Bistable Boron related defect associated with the acceptor removal process in irradiated p-type silicon – electronic properties of configurational transformations*

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Motivation

The **bistable behavior** of a Boron Containing Donor (BCD) related to acceptor removal effect in p-type silicon

**Assignments of BCD:**

1) $\text{B}_i\text{O}_i$ formed via the reactions$^{2-4}$
   $\text{B}_s + \text{Si} \rightarrow \text{B}_i$
   $\text{B}_i + \text{O}_i \rightarrow \text{B}_i\text{O}_i$

2) $\text{B}_s\text{Si}_i$ formed via the reaction$^{5,6}$
   $\text{B}_s + \text{Si} \rightarrow \text{B}_s\text{Si}_i$

**BCD** trapping parameters:

- $\sigma_n = 1.05 \times 10^{-14}$ cm$^2$; $\sigma_p = 2.5 \times 10^{-20}$ cm$^2$
- Due to the Poole Frenkel effect, specific to columbic centers, the defect energy level is lowering with the electric field ($F$)
- $E_t = E_{t,0} - \delta E(F)$

The BCD defect can exist in minimum 2 configurations:

**A-** the ground state in equilibrium conditions, with a donor level at about 0.28 eV from $E_c$ of silicon. In this state the defect is contributing with positive charge to $N_{eff}$.

**B-** the ground state in non-equilibrium conditions (excess of carriers). This state is not electrically active and is indirectly observed via the variations in the A configuration.
Samples

\[ n^{++} - p - p^{++} \] PAD (W5-LGB-72P)

Both PAD and LGAD samples produced on high-resistivity (12kΩ · cm) FZ wafers, by CNM Barcelona, and have been irradiated with \(10^{14} n/cm^2\)

- The samples were annealed for more than 136,000 minutes at 80°C
- The Guardrings were grounded in all the electrical measurements
Methods

• The change of the defect configuration from A to B was achieved by performing a small forward current injection ($I_{Fw} \sim 5.7 \, \mu A$) at temperatures between 243K and 313 K.

• The reverse configurational transformation (from B to A) takes place when the excess of carriers is removed and sample kept in dark

• The defect configurational transformations were studied by means of:
  • C-V/I-V measurements at different temperatures
  • TSC experiments
Results

BCD Configurational transformations as seen in C-V experiments

• **A to B (left Figure):** Upon injecting a $I_{fw} = 5.7 \mu A$ at 293K, an increase of up to 6.3V in depletion voltage has been measured in the PAD and LGAD samples. This corresponds to an increase in $N_{eff}$ in the bulk of the diodes of $\Delta N_{eff} \sim 5 \cdot 10^{12} \text{ cm}^{-3}$.

• **B to A (right Figure):** Removing $I_{fw}$, the $V_{dep}$ is slowly decreasing back to its initial value before the $I_{fw}$ was applied.
Results

BCD Configurational transformations as seen in TSC experiments

- Consecutive TSC measurements, after fully switching the defect from A to B configuration at 293 K, were performed and they show a recovery of the donor level specific to the A configuration. \( T_0 = 10 \text{ K} \); \( I_{\text{fill}} = 350 \mu\text{A} \); \( V_{\text{rev}} = -100 \text{ V} \); \( \beta = 11 \text{ K/min} \)

- The only visible variation in TSC scan is attributed to the change of \( BCD_A^{(0/+)\Dagger} \) to \( BCD_B^0 \)

\[
\Delta BCD_A^{(0/+)} \sim 3.8 \times 10^{12} \text{ cm}^{-3}
\]
Simulation of TSC spectra & evaluation of defect concentrations in PAD

\[
TSC^e(T) = \frac{1}{2} \times q_0 \times A_f \times N_t \times \int_0^d \left\{ e_n^{PF}(x, T) \times \exp\left(-\frac{1}{\beta} \int_{T_0}^T e_n^{PF}(x, T) \, dT\right) \right\} \, dx
\]

where \( e_n^{PF}(T) = e_{n,0} \left( \frac{1}{\gamma^2} \right) (e^\gamma(\gamma - 1) + 1) + \frac{1}{2} \),

\[
\gamma = \frac{q_0}{k_B \times T} \sqrt{\frac{q_0 \times [F(x, T)]}{\pi \times \varepsilon_0 \varepsilon_r}},
\]

\[
F(x, T) = \frac{q_0}{\varepsilon_0 \varepsilon_r} \times N_{eff}(T) \times (d - x) + \frac{V_R - V_{dep}(T)}{d}
\]

\[
e_{n,0}(T) = \sigma_n(T) \times \nu_{th,n}(T) \times N_c(T) \times \exp\left(- \frac{E_c - E_{t,0}}{k_B \times T}\right)
\]

\[
TSC^e(T) \approx 0.286 \, eV, \text{ zero field activation energy of the } BCD \text{ defect in the A configuration}
\]
**A→B transformation via Cyclic CV measurements at different temperatures.** In between the C-Vs a small forward injection, $I_{fw} = 5.7\mu A$, is applied for different times.

\[
\Delta N_{eff}(T) = -\Delta [BCD_A(t)] = BCD_A^{0}(1 - \exp(-k \cdot t))
\]
Electronic properties of A→B transformation

- Because the energy level of the defect lies above the Fermi level, the value of $k_0$ is much smaller than that expected for a free carrier capture (of $10^7$ s$^{-1}$)
- This is due to the position of the fermi energy level, which remains below the donor energy level of defect during the small Fw injection, affecting thus the population of donor defect $^7$

$$k \cong \sigma_n \cdot Nt \cdot v_{th} \cdot \left(1 + \exp \left(\frac{E_t - E_{nF}}{k_B \cdot T}\right)\right)^{-1}$$

$\sigma_n = \text{capture cross-section}$

$v_{th} = \text{electron thermal velocity}$

$E_t = \text{donor energy level}$

$E_{nF} = \text{quasi-Fermi energy level}$
Equation: \( \Delta N_{\text{eff}}(T) = \Delta [BCD_B(t)] = BCD_B^0(\exp(-k \cdot t) - 1) \)

\( \Delta N_{\text{eff}}(T) = \Delta [BCD_B(t)] = BCD_B^0(\exp(-k \cdot t) - 1) \)

Different times after the \( I_{Fw} \) injection has stopped via cyclic CV measurements at different temperatures

\[ N_{\text{eff}}(t) = [BCD_B^0] \cdot (\exp(-k \cdot t) - 1) \]

**BCDB0 (cm\(^{-3}\)):**

- **Equation:** \( BCD_B^0 = (5.8219 \pm 0.017) \times 10^{12} \)
- **R-Square (COD):** 0.99967
- **Adj. R-Square:** 0.99964

**k (s\(^{-1}\)):**

- **Equation:** \( k = (2.305 \pm 0.03766) \times 10^{-5} \)
- **R-Square (COD):** 0.99884
- **Adj. R-Square:** 0.99868

**DNeff (cm\(^{-3}\)):**

- **Equation:** \( N_{\text{eff}}(t) = [BCD_B^0] \cdot (\exp(-k \cdot t) - 1) \)
- **BCDB0 (cm\(^{-3}\)):** \( (4.389 \pm 0.0391) \times 10^{12} \)
- **k (s\(^{-1}\)):** \( (2.8145 \pm 0.0823) \times 10^{-5} \)
- **R-Square (COD):** 0.99884
- **Adj. R-Square:** 0.99868
Electronic properties of $B \rightarrow A$ transformation

- The value of $k_0 = 1.2 \times 10^{12} \text{s}^{-1}$ is in the range for a free carrier emission process.
- The large energy barrier of $E_a = 0.94 \text{ eV}$ also explains the long times required for the full recovery of the $BCD_A$ configuration.
Configuration Coordinate Diagram

for $A \rightarrow B$ transformation
(when electrons in excess are injected)

for $B \rightarrow A$ transformation
(when excess electrons are removed)
Conclusions

• In equilibrium conditions, the BCD defects are found in the A configuration. Through TSC measurements, the corresponding zero field energy level for $BCD_A^{(0/+)}$ donor state has been determined to be at $E_{t,0} \cong 0.286 \text{ eV}$ from the conduction band of silicon.

• In non-equilibrium conditions, when electrons exist in excess in high resistivity samples, the defect can transform in configuration B ($BCD_B^0$) at ambient temperatures, by capturing a free electron and overpassing the energy barrier of $E_{A \rightarrow B} = 0.363 \text{ eV}$. The defect remains in B state as long as there is an excess of electrons.

• Removing the source of excess carriers, the defect returns to its donor state A ($BCD_A^{(0/+)}$) by emitting an electron while surmounting the large energy barrier of $E_{B \rightarrow A} = 0.94 \text{ eV}$.

• The $A \rightarrow B$ defect configurational change, as observed here also in CV measurements, is not detected in low resistivity diodes. In high resistivity samples, the small forward injection current, comparable with the photocurrent generated by the ambient light, is larger than that of injected holes and on longer distances inside the diodes. Therefore, the transformation $A \rightarrow B$ in low resistivity samples is expected to occur in a much smaller volume, causing negligible variations in C-V measurements.
References


Thank you for your attention!
$1^{st}$-order defect kinetics

$$- \frac{\partial [N]}{\partial t} = k [N] \rightarrow [N] = [N]_{t \rightarrow 0} \ast \exp(-k \ast t); \left\{ \begin{array}{l} [N] = \text{concentration of defect} \\ t = \text{time} \\ k = \text{constant rate} \end{array} \right.$$ 

$$k = k_0 \ast \exp \left( - \frac{E_a}{k_B T} \right); \left\{ \begin{array}{l} k_0 = \text{frequency factor} \\ E_a = \text{activation energy} \\ k_B = \text{Boltzmann constant} \\ T = \text{temperature} \end{array} \right.$$ 

$$k_0 \sim \left\{ \begin{array}{l} 10^7 \text{s}^{-1} \rightarrow \text{capture of free carrier by multiphonon emission} \\ 10^{12} \text{s}^{-1} \rightarrow \text{emission of free carriers} \end{array} \right.$$
Poole-Frenkel (PF) Thermally Stimulated Current Signal simulation for electron traps in diodes

\[ TSC_{PF}^e (T) = \frac{1}{2} \cdot q \cdot A \cdot N_t \cdot \int_{0}^{d} e_{n}^{PF} (x, T) \cdot \exp \left( -\frac{1}{\beta} \int_{T_0}^{T} e_{n}^{PF} (x, T') dT \right) dx \]

\[ e_{n}^{PF} (T) = e_n \left( \frac{1}{2} \right) (e^\gamma \cdot (\gamma - 1) + 1) + \frac{1}{2}; \gamma = \frac{q |\vec{F}|}{k_B T \sqrt{\pi \cdot \varepsilon_0 \varepsilon_r}} \]

\[ e_n = \sigma \cdot v_{th} \cdot N_c \cdot \exp \left( -\frac{E_c - E_t}{k_B T} \right) \]

\[ q = \text{elementary charge} \]
\[ d = \text{thickness of the sample} \]
\[ A = \text{active surface of the sample} \]
\[ N_t = \text{defect concentration} \]
\[ \beta = \text{heating rate} \]
\[ T_0 = \text{filling temperature} \]
\[ e_n = \text{electron emission rate} \]
\[ \vec{F} = \text{electric field in sample (sample is fully depleted)} \]
\[ \varepsilon_0 \varepsilon_r = \text{dielectric constant of silicon} \]

In diodes:

\[ F(x, T) = \frac{q_0}{\varepsilon_0 \varepsilon_r} \times N_{eff} (T) \times (d - x) + \frac{V_R - V_{dep}(T)}{d}, \text{for } V>V_{dep} \]
EPI-02-50-65, 50 Ω·cm

\[ \Phi = 1 \times 10^{14} \text{n/cm}^2 \]

CZ-03-100-DS-81, 100 Ω·cm

\[ \Phi = 1 \times 10^{15} \text{n/cm}^2 \]