.10µm, compound corr. 1.00 no penetration

P 460keV, resist 1.10µm, compound corr. 1.00 penetrated fraction: 0.070% of the dose
P 520keV, resist 1.10μm, compound corr. 1.00 penetrated fraction: 3.45% of the dose

P 560keV, resist 1.10μm, compound corr. 1.00 penetrated fraction: 13.6% of the dose

P 580keV, resist 1.10μm, compound corr. 1.00 penetrated fraction: 22% of the dose

P 580keV, resist 1.10μm, compound corr. 1.05 penetrated fraction: 12.5% of the dose

P 460keV, resist 1.00μm, compound corr. 1.00 penetrated fraction: 3.14% of the dose

P 460keV, resist 1.00μm, compound corr. 1.05 penetrated fraction: 1.05% of the dose
B 200keV, resist 1.10µm, compound corr. 1.00
no penetration

B 240keV, resist 1.10µm, compound corr. 1.00
penetrated fraction: 1.22% of the dose

Summary of the simulated penetration fraction for different implant energy
and compound correction

<table>
<thead>
<tr>
<th>Phosphorus energy</th>
<th>Resist thickness</th>
<th>Assumed resist compound correction</th>
<th>Compound correction that matches result of the short-loop experiment</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>1.00</td>
<td>1.05</td>
</tr>
<tr>
<td>P 580keV</td>
<td>1.10µm</td>
<td>22.0%</td>
<td>12.5%</td>
</tr>
<tr>
<td></td>
<td>1.40µm</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
<tr>
<td>P 560keV</td>
<td>1.10µm</td>
<td>13.6%</td>
<td>6.74%</td>
</tr>
<tr>
<td></td>
<td>1.40µm</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
<tr>
<td>P 520keV</td>
<td>1.00µm</td>
<td>22.7%</td>
<td>14.06%</td>
</tr>
<tr>
<td></td>
<td>1.10µm</td>
<td>3.45%</td>
<td>1.17%</td>
</tr>
<tr>
<td></td>
<td>1.40µm</td>
<td>0.00%</td>
<td>0.00%</td>
</tr>
<tr>
<td>P 460keV</td>
<td>1.00µm</td>
<td>3.14%</td>
<td>1.105%</td>
</tr>
<tr>
<td></td>
<td>1.10µm</td>
<td>0.070%</td>
<td>0.00%</td>
</tr>
<tr>
<td>P 430keV</td>
<td>1.00µm</td>
<td>0.51%</td>
<td>0.105%</td>
</tr>
<tr>
<td></td>
<td>1.10µm</td>
<td>0.005%</td>
<td>0.00%</td>
</tr>
</tbody>
</table>

Note that “0.00%” denotes “0” ion penetration from “20000” ions lunched.

Compound correction in range (1.06, 1.10) agrees well with experimental data.

This study provides compound correction of around 1.07 for resist OiR38.
Some results on full-process lots

Lots have been processed in a full CMOS/EE-process flow, with fine splits in resist thickness. The resist thickness is varied from 900nm to 1200nm in steps of 50nm.

Onset of the parasitic penetration through the resist and oxide may be detected by measuring various PCM electrical parameters, in particular on high-voltage part. HV devices are more sensitive to the parasitic penetration due to much lower doping concentration in the wells.

The obtained resist thickness that fully stops the field implants is very close to the thickness measured in the short-loop and which follows from simulations.

Examples:

LOT 5.4195 DX01 M28SPL, NFET LV, Vt extrapolated @Vd=0.1

Dependence of threshold voltage Vt of 10/10 LVNFET (low-voltage) as a function of field-implant resist thickness (P 2.0x10^{13} cm^{-2} @ 430keV). For resist thickness bellow 1000nm phosphorous implantation penetrates through the resist and oxide underneath, thereby lowering Vt.
Vt in HV NFET (high-voltage) for different field-implant resist thickness. HV part is very sensitive to the penetration of phosphorous (P @ 430keV) that occurs for resist thickness less than or equal to 1.050µm.
Breakdown voltage of HV NMOST in EE block for different field-implant resist thickness 
($P @ 430\text{keV}$). The penetration into the bulk occurs for thickness less than $1.050\mu m$. 

**Conclusion**

- Stopping thickness of a Novolac-based photoresist OiR38 is measured by using a fast short-loop 
and surface charge analyzer.

- Implantation into stack “resist/oxide/silicon-bulk” has been simulated by using Monte Carlo 
(MC) simulator SRIM. Novolac-based resist is assumed by its chemical composition. The resist 
density after the bake is measured ($1.20\text{g/cm}^3$).

- Comparison between the experimental penetration fraction (measured in the short-loop) and the 
numerical MC simulation has enabled calibration of the stopping power of the resist. This 
procedure has resulted in compound correction close to $1.07$ (bond and core approach).

- Minimal necessary resist thickness ($1.10\mu m$) is implemented into a real sub-micrometer 
CMOS/EE process. This resist thickness enables the narrowest field-implant opening ($0.35$-
$0.40\mu m$) of this resist type for the given high-energy field implant conditions. 
As a consequence of the optimal resist thickness, minimum design distance between EE cells is 
achieved in the memory array.
References


