Diffusion in Extrinsic Silicon and Silicon Germanium

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Hughes Silvestri, Ian Sharp,
Hartmut Bracht, and Eugene Haller
Berkeley, CA

2002 GOAL: Diffusion measurements on P doped Si to complete comprehensive model of Si diffusion by 9/30/2002.
Motivation

- **Modern device scale**
  (100-nm gate length)
  - Source and drain regions
    - Highly doped: $10^{20}$ atoms/cm$^3$
    - Very shallow: < 30 nm
    - Abrupt profile: 5nm/decade

- **Future device demands**
  (< 100-nm gate length)
  - Source and drain regions
    - Junction depth: < 10 nm
    - Abrupt profile: 2 nm/decade
    - Not yet achievable

- To maintain shallow profile:
  - Control diffusion during further high T (800 -1200 °C) processing steps
    - Understand the Fermi level effect on diffusion and its impact on native defect formation

(P.A. Packan, MRS Bulletin, June 2000)
Our Approach

• Dopant and self-diffusion mediated by native point defects
  \[ D_{Si} = f_I^oC_I^o D_I^o + f_I^+C_I^+ D_I^+ + f_V^-C_V^- D_V^- + K \]
  \( f = \) correlation factor: \( f_V = 0.5, f_I = 0.73 \)
  – Interstitial self-atoms and vacancies
  – Role of native defects in diffusion reactions unresolved

• Device processing can affect native defect properties
  – Ion implantation \( \Rightarrow \) native defect concentration
  – High dopant concentration \( \Rightarrow \) native defect concentration and charge state
  – Effect of non-equilibrium native defect properties on diffusion not fully understood

• Use an isotopically enriched Si heterostructure
  – observation of Si and dopant diffusion simultaneously
### Fermi Level Effect

Heavily doped semiconductors - extrinsic at diffusion temperatures

- Fermi level moves from mid-gap to near conduction (n-type) or valence (p-type) band.

<table>
<thead>
<tr>
<th>Dopant charge state</th>
<th>Native defect charge state</th>
</tr>
</thead>
<tbody>
<tr>
<td>extrinsic n-type</td>
<td>$D_s^+$</td>
</tr>
<tr>
<td>extrinsic p-type</td>
<td>$A_s^-$</td>
</tr>
</tbody>
</table>

- Fermi level shift lowers the formation enthalpy, $H_F$, of the charged native defect

$$C_{V,I}^{eq} = C_{Si}^o \exp \left( \frac{S_{V,I}^F}{k_B} \right) \exp \left( - \frac{H_{V,I}^F}{k_B T} \right), H_{V,I}^F = H_{V,o}^F - (E_F - E_{V-I})$$

- Increase of $C_{I,V}$ affects Si self- and dopant diffusion

$$D_{imp} = C_I D_I + C_V D_V$$

#### Extrinsic p-type

- $E_c$
- $E_v$
- $V_{--/-}$ at 0.11 eV
- $V_{-/o}$ at 0.57 eV
- $V_{o/+}$ at 0.05 eV
- $V_{+/++}$ at 0.13 eV
- $I_{o/+}$ at 0.35 eV

#### Extrinsic n-type

- $E_c$
- $E_v$
- $V_{--/-}$ at 0.11 eV
- $V_{-/o}$ at 0.57 eV
- $V_{o/+}$ at 0.05 eV
- $V_{+/++}$ at 0.13 eV
- $I_{o/+}$ at 0.35 eV
Approach: Isotopically enriched Si heterostructure

- Alternating layers of natural Si (92.2% $^{28}\text{Si}$, 4.7% $^{29}\text{Si}$, 3.1% $^{30}\text{Si}$) and $^{28}\text{Si}$ (99.95% $^{28}\text{Si}$) (UHV-CVD grown at Lawrence Semiconductor Research Laboratory, Tempe, AZ)

- Ion implanted amorphous natural Si cap layer used as dopant source to suppress transient enhanced diffusion (TED) (MBE grown at University of Aarhus, Denmark)

- Stable isotope structure allows for simultaneous Si and dopant diffusion studies
Extrinsic dopant diffusion experiments

Dopant source: ion implantation in a-Si layer:
- **p-type** - Boron - interstitially assisted
- **n-type** - Arsenic - interstitial + vacancy assisted
  - Phosphorus - interstitially assisted

Diffusion: samples sealed in silica ampoules and annealed between 850 °C and 1100 °C

Secondary Ion Mass Spectrometry (SIMS) concentration profiles of $^{11}\text{B}$, $^{28}\text{Si}$, and $^{30}\text{Si}$ (Accurel Systems, CA)

Computer modeling of dopant and $^{30}\text{Si}$ concentration profiles
- comparison to experimental results
- determination of mechanism and diffusivity
Extrinsic n-type: As diffusion results

- **Implant As into amorphous layer:** $0.7 \times 10^{16}$ cm$^{-2}$ at 130 keV, $1.0 \times 10^{16}$ cm$^{-2}$ at 160 keV
- **Anneal:** $950 \, ^\circ\mathrm{C} < T < 1100 \, ^\circ\mathrm{C}$
- **Secondary Ion Mass Spectrometry (SIMS)**

Reactions for simulation:
- **Vacancy mechanism**
  \[(AsV)^0 \leftrightarrow As_s^+ + V^-\]
- **Interstitialcy mechanism**
  \[(AsI)^0 \leftrightarrow As_s^+ + I^0 + e^-\]

$V^-$ and $I^0$ control Si self-diffusion under n-type extrinsic doping.
Extrinsic n-type: As simulation results

No supersaturation of $I^0$ or $V^-$ during As diffusion

Enhancement of As and Si self-diffusion under extrinsic conditions is entirely due to Fermi level effect.
Native defect contributions to Si self-diffusion

Diffusion coefficients of individual components add up accurately:

\[ D_{Si}(n_i)_{tot} = f_{I^0} C_{I^0} D_{I^0} + f_{I^+} C_{I^+} D_{I^+} + f_{V^-} C_{V^-} D_{V^-} = D_{Si}(n_i) \]

(Bracht, et al., 1998)
Extrinsic n-type: P diffusion results

- Phosphorus diffusion - Interstitially assisted I⁻ concentration enhanced

Annealed 950 °C for 30 hrs

Reduced Si self-diffusion enhancement under extrinsic conditions
Diffusion in SiGe alloys: Isotope heterostructure

- SiGe alloys: important new material for next generation electronic devices.
- Understanding dopant and native defect diffusion properties important for SiGe alloy device engineering.
  - Limited knowledge of diffusion mechanisms in SiGe alloys

- Use same experimental technique to study self-diffusion in $\text{Si}_{1-x}\text{Ge}_x$ alloys.
- Proposed isotope heterostructure (MBE-grown):

<table>
<thead>
<tr>
<th>Depth (nm)</th>
<th>Composition</th>
</tr>
</thead>
<tbody>
<tr>
<td>200</td>
<td>nat. $\text{Si}_{1-x}\text{Ge}_x$</td>
</tr>
<tr>
<td>400</td>
<td>$^{28}\text{Si}_{1-x}^{70}\text{Ge}_x$</td>
</tr>
<tr>
<td>200</td>
<td>nat. $\text{Si}_{1-x}\text{Ge}_x$</td>
</tr>
<tr>
<td></td>
<td>SiGe graded buffer layer</td>
</tr>
<tr>
<td></td>
<td>Si substrate</td>
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Proposed as-grown depth profile
Current / Future Developments

- **Enriched Silicon Isotope Heterostructure**
  - Simultaneous analysis of Si self-diffusion and dopant diffusion.

- **Boron diffusion** - via the kick-out mechanism - $B_i^0 \leftrightarrow B_s^- + I^{0,+}$

- **As diffusion** - via interstitialcy and vacancy mechanisms:
  
  $$(AsI)^0 \leftrightarrow As_s^+ + I^0 + e^- \quad (AsV)^0 \leftrightarrow As_s^+ + V^-$$

- **Determine contributions of native defect charge states to Si self-diffusion.**
  - Activation enthalpy for self-diffusion due to $I^0, I^+, V^-$

D_{Si}(I^0): Q=(4.32 \pm 0.15) eV, \quad D_{Si}(I^+): Q=(4.74 \pm 0.13) eV, \quad D_{Si}(V^-): Q=(5.18 \pm 0.13) eV

**2002 and 2003 Goals:**

- **Diffusion measurements on P doped Si to complete comprehensive model of Si diffusion by 9/30/2002.**

- **Use isotope multilayer structure for diffusion studies in SiGe by 9/30/2003.**