Simulation of defect formation in different hadron irradiation environments

Mika Huhtinen

CERN EP

For details see ROSE/TN/2001-02, submitted to NIM
Motivation

Reasons for this simulation study

No really microscopic NIEL simulation exists

NIEL scaling seems to be often misinterpreted.

Modern simulation codes allow to attempt a truly microscopic NIEL calculation.

Experimental data from the ROSE (CERN RD48) collaboration shows NIEL violation in some cases.

Especially,

Oxygen enriched silicon behaves differently under neutron and proton irradiation when compared to standard Si.

Understanding of possible NIEL violation and effects of oxygen can be significant for LHC and other forthcoming experiments.
Recoil spectra of $>20$ MeV hadrons on Si

- 19 MeV neutron ($Z \geq 10$)
- 20 MeV neutron ($Z \geq 10$)
- 60 MeV neutron ($Z \geq 10$)
- 200 MeV neutron ($Z \geq 10$)
- 200 MeV neutron ($2 < Z < 10$)

Typical recoil energies up to few tens of MeV
Stopping of nuclear fragments in Si

**Calculated dE/dx for various ions in Si**

NIEL is important only at low ion energies → saturation
Schematic of Atomic Cascade

- Phonons
- Interstitials
- Dislocations
TRIM simulation of full atomic cascade

Generate explicitly all recoils above dislocation threshold $E_D = 20$ eV

\[ \downarrow \]

Exact knowledge of all vacancy and interstitial positions (except lattice structure) created by the h-Si interaction

\[ \begin{align*}
Z = 14, \ A = 28 \\
E = 50 \text{ keV} \\
505 \text{ Vacancies}
\end{align*} \]
Vacancy densities at high fluences

Projections of vacancy positions

Project through 1 $\mu$m of depth after fluence $10^{14}$ cm$^{-1}$

10 MeV Proton  
24 GeV/c Proton  
1 MeV Neutron

10 MeV protons  
Mainly isolated point defects (remember depth dimension)

24 GeV/c protons  
Isolated point defects and clusters

1 MeV neutrons  
Almost only clusters
NIEL of Neutrons

DEFINEd value for 1 MeV neutrons:
NIEL Xsec = 95 MeV mb
Agreement with previous work / expt. at high energy
Consistent with pion data at $\Delta$-resonance
Lower than older work for low-energy protons.
Partitioning of NIEL

NIEL itself is further partitioned into

- dislocations (≈20 eV per case)
- phonons (all collisions transferring less than 20 eV)

**Kinchin-Pease:**

\[
\begin{align*}
\nu &= 1 & \text{if } E_D < E_\nu < 2.5E_D \\
\nu &= \frac{E_\nu}{2.5E_D} & \text{if } E_\nu > 2.5E_D
\end{align*}
\]

\[
E_\nu=\text{NIEL}, \quad \nu=\text{Number of dislocations}.
\]

⇒ 40% of NIEL goes into dislocations (=damage).

**These simulations:**

<table>
<thead>
<tr>
<th></th>
<th>10 MeV proton</th>
<th>24 GeV/c proton</th>
<th>1 MeV neutron</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total NIEL Xsec</td>
<td>292</td>
<td>47.2</td>
<td>76.9</td>
</tr>
<tr>
<td>Phonons</td>
<td>147</td>
<td>27.2</td>
<td>44.1</td>
</tr>
<tr>
<td>Displacements</td>
<td>145</td>
<td>20.0</td>
<td>32.8</td>
</tr>
<tr>
<td>Displace./Total</td>
<td>50 %</td>
<td>42 %</td>
<td>43 %</td>
</tr>
</tbody>
</table>

Possibly slight dependence on type of irradiation
Vacancies and interstitials migrate and recombine with each other and with impurities

Different recombination probabilities $P(X, Y)$ for all defect (impurity) pairs, i.e. reaction $X + Y \rightarrow XY$

Relative formation rate of defect $XY$:

$$\frac{P(X, Y)[Y]}{\sum_i P(X, Z_i)[Z_i]}$$

$[Y], [Z_i]$ = concentration of $Y$ and $Z_i$.

Reasonable model if defects uniformly dispersed

Not applicable in clusters with varying density
After hadron irradiation the defects tend to be clustered

\[ \Rightarrow \]

Assumption of uniform dispersion not valid

\[ \Rightarrow \]

Treat each defect initially as a random walker which jumps from one lattice site to the other.
Some assumptions of the model

- Interstitial diffuse $1000 \times$ faster than vacancies
- The $P(X, Y)$-values implicitly account for interactions between the defects
- Values of $P(X, Y)$ are the same within and outside cluster.
- $P(X, Y)$ values extracted from fits to DLTS data.

Basic simulation procedure

1. Take final vacancy/interstitial constellation after TRIM
2. Allow for immediate recombinations (randomly in order of inter-defect distance)
3. Random walk the defects – after each step check recombination
4. Defects which escape cluster undergo Davies’ treatment (assuming uniform distribution of previously produced defects)
5. Proceed in fluence steps (16 steps from $10^{12}$ to $10^{15}$ cm$^{-2}$)
Defect Densities after Migration

Projections of V2 and V3 positions

Project through 1 µm of depth after fluence $10^{14}$ cm$^{-1}$

Some degree of clustering still remaining

Fraction of vacancies ending up in different composite defects:

<table>
<thead>
<tr>
<th>Irradiation type</th>
<th>$\text{[VO]/[V]_{ini}}$</th>
<th>$2 \times \text{[V2]/[V]_{ini}}$</th>
<th>$3 \times \text{[V3]/[V]_{ini}}$</th>
<th>$N \times \text{[V_N]/[V]_{ini}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>10 MeV proton</td>
<td>0.0133</td>
<td>0.0191</td>
<td>0.0075</td>
<td>0.0025</td>
</tr>
<tr>
<td>24 GeV proton</td>
<td>0.0105</td>
<td>0.0231</td>
<td>0.0119</td>
<td>0.0041</td>
</tr>
<tr>
<td>1 MeV neutron</td>
<td>0.0064</td>
<td>0.0227</td>
<td>0.0150</td>
<td>0.0056</td>
</tr>
</tbody>
</table>

M. Huhtinen Si-RadHard Workshop, CERN: 29 November 2001
Evolution of Defect Densities

Open symbols \([O]=5 \times 10^{17} \text{ cm}^{-3}\), Solid symbols \([O]=5 \times 10^{15} \text{ cm}^{-3}\)

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*Si-RadHard Workshop, CERN: 29 November 2001*
Shockley-Read-Hall predictions

Defect occupancies can be calculated from standard SRH theory

However,

Significant uncertainties in
- defect energy levels
- capture cross sections for \( e \) and \( h \)

Reasonable guess \( \sigma_p = \sigma_h = 2 \times 10^{-15} \text{ cm}^{-2} \)

<table>
<thead>
<tr>
<th>Defect type</th>
<th>Energy (eV)</th>
<th>( f_i )</th>
<th>( I_{\text{leak}} ) (( \mu \text{A/defect} ))</th>
</tr>
</thead>
<tbody>
<tr>
<td>( V_2 )</td>
<td>( E_c-0.42 )</td>
<td>( 2 \times 10^{-5} )</td>
<td>( 9 \times 10^{-14} )</td>
</tr>
<tr>
<td>( V_3 )</td>
<td>( (E_c-0.47) )</td>
<td>( 7 \times 10^{-4} )</td>
<td>( 6 \times 10^{-13} )</td>
</tr>
<tr>
<td>( V_{2O} )</td>
<td>( (E_c-0.55) )</td>
<td>0.3</td>
<td>( 1 \times 10^{-11} )</td>
</tr>
</tbody>
</table>

\[
N_{\text{eff}} = \left| [P] - f_1 \times [V_{2O}] - f_2 \times [V_2] - f_3 \times [V_3] \right|
\]

With above SRH values and simulated defect concentrations \( N_{\text{eff}} \) and \( I_{\text{leak}} \) are orders of magnitude too low
Effect of clustering

V2 and probably V3 have 3 charge states in the band-gap

If defects are clustered, transitions between defect levels can amplify the occupancies predicted by simple SRH theory

Effect predicted to be seen at local densities of $10^{16}$ – $10^{18}$ cm$^{-3}$
Cluster Enhancement over SRH

Use local density within radius $R$ around each defect

<table>
<thead>
<tr>
<th>Defect type</th>
<th>R (Å)</th>
<th>$f_c^i$</th>
<th>$E_i$</th>
<th>$f_c^i$</th>
<th>$E_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_2$</td>
<td>100</td>
<td>0.70</td>
<td>288</td>
<td>0.51</td>
<td>277</td>
</tr>
<tr>
<td>$V_3$</td>
<td>100</td>
<td>0.65</td>
<td>281</td>
<td>0.57</td>
<td>274</td>
</tr>
<tr>
<td>$V_2$</td>
<td>200</td>
<td>0.87</td>
<td>64</td>
<td>0.64</td>
<td>58</td>
</tr>
<tr>
<td>$V_3$</td>
<td>200</td>
<td>0.85</td>
<td>62</td>
<td>0.74</td>
<td>58</td>
</tr>
</tbody>
</table>

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<thead>
<tr>
<th>Defect type</th>
<th>R (Å)</th>
<th>$f_c^i$</th>
<th>$E_i$</th>
<th>$f_c^i$</th>
<th>$E_i$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_2$</td>
<td>100</td>
<td>0.35</td>
<td>269</td>
<td>0.56</td>
<td>279</td>
</tr>
<tr>
<td>$V_3$</td>
<td>100</td>
<td>0.51</td>
<td>271</td>
<td>0.59</td>
<td>276</td>
</tr>
<tr>
<td>$V_2$</td>
<td>200</td>
<td>0.41</td>
<td>55</td>
<td>0.70</td>
<td>59</td>
</tr>
<tr>
<td>$V_3$</td>
<td>200</td>
<td>0.64</td>
<td>56</td>
<td>0.77</td>
<td>59</td>
</tr>
</tbody>
</table>

$\downarrow$

Split $V_2$ and $V_3$ in clustered and non-clustered components

$$N_{\text{eff}} = |[P] - f_1[V_2O] - f_2\{ E_2f_c^2 + (1 - f_c^2) \}[V_2] - f_3\{ E_3f_c^3 + (1 - f_c^3) \}[V_3]|$$

Best fit to data with R=100 Å values.
Experimentally observed effect of oxygen reproduced (although not quite as pronounced as in experiments)

M. Huhtinen Si-RadHard Workshop, CERN: 29 November 2001
$N_{\text{eff}}$ for 10 MeV protons

Assume simulated hardness factors

$H(10 \text{ MeV p})/H(24 \text{ GeV/c p}) = 6.2$

Large oxygen effect for 10 MeV protons, scaling violation
Changes of $I_{\text{leak}}$

Assume simulated hardness factors
$H(10 \text{ MeV p})/H(24 \text{ GeV/c p})=6.2$

Symbols = std.Si, Lines = oxy.Si

- $\bullet$ = 1 MeV neutrons
- $\triangle$ = 200 MeV pos. pions
- $\circ$ = 24 GeV/c protons
- $\star$ = 10 MeV protons

Apparent NIEL violation – but maybe correct!

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Si-RadHard Workshop, CERN: 29 November 2001
NIEL scaling violation?

NIEL cannot be directly measured
&
Neutron damage at 1 MeV varies rapidly

\[ \downarrow \]
Experimental uncertainty for 1 MeV neutrons

Recent experiments (Bechevet et al) for relative damage ($\alpha$ and $\beta$) show NIEL violation in standard Si.

<table>
<thead>
<tr>
<th>Energy</th>
<th>$\alpha$</th>
<th>$\beta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>9 MeV p</td>
<td>13.3</td>
<td>4.3</td>
</tr>
<tr>
<td>10 MeV p</td>
<td>9.9</td>
<td>3.4</td>
</tr>
<tr>
<td>24 GeV/c p</td>
<td>2.54</td>
<td>0.56</td>
</tr>
<tr>
<td>Ratio</td>
<td>3.9–5.2</td>
<td>6.1–7.7</td>
</tr>
</tbody>
</table>

These are fairly consistent with the simulations.
Is NIEL violation reasonable?

- The prediction that NIEL is violated arises from a few almost model-independent facts

- Concentrations of defects (V2, V3, ...) are fixed by experimental DLTS data and 'cannot' be wrong by orders of magnitude

- Need a mechanism to amplify level occupancies above SRH theory
  - Intercenter charge transfer seems a natural candidate

- The presumably dominant defect V2 scales with NIEL &
  - Different degree of V2 (and V3) clustering for various irradiation types

- NIEL scaling violation
Conclusions I

NIEL scaling usually OK within factor of $\sim 2$

but do not trust it blindly because

It can fail badly for oxygenated silicon

It does not seem to be exact for standard silicon either

Discrepancies seem to be largest for low-energy protons especially

Measured 1 MeV neutron damage values should be treated with care

Would be better to use 24 GeV/c protons as reference
Model predictions are consistent with experiments on standard and oxygenated silicon

The V2O defect and SRH enhancement due to clustering of V2 are both needed for this

However, there are several assumptions, which can be considered as almost free parameters.

The present assumptions seem reasonable, but one can easily think of others which would not provide the same consistency

Can check model and assumption with

- 10 MeV proton data for std and oxy silicon
- $N_{\text{eff}}$ data immediately after (cold) irradiation