Secondary Ion Mass Spectrometry (SIMS)

Thomas Sky
Characterization of solar cells

Characterization
• Optimization of processing
• Trouble shooting
Characterization of device structure

- Atomic concentration (cm$^{-3}$)
- Depth (um)

- Si$_{0.7}$Ge$_{0.3}$
- B
- P
- As

Graph showing atomic concentration versus depth with specific concentrations labeled.

Diagram illustrating device structure with components labeled:
- B
- E
- C
- p$^+$ polysilicon
- n$^+$ polysilicon
- Pedestal collector
- n$^+$ subcollector
- Polysilicon-filled deep trench isolation
- Field oxide

Intel Core i7 Extreme quad-core processor as an example device.
Assignment of electrically active defects

- Assignment of an impurity to an electrically active deep level defect in ZnO

**SIMS** (impurities) vs. **DLTS** (electrically active defects)

Outline

• Basic principle and characteristic features
• Physical processes
  – Sputtering
  – Ionization
• SIMS instrumentation
  – Types of mass spectrometers
  – Measurement modes: Mass spectra, Depth profiling, Ion imaging
Outline

- Basic principle and characteristic features
- Physical processes
  - Sputtering
  - Ionization
- SIMS instrumentation
  - Types of mass spectrometers
  - Measurement modes: Mass spectra, Depth profiling, Ion imaging
Analytical Resolution versus Detection Limit

- Physical limit for 0.3 nm Sampling Depth
- Physical limit for 3 nm Sampling Depth
- Physical limit for 30 nm Sampling Depth

Detection Range (Atoms/cm²)
- 100 at%
- 10 at%
- 1 at%
- 0.1 at%
- 100 ppm
- 10 ppm
- 1 ppm
- 1 ppb
- 10 ppb
- 100 ppb
- 100 ppt
- 10 ppt

Analytical Spot Size
- 0.1 nm
- 1 nm
- 10 nm
- 100 nm
- 1 μm
- 10 μm
- 100 μm
- 1 mm
- 1 cm

Techniques:
- Imaging
- RTX
- ICP
- TGA/DTA/DC
- GAMS
- GSMS
- InG

Chemical bonding/molecular information
Elemental information
Imaging information
Thickness and Density information only (no composition information)
Physical Properties

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Secondary Ion Mass Spectrometry

**Diagram:**
- **ION SOURCE**
- **ENERGY ANALYZER**
- **MASS SPECTROMETER**
- **DETECTOR**
- **SAMPLE**
- **SECONDARY IONS**
- **IMAGE**

**Graphs:**
- Mass spectrum showing elements like Na, Cr, ZnO, ZnO₂.
- Depth profile graph showing atomic concentration (cm⁻³) against depth (μm) for Si₀.₇Ge₀.₃.

**Equations:**
- Counts/sec
- Mass (AMU)
- Atomic concentration (cm⁻³)
- Depth (μm)
SIMS – Basic principle

- Ion source
- Mass spectrometer
- Sputter time (sec)
- Intensity (counts/sec)
- Primary beam
- Secondary beam
Characteristic features

- Quantitative chemical analysis
- High detection sensitivity
  - $10^{16} - 10^{12}$ atoms/cm$^3$ (ppm-ppb)
  - Can measure H
- Large dynamic range
  - > 5 orders of magnitude
- Very high depth resolution
  - Resolution < 20 Å can be obtained
- Ion microscopy
  - Lateral resolution < 0.5 μm
    (NanoSIMS ~ 60nm)

But,
- Limited to concentration <1-5%
- Samples must be vacuum compatible
- Samples must be partially conductive
- Destructive technique
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SIMS – Basic principle

- Ion source
- Primary beam
- Secondary beam
- Mass spectrometer

Graph:
- X-axis: Sputter time (sec)
- Y-axis: Intensity (counts/sec)

Legend:
- 0
- 10
- 100
- 1000
- 10000
Energy is transferred from the energetic primary ions to atoms in the sample. Some of these receive enough energy to escape the sample.

Primary ions are accelerated by an applied sample voltage.

Ion – solid interaction
Sputtering

Sputtering Yield:
number of sputtered atoms per incoming ion

\[
S(E_i) = \frac{K_{it}}{U_0} S_n \left( \frac{E_i}{E_{it}} \right)
\]

Sputtering is a multiple collision process involving a cascade of moving target atoms, this cascade may extend over a considerable region inside the target.

Nuclear stopping cross-section:

\[
S_n(\xi) = 0.5 \ln(1 + \xi) / \left\{ \xi + (\xi / 383)^{3/8} \right\}
\]

\[
E_{it} = \left( 1 + \frac{M_i}{M_t} \right) Z_i Z_t \left( Z_i^{2/3} + Z_t^{2/3} \right)^{1/2} / 32.5 \quad [\text{keV}]
\]

\[
K_{it} \approx \left( Z_i Z_t \right)^{5/6} / 3 \quad \text{for} \quad 0.05 \leq Z_i Z_t \leq 5
\]

\[ M_i, Z_i: \text{Ion mass and atomic number} \]
\[ M_t, Z_t: \text{Target mass and atomic number} \]
\[ U_0: \text{Surface escape barrier in eV} \]
\[ E_i: \text{Ion energy} \]
Sputtering

- Dependence of ion yield

![Graph showing sputtering yield vs. energy](image)

- Dependence of target on sputtering yield: \((\text{Si}_{1-x}\text{Ge}_x)\)

![Graph showing normalized ion yield vs. Ge content](image)

- Sputtering of polycrystalline Fe surface
- The erosion rate is different for the different grains: Sputtering yield vary with the crystal orientation
Sputtering

• Example of sputtering yield:

Current: 200 nA
Sputtering time: 700 sec

200 µm
Sputtering

• Example of sputtering yield:

Current: 200 nA
Sputtering time: 700 sec

Material removed: $1 \times 200 \times 200 \, \mu^3 = 4 \times 10^{-8} \, \text{cm}^3 \approx 2 \times 10^{15} \, \text{atoms}$

Incoming ions: $200 \times 10^{-9} \, \text{A} \times 6.24 \times 10^{18} \, \text{ions/C} \times 700 \, \text{sec} = 9 \times 10^{14} \, \text{ions}$

Sputtering Yield = 2.2 atoms/ion
Energy distribution of secondary ions

- Accelerated further (5kV) by an external field in SIMS
Ionization

- **Ion yield/ionization efficiency**: The fraction of sputtered ions that becomes ionized
- Ion yield can generally not be predicted theoretically
- Ion yield can vary by several orders of magnitude depending on element and chemistry of the sputtered surface
- Oxygen on the surface will increase positive ion yield
- Cesium on the surface will increase negative ion yield
Ionization

Positive Ion Yield \( \propto \exp\left(- C^+ (E_i - \phi) / v \right) \)

Negative Ion Yield \( \propto \exp\left(- C^- (\phi - A) / v \right) \)

C\(\pm\): Constants

\(v\): velocity perpendicular to surface

\(\phi\): work function

\(A\): Electron affinity (eV)

\(E_i\): Ionization potential (eV)

\(C^+\): Positive secondary

\(C^-\): Negative secondary

\(\phi\): Work function

\(A\): Electron affinity

\(E_i\): Ionization potential

\[\text{Table of Elements}\]

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Ionization

Mass spectrum of ZnO, Zn peaks

Positive mode

Negative mode

$^{64}\text{Zn}$ (48.6%)

$^{66}\text{Zn}$ (27.9%)

$^{67}\text{Zn}$ (18.8%)

$^{70}\text{Zn}$ (0.6%)

$^{64}\text{Zn}$, $^{66}\text{Zn}$, $^{68}\text{Zn}$, $^{70}\text{Zn}$ peaks
Ionization

- Limits the quantification procedure:
  - SIMS is mainly a tool for measuring small concentrations in a given matrix
General Yield

• Measured intensity $I_t$ for a specific target atom

$$I_t = I_P Y [C_t] \gamma_t T$$

$I_P$: Primary ion current
$Y$: Sputtering yield
(number of sputtered particles per impinging primary ion)
$[C_t]$: Concentration of species $t$
$\gamma_t$: Secondary ion formation and survival probability
(ionization efficiency)
$T$: Instrument transmission function

$\gamma_t$ is highly dependent on species and matrix
General Yield

- Measured intensity $I_t$ for a specific target atom

$$I_t = I_P Y [C_t] \gamma_t T$$

$$[C_t] = RSF \cdot I_t$$

From calibration

- $I_P$: Primary ion current
- $Y$: Sputtering yield
- $[C_t]$: Concentration of species $t$
- $\gamma_t$: Secondary ion formation and survival probability (ionization efficiency)
- $T$: Instrument transmission function
Outline

• Basic principle and characteristic features
• Physical processes
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  – Ionization
• SIMS instrumentation
  – Types of mass spectrometers
  – Measurement modes: Mass spectra, Depth profiling, Ion imaging
The SIMS instrument

Focused ion beam

Mass Spectrum

Depth Profile

Image
Types of SIMS instrument

- Instruments are usually classified by the type of mass spectrometer:
  - Quadrupole
    - Low impact energy
  - Time of Flight
    - Simultaneous detection of many elements
    - High transmission
    - Measures large molecules
  - Magnetic Sector
    - High mass resolution
    - High transmission
    - Low detection limit

MiNaLab/NICE since 2012

UiO-MiNaLab since 2004
Quadrupole SIMS

Physical Electronics

Quadrupole Mass Analyzer
90° Electrostatic Analyzer
Electron Multiplier Detector
Ion Source
Sample Viewing Microscope
Electron Gun
Sample Manipulator
Ion Pump

\[ \Delta x = U \]
\[ rf = V \cos \omega \]
Time Of Flight-SIMS (TOF-SIMS)
TOF-SIMS

• Analysis is performed by a short pulse length and small spot size ion beam
• Sputtering is achieved by a beam of reactive species (e.g. $O_2$ or Cs)
• Sputter beam and analysis beam conditions are optimized independently!
Magnetic sector - mass spectrometer

Electrostatic sector analyser

\[ qE_0 = \frac{mv^2}{r_e} \]

Magnetic sector analyser

\[ qvB = \frac{mv^2}{r_m} \]

Centripetal force:

\[ \mathbf{F} = -\frac{mv^2}{r} \mathbf{r} \]

Lorenz’ force:

\[ \mathbf{F} = qE + q(\mathbf{v} \times \mathbf{B}) \]
Secondary ion mass spectrometry

\[ \frac{m}{q} = \left( \frac{r_m B}{r_e E_0} \right)^2 \]
Magnetic sector vs. TOF-SIMS

- Superior detection limit (~ppb)
- Better depth limit (>50um)
- Better mass resolution
- Faster depth profiling

- Better lateral resolution (<130nm)
- Simultaneous mass spectra
- Measures large molecules (<10 000 amu)
- Better for insulating samples
- Can provide molecular information
Instrumentation:
- ion sources
- electrostatic sector analyser
- magnetic sector analyser
- sample chamber
- detectors
Mass spectrum of a ZnO-sample with traces of Li, Na, K, and Cr.
# Isotopic abundance

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Secondary intensity (cps)

Mass (AMU)

Mass spectrum of graphite

91.6% 8.4%
Mass interference

- Several ions/ionic molecules have similar mass to charge ratio:

\[
\begin{align*}
10^\text{B} & - 30^\text{Si}^{3+} & = 10 \text{ amu} \\
75^\text{As} & - 29^\text{Si}30^\text{Si}16^\text{O} & = 75 \text{ amu} \\
31^\text{P} & - 30^\text{Si}1^\text{H} & = 31 \text{ amu}
\end{align*}
\]

The measured SIMS intensity is the sum of the intensity from each element.
Mass interference

• Several ions/ionic molecules have similar mass to charge ratio:

\[ \frac{m}{q} = \left( \frac{r_m B}{r_e E_0} \right)^2 \]

\[ ^{10}\text{B} - ^{30}\text{Si}^{3+} \]
Isotopic abundance

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Mass spectrum of graphite

- Ne*: 91.6%
- K*: 8.4%
Mass interference

- Several ions/ionic molecules have similar mass to charge ratio:

\[ ^{10}\text{B} - ^{30}\text{Si}^{3+} \]

\[ ^{75}\text{As} - ^{29}\text{Si}^{30}\text{Si}^{16}\text{O} \]

\[ \frac{m}{q} = \left( \frac{r_m B}{r_e E_0} \right)^2 \]

Monitor \( ^{11}\text{B} \)
Energy selection

electrostatic sector analyser

Energy selection slit

Increasing kinetic energy

Secondary beam

\[ qE_0 = \frac{mv^2}{r_e} \]

Ejection energy (eV)

log (ion intensity)

\[ ^{75}\text{As} \]

\[ ^{29}\text{Si}^{30}\text{Si}^{16}\text{O} \]
Mass interference

• Several ions/ionic molecules have similar mass to charge ratio:

\[ ^{10}\text{B} - ^{30}\text{Si}^{3+} \]

Monitor \(^{11}\text{B} \)

\[ ^{75}\text{As} - ^{29}\text{Si}^{30}\text{Si}^{16}\text{O} \]

Energy selection

\[ ^{31}\text{P} - ^{30}\text{Si}^{1}\text{H} \]
High mass resolution

magnetic sector analyser

Discriminating between $^{31}\text{P}$ and $^{30}\text{Si}^1\text{H}$:

$M(^{31}\text{P}) = 30.973761$

$M(^{30}\text{Si}^1\text{H}) = 30.98160$

$qvB = \frac{mv^2}{r_m}$

Exit slit

$\Delta M/M = 4000$
Mass interference

- Several ions/ionic molecules have similar mass to charge ratio:

- $^{10}\text{B} - ^{30}\text{Si}^{3+}$  Monitor $^{11}\text{B}$

- $^{75}\text{As} - ^{29}\text{Si}^{30}\text{Si}^{16}\text{O}$  Energy selection

- $^{31}\text{P} - ^{30}\text{Si}^{1}\text{H}$  High mass resolution
Isotopes

Mass spectrum of graphite

High mass resolution

Primary isotopes:
- Carbon: 12 (98.9%), 13 (1.1%)
- Hydrogen: 1 (91.6%), 2 (8.4%)

Secondary isotopes:
- Nitrogen: 14
- Oxygen: 16
- Fluorine: 19
- Argon: 40
- Potassium: 39
- Calcium: 40
Depth resolution

Limited by

- Surface roughness
- Sputter rate
  - For large sputter rates or many elements
    • Sputter rate/ measurement cycle
- Primary beam energy
  - 10-15 keV $O_2^+/Cs^+ \rightarrow 5-10$ nm
  - 500 eV $O_2^+ \rightarrow \sim 2$ nm

First 2-10 nm gives an artificial signal (Dynamic SIMS)
Calibration of depth profiles

"Raw" phosphorus profile

Depth calibration

Sputter time: 700 sec

Depth: 9310 Å

Erosion rate: 13,3 Å/sec
Calibration of depth profiles

"Raw" phosphorus profile

\[ I_t = I_P Y [C_t] \gamma T = \left( \frac{1}{S} \right) [C_t] \]

\( S \): Sensitivity factor

Concentration calibration

Ion implanted sample:
P dose 1e15 P/cm²

Sensitivity factor:
Relate the intensity to atomic concentration

\[ S = \frac{\text{Dose}}{\int I(x) \, dx} \]

Sensitivity factor:
1 count/sec = \(3,4 \times 10^{15}\) P/cm³
Calibration of depth profiles

"Raw" phosphorus profile

Calibrated phosphorus profile

Erosion rate: 13.3 Å/sec

Sensitivity factor:
1 count/sec = 3.4 × 10^{15} P/cm^3
Ion imaging

Intensity recorded as a function of primary beam position

Sample Surface

Distribution of given atoms at the surface
Ion imaging
‘Summary’