Properties of Vacancies in Silicon Determined from Laser-Annealing Experiments

Peter Pichler

Fraunhofer IIS
Institut Integrierte Schaltungen
Contents

Introduction
Experimental Conditions
Model and Simulation Strategy
Results and Discussion
Conclusions
Contents

Introduction
Experimental Conditions
Model and Simulation Strategy
Results and Discussion
Conclusions
### Introduction (I)

<table>
<thead>
<tr>
<th>Diffusion</th>
<th>Selfdiffusion and dopant diffusion in silicon requires the interaction with intrinsic point defects:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Vacancies</td>
<td>Missing silicon atoms</td>
</tr>
<tr>
<td>Self-Interstitials</td>
<td>Silicon atoms on sites between regular lattice sites</td>
</tr>
<tr>
<td>Important parameters</td>
<td>Equilibrium concentration</td>
</tr>
<tr>
<td></td>
<td>Diffusion coefficient</td>
</tr>
<tr>
<td>Determination</td>
<td>No reliable information from direct methods:</td>
</tr>
<tr>
<td></td>
<td>Simmons-Balluffi experiment, quenching</td>
</tr>
<tr>
<td>Indirect methods:</td>
<td></td>
</tr>
<tr>
<td></td>
<td>• Formation of extended defects during crystal growth</td>
</tr>
<tr>
<td></td>
<td>• Dopant diffusion under non-equilibrium conditions</td>
</tr>
<tr>
<td></td>
<td>• Metal diffusion</td>
</tr>
</tbody>
</table>
Introduction (II) - Vacancy Equilibrium Concentration

8 orders of magnitude
Introduction (III) - Vacancy Diffusion Coefficient

10 orders of magnitude
Introduction (IV) - Reasons for the Discrepancies

What is the problem? Diffusion experiments are usually only sensitive to the products $D_V^*C_v^{eq}$ and $D_i^*C_i^{eq}$

Recombination of I and V results in an effective diffusion coefficient

Interactions with carbon reduce the effective diffusivity of self-interstitials

There may be interactions with other impurities with similar effects
Introduction (V) - Quenching

What is the problem? Vacancies and self-interstitials diffuse in silicon already at room temperature
                 Vacancies and self-interstitials will diffuse to the surface or form complexes
                 Whatever remains is hard to identify (sometimes related to iron rather than to intrinsic point defects)

Exception Work of Chantre et al.
                 Complexes identified as E-centers (vacancy-phosphorus pairs)
Contents

Introduction

Experimental Conditions

Model and Simulation Strategy

Results and Discussion

Conclusions
Experimental Conditions (I) - Heating

Chantre et al.
Physica B 116, 547 (1983),

Scanning cw argon laser annealing
95% of power needed for local melting
Beam diameter 50 µm
Scan speeds between 1 and 50 cm/s

Temperature gradient at surface:
-120 K/µm
Experimental Conditions (II) - Depth Profiling

DLTS measurements of an acceptor state at $E_c - 0.45 \text{ eV}$

Identified as E-center (Phosphorus-vacancy pair)
Contents

Introduction
Experimental Conditions
Model and Simulation Strategy
Results and Discussion
Conclusions
Model and Simulation Strategy (I) - General Concept

During heating-up

\[ C_V < C_V^{eq}, C_I < C_I^{eq} \]

 UITableViewCell

- Vacancies and self-interstitials are generated at the surface and diffuse into the bulk

After the peak temperature is exceeded

\[ C_V > C_V^{eq}, C_I > C_I^{eq} \]

- Vacancies and self-interstitials recombine
- Vacancies and self-interstitials diffuse to the surface
- Vacancies form complexes with phosphorus atoms

Important reactions

\[ V + P \leftrightarrow E \]

\[ I + V \leftrightarrow 0 \]

\[ I + E \leftrightarrow P \]
Model and Simulation Strategy (II) - Temperature Gradients

Ludwig-Soret Effect

\[ J_{I,V} = -D_{I,V} \nabla C_{I,V} + Q^* C_{I,V} D_{I,V} \frac{q}{kT^2} \nabla T \]

$Q^*$

Heat of transport
needed especially in models for crystal growth

Assumptions

Ludwig-Soret Effect is negligible

or

$Q^* q = E^f$

Simulations with $Q^*$

\[ J_{I,V} = -D_{I,V} C_{eq}^{I,V} \nabla \frac{C_{I,V}}{C_{eq}^{I,V}} \]
Model and Simulation Strategy (III) - Important Parameters

Temperature dependence

\[ X(T) = X(1550 \text{ K}) \cdot \exp\left(\frac{E_X}{k} \cdot 1550 \text{ K} - \frac{E_X}{kT}\right) \]

- \( D_I(1550 \text{ K}), E^m_I \)
  - from literature (negligible influence)
- \( C_i^{eq}(1550 \text{ K}), E^f_I \)
  - from literature (negligible influence)
- \( E^m_V \)
  - 0.35 eV from literature (negligible influence)
- \( E^f_V \)
  - varied form 3.8 to 4.6 eV (contains all literature values)
- \( E_B \) (binding energy of E-center)
  - varied form 0.85 to 2.2 eV (contains all literature values)
- \( D_V(1550 \text{ K}) \)
  - from backward simulation
- \( C_v^{eq}(1550 \text{ K}) \)
  - from backward simulation
Results and Discussion (I) - Influence of Self-Interstitials

<table>
<thead>
<tr>
<th>Self-interstitial parameters</th>
<th>No influence found</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reasoning</td>
<td>Recombination between I and V or I and E simply too slow</td>
</tr>
<tr>
<td></td>
<td>Estimated time constant 1.5 ms</td>
</tr>
<tr>
<td></td>
<td>Only about 0.2 s above 1000 °C</td>
</tr>
</tbody>
</table>
Results and Discussion (II) - Parameter Extraction

Increase in $C_{eq}^V$
  shifts the curve upwards

Increase in $D_V$
  makes the curve broader

Both parameters can be determined individually
Results and Discussion (III) - Optimum Values
Results and Discussion (IV) - $C_{eq\gamma}$

[Graph showing the relationship between temperature (°C) and vacancy equilibrium concentration (cm$^{-3}$). The graph includes data points and lines indicating various studies and authors (e.g., Fairfield & Masters, Yoshida & Sallo, Bracht et al., et al.).]

---

This work

---

Fraunhofer Institut
Integrierte Schaltungen
Results and Discussion (V) - $D_V$

![Graph showing $D_V$ vs. temperature and 1000/Temperature (1/K)]

- Fairfield & Masters
- Masters & Corey
- Voronkov
- Chantre et al.
- Tan & Gösele
- Wada & Inoue
- Budil et al.
- Brabec et al.
- Griffin
- Zimmermann et al.
- Budil et al.
- Griffin et al.
- Zimmermann
- Law
- Dunham
- Park & Law
- Okino
- Okino
- Gossmann et al.
- Habu et al.

- Okino & Onishi
- Bracht et al.
- Ghaderi et al.
- Ghaderi et al.
- Shimizu et al.
- Habu & Tomiura
- Mogi et al.
- Knowlton et al.
- Sinno et al.
- Chakravarthi & Dunham
- Waiton et al.
- Giese et al.
- Giese et al.
- Bornberger et al.
- Voronkov & Falster
- Voronkov & Falster
- Scholz et al.
- Falster et al.
- Falster et al.
- Ngau et al.

---

This work

---
Results and Discussion (VI) - Fraction of Self-Diffusion via I

\[ f_I \] vs. Temperature (°C)

- Morehead et al.
- Gósele and Tan
- Griffin
- Habu et al.
- Okino
- Okino & Onishi
- Bracht et al.
- Ghaderi et al.
- Habu & Tomiura
- Knowlton et al.
- Sinno et al.
- Walton et al.
- Okino et al.
- Chakravarthi & Dunham
- Bracht et al.
- Bracht et al.
- Ural et al.
- Dornberger et al.

--- This work
# Results and Discussion (VII) - Uncertainties

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature profile</td>
<td>Just estimated in the original work</td>
</tr>
<tr>
<td>Geometry of scanning beam</td>
<td>3-D problem including overlap of scans</td>
</tr>
<tr>
<td>E-center profile</td>
<td>Accuracy of measurements, no points near surface</td>
</tr>
</tbody>
</table>


Contents

Introduction
Experimental Conditions
Model and Simulation Strategy
Results and Discussion
Conclusions
Conclusions

Laser annealing
Fast quenching process, no significant interactions with self-interstitials

DLTS
Allows unambiguous identification of vacancy complexes

Extracted values
Independent determination of $C_{eq}^V$ and $D_V$
Support values predicted from crystal growth

But
Problems with the process temperature and with the scanning of the beam
## Conclusions

<table>
<thead>
<tr>
<th>Laser annealing</th>
<th>Fast quenching process, no significant interactions with self-interstitials</th>
</tr>
</thead>
<tbody>
<tr>
<td>DLTS</td>
<td>Allows unambiguous identification of vacancy complexes</td>
</tr>
<tr>
<td>Extracted values</td>
<td>Independent determination of $C_{eq}^V$ and $D_V$</td>
</tr>
<tr>
<td></td>
<td>Support values predicted from crystal growth</td>
</tr>
<tr>
<td>But</td>
<td>Problems with the process temperature and with the scanning of the beam</td>
</tr>
</tbody>
</table>