Can cluster physics shed some light on the puzzles of our Experimental findings with energetic particles?

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Introduction

Leakage current / 
Carrier removal / ???clusters???
Annealing / 

1. Cluster formation
(Vinetskii and Kondrachuk in Rad. Effects 1975, vol.30 p227)

first stage: high-energy particles displace matrix atoms
point defects: vacancies(V), interstitials(I)

second stage: diffusion of vacancies and interstitials
quasimolecules (secondary radiation defects)

Model for second stage:
Mobility of I >> V
2 reactions 

\[ V + V \rightarrow D \quad \text{reaction constants} \]
\[ V + O \rightarrow A \quad \alpha_D, \quad \alpha_A \]

Diffusion equation for vacancies and reaction equation for Oxygen and initial conditions at center of cluster \( N_0 \)
system of nonlinear equations
dimensionless parameter

\[ E = \frac{D_v}{\alpha_D N_0 L^2} \]

L characteristic size of cluster
\( N \) and \( L \) depend on incident particle, while Depend on crystal properties

\( a) \quad E < < 1 \quad \text{low vacancy diffusion} \rightarrow \text{congealing cluster} \\
\quad \text{shape of D-cluster} \sim \text{V-cluster (original)} \\
\( b) \quad E >> 1 \quad \text{high vacancy diffusion} \rightarrow \text{spreading cluster} \]
belt of A centers around D-cluster
energy threshold of knock-on atom between 2 cases 10keV

2. Properties of cluster

2.1 structure
central region (core): vacancies +
interstitial associations

peripheral region (impurity defect shell)
bell shape of distribution

2.2 electrical field
center: charged D depending on Fermi level
periphery: charged impurity defects
local charge neutrality: (acceptors, donors,
free carriers)
Poisson equation + charge neutrality → selfconsistent system
which yields occupation probability of acceptors $f_i$
and potential barrier $\psi_0$ between matrix and center of cluster
Approximate solution of Poisson equation

$$\psi_0 \approx \frac{2\pi e^2 r^2}{\varepsilon} \sum_i N_i f_i - \frac{kT}{3}$$

$$f_i = \frac{1}{1 + N_e / n_g \exp \left[ \frac{\psi_0 - \Delta E_i}{kT} \right]}$$

where $r$ is radius of cluster and $\Delta E_i$ energy position of
defect in forbidden bandgap
$N_i$ density of defect
2.3 Parameter description

Kuznetsov and Lugakov, phys.stat.sol(a) vol.79, p381 (1983)
Temperature dependencies of Hall coefficient + nature of defect

Defect cluster parameters in n-Si

<table>
<thead>
<tr>
<th>irradiation</th>
<th>material n₀ (10¹³ cm⁻³)</th>
<th>core</th>
<th>periphery</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>ψ (eV)</td>
<td>radius (Å)</td>
</tr>
<tr>
<td>neutrons</td>
<td>float-zone 3</td>
<td>≈0.14</td>
<td>≈130</td>
</tr>
<tr>
<td>neutrons</td>
<td>pulled</td>
<td>2</td>
<td>≈0.14</td>
</tr>
<tr>
<td>protons</td>
<td>float-zone 1</td>
<td>1</td>
<td>0.11</td>
</tr>
<tr>
<td>protons</td>
<td>float-zone 3</td>
<td>3</td>
<td>0.11</td>
</tr>
<tr>
<td>protons</td>
<td>float-zone 8</td>
<td>8</td>
<td>0.11</td>
</tr>
<tr>
<td>protons</td>
<td>float-zone 1.6</td>
<td>1.6</td>
<td>0.11</td>
</tr>
<tr>
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<td>pulled</td>
<td>2</td>
<td>0.11</td>
</tr>
<tr>
<td>protons</td>
<td>pulled</td>
<td>5</td>
<td>0.11</td>
</tr>
<tr>
<td>protons</td>
<td>pulled</td>
<td>30</td>
<td>0.11</td>
</tr>
</tbody>
</table>

2.4 Strain field
Deposited energy ~10000 eV in a cluster volume ~10⁻¹⁸ cm⁻³
Temperatur diff ~1000 K
Fast cooling in ~10⁻¹⁰ s
Pressure ~10⁰⁻⁰ bar

2.5 Divacancy levels in cluster

For locally inhomogeneous distribution of deep levels

\[ \bar{N}_d = N_\tau \int M F(\tau, E_F - E_d) dV \]
where \[ \int F(+) \, dV = I \]

and \[ f(T, E_p - E_d) \] occupancy

\[ \overline{N_d} \] Volume average concentration of charged center

\[ N_r \] Concentration of local region

Analysis performed with following assumptions
- homogeneous distribution of D in matrix + embedded local regions with M divacancies in it.
- bell shape of initial cluster

\[ F(r) = \frac{1}{\pi^{3/2}} \frac{1}{L^3} \, \exp\left( - \frac{r^2}{L^2} \right) \]

only divacancy level \[ E_c - 0.39 \text{ eV} \] considered
- \( N \) depends linearly on dose

A.V. Varlev et al.


20 p 465 (1986)

FIG. 1. Values of \( \Delta n/\Phi \) obtained at temperatures 250-450 K for zone-grown (1) and crucible-grown (2-4) samples. Radiation dose \( \Phi (10^{12} \text{ cm}^{-2}) \):
1), 2) 0.5; 3) 1.0; 4) 1.5. The experimental points were taken from Ref. 7. The continuous curves are theoretical dependences calculated on the assumption of a locally inhomogeneous distribution of divacancies in a crystal (Table II).

\[ \alpha = 5 \times 10^{-13} \]

\[ \alpha \approx 6.3 \text{ MeV} \]

\[ m = \text{specific} \]
3. Consequences for ROSE problems

3.1 Carrier Recombination

Most likely recombination centers are D
Problem of capture coefficient for free carriers
If there is a potential barrier built-up inside cluster:
Holes attracted into interior
Electrons pushed to matrix depletion

Then effective capture cross section for holes

\[ \sigma_p^* = \sigma_p \exp\left( \frac{\psi}{kT} \right) \cdot K_s \]

\( K_s \) is a factor for fact that potential barrier \( \psi \) is not abrupt but extends to a Debye screening length
for the case that this length is smaller than outer cluster radius

\[ K_s \sim \text{vol of total cluster / volume of negative charge} \]

For \( n_0 \approx 3 \times 10^{13} \text{ cm}^{-3} \quad K_s \exp\left( \frac{\psi}{kT} \right) \approx 30 \)

find

\[ \frac{\sigma_p}{\sigma_\nu} \approx 150 \quad \text{for clusters} \]

and \[ \frac{\sigma_p}{\sigma_\nu} \approx 22 \quad \text{electron irradiated Si} \]

This yields \( K_s \exp\left( \frac{\psi}{kT} \right) \) for 2kOhmcm Si

M. Moll needs 6
3.2 DLTS measurements

Careful with interpretation, since charging of traps in potential well of clusters not guaranteed
Capture rate of carriers $\gg$ thermal release of carriers
Broadening + temperature shift of $E_1$ peak

reactor neutrons

\[ B \quad (-0.39 \text{ eV}) \]

\[ t_1 = 1 \text{ ms} \quad t_2 = 0.1 \text{ ms} \quad t_3 = 0.01 \text{ ms} \]


Fig. 1. DLTS spectra of non-irradiated sample (a); irradiated with a fluence of $5.5 \times 10^{11}$ n/cm$^2$ (b); and with a fluence of $1.0 \times 10^{12}$ n/cm$^2$ (c)
<table>
<thead>
<tr>
<th></th>
<th>E1</th>
<th>E2</th>
<th>E3</th>
<th>E4</th>
<th>$\sigma_e \text{ cm}^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Before radiation</td>
<td>0.21</td>
<td>0.31</td>
<td>0.49</td>
<td></td>
<td></td>
</tr>
<tr>
<td>After 5.5 $10^4 E11$</td>
<td></td>
<td></td>
<td></td>
<td>0.43</td>
<td>2.E-15</td>
</tr>
<tr>
<td>After 10 $E12$</td>
<td></td>
<td></td>
<td></td>
<td>0.33</td>
<td>2.E-17</td>
</tr>
</tbody>
</table>

Extend of cluster space charge layer (CSCL) ~ 3 microns Debeye length

Overlap of CSCL after a fluence 10E12 cm-2 Fabrication defects (shallow) masked by local potential

3.3 Annealing of D in Si containing clusters


\[
\begin{align*}
CZ & \quad nt. 3.5 \times 10^{14} \\
\phi & \quad 4.4 \times 10^{-14} \text{ cm}^{-2} \\
D & \quad 95 \\
R_e & \quad 220 \AA
\end{align*}
\]
observation: anneal in 2 stages

$250 - 350^\circ C$ classical $E_d = 1.5eV$

$100 - 200^\circ C$ smooth \textit{different} mechanism

at $120^\circ C$

$I_0 \rightarrow I + I$

$I + C_5 \rightarrow C_i$

$c_i \rightarrow \text{cluster (strain)}$

3.31 Peculiar observations

PECULIARITIES OF DIVACANCY ANNEALING

\[ C_i_0 (E_e - 0.17 \text{eV}) \]

\[ \text{Defect Concentration, } N \times 10^{-12} \text{ cm}^{-3} \]

\[ \begin{align*}
\text{Indirect proof of } & C_i \text{ annealing: more than 2 times of } C_i \text{ goes into cluster} \\
\text{Effect of strain field: } & C_i \text{ cause lattice compression} \\
& D_i \text{ cause lattice tension}
\end{align*} \]

3.3 Annealing of ROSE detectors

Z. Li et al. NIM A 385 p321 (1997)
4. Model for positive and negative annealing

Be cautious!! Might be crab!!

Suppose: main defect D distributed as point defects in matrix or forming a cluster potential barriers and strain field around cluster

irradiation produces Interstitials which go to sinks

\[
\begin{align*}
\text{Sinks} & \quad I + C_5 \quad \rightarrow \quad C_i \\
& \quad I + O_2 \quad \rightarrow \quad O_i \\
& \quad I + V_2 \quad \rightarrow \quad V \\
& \quad I + P \quad \rightarrow \quad P_i
\end{align*}
\]

\( C_i \) are mobile and get eventually settled in

\[
\begin{align*}
\text{Sinks} & \quad C_i C_5 \\
& \quad C_i O_2 \\
& \quad D \text{ in cluster} \\
& \quad D \text{ in matrix (??)}
\end{align*}
\]

4.1 Positive annealing: destruction of D in vacancies by C

4.2 Negative annealing: destruction of D in clusters by C

Why??

Because destruction of D lowers potential barrier and more Charged D become visible

\[ \frac{dW}{d\Phi}, \text{cm}^{-1} \]

\[ V_2 \text{ DLTS} \]

\[ R, \text{Å} \]

\[ \text{temperature dependence of DLTS peak} \]


\[ T_1 < T_2 < T_3 \]

\[ \delta, \text{rel. units} \]

\[ M, \text{rel. units} \]

have shown that \( \psi_{\text{max}} \sim \ln D \)

if D goes down D goes up

since \( \Delta \psi_{\text{max}} \sim \frac{\Delta D}{D} \)

\( \Delta \psi_{\text{max}} \) changes strongly when few D left

this is reason why negative annealing delayed

4.3 Some experimental facts in favor of model

4.3.1 decrease of overall D measured by positron lifetime and infrared technique during annealing

4.3.2 Thesis M. Moll (1999) p198

peak H(116K) \( \uparrow \) assignment to \( C_4^i \)
because C pushed in by strain field and gets immobile

appearance of small peak \( V_2 \)

\( C_4^i \) and probably \( C_4^i C_5 \) go up

Unexplained time behavior of reverse annealing

5. Conclusion and Outlook

some properties of clusters are able to explain peculiar behavior of our measurements; it has to be proven that clusters produced in ROSE detectors behave as the ones found in low resistivity material
in particular geometrical complications are expected due to the
great Debeye length in ROSE detectors. (merging of the periphery
of clusters)

qualitative picture: further thinking if correct; refine or amend

quantitative model: needs description of primary cluster with
input from experiment (probably dedicated)
since cluster shape depends also on chemical impurities whole kinetic of
V and I- diffusion must be implemented
Calculate cluster size and number of D
Do point defect kinetics in periphery of cluster