Radiation damage in Si and SiC based sensors / RADASS - 2025

- The project is embedded as part of the research efforts in DRD3 working groups
  - *WG3 – Radiation damage characterization and sensor operation at extreme fluences*,
  - *WG4: Simulation*
  - *WG6 – Wide Band Gap (WBG) and innovative sensor materials*.
- The work directly map into the work package ***WP3- Sensors for extreme fluences*** covering the Roadmap DRDT 3.3. on extreme fluence operation and reaches into all four Roadmap DRDTs for solid-state detectors wherever radiation damage is of concern.

Partners: NIMP (CO), NIPNE(P1), ISS(P2), UB(P3)

Aim

to *achieve a fundamental scientific understanding of radiation damage processes in Si and SiC detector materials at low, high, and extreme radiation levels*

Objectives

O1) Characterize the radiation damage at the microscopic level in SiC and contribute to building up the data sets on radiation induced defects.

O2) Establish the role of B, C, O and P in the formation of electrically active defects in Si PiN diodes exposed to irradiation fluences above 10^{15} n_{eq}/cm^2. Defect engineered diodes mimicking the gain layer in LGADs will be studied for this purpose.

O3) Model the defects formation, dynamics and metastabilities in irradiated Silicon in connection with doping and extrinsic impurities, starting from Geant4 simulations to molecular dynamics (MD) with LAMMPS and further a*b initio* calculations with SIESTA packages.

O4) Device modeling and parametrization of radiation effects in Si sensors over a large fluence range, from low to high, starting from the characterization of radiation induced defects and an evaluation of the device's performance, based on impurity content, fluence, annealing and simulations.

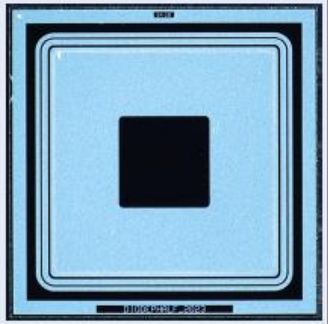
Main activities

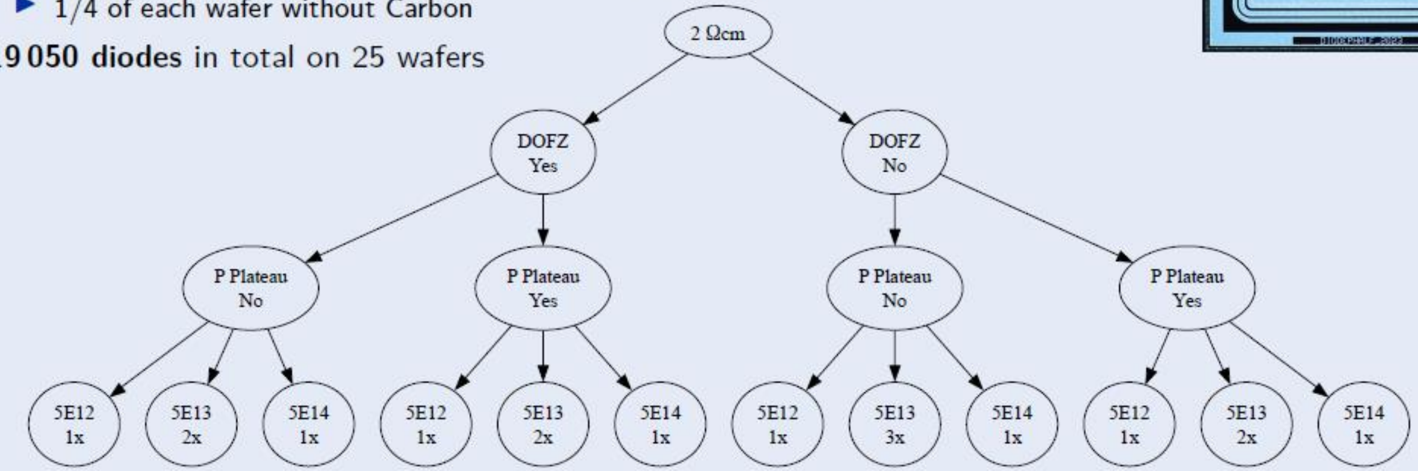
- **Electrical and structural investigations (NIMP)**
  - IV/CV/DLTS/TSC/Hall/FTIR
- **Modeling and Simulations - all partners**
  - MathCad (NIMP), Geant4 (ISS), LAMMPS (UB), SIESTA (NIPNE)
- **Dissemination and outreach- all partners**

Radiation damage in Silicon - experimental

- Start measurements on diodes mimicking the gain layer in LGADS

- *p*-type Silicon pad diodes, FZ and DOFZ wafers
- $2\,\Omega\,\text{cm}$ ($6.5 \cdot 10^{15}\,\text{cm}^{-3}$) and $10\,\Omega\,\text{cm}$ ($1.3 \cdot 10^{15}\,\text{cm}^{-3}$) wafers, 250 µm and 525 µm thickness respectively
- Large diodes $6.25\,\text{mm}^2$, small diodes $1.56\,\text{mm}^2$
- Phosphorus plateau co-doping for some wafers
- 3 Carbon implantation doses: $5 \cdot 10^{12}\,\text{cm}^{-2}$, $5 \cdot 10^{13}\,\text{cm}^{-2}$ and $5 \cdot 10^{14}\,\text{cm}^{-2}$
  - 1/4 of each wafer without Carbon
- **19 050 diodes** in total on 25 wafers



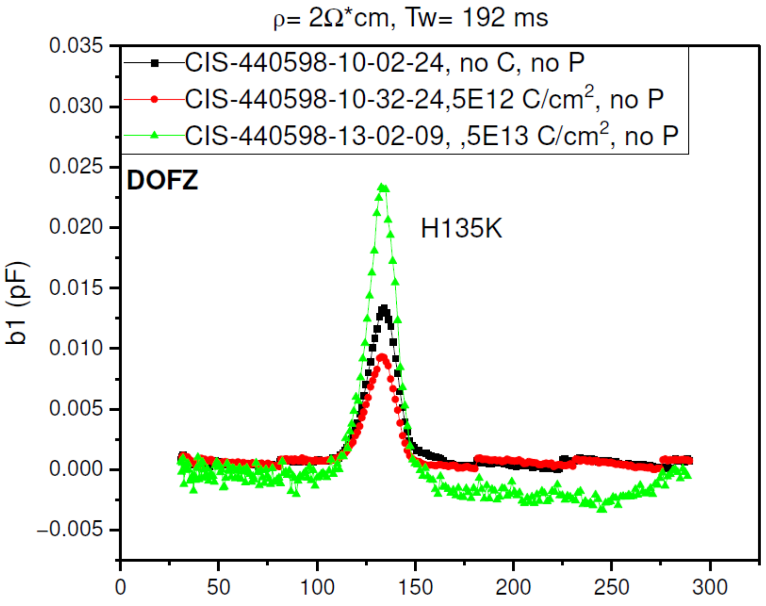


- IV, CV and DLTS measurements were performed on the unirradiated diodes
- SIMS measurements were carried out on dedicated diodes of all flavours
- Hall measurements started
- Fourier-transform infrared spectroscopy (FTIR) at RT measurements ongoing
- First irradiation campaign was carried out at CERN, $2 \cdot 10^{14}$ p/cm2 at PS-IRRAD
- DLTS measurements ongoing
- Measuring multiple annealing steps

- All measurements show that the diodes are of excellent quality
- No early breakdowns, expected depletion behaviour

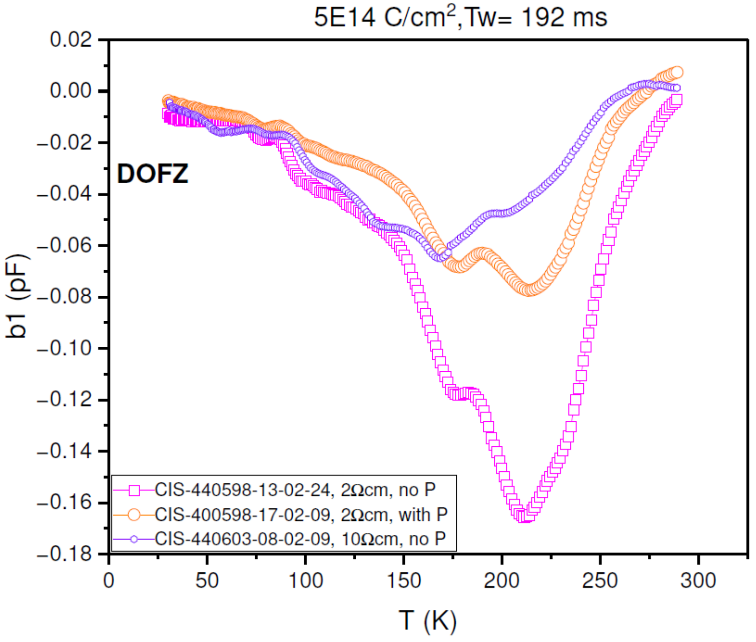
Before irradiation - DLTS

- The spectra look more or less identical for all flavours
- All diodes have the hole trap *H135K*
- Not yet identified with a known defect, activation energy is too small ~ 0.27 eV to influence on leakage current generation
- Concentration affected by flavor and Carbon concentration not consistently



Problems with the highest Carbon dose

- Observed only for largest Carbon dose $5 \cdot 10^{14}$ cm^{-2}
- Negative peaks are measured (shouldn't happen)
- Appears irrespective of flavor
- Not understood why this happens



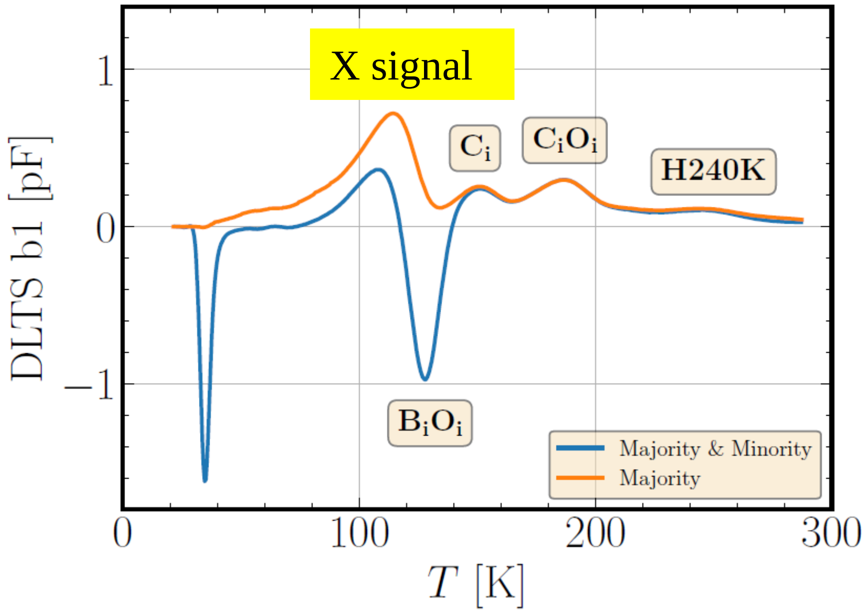
- SIMS measurement show weird peak in Oxygen concentration
- Hall measurements show weird results
- Doping profiles from CV measurements show weird peaks
- Unirradiated DLTS has minority carrier peaks for majority carrier injection ⇒ Further investigations needed

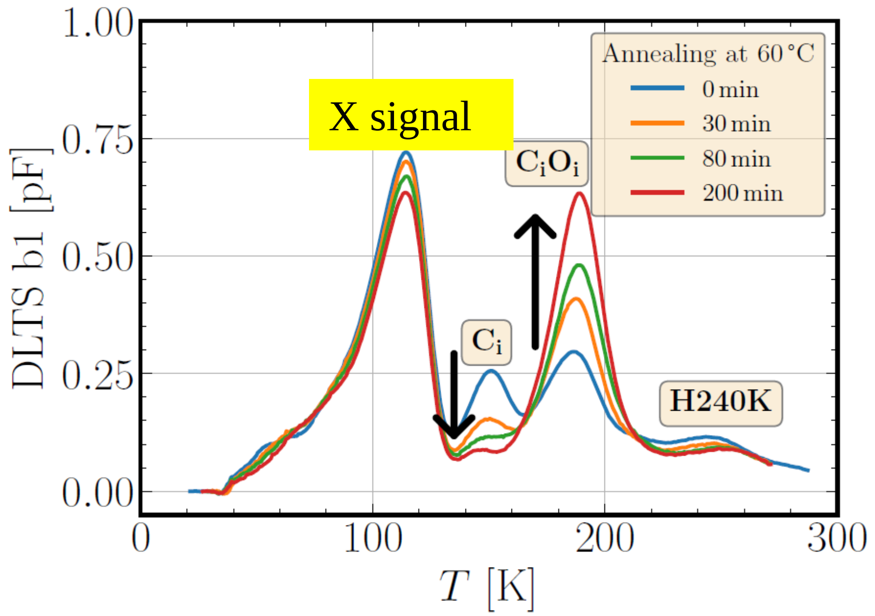
Proton irradiation - DLTS

- Test campaign to gauge proper fluence levels for DLTS measurements
- Set of all flavours irradiated to **2 ▪ 10^{14} p/cm^2 (23 GeV protons)**
- For each flavour, one diode with and one without Carbon (only 5 ▪ 10^{13} cm^{-2})

Both resistivities were irradiated

- For the 10Ω cm diodes, fluence level was too high for DLTS measurements
- All (2Ωcm) diodes were measured after irradiation with DLTS
- Before annealing, after annealing at 60 ◦C for 30, 60 ◦C, 80 min and 200 min





- Comparison of annealing times at 60 ◦C
- Ci shrinks, CiOi increases
- Concentration of Ci goes into CiOi
- X signal, belonging to a center with enhanced field emission – identified as the donor state of the V_2

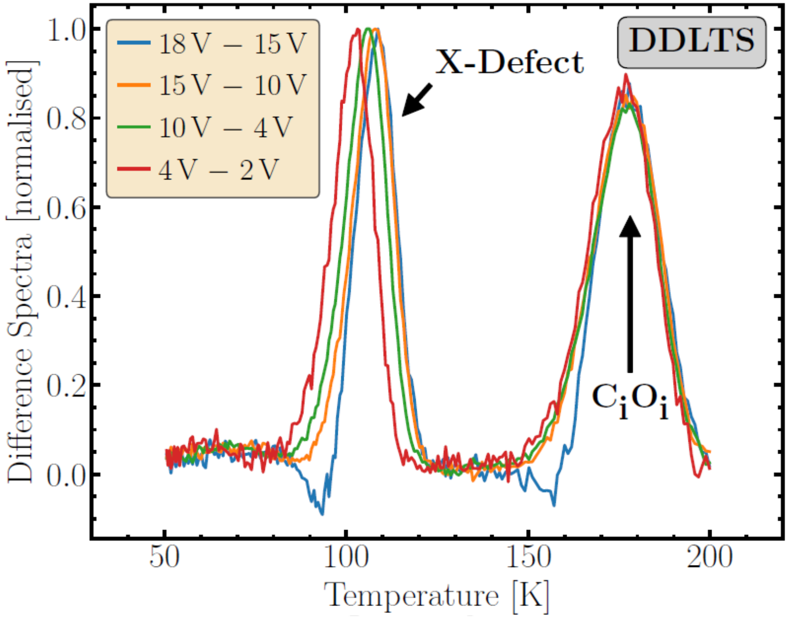
Identification of the X defect as $V_2(0/+)$: Niels Sorgenfrei et al.: *On the nature and charge state of the X-Defect, a radiation-induced Silicon defect with field-enhanced charge carrier emission* 10.1016/j.nima.2025.171133

The X defect

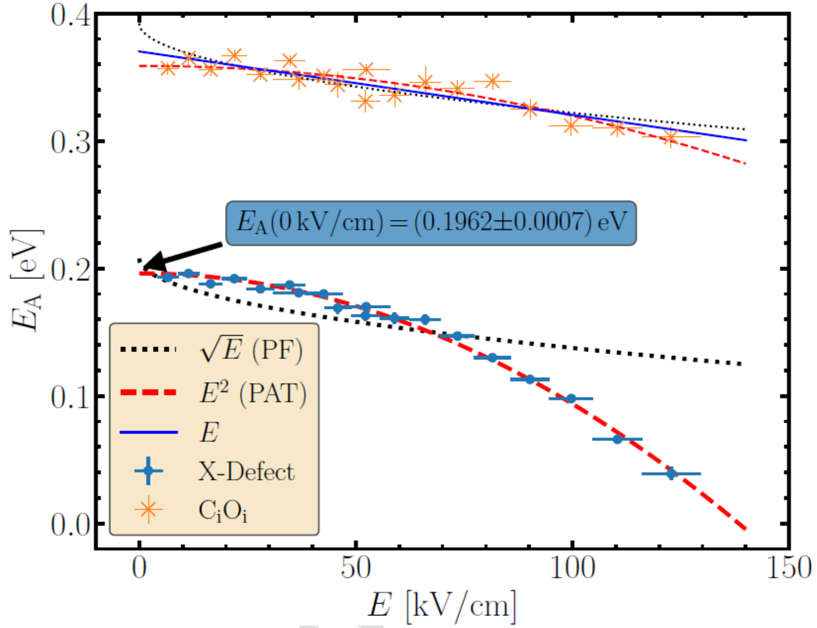
- Reported previously from TSC exp. as having an electric field enhanced emission of holes associated with Poole Frenkel (PF) mechanism → The defect should fully impact N_{eff}

However, no change in N_{eff} was observed calling for further studies:

- Check the dependence on electric field: $\sim E^{1/2}$ for PF or E^2 a phonon-assisted tunnelling (PAT) mechanism

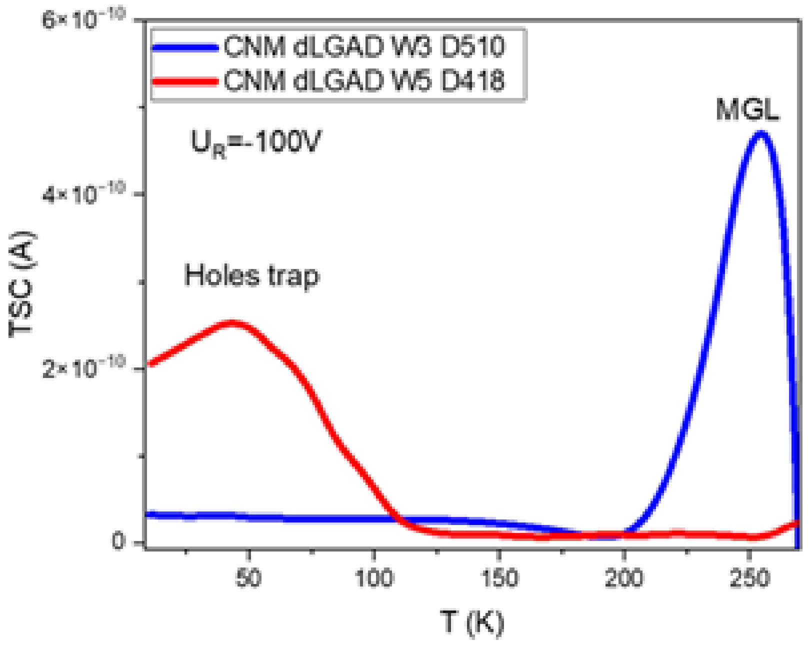


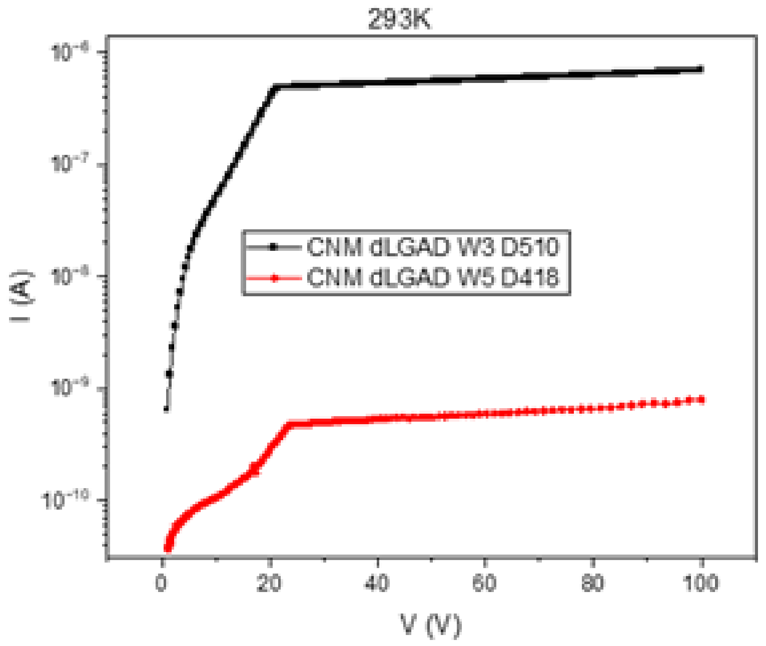
- A clear quadratic dependence was found ($\sim E^2$), providing evidence that a PAT mechanism prevails rather than the PF effect.
- This finding is in-line with the previous observation that the X-defect is not contributing to N_{eff}, the center being electrically neutral at ambient temperatures.
- **The measured characteristics of the X-Defect are in good agreement with literature values for the donor charge state of the singly charged di-vacancy, $V_2(+/0)$.**

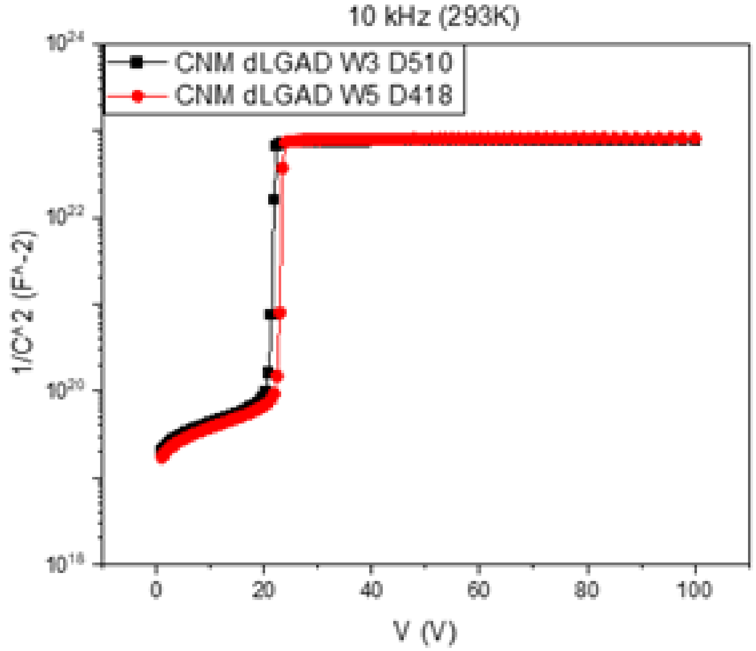


Start studies on LGADs - from DRD3 Colaborators (CNM Barcelona, PSI)

Deep p-type LGADs from CNM with/without Carbon implantation



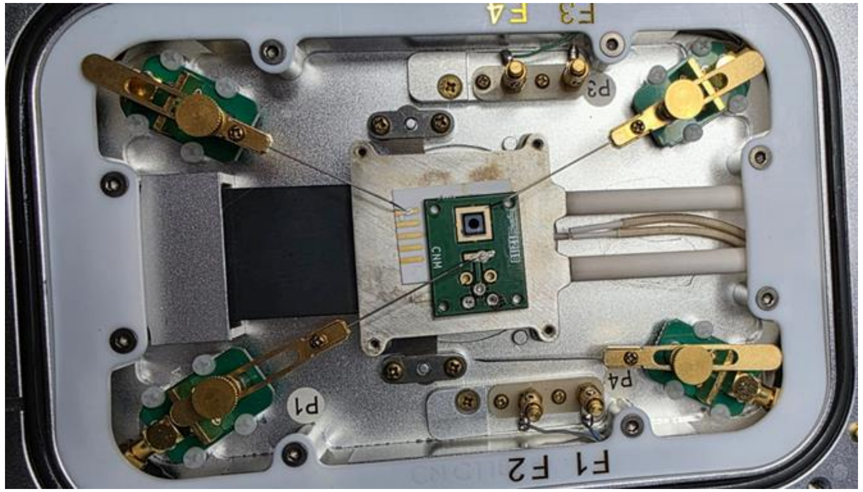


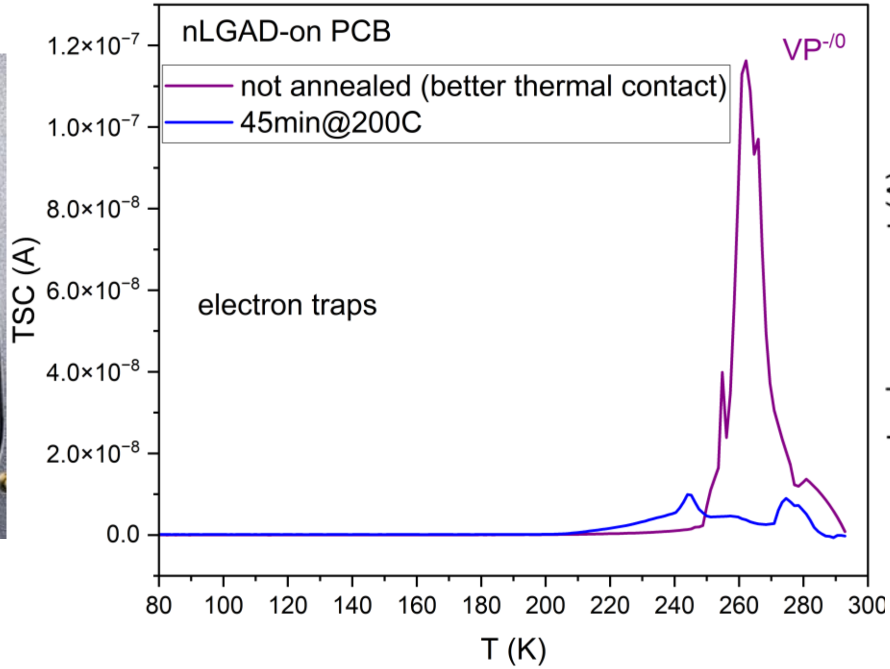


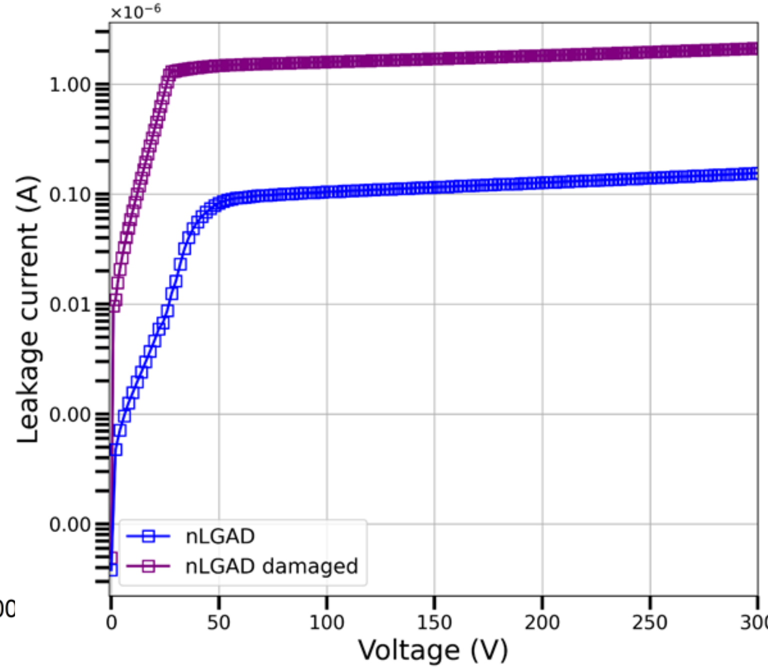
- Carbon implantation generates mid-gap levels in dLGADs (W3 wafer) → generates large leakage currents

n-type LGADs from CNM exposed to short-range Ga ions beams (1.285 MeV)

- **Global gain quenching** even at modest ion fluences of ~ 10^9 ions/cm^2 **due to a donor removal effect**



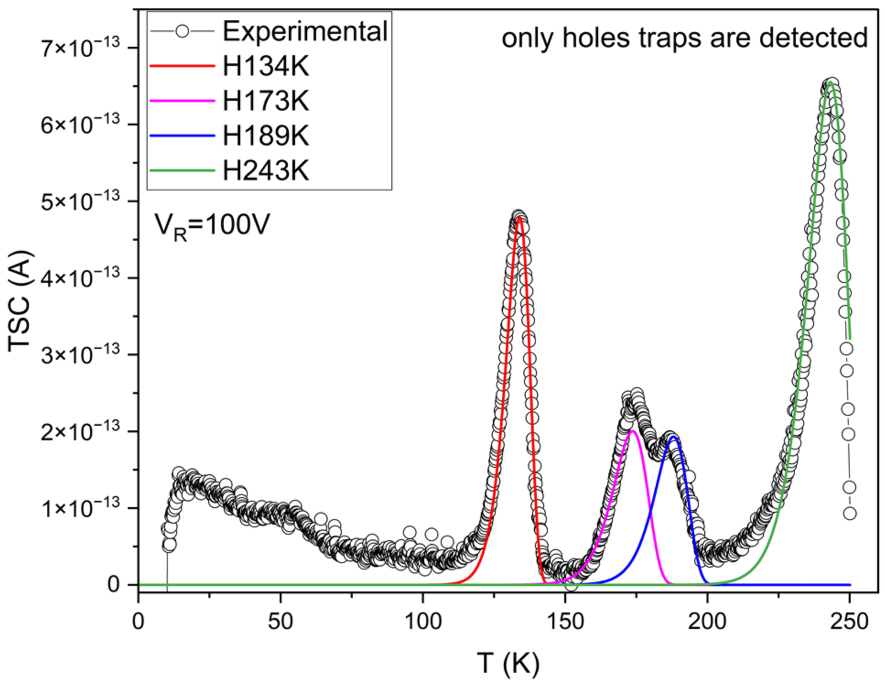


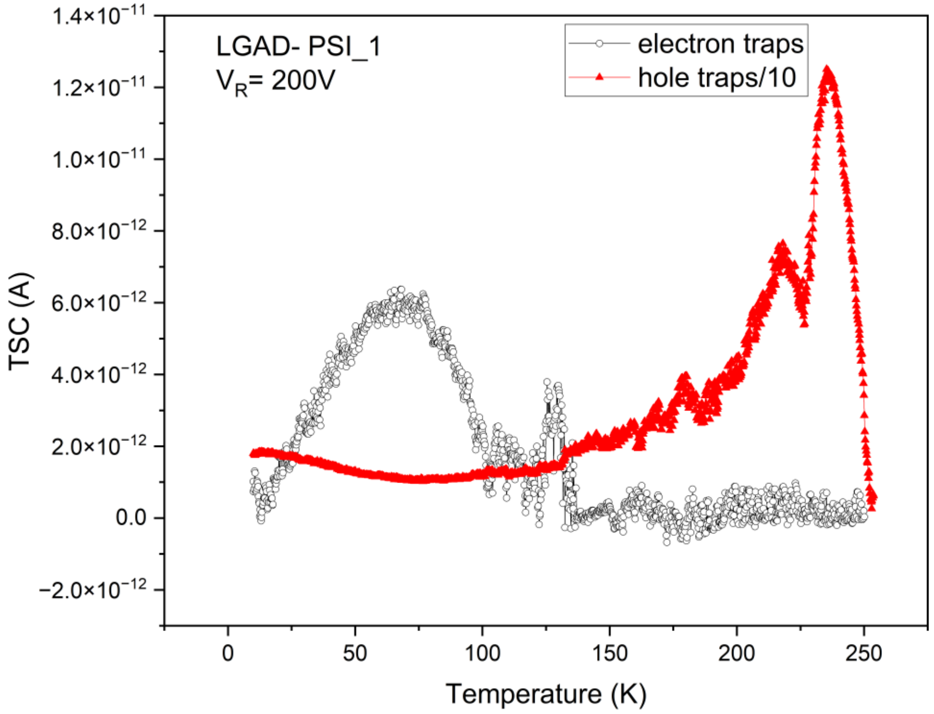


- Recovery after annealing at 200 ^{o}C indicates that VP center is generated in high concentrations via the reaction V+P, the calculated number of vacancies induced by Ga ion-beams being in the order of Phosphorous doping

As fabricated p-type PiN and LGADs from PSI

- **Gain suppression after exposure to X-ray photons (2 keV)** indicating a pre-existing population of defects in the gain layer





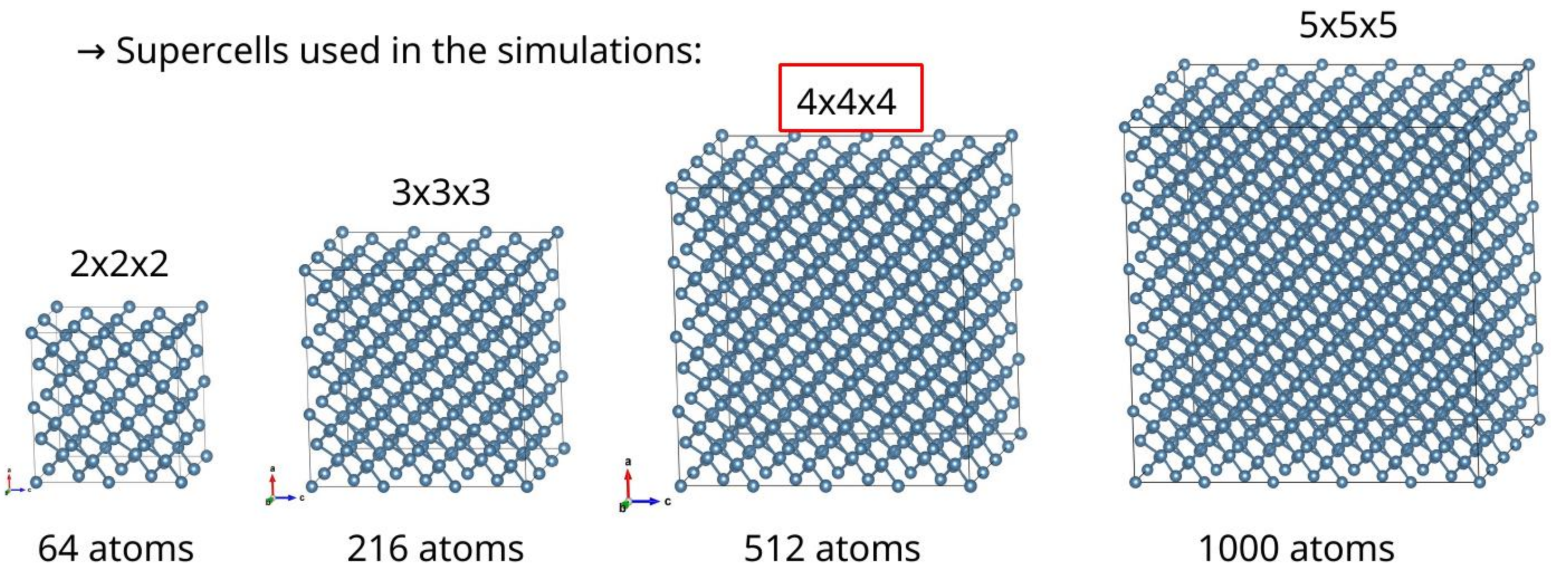
Only holes traps are detected in PiN diodes

H134K: E_a = 0.338 eV; σ_p= 2.75x10^{-15} cm^2, N_t= 3.75x10^{11} cm^{-3}
H173K: E_a = 0.43 eV; σ_p= 6x10^{-16} cm^2, N_t= 2.1x10^{11} cm^{-3}
H189K: E_a = 0.475 eV; σ_p= 1x10^{-15} cm^2, N_t= 2.1x10^{11} cm^{-3}
H134K: E_a = 0.68 eV; σ_p= 9x10^{-15} cm^2, N_t= 8.5x10^{11} cm^{-3}

Much larger defect concentrations in gain layer of LGADs after exposure to X-rays

- **hole traps ~ 1.5 10^{14} cm^{-3}**
- **Shallow electron traps ~ 10^{13} cm^{-3} (possible BCD)**

Radiation damage in Silicon – *Ab initio* modeling of charged defects



Several types of defects are used in the simulations:

- single-atom defects: vacancies, intersititials, B/C/P substitutions (used for calibration)

- double-atom defects (e.g. $B_{Si}Si_i$, B_iO_i, C_iO_i in different metastable configurations)

→ **SIESTA code:** Linear scaling of the computational time with the system size (employs numeric atomic orbitals as basis sets, pseudopotentials)

→ Formation energies of charged defects:

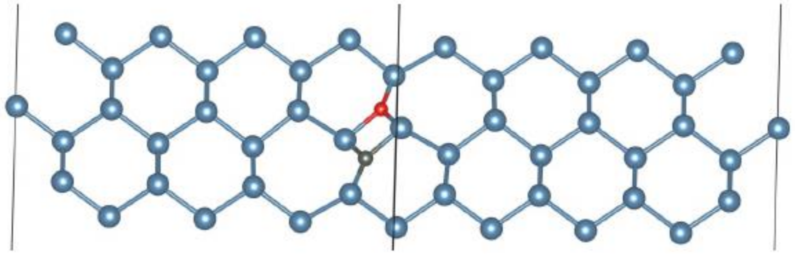
$$E^{\mathrm{f}}[X^q] = E_{\mathrm{tot}}[X^q] - E_{\mathrm{tot}}[ideal] - \sum_i n_i \mu_i + q\left(E_{\mathrm{VBM}} + E_F\right) + E_{\mathrm{corr}}(q)$$

→ Transition energy levels:

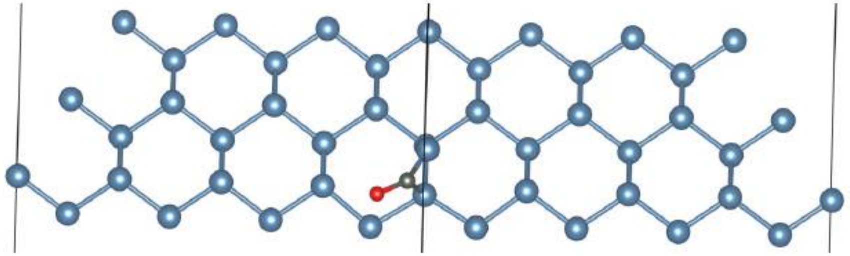
$$\epsilon(q/q') = \frac{E^f[X^q] - E^f[X^{q'}]}{q' - q}$$

Radiation damage in Silicon – *B_iO_i metastable states*

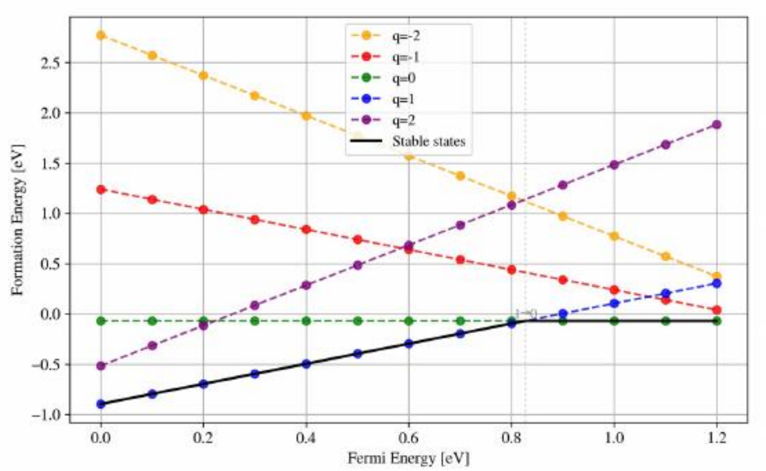
Two configurations of the B_iO_i defect, revealing different behaviors:



Configuration A (standard)

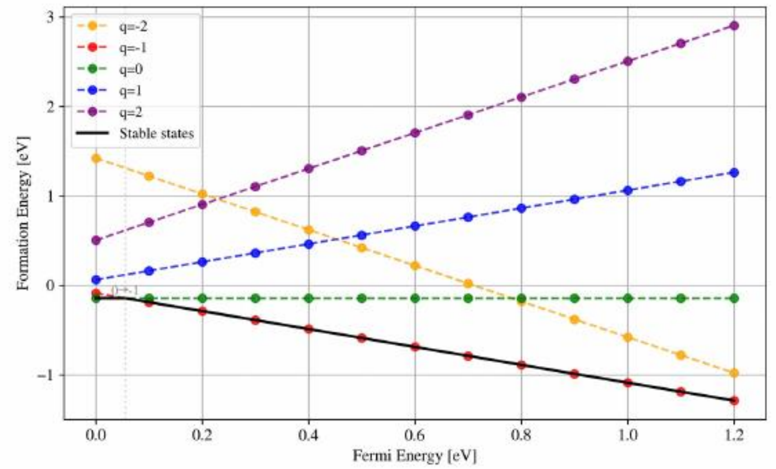


Configuration B



Interstitial boron – interstitial oxygen (A) – B_iO_i (our result)

→ mostly donor character



Interstitial boron – interstitial oxygen (B) – B_iO_i (our result)

→ acceptor character

Compared to the standard configuration, we identified another metastable state, with a different structural configuration, presenting boron and oxygen atoms in close proximity,

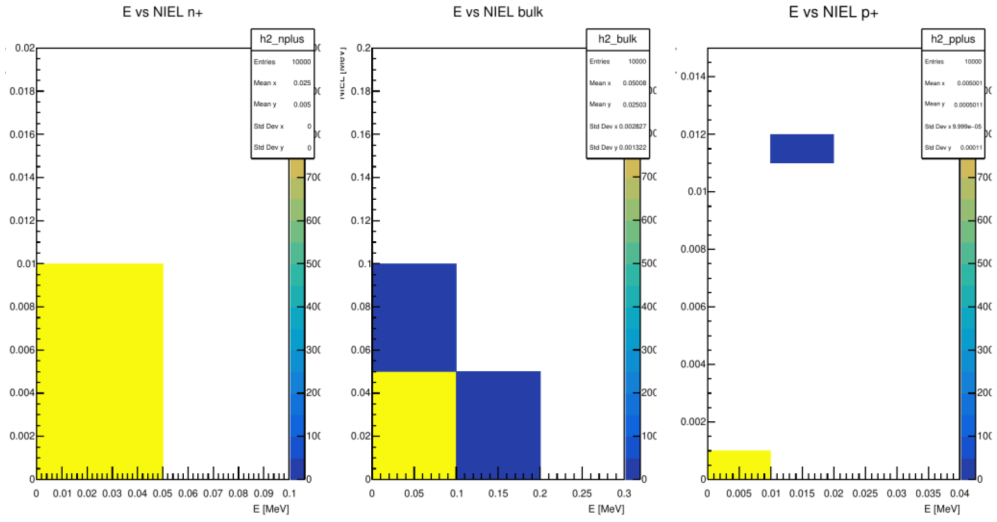
Further explorations of metastable states would provide a deeper understanding of the donor/acceptor character under different doping conditions and could indicate ways to mitigate ARP.

These results were presented within the 4th DRD3 week on Solid State Detectors R&D, CERN, 10-14 November.

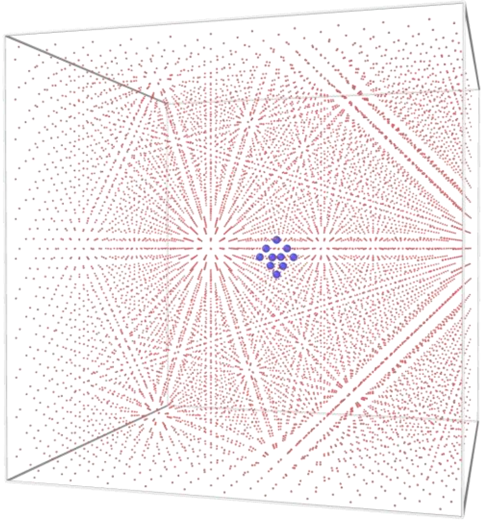
Radiation damage in Silicon – *Geant4 & Molecular dynamics simulations*

→ High fluences are prone to generate rather complex defects, beyond the few-atom defects considered so far.
→ Geant4 simulations can be used to simulate the initial configuration of complex defects.
→ The evolution of such complex defects is assesed using molecular dynamics (MD) simulations on large silicon supercells (10000 atoms), using the LAMMPS package.
→ Vacancies are induced in the ideal system by displacing a cluster of Si atoms.
→ Canonical conditions were used, at fixed temperature (T=253K).

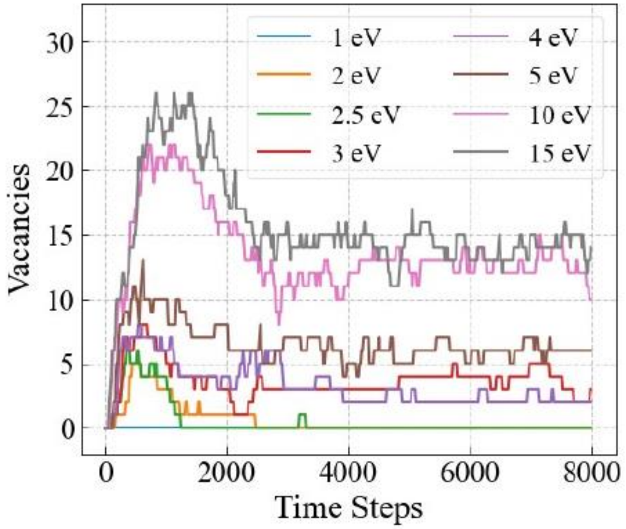
Geant4 simulation for a n+/p+ junction irradiated with 1MeV neutrons: NIEL vs. energy plots for each region.



Simulation box containing 10000 atoms

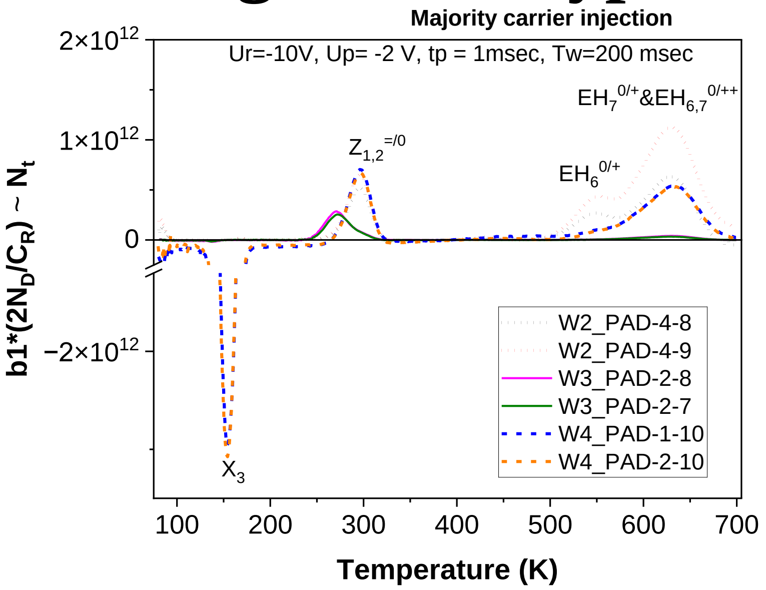


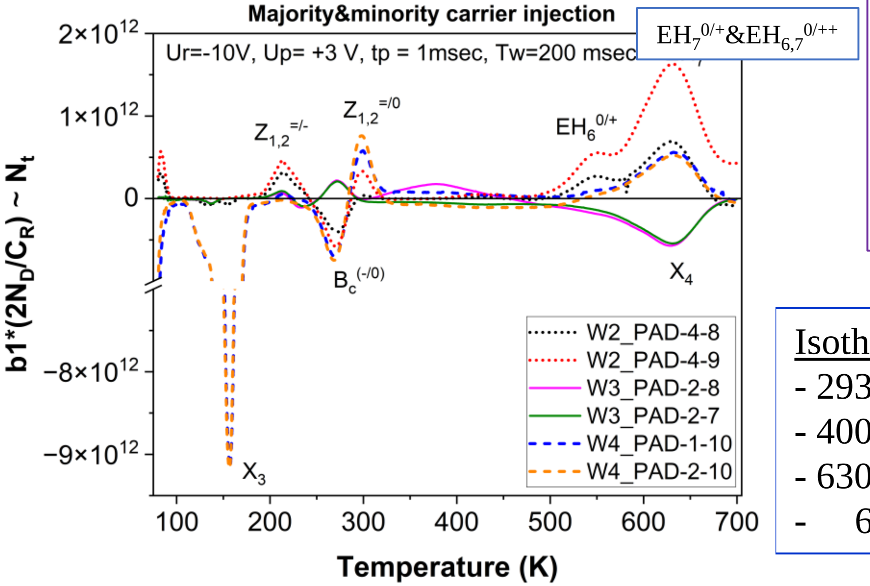
Vacancy-interstitial recombination after inducing the cluster defect



Radiation damage in SiC - experimental

As grown n- type SiC p$^+$-n diodes – from DRD3 Collaboration





N_{eff} at RT:

W2_PAD_4_8: 4.85 x 10^{13} cm^{-3}
W2_PAD_4_9: 1.19 x 10^{14} cm^{-3}
W3_EPI_50_PAD_2_7: 3.57 x 10^{13} cm^{-3}
W3_EPI_50_PAD_2_8: 4.43 x 10^{13} cm^{-3}
W4_EPI_100_PAD_1_10: **7.02 x 10^{14} cm^{-3}**
W4_EPI_100_PAD_2_10: **6.82 x 10^{14} cm^{-3}**

Defect level		W2_PAD_4-8	W2_PAD_4-9	W3_PAD_2-8	W3_PAD_2-7	W4_PAD_1-10	W4_PAD_2-10
Minima X3	Energy (eV)	0.346	-	0.371	0.332	0.342	0.336
	Nt (cm^{-3})	9.97E+11	-	9.59E+12	1.09E+13	8.17E+13	8.10E+13
Minima B_C (-/0)	Energy (eV)	0.653	0.650	0.625	0.643	0.635	0.633
	Nt (cm^{-3})	5.48E+12	1.30E+13	5.81E+11	2.44E+12	6.35E+12	6.83E+12
Minima X4	Energy (eV)	-	-	1.521	1.493	-	-
	Nt (cm^{-3})	-	-	6.03E+12	5.69E+12	-	-
Maxima $Z_{1/2}$ (=/0)							
	Nt (cm^{-3})	3.21E+12	6.65E+12	1.31E+12	1.48E+12	3.28E+12	3.18E+12
Maxima EH_4	Energy (eV)	1.039	1.064	-	-	-	-
	Nt (cm^{-3})	4.34E+11	3.72E+11	-	-	-	-
Maxima EH_6(0/+)	Energy (eV)	1.444	1.453	-	-	-	-
	Nt (cm^{-3})	3.19E+12	6.39E+12	-	-	-	-
Maxima EH_7(0/+)	Energy (eV)	1.536	1.572	-	-	1.549	1.586
	Nt (cm^{-3})	7.65E+12	1.70E+13	-	-	5.34E+12	5.29E+12
Maxima $EH_{6,7}$	Energy (eV)	-	-	1.626	1.697	-	-
	Nt (cm^{-3})	-	-	4.46E+11	3.77E+11	-	-
Minima X4	**Energy (eV)**	-	-	**1.521**	**1.493**	-	-
	Nt (cm^{-3})	-	-	6.03E+12	5.69E+12	-	-

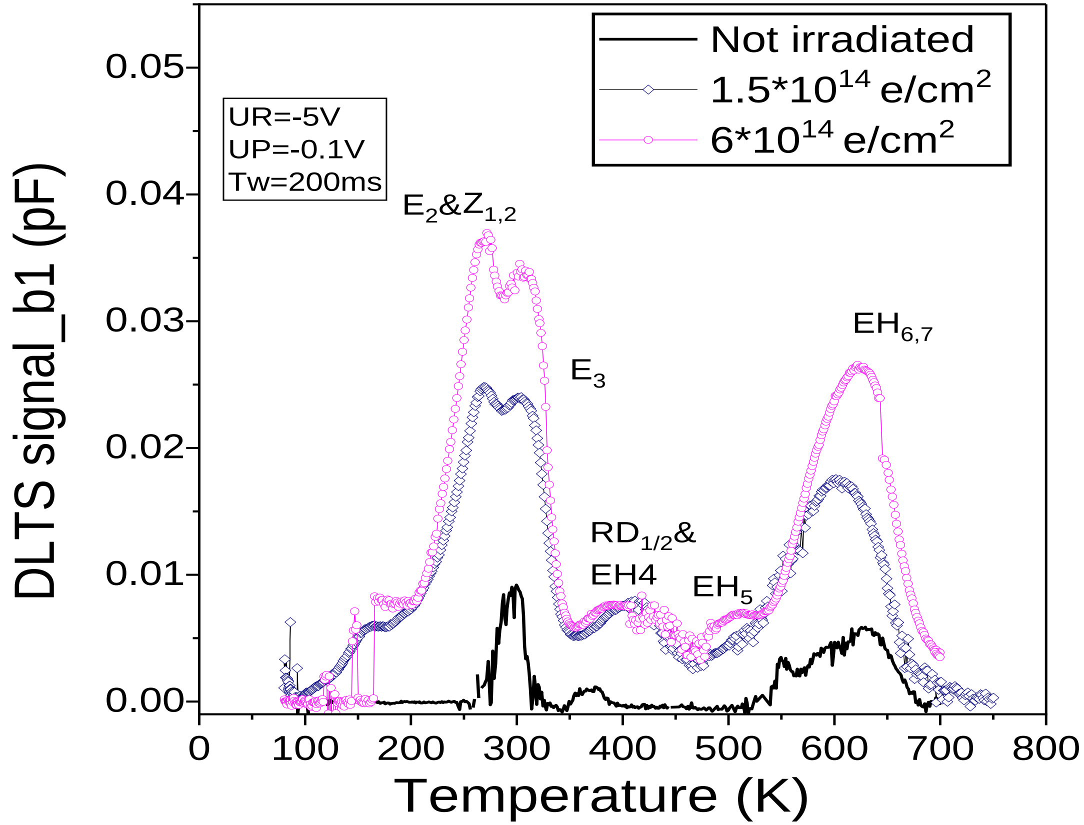
- X_3 - may originates from the ion-implanted (Al^+) p+ region. *Raja, P.V., et al, J Mater Sci: Mater Electron 34, 1383 (2023)* *https://doi.org/10.1007/s10854-023-10813-z*
- B_c - Boron incorporation on Carbon sites (unintentional during CVD growth) *T. Knezevic et al, Materials 16, 3347 (2023)*

The ratio $Z_{1,2}/EH_{6,7}$ –vary from sample to sample, from ~ 0.3 to 3 indicating that $Z_{1,2}$& $EH_{6,7}$ signals cannot be attributed to different charge states of the same defect (V_C), as presently proposed in the literature

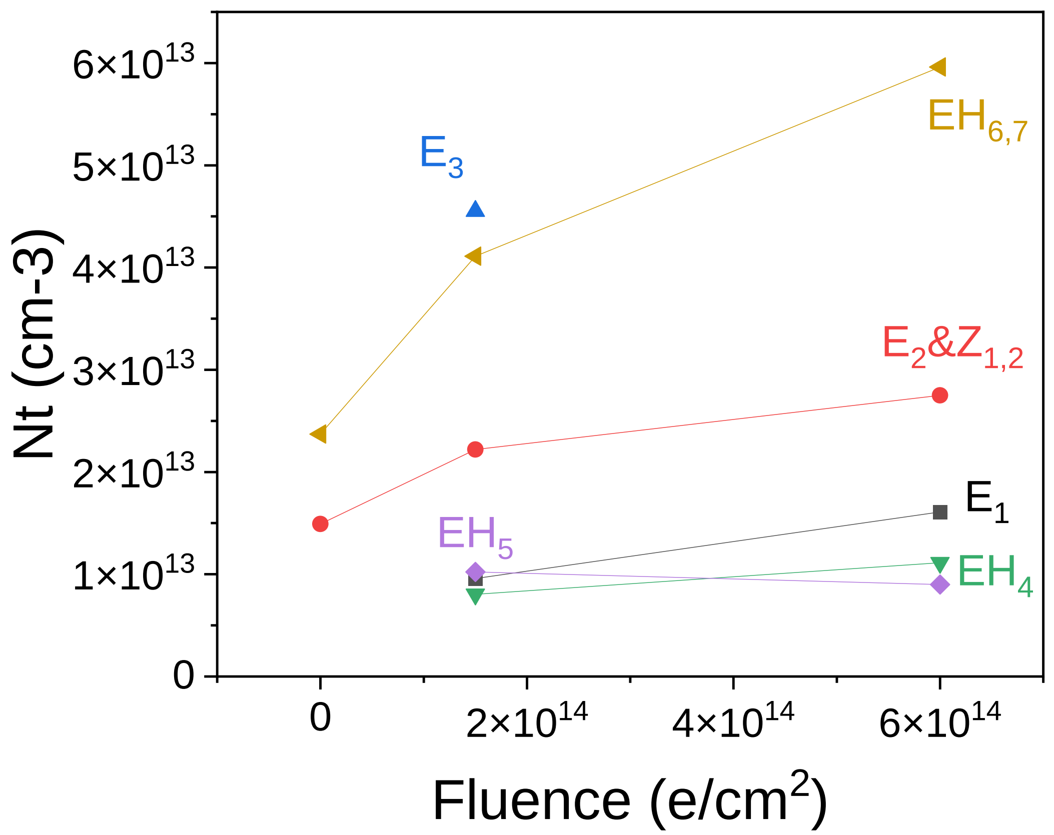
Isothermal, **W3_PAD_2-8**:
- 293 K ($Z_{1/2}$): **σ_n = 3.51 x 10^{-16} cm^2**
- 400 K (EH_4): **σ_n = 8.83 x 10^{-22} cm^2**
- 630 K (EH_7): **σ_n = 7.27 x 10^{-16} cm^2**
- 630 K (X_4): **σ_n = 6.68 x 10^{-16} cm^2, σ_p = 1.16 x 10^{-20} cm^2**

n- type SiC Schottky diodes irradiated with 6 MeV electrons

- Detect the defects induced by irradiation
- focus on the identity of the most prominent signals $Z_{1,2}$ (carrier life-time killer in SiC) and $EH_{6,7}$ proposed in the literature to be different charge states of the same defect - V_C

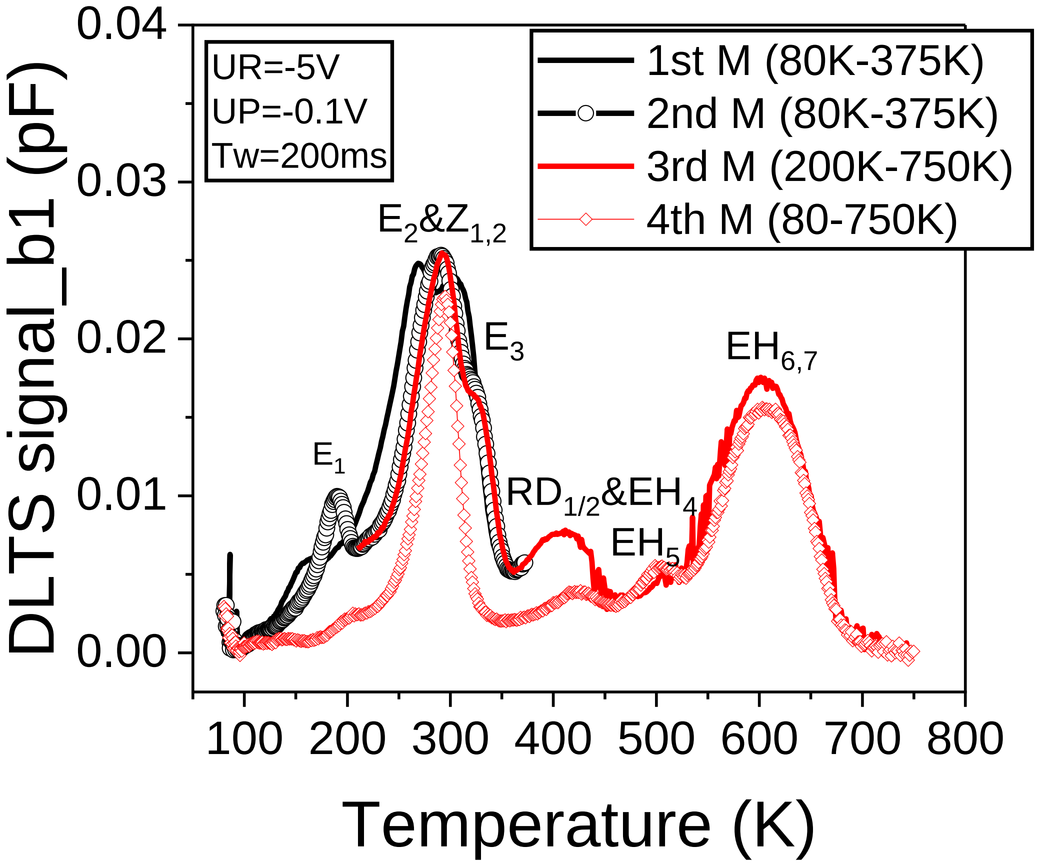


Continuous measurements 80K-750K



Annealing effects

DLTS results after irradiation with $1.5 * 10^{14} e/cm^2$ (6 MeV)

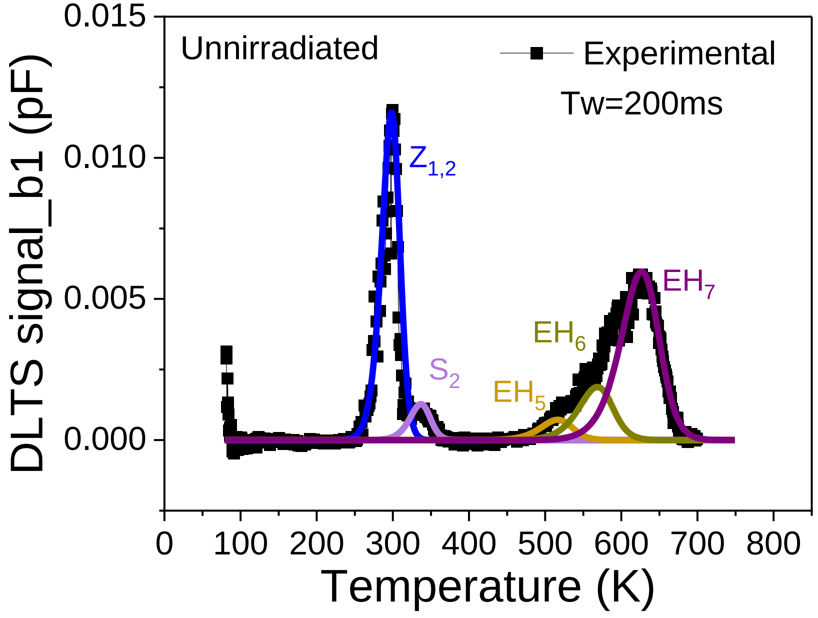


1st measurement (80K-375K)
2nd measurement (80K-375K)
3rd measurement (200K-750K)
4th measurement (80K-750K)

Same radiation induced defects are detected and **with similar annealing behaviour** as for irradiation with lower fluence

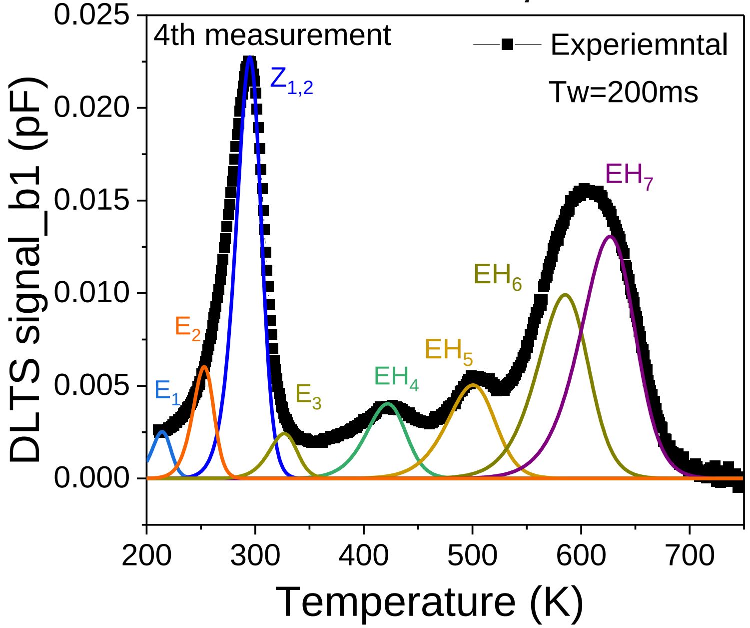
- $\mathbf{E_1}$ is initially annealing in after the 1st heating at 375K and then anneals out after the heating at 750K
- $\boldsymbol{E_2}$ **and** $\boldsymbol{E_3}$ – annealed out after heating up to **375 K**
- $\boldsymbol{EH_4}$ **and** $\boldsymbol{RD_{1/2}}$ – significantly reduced after heating up to **750 K**
- $\boldsymbol{EH_5}$ – remained unchanged within this temperature range

Following $Z_{1,2}$:EH_7 ratio, whether approaches **≈ 1** after annealing-out of other radiation induced defects.



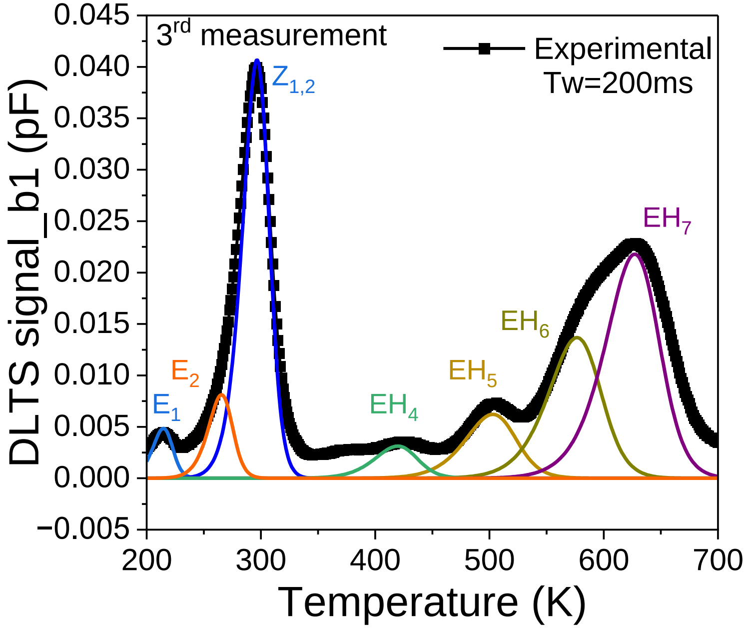
$Z_{1,2}/EH_7$= **0.43**

$1.5 * 10^{14} e/cm^2$



$Z_{1,2}/EH_7$= 1.16

$6 * 10^{14} e/cm^2$



$Z_{1,2}/EH_7$= 1.01

	$E_c - E_t\ (eV)$	$\sigma\ (cm^2)$	$N_t\ (cm^{-3})$
$Z_{1,2}$	0.68	$2 * 10^{-14}$	$1.8 * 10^{12}$
EH_6	1.3	$3 * 10^{-15}$	$1.25 * 10^{12}$
EH_7	1.422	$3 * 10^{-15}$	$4.1 * 10^{12}$

	$E_c - E_t\ (eV)$	$\sigma\ (cm^2)$	$N_t\ (cm^{-3})$
$Z_{1,2}$	0.687	$1.6 * 10^{-14}$	$1 * 10^{13}$
EH_6	1.35	$1.5 * 10^{-15}$	$7.4 * 10^{12}$
EH_7	1.4	$1 * 10^{-15}$	$8.6 * 10^{12}$

	$E_c - E_t\ (eV)$	$\sigma\ (cm^2)$	$N_t\ (cm^{-3})$
$Z_{1,2}$	0.682	$1.27 * 10^{-14}$	$1.32 * 10^{13}$
EH_6	1.3	$2 * 10^{-15}$	$9.2 * 10^{12}$
EH_7	1.51	$1 * 10^{-14}$	$1.3 * 10^{13}$

→ $Z_{1,2}$ and $EH_{6,7}$ cannot belong to the same defect (V_C)

Dissemination

- ***3 publications:***

1) *Defects and acceptor removal in 60Co γ-irradiated p-type silicon*, A. Himmerlich et al, co-authors A. Nitescu and I. Pintilie, Nuclear Instruments and Methods in Physics Research A 1081 (2026) 170886, https://doi.org/10.1016/j.nima.2025.170886
2) *Gain Response and Ion Beam-Induced Donor Removal in nLGAD Detector: Global Gain Quenching*, Miloš Manojlović et al, co-author I. Pintilie, IEEE Sensors Journal (Early Access), 10.1109/JSEN.2025.3624206
3) *On the nature and charge state of the X-Defect, a radiation-induced Silicon defect with field-enhanced charge carrier emission*, N. G. Sorgenfrei et al, co-author I. Pintilie, Nuclear Inst. and Methods in Physics Research, A (2025), https://doi.org/10.1016/j.nima.2025.171133

- ***3 talks during the 3rd DRD3 workshop held in Amsterdam (2-6 June 2025) and 4 talks during the 4th DRD3 week held at CERN (10-14 November 2025):***

1) *Hunting the X-Defect*, N. Sorgenfrei et al, co-author I. Pintilie, Jörn Schwandt, on behalf of the DRD3 WG3- Acceptor Removal Team ***(3rd DRD3 week)*** - https://indico.cern.ch/event/1507215/contributions/6539534/
2) *Characterization of electrically active defects in unirradiated epitaxial 4H-SiC p+-n diodes*, C. Besleaga, R. E. Patru, G.A. Boni, A. Nitescu, N. G. Sorgenfrei, Y. Gurimskaya, F. Rizwan, M. Moll, I. Pintilie ***(3rd DRD3 week)*** https://indico.cern.ch/event/1507215/contributions/6539557/
3) *Update on the "Defect engineering in PAD diodes mimicking the gain layer in LGADs" project, J. Schwandt, I. Pintilie, K.Lauer, M. Moll,* ***(3rd DRD3 week)-*** https://indico.cern.ch/event/1507215/contributions/6539553/
4) *Gain-Layer Project*, Niels Sorgenfrei et al, co-authors: C.Besleaga, G. A. Boni, C. Chirila, D. Geambasu, L. Nedelcu, A. Nitescu, R. Patru, G. Stan and I. Pintilie ***(4th DRD3 week)*** https://indico.cern.ch/event/1581713/contributions/6765826/
5) *Investigation of point defects in silicon supercells using density functional theory*, N. Filipoiu, M. Coasinschi, C. A. Pantis-Simut, A.T. Preda, I. Pintilie, G. A. Nemnes, A. Danu, ***(4th DRD3 week),*** https://indico.cern.ch/event/1581713/contributions/6765861/
6) *Donor removal and Global Gain Quenching (GGQ) in nLGAD detectors*, Milos Manojlovic et al, co-authors: A. Nitescu, C. Besleaga, and I. Pintilie ***(4th DRD3 week),*** https://indico.cern.ch/event/1581713/contributions/6765863/
7) *Defect investigation on n-type Schottky diodes based on 4H-SiC before and after irradiation with 5 MeV electrons*, A. G. Boni, A. Nitescu, C. Besleaga, D. Geambasu, R.E. Patru and I. Pintilie ***(4th DRD3 week),*** https://indico.cern.ch/event/1581713/contributions/6765865/

Outreach activities

- 13 visits in DUROCERN centre;
- „European Researcher Night 2025" in Magurele (26.09.2025) and Bucharest (27.09.2025)
- participation in the organisation of the 5th EPS-TIG hands-on session “Frontier of Quantum Technologies” – satellite event at the 12th Congress of the Balkan Physical Union, 9-12 July 2025 (https://bpu12.ucv.ro/wp-content/uploads/2025/05/5thEPS-TIG_Romania.pdf);
- material/device/scientific support for 5CBees team applying for “beamline for schools, cern.ch/bl4s” with application “5CB Liquid Crystal Particle Detector”. The team was selected among the shortlist of 50 teams, receiving a special prize including a do-it-yourself kit to build their own particle detector and BL4S T-shirts (chrome-extension://efaidnbmnnnibpcajpcglclefindmkaj/https://beamline-for-schools.web.cern.ch/sites/default/files/BL4S_all-winners_2025.pdf)

Involvement in DRD3 management and strategic projects

- I. Pintilie endorsed by DRD3-CB in June 2025 for a 3 years mandate as joint Convener of WG3 (*Radiation damage characterization and sensor operation at extreme fluences)* and Leader of WP3 (*Sensors for extreme fluences)*
- WP3 *“Radiation damage in Si PiN and LGAD sensors”* (project leader I. Pintilie, NIPNE and ISS team members); “*SiC-LGAD Detectors*”, (team member -NIMP),

Thank you for your attention !