RTA Simulation Using \(</311>\) Cluster Models
• Standard Diffusion Models in Athena
  • Fermi
  • Two.Dim
  • Full.Cpl
  • Simple Point Defect Damage
• Advanced Diffusion Models in Athena
  • Implant Damage
  • Stanford High Concentration Model
  • Peter Griffins RTA Model
    • <311> Cluster Injection
    • Dislocation Loop Sinks
• Examples and Calibration of Advanced Diffusion Models
• Fermi - Simple Numerical model with constant level of point defects (default)
• Two.Dim - Two Dimensional Distribution of Point Defects
• Full.Cpl - Simple Fully Coupled Diffusion Model
• Simple Point Defect Damage
• Fermi
  • FERMI is Default Model, good for:
    • Low or moderate concentrations
    • Low level of point and/or extended defects
    • No or very little oxidation/silicidation
  • Tuning parameters: Dix.0/Dip.0, but not recommended for wide variation
Standard Diffusion Models (con’t)

Figure 1. FERMI diffusion model.
Two.Dim - Two Dimensional Distribution of Point Defects

- Method TWO.DIM solves two-dimensional distribution of point defects
- Takes into account point defect generation during implant or oxidation
- Allows coupling of point defects and dopant diffusion
- Suitable for oxidation/silicidation enhanced diffusion and low dose implants
- Tuning parameters for OED:
  - Point defect generation during oxidation Theta.0
  - Point defect surface recombination Ksurf.0
• FULL.CPL - Simple Fully Coupled Diffusion Model
  • Fully coupled (FULL.CPL) model takes into account coupling between point defects and individual dopants
  • It is not completely comprehensive because it ignores reactions between defects and defect-dopant pairs
  • Can be used for simulation of various transient diffusion phenomena including RTA, low-temperature diffusion, co-diffusion of dopants (emitter push effect)
  • Figure 2 shows that most of transient enhanced diffusion happens during first 2-5 seconds of a low-temperature anneal
Standard Diffusion Models (con’t)

Figure 2. Low temperature boron transient enhanced diffusion.
Current Diffusion Models (con’t)

• Simple Point Defect Damage
  • Damage Described as a simple distribution of both types of Point Defects
    • Command line flag:
      ▪ Unit.damage
    • Command line scaling parameter:
      ▪ Dam.factor=0.01 (default)
      ▪ Dam.factor is a good tuning parameter, given this limited description of damage
  • The figure on the following page shows effect of implant damage factor on RSCE
Current Diffusion Models (con’t)

Figure 3. Effect of implant damage on threshold voltage for different gate lengths
Advanced Diffusion Models: Overview

- Extensions to Control Implant Damage Profiles
- Peter Griffin and Scott Crowder Advanced Diffusion Models, Stanford University
  - High Dose Effect extensions to the Fully Coupled Diffusion Model
  - $<311>$ Cluster Distribution with Bulk Point Defect Injection
  - Dislocation Loop Interstitial Sinks
The original FULL.CPL Model does not include the effects of dopant/defect pairs interaction with other defects and with interfaces. The model takes these effects into consideration. The high dose Stanford diffusion model can be specified by the following statement:

```plaintext
METHOD FULL.CPL HIGH.DOSE
```

The main area of application is furnace and RTA diffusion at high concentration levels (above $1020 \text{cm}^{-3}$).
• It was observed that \<311\> cluster distribution is introduced during ion implantation \cite{1}

• The model \cite{2}-\cite{4} suggests that the clusters dissolve in time, injecting point defects as they disappear \cite{2}

• The model considers this transient release of point defects as bulk injection process

• Then dopant diffusion is coupled with the resultant injected interstitials

• Main application: RTA after medium dose implant (LDD profiles)

\begin{enumerate}
    \item C.S. Rafferty, IEDM 93, p. 311
    \item S. Crowder, IEDM 95, p. 427
    \item P.A. Stolk Appl. Phys. Lef v. 66, p. 568, 1995
\end{enumerate}
Interstitials released from <311> clusters are injected into the bulk over a short time period and couple with the dopant.
The model is switched on as follows

METHOD CLUSTER.DAM FULL.CPL

The number of interstitials released into silicon is

\[ l_r = f(x) \left( \frac{1}{t} \right) \exp \left( -\frac{t}{\tau} \right) \]

\( t \) is the diffusion time;

\( f(x) \) is the as-implanted profile of <311> clusters which can be scaled to the dopant profile using the CLUSTER statement;

\( \tau \) is the time constant (in seconds) calculated

\[ \tau = TAU.311.0 \exp \left( -TAU.311.E/KT \right) \]
Dislocation Loop Sinks

- Dislocation Loop Interstitial Sinks
  - This model is a first order approximation for dislocation loop interaction with point defects
  - Point defects recombine faster in the region of the loops which acts as a static interstitial sink
  - The model is switched on as follows:
    ```
    METHOD ILOOP.SINK FULL.CPL
    ```
  - Recombination rate of interstitials is proportional to local non-equilibrium interstitial concentration
    
    \[ R_{\text{loop}} = \text{damalpha} \cdot (C_I - C_I) \]

    where \( \text{damalpha} \) is specified on the INTERSTITIAL statement.
Dislocation Loop Sinks (con’t)

Concentration

Doping Profile

Cluster Profile (Initially Scaled to the Implant)

Injected Interstitials

Dislocation Loop Sinks

Max.loop.conc

Min.loop.conc

Amorphous Region

Interstitial Recombination

C_t

Depth
• Extensions to Control Implant Damage Profiles
  • In order to implement advanced diffusion models more flexible control of Implant Damage generation is needed
  • Several extensions to the Unit Damage model are included
  • 
    -<311> cluster distribution is sealed to ion implant profile using:
      CLUSTER CLUST.FACT=1.4  MIN.CLUST = 1e17
      MAX.CLUST = 1e19  PHOS
  • Region where dislocation loop recombination takes place is also related to ion implant profile:
    DISLOC min.loop.c = 1e15  max.loop.c = 1e16  PHOS
Implant Damage (con’t)

Figure 4. Distribution of phosphorus and defect after ion implantation.
Applications and Calibration of the <311> Cluster Model

• <311> Cluster Model is applicable to all processes which involve transient enhanced diffusion
• TED is anomalous diffusion which is driven by a excessive amount of point defects generated during ion implantation
• The dopant diffusivity during TED could be very large up to several thousand times higher that normal diffusion
• TED process time varies with temperature from a portion of a second up to hundreds of hours
### Applications and Calibration of the $<311>$ Cluster Model (con’t)

<table>
<thead>
<tr>
<th>Anneal Temperature</th>
<th>Time to Complete 95% of TED</th>
</tr>
</thead>
<tbody>
<tr>
<td>600</td>
<td>390 hours</td>
</tr>
<tr>
<td>700</td>
<td>3.3 hours</td>
</tr>
<tr>
<td>750</td>
<td>30 minutes</td>
</tr>
<tr>
<td>800</td>
<td>3.7 minutes</td>
</tr>
<tr>
<td>850</td>
<td>43 seconds</td>
</tr>
<tr>
<td>900</td>
<td>8.3 seconds</td>
</tr>
<tr>
<td>950</td>
<td>1.9 seconds</td>
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<tr>
<td>1000</td>
<td>0.48 seconds</td>
</tr>
<tr>
<td>1050</td>
<td>0.13 seconds</td>
</tr>
</tbody>
</table>

Table 1. Simulated length of transient enhanced diffusion versus anneal temperature based on $<311>$ cluster decay kinetics, for a 50eV, 1e14 implant.
• If all excess or free potential defects are generated right after implant then TED process would be always very short because of fast defect recombination and diffusion (see Figure on page 8 for FULL.CPL model)

• Therefore, only when <311>-CLUSTERS are taken into consideration proper time temperature relations for TED process can be achieved

• The next two figures show that interstitials released from <311> clusters are responsible for TED of “buried” boron marker layer
Applications and Calibration of the <311> Cluster Model (con’t)

Figure 5. RTA diffusion of boron and phosphorus.
Applications and Calibration of the $<$311$>$ Cluster Model (con’t)

Figure 6. Movie of interstitial generation, recombination and re-distribution.
The following examples based on experiments of M. Giles “J. Electronchem Soc.” v.138, p1160 (1991) shows that the <311> - cluster model adequately describes RTA diffusion for medium dose phosphorus implant. It is very important for LDD engineering of modern MOS devices (next figure)

Simulation is very close to experiment which shows that TED extends over several minutes at low temperatures ~ 800°C

The second figure shows that the time constant of cluster dissolution τ should be main parameter when calibrating the <311>-cluster model
RTA Simulation Matched to Experimental Data in [3]

Figure 7. RTA simulation matched to experimental data in [3].
Simulation From Figure 1 with Lower TAU.311.0

Figure 8. Simulation From from Figure 7 with lower TAU.311.0.
Conclusion

- The <311> cluster model developed at Stanford University is implemented into Athena
- This model allows simulation of TED effects over a wide range of temperatures and diffusion times
- It can be successfully used for simulation of RTA processes as well as temperature thermal cycles which are widely used in modern MOS technologies