The aim of this programme is to prepare, evaluate and optimise Total Dielectric Isolated (TDI) structures in order to develop the technology for the preparation of substrates for circuits which exhibit improved radiation tolerance.

The work carried out during this reporting period has provided a sound base for this project. Successful experiments include the preparation of device worthy substrates in variously patterned wafers, identification of the microstructure of TDI wafers by cross-sectional transmission electron microscopy (XTEM) and the successful implementation of a new predictive software package (IRIS). In addition a new halogen lamp heated wafer holder (funded under another contract) has been commissioned and used to prepare substrates with pre-heating and background heating up to 680°C. Keywords: Silicon
UNIVERSITY OF SURREY

DEPARTMENT OF ELECTRONIC AND ELECTRICAL ENGINEERING

TOTAL DIELECTRIC ISOLATION (TDI) OF FULLY DEPLETED DEVICE STRUCTURES

AFOSR-88-0356 Programme Manager:
P L F Hemment Dr D Eirug Davies
July 1990

INTERIM SCIENTIFIC REPORT

SUMMARY

SIMOX is the most mature SOI technology and many laboratories in the USA, Japan and Europe are developing radiation hard and high speed CMOS/SIMOX circuits. However, circuits fabricated on conventional SIMOX substrates still require additional processing (eg MESA etching or LOCOS) to achieve lateral device isolation.

The innovative programme of work undertaken at the University of Surrey is designed to take SIMOX technology a stage further by achieving both vertical and lateral isolation during a single O⁺ ion implantation stage. The process being developed, known as Total Dielectric Isolation (TDI), achieves this goal by implanting into a patterned wafer and thereby synthesising a non-planar buried layer of SiO₂, which completely isolates the silicon island from the underlying substrate. The technique has already been demonstrated and dielectrically isolated islands have been formed.

The principal achievements during the current period are (i) results of microstructural analysis of TDI structures by cross-section transmission electron microscopy (XTEM), (ii) completion of a computer model which permits the dimensions (tₜ₁, t₂₁) to be predicted in both “as implanted” and annealed substrates, and (iii) first results of experiments to planarise the top (free) silicon surface.

The project has benefitted from close collaborative links with staff at NRL, Washington DC, and IBIS Technology Corp, Danvers, MA.
1. REPORT OF WORK COMPLETED

A novel isolation technique (total dielectric isolation - TDI) to replace MESA etching and LOCOS isolation has been developed at the University of Surrey, which has twelve years experience in SIMOX technology. The TDI process is an extension of SIMOX technology and entails O\(^+\) implantation through a patterned masking layer (SiO\(_2\)). As the ions lose energy within the mask, a non-planar layer of SiO\(_2\) may be synthesised which, by careful optimisation of the processing parameters, provides lateral and vertical isolation of the silicon device islands. The dimensions of the silicon islands are freely defined across the wafer by lithography from \(\mu\)m to mm. The islands are delineated by Si/SiO\(_2\) interfaces which are formed by internal oxidation and have a topography quite different from previous structures and, thus, offer the prospect of forming novel structures and achieving improved radiation tolerance, which currently is necessary to meet system requirements. The dielectric isolation will also ensure circuit operation in high temperature environments, as reported for conventional SOI/CMOS.

The aim of the DOD programme is to prepare, evaluate and optimise TDI substrates for circuits with improved radiation hardness and substrates have been prepared and sent to NRL, Washington DC. The grant supports an experienced research fellow (Dr U Bussmann) and at the start of the project he was able to quickly define structures for the first round of experiments. Masked wafers were prepared by NRL, implanted at Surrey and returned to Washington for processing. In parallel the research fellow has developed techniques and expertise to enable him to optimise the TDI structures. This work has entailed the use of cross-sectional TEM to determine the lateral dimensions and microstructure of the silicon islands and interfaces, surface analysis techniques for composition and thickness determinations and development of a computer model (IRIS) to simulate the evolution of the oxide layer. The ideal TDI wafer will have a planar surface and this model, which incorporates swelling, sputtering and diffusion, has been used to determine the optimum values of the processing parameters (energy, dose, mask thickness and etch back) to achieve this end.

The accomplishments and research progress during this period fall under
the following headings.

1.1 Preparation of Substrates

Wafers were received from NRL with patterned masking layers and were implanted over a range of $O^+$ doses at 200 keV and substrate temperature of 550°C. These were used for materials science experiments. Further substrates with FET test patterns etched in the poly-silicon masking layer have been prepared and returned to NRL for annealing and fabrication of test devices.

Additional wafers with a LOCOS patterned masking layer have been implanted and studied in order to optimise the processing to achieve a planar surface after $O^+$ implantation.

1.2 Heated Sample Holder

Extensive testing of a new heated sample holder (funded under a separate contract) have been successfully completed and the facility is now available for implants in the temperature range 300°C to 700°C into 3" and 6" wafers.

The temperature has been calibrated and the facility is now used routinely to prepare substrates.

1.3 Materials Science Experiments

The microstructure of both "as implanted" and high temperature annealed samples have been studied by cross-sectional transmission electron microscopy (XTEM). A wide range of experimental conditions have been explored including implantations into thick and thin masking layers and the use of poly-silicon and oxide masks. The output from this work has been used to optimise the processing of wafers for test devices and as input to the computer simulation software.

1.4 Computer Simulations

The computer programme, IRIS, developed as part of this project, has been further extended to model the effect of high temperature annealing when the evolved oxygen depth profile is transformed into a rectangular distribution. This software is now running and has been used extensively to accurately predict the structure of device grade substrates.
2. FUTURE WORK

Priorities during the next period will be:

(i) description of the microstructure of TDI structures formed on LOCOS masked wafers,
(ii) optimisation of the processing conditions,
(iii) direct formation of thin film SIMOX/TDI substrates using lower energy $^{16}O^+$ ions and the heated sample holder, and
(iv) refinement of the computer model (IRIS) to extend the working range.
PUBLICATIONS


2. U Bussmann and P L F Hemment, "Layer Thickness Calculations for SOI Structures Formed by Oxygen Implantation", Accepted for publication in Appl Phys Letts.


4. U Bussmann, A K Robinson and P L F Hemment, "Energy and Dose Dependence of Si Top Layer and Buried Oxide Layer Thicknesses in SIMOX Substrates", Accepted by IIT'90, University of Surrey, July 1990.


APPENDIX

- Reference 1 (above).
- Progress Reports 1, 2 and 3.
**OBJECTIVE**

The aim of this programme is to prepare, evaluate and optimise TDI structures as quickly as possible in order to develop the technology for the preparation of substrates which exhibit improved radiation tolerance.

**TECHNICAL PROGRESS**

The Research Fellow (Dr U Bussmann), supported by this contract, was appointed on time and rapid progress has been made in developing expertise and carrying out initial experiments. Technical progress will be reported under separate headings.

**Computer Modelling**

It is important to have predictive models to describe the movement of the free surface and buried interfaces during O⁺ ion implantation. Software has been written which enables these movements to be followed in both the "window" and "field" regions of the structures, which are characterised by different sputtering rates.

The model uses an iterative procedure to simulate the evolution of the implanted oxygen depth profile. Input data is in the form of the concentration depth profile, either experimental or calculated using TRIM, of incremental doses of O⁺ ions and the redistribution due to diffusion (if x > 2), swelling and sputtering is calculated after the addition of each increment of value, typically, \( 1 \times 10^{15} \) O⁺ cm⁻². The iterations are continued until the required dose has accumulated. Figures 1(b), (c) and (d) are calculated depth profiles of \( 1 \times 10^{15} \) O⁺ cm⁻², \( 1.4 \times 10^{16} \) O⁺ cm⁻² and \( 1.8 \times 10^{15} \) O⁺ cm⁻² implanted into silicon at an energy of 200 keV. Figures 1(f), (g) and (h) are the analogous profiles when the O⁺ ions are implanted through a masking oxide of thickness 3200 Å. The rapid sputter erosion of the mask modifies the shape of the final distribution and increases the value of the critical dose required to achieve a stoichiometric oxide. These profiles, which have been calculated using values of the system variables derived from experiment, show good agreement with experimental profiles reported in the literature. Figures 1(a) and 1(e) show the oxygen distributions for a low dose of \( 1 \times 10^{14} \) O⁺ cm⁻².
2.2 Determination of Microstructure

The Research Fellow has access to a JEOL 200CX transmission electron microscope and an Ion Tech Fast Atom Beam Miller for detailed cross-sectional TEM (XTEM) studies of the TDI structures. A procedure for sample preparation has been developed and proven using TDI samples used in earlier experiments. The preparation of XTEM samples from the first batch of wafers will commence immediately after their return to Surrey after high temperature (1300°C, five hours) annealing at NRL.

The seventeen stage preparation procedure, resulting in samples of two different materials, is as follows:

<table>
<thead>
<tr>
<th>Period</th>
<th>Action</th>
<th>Working Time (hours)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Day 1</td>
<td>1 Cleaving (15 - 20 pieces, 3 mm)</td>
<td>1.5</td>
</tr>
<tr>
<td></td>
<td>2 Cleaning - Acetone + Methanol + Toluene</td>
<td></td>
</tr>
<tr>
<td></td>
<td>3 Gluing - epoxy resin</td>
<td>1.5</td>
</tr>
<tr>
<td>Day 2</td>
<td>4 Mount between glass on stubs</td>
<td>1.5</td>
</tr>
<tr>
<td></td>
<td>5 Coarse Polishing</td>
<td>2</td>
</tr>
<tr>
<td></td>
<td>6 Fine Polish (SiC)</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>7 First Diamond Polish (1 μm)</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>8 Optical Check</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td>9 Reverse Sample Mount, Between Cover Slips</td>
<td>1.5</td>
</tr>
<tr>
<td>Day 3</td>
<td>10 Coarse Polishing</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td>11 Fine Polish (SiC)</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>12 Fine Polish (1 μm)</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>13 Optical Check</td>
<td>0.5</td>
</tr>
<tr>
<td></td>
<td>14 Mount First Copper Grid</td>
<td>1</td>
</tr>
<tr>
<td>Day 4</td>
<td>15 Remove from Stub</td>
<td>1.5</td>
</tr>
<tr>
<td></td>
<td>16 Mount Second Copper Grid</td>
<td>1.5</td>
</tr>
<tr>
<td></td>
<td><strong>TOTAL</strong></td>
<td><strong>18.5</strong></td>
</tr>
<tr>
<td>Day 5</td>
<td>17 Commence Ion Milling (10 - 20 hours for each sample)</td>
<td><strong>-x--</strong></td>
</tr>
<tr>
<td></td>
<td><strong>Select sample for analysis</strong></td>
<td><strong>-x--</strong></td>
</tr>
</tbody>
</table>
2.3 Implantation of Masked Wafers

A set of twelve 3" wafers has been received from the Naval Research Laboratory (NRL) which have patterned polysilicon masking layers of thickness 0.25 μm and 1.5 μm. Areas are defined which are suitable for analysis by Rutherford backscattering, SEM and TEM. The first batch of four wafers have been implanted at -550°C with 200 keV O⁺ ions over the dose range $0.3 \times 10^{10} \text{ cm}^{-2}$ to $2.4 \times 10^{10} \text{ cm}^{-2}$. Two of these implanted wafers have been sent to the NRL for capping and high temperature annealing and will be returned to Surrey for analysis.

2.4 Materials Science

A novel feature of the patterned TDI structures is that the formation of the synthesised dielectric layer can be dominated by different mechanisms in the window and field regions. If the sputter rate is high (eg SiO₂, masking layer) then the final oxygen depth distribution will be a "sputter limited profile" which may not achieve an adequately high volume concentration to directly form the stoichiometric silicon dioxide. It is important, therefore, to determine the dependence of the volume concentration upon sputter rate as this information is input data for the computer model (Section 2.1).

Figures 3(a) and (b) are the backscatter energy spectra of 1.5 MeV He⁺ from a SIMOX sample $(1.8 \times 10^{18} \text{ O}^+ \text{ cm}^{-2})$ and a masked sample $(3200 \text{ Å of SiO₂})$ implanted with a dose of $1.7 \times 10^{18} \text{ O}^+ \text{ cm}^{-2}$, respectively. The oxygen depth distributions and the composition of the buried oxide (SiOₓ) can be inferred from the yield deficiency between channels 150 and 250, which is due to the included oxygen. These preliminary results suggest that the oxide formed beneath the mask (Figure 3(b)) is sub-stoichiometric, which is consistent with previous SIMS analyses. Further analyses will be carried out to improve the statistical significance of the results.

2.5 Heated Sample Holder

This TDI project draws upon the expertise of staff at Surrey and requires access to the ion implantation facilities. New equipment, which has recently been ordered and will be used by Dr Bussmann, includes a lamp heated sample holder. This unit will enable the wafer to be pre-heated to 500°C - 600°C and will provide background heating to maintain the wafer at a constant temperature during the three hours to five hours of implantation time. Dr Bussmann has participated in design and technical discussions with the manufacturer.

3. FUTURE WORKPLAN (APRIL - JUNE 1989)

The initial implantations have been carried out on time and during the next reporting period (April 1989 - June 1989) it will be possible to evaluate the TDI structures. This will entail the following activities.
FIGURE CAPTIONS

Figure 1: Calculated depth profiles of \(1 \times 10^{18} \text{ O}^+ \text{cm}^{-2}\), \(1.4 \times 10^{18} \text{ O}^+ \text{cm}^{-2}\) and \(1.8 \times 10^{18} \text{ O}^+ \text{cm}^{-2}\) implanted at 200 keV into bulk silicon [(a), (c) and (d)] and into silicon through an \(\text{SiO}_2\) mask of thickness 3200 Å [(f), (g) and (h)], respectively. Figures 1(a) and 1(e) show the low dose depth profiles.

Figure 2: Backscatter energy spectra of 1.5 MeV \(\text{He}^+\) ions from (a) a SIMOX sample \((1.8 \times 10^{18} \text{ O}^+ \text{cm}^{-2}, 200 \text{ keV})\) and (b) a masked sample \((3200 \text{ Å, SiO}_2)\) implanted with a dose of \(1.7 \times 10^{18} \text{ O}^+ \text{cm}^{-2}\), respectively. The residual oxide (+500 Å) on the surface of the masked sample was removed before carrying out the analysis.
FIGURE 2(b)

Counts

Channel Number

0  50  112  174  236  300

0  1150  2300  3450  4600

Counts vs Channel Number
FIGURE 2(a)
UNIVERSITY OF SURREY

DEPARTMENT OF ELECTRONIC AND ELECTRICAL ENGINEERING

Total Dielectric Isolation (TDI) of Fully Depleted Device Structures

P L F Hemment
July 1989

SECOND PROGRESS REPORT

ABSTRACT

The initial experiments described in the First Progress Report have provided a sound base for this project and further good progress has been made during this second reporting period in the areas of preparation of substrates, cross-sectional TEM analysis, computer modelling and materials science experiments. Delivery from the manufacturers of the heated sample holder is a few weeks behind schedule due to late delivery of components from a sub-contractor.

1. OBJECTIVE

The aim of this programme is to prepare, evaluate and optimise TDI structures as quickly as possible in order to develop the technology for the preparation of substrates for circuits which exhibit improved radiation tolerance. TDI structures incorporating N⁺ implantation will additionally be examined.

2. TECHNICAL PROGRESS (April 1989 - June 1989)

2.1 Preparation of Substrates

A further two patterned 3" (100) silicon substrates have been successfully implanted. These have TDI FET test patterns etched in the poly-silicon masks of 0.25 μm (transparent to 200 keV O⁺ ions) and 1.5 μm (opaque) thicknesses. These substrates have been returned to NRL, Washington, for capping, annealing and fabrication of test devices.

New materials science experiments have been started with the aim of evaluating TDI structures formed by the synthesis of a Si₃N₄ layer. This is supported by 200 keV N⁺ implants into SiO₂ masked wafers. The patterned oxide layers are 0.31 μm and 0.47 μm thick and the implanted doses are 0.4 x 10¹⁸ N⁺ cm⁻², 1.0 x 10¹⁸ N⁺ cm⁻² and 1.4 x 10¹⁸ N⁺ cm⁻².

2.2 Microstructure of "as Implanted TDI Structures"

Cross-sectional samples prepared from an "as implanted" (no post implantation anneal) wafer (NRL Wafer Number 5) have been examined in a JEOL 200CX TEM. This wafer has a patterned poly-silicon mask of nominal thickness 2500 Å above a Si₃N₄ buffer layer of thickness 320 Å. These were deposited on a screen oxide of nominal thickness 210 Å.
Figure 1 shows a schematic of the actual structure together with a cross-sectional micrograph from which the layer thicknesses were determined. The edge of the mask is non-ideal having a slope of $45^\circ$ in the lower part but is steeper near the top surface. The Si$_3$N$_4$ has been incompletely etched and extends about 0.45 $\mu$m into the window region.

An unannealed TDI structure formed by a dose of $1.8 \times 10^{14}$ O/cm$^2$ is shown in Figure 2, which includes a schematic of a typical structure and TEM micrographs from representative areas. Surprisingly, within the window region the silicon surface is $500$ Å below the plane of the original surface which is still preserved and can be seen under the field mask. Within the field region the structure consists of 1400 Å of polysilicon, about 600 Å of buffer layer, 1400 Å of defective but crystalline silicon, 2900 Å of amorphous oxide and 2000 Å of highly defective silicon above the silicon substrate. As a negligible amount of oxide is deposited in the polysilicon the change in thickness is due solely to sputtering which gives a sputtering coefficient for 200 keV O$^+$ ions at 550$^\circ$C of 0.22 atoms/ion. Within the window region the structure consists of 3500 Å of defective single crystal silicon, 2900 Å of amorphous oxide, about 2000 Å of damage silicon above the silicon substrate. As predicted the amorphous oxide layer has the same thickness (2900 Å) in both the field and window regions.

The edge of the window shows a smooth transition between the geometries of the field and window structures. It is noted that sputtering of the mask has reduced the slope of the mask edge. Finger like protrusions of defective silicon penetrate into the synthesised layer of SiO$_2$. A silicon rich region has been reported previously in wafers with an oxide mask and this phenomena is associated with the lateral movement of the window edge due to sputtering. The effect is less pronounced in this polysilicon masked wafer and it is anticipated that oxygen segregation during high temperature annealing will achieve good dielectric isolation between the silicon device island and substrate.

Conclusions which may be drawn from these experiments include:

(a) desirability of a thicker polysilicon mask (3000 Å) to achieve a field oxide extending up to the silicon surface,

(b) sputter coefficient for 200 keV O$^+$ in polysilicon (550$^\circ$C) is 0.22 atoms per ion (the measured rate for SiO$_2$ is 1.1 atom per ion with theoretical (TRIM) values of 0.18 and 0.38, for Si and SiO$_2$, respectively),

(c) the improved edge structure may be due to the lower sputtering rate of polysilicon compared to SiO$_2$,

(d) it is desirable to have vertical mask edges, and
(e) the Si$_3$N$_4$/SiO$_2$ buffer layer maintains its integrity during O$^+$ implantation.

Additional specimens implanted with a higher dose ($2.4 \times 10^{18}$ O$^+ \text{cm}^{-2}$) have been thinned and are ready for examination in the TEM.

2.3 Materials Science Experiments

2.3.1 Stoichiometry

Previous analyses by SIMS of oxides formed beneath an oxide mask have suggested that the layer is not stoichiometric SiO$_2$ but rather SiO$_x$ where $x = 1.7$. Preliminary RBS analysis, recorded in the first report, seemed to support the SIMS data. During this reporting period very detailed RBS analyses have been carried out to achieve a more reliable measure of the value of $x$ and to support the computer modelling (Section 2.4). It is important to note that this new data clearly shows the oxide is stoichiometric ($x = 2.00 \pm 0.05$) to within experimental errors. The reason for the discrepancy between SIMS and RBS analyses is not obvious but as ion yields are known to be influenced by the matrix it is reasonable to accept the new RBS data described below.

Figure 3 shows 1.5 MeV He$^+$ RBS spectra from a thick polysilicon layer (1.5 µm), a standard SIMOX sample implanted with $1.8 \times 10^{18}$ O$^+ \text{cm}^{-2}$ at 200 keV and a TDI test structure in which $1.8 \times 10^{18}$ O$^+ \text{cm}^{-2}$ were implanted through an SiO$_2$ mask of thickness 3200 Å. Figure 4 shows RBS simulation spectra for (i) bulk silicon, (ii) 3000 Å silicon on 3000 Å SiO$_2$ on silicon, and (iii) 2000 Å silicon on 3000 Å SiO$_2$ on silicon. The data is consistent and by taking ratios of yields it is concluded that the oxide in the TDI sample has a stoichiometric composition ($\pm 2.5\%$).

2.3.2 Implantation into Polysilicon

Figure 5 shows 1.5 MeV He$^+$ RBS spectra from a wafer with a thin polysilicon mask (0.25 µm) and a Si$_3$N$_4$/SiO$_2$ buffer layer. The regions are labelled in the figure. The buffer layer has been used as a shallow buried marker and enables the sputtering coefficient of 200 keV O$^+$ into polysilicon to be estimated (0.22 atoms per ion).

Figure 6 confirms the formation of a buried layer of SiO$_2$ in the thick polysilicon film (1.5 µm) after implantation of $1.8 \times 10^{18}$ O$^+ \text{cm}^{-2}$.

2.4 Computer Modelling

Further refinements have been made to the computer model and simulations have been run to determine the sensitivity of the structure to the diffusion of excess oxygen in the buried oxide.

Figure 7 shows the evolution of the oxygen depth profile in bulk silicon over the dose range $0.6 \times 10^{18}$ O$^+ \text{cm}^{-2}$ to $2.6 \times 10^{18}$ O$^+ \text{cm}^{-2}$. The sputter rate is 0.2 and excess oxygen is allowed to move to the upper (near surface) Si/SiO$_2$ interface. As expected this interface advances towards the surface and rapidly becomes more abrupt.
Figure 8(a), (b) and (c) show the evolution of the oxide profiles in samples with an oxide mask of thickness 3200 Å. The sputtering coefficient is 1.1 atoms per ion. Figures 8(a), (b) and (c) show profiles when excess oxygen diffuses to the lower interface, distributes equally and diffuses to the upper interface, respectively.

The following conclusions may be drawn:

(a) in SIMOX structures the oxygen peak moves away from the surface with increasing dose,

(b) for TDI samples the oxygen peak moves towards the free (upper) surface, the effect is independent of the direction of oxygen diffusion being dominated by sputtering of the mask, and

(c) the critical dose just to achieve a stoichiometric oxide is $1.35 \times 10^{18}$ O$^+$ cm$^{-2}$ for SIMOX and $1.57 \times 10^{18}$ O$^+$ cm$^{-2}$ for TDI structures.

2.5 Heated Sample Holder

Delivery of the heated sample holder (funded under another contract) has been delayed due to late delivery of components from a sub-contractor. Acceptance tests will be carried out during early August 1989 and it is planned to implant wafers using preheating during the next reporting period.

3. FUTURE WORKPLAN

Priorities during the next period will be:

(a) cross-sectional TEM analysis of annealed TDI structures,

(b) implantation of additional wafers for the fabrication of CMOS test structures at NRL,

(c) refinements to the computer model, to include thermal segregation,

(d) materials science, further measurements to quantify the effects of swelling and sputtering.

REFERENCES

XTEM analysis of the first batch of wafers annealed at Naval Research Laboratories.

O⁺ ion implantation.

Sample preparation and XTEM analysis.

Computer modelling.

Definition of new structures.

Commission heated sample holder.

Materials science experiments (e.g., RBS).

Electrical evaluation (NRL).

Discussion will be held with our sponsors/collaborators to define improved structures and to agree upon future experiments to assess the electrical characteristics and radiation tolerance of the structures.

P L F Hemment
July 1989
FIGURE CAPTIONS

1. XTEM micrograph showing the edge of the thin polysilicon mask.

2. XTEM micrograph shown as-implanted structure (D = 1.8 x 10¹⁸ O⁺ cm⁻², E = 200 keV, Tᵢ = 550°C) in mask, transition and window region.

3. RBS profiles after implantation (D = 1.8 x 10¹⁸ O⁺ cm⁻², E = 200 keV, Tᵢ = 550°C) into silicon and through a 320 nm thick SiO₂ mask (remainder of oxide mask removed). The profile of the thick polysilicon mask is taken as a reference.

4. Theoretically expected RBS profiles for the layered structures shown in the schematics.

5. RBS profiles of the thin polysilicon sample (see schematic) before and after implantation (D = 1.8 x 10¹⁸ O⁺ cm⁻², E = 200 keV, Tᵢ = 550°C).

6. RBS profiles of the thick polysilicon sample (1.5 μm) before and after implantation (D = 1.8 x 10¹⁸ O⁺ cm⁻², E = 200 keV, Tᵢ = 550°C) in comparison to an implantation into bulk silicon.

7. Calculated θ-profiles for the implantation of different doses into silicon (E = 200 keV) with diffusion directed to upper interface.

8. Calculated θ-profiles for the implantation of different doses through a 320 nm thick SiO₂ mask. The diffusion is directed to (a) lower interface, (b) both interfaces, and (c) upper interface.
Figure 3

- Implantation through oxide mask
- Thick poly-Si reference
- Standard SIMOX
FIGURE 4

(a) 300 nm Si
    300 nm SiO₂
    bulk Si

(b) 200 nm Si
    300 nm SiO₂
    bulk Si

structure (a)
structure (b)
210 nm poly-Si
30 nm Si$_3$N$_4$
25 nm SiO$_2$
bulk Si

**FIGURE 5**
implantation into poly-Si
standard SIMOX

FIGURE 6
FIGURE 7
FIGURE 8
PROGRESS REPORT

1. REPORT FOR THE LAST PERIOD

Extensive testing of the heated sample holder, which was purchased under a separate contract has been carried out. 3" to 6" wafers can now be implanted in the temperature range 200 - 700°C (calibrated). The system is now in routine use for substrate preparation.

1.1 Heated Sample Holder
- Extensive testing: ok.
- Temperature calibration.
- Now in routine use for substrate preparation.

1.2 Substrate Preparation

A new set of twenty-one masked and patterned substrates has been fabricated by the NRL for materials science experiments: LOCOS oxide masks of 1920, 2565 and 3760 Å; SiO₂ masks of 2370, 3685 and 4389 Å; poly-Si masks of 2450 Å.

When the oxide mask is formed in a LOCOS process 55% of this masking layer is located above and 45% below the silicon surface level. As shown by simulations, a planar surface can then be achieved after implantation (see schematic in Figure 1). Also, the transition between the buried oxide layers in the mask and window regions will be smoother. Therefore, a structural improvement of the critical transition region is expected.

A different approach uses relatively low implantation energies to avoid steep steps between the oxides in the transition region. The lower flank of the implantation profile itself in the mask region as well as in the window region will be steeper due to the reduced straggle of the ion distribution. This may lead to the absence of silicon inclusions at the lower interface, which are always found under standard implantation conditions. The necessary wafer temperature can now be maintained by the background heating using the new sample holder. An additional advantage is the formation of a thinner silicon overlayer for fully depleted device areas.
A wafer with a LOCOS oxide pattern of 3760 Å has been implanted with 0.4, 1.8 and 2.2 \( \times 10^{10} \) O cm\(^{-2} \) at the standard energy of 200 keV/atom at the elevated temperature of 700°C, with background heating from an array of halogen lamps.

Wafers with a 2370 Å SiO\(_2\) pattern and a 2450 Å SiO\(_2\) pattern were implanted at a relatively low energy of 100 keV/atom with 0.3, 1.2 and 1.5 \( \times 10^{10} \) O cm\(^{-2} \).

The wafers were sent to the NRL for capping and annealing.

1.3 Materials Science Results

Microstructure of annealed samples (poly-Si masks)

- "thin" poly-Si mask
  
  (energy 200 keV, annealing 1310°C for five hours)
  
  Polycrystalline silicon masks have been successfully used to form continuous non-planar buried oxide layers. As an example Figure 2 shows the result of a 1.8 \( \times 10^{10} \) O cm\(^{-2} \) implantation through a 250 nm mask. As expected, after annealing dislocations are found in the silicon top layer and silicon inclusions in the oxide close to the lower interface. In addition a vertical chain of inclusions appears in the transition region. These inclusions might be avoided by decreasing the slope of the mask edge. A thin superficial silicon overlayer is left underneath the mask, which can be used as an etch stop when removing the remainder of the masking material.

- "thick" poly-Si mask
  
  (energy 200 keV, annealing 1310°C for five hours)
  
  Figure 3 shows the transition region of a sample implanted with 1.8 \( \times 10^{10} \) O cm\(^{-2} \) after annealing. Silicon islands are formed, which are disconnected from the bulk material, although many silicon inclusions still exist in the transition region. In the mask region all the oxygen is stopped in the upper half of the thick poly-Si layer forming a continuous oxide. After removal of the thick poly-Si (including its "buried" oxide layer) such silicon islands could be used for building devices.

- LOCOS oxide mask
  
  (energy 200 keV, annealing 1300°C for four hours, oxide cap)
  
  A wafer with a LOCOS oxide mask was obtained, under alternative funding, for a test implantation. Figure 4 shows first results after implantation of 1.8 \( \times 10^{10} \) O cm\(^{-2} \), subsequent capping and annealing. Compared to the previous implantations using poly-Si masks less Si-inclusions are found on that "vertical chain". However, the edge of the mask region contains a high number of inclusions, although probably these would not be detrimental for the performance of devices built in the silicon islands. Apart from the surface dip in the transition region itself a nearly planar surface has been
achieved. A more detailed study of the resulting structures is on the way using masking patterns designed and prepared in collaboration with the NRL.

1.4 Computer Simulation

The programme IRIS (U Bussmann and P L F Hemment, Nucl Inst & Meths B47, 22, 1990) has now been further developed to model the effect of very high temperature (>1300°C) annealing when the implantation profile is transformed into a rectangular profile. It has been shown, that oxygen transport occurs up the macroscopic concentration gradient as the system moves to reduce the total energy through the growth of large SiO₂ precipitates at the expense of small precipitates and eventually reaches thermal equilibrium with the segregation of all of the implanted oxygen at the buried oxide layer. This layer, thus, may be considered as a planar precipitate of infinite radius. The phenomenological approach used here does not attempt to simulate processes on an atomic scale, which lead to the thermal segregation. In our calculations all the implanted oxygen (i.e., the total fluence minus the small amount of oxygen, which is deposited close to the surface and subsequently lost by surface erosion) is bound within a stoichiometric SiO₂ layer. The justification for neglecting out-diffusion is that there is good agreement between predicted and measured layer thicknesses in structures which have been well characterised.

Profiles have been calculated over a wide range of fluences. Figures 5 and 6 summarize the resulting layer thicknesses for 200 keV and 150 keV ions. Experimental layer thicknesses, as determined from XTEM micrographs or SIMS profiles from the literature, have been included for comparison. Taking into consideration the scatter of the experimental data, there is good agreement between experiment and simulation.

An important method for producing low defect density silicon top layers involves sequential implantation and annealing. The programme IRIS has been used to make predictions of layer thicknesses after multiple step implantations in comparison with single step implantations. The implantation of \(1.8 \times 10^{18}\) O⁺ cm⁻² in three equal steps will be considered as an example. Figure 7a shows the implantation profile for a fluence of \(0.6 \times 10^{18}\) O⁺ cm⁻² together with the rectangular profile after thermal segregation during high temperature annealing. This layer structure is the target for the second implantation stage with the same fluence, resulting in the distributions shown in Figure 7b (before and after annealing), while the final oxygen distributions after the third implantation and annealing are shown if Figure 7c. For comparison, the implantation of \(1.8 \times 10^{18}\) O⁺ cm⁻² in a single step is included as Figure 7d. Using multiple implantation and annealing leads to steeper flanks in as-implanted profiles due to the previous thermal segregation. The simulation also shows that the buried oxide layer is shifted 35 nm towards the surface. This shift is due to the early existence of a stoichiometric layer, which leads to an increase of the amount of oxygen being
2. FUTURE WORKPLAN

Priorities during the next period will be:

(a) Cross-sectional TEM analysis of TDI structures formed by implants through LOCOS oxide masks.

(b) Fabrication of additional wafers for the optimisation of the structural properties.

(c) Lower energy (100 keV) implants using the heated sample holder.

(d) Refinements of the computer model to extend the energy range to 50 - 300 keV (especially important for the simulations of the planned lower energy implantations).

3. FIGURE CAPTIONS

Figure 1: LOCOS oxide mask (schematic): Expected structure of the periphery of the window before and after implantation and annealing.

Figure 2: "Thin" poly-Si mask: Resulting structure of the transition region after implantation (1.8 x 10^16 O' cm^-2) and annealing (13100°C for five hours).

Figure 3: "Thick" poly-Si mask: Resulting structure of the transition region after implantation (1.8 x 10^16 O' cm^-2) and annealing (13100°C for five hours).

Figure 4: LOCOS oxide mask: Resulting structure of the transition region after implantation (1.8 x 10^16 O' cm^-2) and annealing (1300°C for four hours).

Figure 5: Calculated depth of the maximum oxygen concentration (Rmax) and interface positions for 200 keV implantations into silicon in comparison to experimental data from the literature (symbols).

Figure 6: Calculated depth of the maximum oxygen concentration (Rmax) and interface positions for 150 keV implantations into silicon in comparison to experimental data from the literature (symbols).

Figure 7: Calculated oxygen concentration profiles after implantation (histograms) and high temperature annealing (rectangular profiles):

(a) 0.6 x 10^16 O' cm^-2
(b) 2 x (0.6 x 10^16 O' cm^-2)
(c) 3 x (0.6 x 10^16 O' cm^-2)
(d) 1.8 x 10^16 O' cm^-2, single implantation stage
Figure 1

Before implantation

Si

SiO₂

After implantation

Si

SiO₂
Figure 2
Si island
buried oxide

thick poly-Si mask
with implanted oxide

Figure 3
Figure 5
Figure 6
a) annealed
b) as-implanted
c)
d) 135 nm