Positron beam study on the ion-implanted Si

At Halle, 04-AUG-03

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1. Depth resolution-enhanced VEPAS
2. O ion implanted Si
3. Noble-gas ion implanted Si (He+ & Ar+)
4. Summary
Acknowledgments

T. Miyagoe (Univ. of Tokyo)
T. Akahane (NIMS)
R. Suzuki (AIST)
T. Ohdaira (AIST)
1. Depth resolution-enhanced VEPAS

VEPAS: Variable-energy positron annihilation spectroscopy

- 0–50 keV
- e\(^+\), Positrons
- Thermalization
- Diffusion
- Trap at defects
- Annihilation
- Emission of 511 keV γ-rays
- Doppler broadening
- Lifetime
- Coincidence Doppler broadening, CDB
Information from positron data

**Lifetime**
- Electron density
- Defect size

**Doppler broadening**
- Low electron momentum
- Amount of defects

**CDB**
- High electron momentum
- Chemical analysis of defects

**Graphs:**
- Lifetime vs. Number of vacancies
- Counts vs. $\gamma$-ray energy, keV
- Log (Counts) vs. $\gamma$-ray energy, keV
- $\gamma$-ray energy, keV with a highlighted area
S-E, CDB and lifetime measurements using e+ beam

Determine the depth; the fixed e+ energy

Chemical information

Size information
AIM

Interaction of vacancy-impurity complexes in Si with positrons

Introduction of impurity and vacancies

Suitable specimens: Ion irradiated Si

V-oxygen: One of the most important impurities in Si
    1x10^{18} O/cm^{3} in CZ-Si, SIMOX wafers

V-helium: Bubble formation

V-argon: Bubble formation

Methodology

- Enhanced depth resolution → layer-by-layer analysis
- V-impurity complexes → CDB ratio curves
Depth dependence of the induced defects

The induced defects and their anneal behavior are strongly influenced with the content of impurities as well as the element. Resolution enhanced VEPAS is required.
Positron implantation profile

Mean implantation depth

\[ P(z, E) = \frac{mz^{m-1}}{z_0^m} \exp \left[-\left(\frac{z}{z_0}\right)^m\right] \]

Mean implantation depth

\[ \bar{Z} = \frac{A}{\rho} E^{1.6} \]
\[ \rho = 2.3 \text{ g/cm}^3 \]
\[ A = 3.6 \text{ mg/cm}^2\text{keV}^{-1.6} \]

\[ Z_0 = \frac{\bar{z}}{\Gamma\left(1 + \frac{1}{m}\right)} \]
\[ m = 2 \]

> 5 keV

Diffusion length of e\(^+\) in Si = FWHM of incident e\(^+\) profile

Usual analysis has a limited on depth resolution.
Combination of e\(^+\) measurement and etching of the surface layer

**Fujinami et al.**  
Chemical etch in Si (1993, JAP)

**Coleman et al.**  
Anodic oxidation + etch in Si (1998, SLOPOS-8)

**Krause-Rehberg et al.**  
Ar\(^+\) sputtering at 2 keV in Si (2000, APL)

**Krause-Rehberg et al.**  
Wedge-shaped polished sample & micro positron beam (1-2 \(\mu\)m\(\phi\)) (2001, SLOPOS-9)

To determine the precise defect depth profile.
Analysis of CDB

The reference specimen for the CDB ratio curve

*Most of previous reports: Bulk Si*

Every sample has a peak at $10 \times 10^{-3} \text{ m}_0\text{c}$ in Si.

**Problem:**

- The boundary of Jones zone around $10 \times 10^{-3} \text{ m}_0\text{c}$
- The effect of the positrons trapped at the surface
- The different fraction of the annihilation rate with electrons of core shells

**Proposal:**

*Divacancies, V$_2$: self-ion implanted FZ-Si*
S-E curves in self-ion implanted Si

2x10^{14} \text{Si}^+/\text{cm}^2 \text{ at } 100 \text{ keV}

2x10^{15} \text{Si}^+/\text{cm}^2 \text{ at } 100 \text{ keV}

Virgin-Si

As-implanted

600°C

300°C

Larger vacancy clusters above 600°C

V_2 \text{ in crystalline phase}

700°C

800°C

600°C

Amorphous phase

Larger vacancy clusters above 300°C

The dominant defects are simple vacancy clusters.
CDB ratio curves in self-ion implanted Si
Normalized by bulk Si

- Some peaks appear in this momentum region.
- No structures in the ratio curves
- Influence of the top surface

Bulk Si at 4 keV

Boundary at Jones Zone

Ratio to bulk Si vs. Momentum, $x10^{-3} m_0 c$
CDB ratio curves in self-ion implanted Si
Normalized by $V_2$ in Si

Bulk Si at 30 keV
Bulk Si at 4 keV

No structures in the ratio curves

Simple vacancy cluster, $V_x$
A linear combination of bulk Si and $V_2$ in CDB at the fixed $e^+$ energy.
It is easy to distinguish a slight change around $10x10^{-3} \, m_0c$. 
Experiment

- The ion implanted Cz-Si:
  - O ion  \(2 \times 10^{15} \text{ /cm}^2\), 180 keV
  - He ion  \(1 \times 10^{15} \text{ /cm}^2\), 60 keV
  - Ar ion  \(1 \times 10^{15} \text{ /cm}^2\), 100 keV

- Chemical etch: KOH solution
  - The thickness of a removal was estimated by a weight change.

- Positron measurements:
  - S-E curves
  - CDB ratio curves
  - Lifetime
2. Vacancy-oxygen complexes in Si

Si implanted with $2 \times 10^{15}$ O$^+$/$\text{cm}^2$ at 180 keV

O and Vacancy profiles in depth
S-E curves and lifetime for Si implanted with $2 \times 10^{15}$ O+/cm$^2$

**S-E curves**

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Lifetime at 6.5 keV, ps</th>
</tr>
</thead>
<tbody>
<tr>
<td>Virgin Si</td>
<td>220</td>
</tr>
<tr>
<td>As-implanted</td>
<td>294</td>
</tr>
<tr>
<td>600$^\circ$ C</td>
<td>330</td>
</tr>
<tr>
<td>800$^\circ$ C</td>
<td>322</td>
</tr>
</tbody>
</table>

*Lifetime in Si*

- Bulk: 220 ps
- $V_2$: 300 ps
- $V_4$: 330 ps
CDB ratio curves for O-implanted Si

3 keV positron energy = top surface - 300 nm depth

Characteristics: peak at $12 \times 10^{-3}$ m$_0$c

- As-implanted
- Virgin Si
- Temperature: 800°C, 600°C, 500°C

Graphical representation showing changes in ratio with momentum for different depths and temperatures.
First-principles calculation for V-O in Si

# Behavior of V-O complexes in Si

<table>
<thead>
<tr>
<th>Temperature</th>
<th>V-Complex</th>
<th>O-Complex (x-y)</th>
<th>Lifespan</th>
<th>Structure in CDB</th>
</tr>
</thead>
<tbody>
<tr>
<td>As-implanted</td>
<td>$V_2$</td>
<td></td>
<td>300 ps</td>
<td>No structure</td>
</tr>
<tr>
<td>500°C</td>
<td>$V_4$</td>
<td>$V_{xO_y}$ (x-y=1)</td>
<td>275 ps</td>
<td>Weak structure</td>
</tr>
<tr>
<td>600°C</td>
<td>$V_4$</td>
<td></td>
<td>275 ps</td>
<td>Strong structure</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>O diffusion takes place.</td>
</tr>
<tr>
<td>800°C</td>
<td>$V_{xO_y}$ (x-y=4)</td>
<td>$V_{xO_y}$ (x-y=4)</td>
<td>322 ps</td>
<td>Strong structure</td>
</tr>
</tbody>
</table>

**top surface - 300 nm  300 - 600 nm depth**
3. Vacancy-noble gas atoms complexes in Si

Vacancy-noble gas atom complexes

Initial stage of bubble formation in Si

A positron is suitable probe in the initial stage of defect evolution.

He ions Ar ions

- Can a positron detect noble gas atoms in vacancies?
- Is a positron sensitive to passivate vacancies?

For example: V-H defects in Si → Low S

Positron is not sensitive to H-passivated defects.
3. Vacancy-noble gas atoms complexes in Si

Vacancy-noble gas atom complexes

Initial stage of bubble formation in Si

A positron is suitable probe in the initial stage of defect evolution.

He ions  Ar ions

✓ Can a positron detect noble gas atoms in vacancies?
✓ Is a positron sensitive to passivate vacancies?

For example: V-H defects in Si  Long lifetime 280 ps

Positron is sensitive to H-passivated defects.

Lifetime & CDB measurements is necessary.
S-E curves for He implanted Si

He: $1 \times 10^{15}$ /cm$^2$ at 60 keV
Mean projected range: 560 nm
Straggling range: 140 nm

S-E curves

S parameter vs. Positron energy, keV

- no - etch
- 250 nm etch
- 420 nm etch
- 750 nm etch
- virgin Si
The defect, $V_2$, profile for He implanted Si

He: $1 \times 10^{15} / \text{cm}^2$ at 60 keV

V-rich region  V-He region

V$_2$ (S-E curves)  He profile (TRIM)

300 nm etch sample

Layer-by-layer analysis: Lifetime & CDB
Positron lifetime for He implanted Si

<table>
<thead>
<tr>
<th>Defect</th>
<th>lifetime</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bulk</td>
<td>218 ps</td>
</tr>
<tr>
<td>V</td>
<td>275 ps</td>
</tr>
<tr>
<td>$V_2$</td>
<td>300 ps</td>
</tr>
<tr>
<td>$V_4$</td>
<td>330 ps</td>
</tr>
</tbody>
</table>

Positron energy: 4 keV

**V-He region**
- Positron trap site with one vacant

Speculation: V-He complexes such as $V_2$He
CDB ratio curve for He implanted Si

Positron energy: 4 keV

Virgin Si- 4 keV

Virgin Si- 30 keV

V-He region

V-rich region

Characteristic peak at 11x10^{-3} m_0c

Electrons due to He?

The theoretical calculations are needed.
S-E curves for He implanted Si after annealing

Low S at 300°C and high S at 500°C.
CDB ratio curve for the annealed samples

V-rich region

- 300°C
- 500°C
- As-implanted

V-He region

- 300°C
- As-implanted
- 500°C

Ratio to $V_2$ in Si vs. Momentum, $x10^{-3} m_0 c$
CDB ratio curve & lifetime in V-He region

<table>
<thead>
<tr>
<th></th>
<th>as-implanted</th>
<th>300°C</th>
<th>500°C</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lifetime</td>
<td>285 ps(98%)</td>
<td>276 ps(98%)</td>
<td>324 ps(98%)</td>
</tr>
</tbody>
</table>

300°C
- Single vacant
- Large He fraction
- \( V_2\text{He} \)
- He diffusion

500°C
- Four vacant
- No He fraction
- \( V_4\text{He}_3 \)?
V-He complexes behavior in Si

as-implanted $\rightarrow$ 300 $\uparrow$ $\rightarrow$ 500 $\uparrow$

V-rich region

300 nm

V-He region

V$_2$ 302 ps

V$_2$He 285 ps

V$_4$He$_3$ 285 ps

V$_4$He$_3$ 276 ps

V$_4$ 337 ps

V$_4$ 324 ps
Vacancy-argon complexes in Si

$1 \times 10^{15}$ Ar$^+$ / cm$^2$, 100 keV

> The critical dose for amorphization
Mean projected range: 114 nm
Straggling range: 41 nm

S-E curves for the as-implanted sample
Vacancy profile in Ar ion-implanted Si

Defects are induced beyond the implantation profile.

Lifetime & CEB measurements
Lifetime & CDB ratio curves in Ar ion-implanted Si

Positron lifetime @ 3 keV

**Ar ion implanted region:**
- Top surface – 200 nm: 302 ps (98%)
  - Size: Divacancies
- Beyond the implanted region:
  - 200 nm – 400 nm depths: 301 ps (92%)
  - Size: Divacancies

CDB ratio spectra @ 3 keV

In the implanted region: Amorphous
Passivation by Ar atoms?

Beyond the implanted range: Divacancies

Due to Ar atoms?
S-E curves for the Ar ion implanted Si after annealing

$1 \times 10^{15} \text{Ar}^+ / \text{cm}^2, 100 \text{ keV}$

**No etch sample**

**200 nm-etched sample**

As-implanted
CDB and lifetime for Ar ion-implanted Si
200 nm - 400 nm

@ 3 keV positrons

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Lifetime (Size)</th>
<th>S parameter</th>
<th>Peak intensity at 10x10^{-3} m_0c</th>
<th>Peak intensity at 10x10^{-3} m_0c</th>
</tr>
</thead>
<tbody>
<tr>
<td>500°C</td>
<td>330 ps, 72%</td>
<td>High S</td>
<td>None</td>
<td>None</td>
</tr>
<tr>
<td>600°C</td>
<td>338 ps, 53%</td>
<td>Low S</td>
<td>None</td>
<td>None</td>
</tr>
<tr>
<td>700°C</td>
<td>318 ps, 52%</td>
<td>Low S</td>
<td>None</td>
<td>None</td>
</tr>
<tr>
<td>800°C</td>
<td>291 ps, 65%</td>
<td>Low S</td>
<td>None</td>
<td>None</td>
</tr>
</tbody>
</table>

Beyond the implantation range: anneal out at 600°C
CDB and lifetime for Ar ion-implanted Si
Top surface - 200 nm

Due to Ar atoms?

<table>
<thead>
<tr>
<th>Temperature</th>
<th>Lifetime (Size)</th>
<th>S parameter</th>
<th>Peak intensity at 10x10^{-3} m_0c</th>
</tr>
</thead>
<tbody>
<tr>
<td>500°C</td>
<td>298 ps, 98%</td>
<td>High S</td>
<td>Medium</td>
</tr>
<tr>
<td>600°C</td>
<td>297 ps, 98%</td>
<td>High S</td>
<td>Medium</td>
</tr>
<tr>
<td>700°C</td>
<td>370 ps, 79%</td>
<td>Higher S</td>
<td>Strong</td>
</tr>
<tr>
<td>800°C</td>
<td>408 ps, 83%</td>
<td>Higher S</td>
<td>Strong</td>
</tr>
</tbody>
</table>
V-Ar complexes behavior in Si

as-implanted $\rightarrow$ 600 $^\circ$C $\rightarrow$ 700 $^\circ$C $\rightarrow$ 800 $^\circ$C

1. A-C trans. temp. is higher. (Usual around 600$^\circ$C)
2. Ar atoms are not released from the sample.
CEB ratio curves for V-impurity complexes in Si
- Reference $V_2$ in Si -

![Graph showing CEB ratio curves for various impurities in Si. The x-axis represents Momentum, $x10^{-3} m_0c$, and the y-axis represents Ratio to $V_2$ in Si. The graph includes curves for V-O, V-He, Surface, Bulk, and V-Ar.]
4. Summary

Various V-impurity complexes in Si have been investigated by S-E, CDB, and lifetime measurements using a positron beam.

1. These techniques are useful to identify V-I complexes in Si.
2. Depth resolution-enhanced VEPAS enables us to carry out the layer-by-layer analysis.
3. Much attention should be paid in the analysis of CDB data using a positron beam.
4. The theoretical approach is needed to identify the structure of V-I complexes in Si.