WP3 Project Title: Radiation damage in Si PiN and LGAD sensors

Project Description

The project addresses both, experimental and theoretical aspects related to radiation induced damage in Silicon, covering the full range from low to high and extreme fluences beyond $2x10^{16}$ n_{eq}/cm^2. It contributes to several of the research goals of WG3 and WG4 (RG 3.2, RG3.3, RG3.4, RG4.2, RG 4.3, RG 4.4). The final goal of the project is to *achieve a fundamental scientific understanding of radiation damage processes in Si detector material at low (<few 1e14 cm^{-2}), high (< 1e16 cm^{-2}), and extreme (>few 1e16 cm^{-2}) radiation levels.* For this, several **specific objectives** (***O***) has to be reached: ***O1)*** *Understand the gain loss in Silicon LGADs exposed to irradiation fluences above 10^{15} n_{eq}/cm^2;* ***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 and find ways to improve the Si based devices*; ***O3)*** *Model the defects formation in Silicon, dynamics and metastabilities* ***(***observed experimentally but not understood so far) *in connection with doping and extrinsic impurities;* ***O4)*** *Device modeling and parametrization of radiation effects in Si over a large fluence range and in connection with doping and extrinsic impurities;* ***O5)*** *Improve LGAD radiation resistance up to $1 \cdot 10^{16}$ n_{eq}/cm^2* . The work in the project addresses both, experimental and theoretical aspects and covers the full fluence range mentioned above..Various defect engineered samples will be fabricated for this purpose. They will be subject of electrical and structural characterizations, by employing a large spectrum of experimental methods, suitable for defect investigations in samples exposed to different levels of irradiation. The parameters determined from experiments will be used as reference values or inputs for modeling both, the defect generation and kinetics, and the device properties. For theoretical modeling a multi-scale approach is employed aiming to understand the fundamental processes which occur in irradiated Silicon and corresponding devices. The acquired knowledge will enable further improvements of the radiation hardness of Silicon based sensors.

Motivation and goals

- main motivation: Future upgrades beyond LHC phase-II
- strategic goals directly addressed in project as specified in WP3, DRDT 3.2, -Sensors for 4D-tracking and WP3, DRDT3.3 -Sensors for extreme fluences

Execution of the project (description, *list of things to be included*)

While comprehensive investigations of radiation induced defects can be achieved with specific techniques based on capacitance or current measurements (e.g. Deep Level Transient Spectroscopy -DLTS, Thermally Stimulated Current/Capacitance -TSC/ TSCap), such methods can only be successfully applied on standardly fabricated Silicon sensors up to fluences of about 10^{15} n_{eq}/cm^2. In addition, as the extrapolation of damage parameters to higher fluences does not resemble the measured performance of the devices, further experimental and modelling work is required, including the employment of other techniques applicable after higher irradiation fluences, as Fourier Transformed Infrared (FTIR) spectroscopies, and/or fabrication of special designed samples. Moreover, the changes of the fundamental semiconductor properties (e.g., carrier mobilities, lifetime) at extreme fluences are poorly known, although they are needed for any detector design. The present consortium had prepared for addressing these challenges for Silicon sensors by bringing together their experimental and theoretical expertise. Specific activities in the project are:

(i) fabrication of defect engineered silicon sensors:

a. planar n^{++}-p^{+}-p^{++} diodes mimicking the gain layer in LGADs with different C, B, P and O content. They are processed on Standard and Oxygenated float-zone Silicon (STFZ and DOFZ) wafers of 1.5 and 15 Ω cm resistivity (p^{+}) and can be thoroughly investigated from microscopic point of view over a large fluence range, either with DLTS and TSCap (no need to fully deplete the samples) or with TSC (need to fully deplete the p^{+} region of the diodes). For measurements where the active $^{p+}$ region has to be fully depleted, diodes with thin p^{+} layers will fabricated by compensating with successive P implantations of different energies on 1.5 Ωcm wafers resulting in a 2 µm p^{+} thin layer of 15 Ωcm.

b. LGADs with different Carbon implantations in the gain layer

(ii) irradiations over a large fluence range, from 10^{12} to $>10^{17}$ n_{eq}/cm^2

(iii) electrical and structural characterization of radiation induced defects by employing a large spectrum of experimental methods, suitable for defect investigations in samples exposed to different levels of irradiation, from DLTS - up to 10^{15} n_{eq}/cm^2, to TSC/TSCap - up to 10^{16} n_{eq}/cm^2 and further to FTIR (above 10^{16} n_{eq}/cm^2) - for extreme high irradiation fluences;

(iv) electrical characterization of the fabricated silicon sensors (CV/IV, CCE, TCT, carrier lifetime, Van der Paw resistivity and Hall mobility);

(v) modeling - the parameters determined from experiments will be used as reference values or inputs for modeling both, the defect generation and kinetics, and the device properties. For theoretical modeling a multi-scale approach is employed aiming to understand the fundamental processes which occur in irradiated material and devices, which combines tools designed to study the passage and impact of particles through matter (Geant4, TRIM), molecular dynamics (LAMMPS), first principle calculations (SIESTA), device simulation (e.g. TCAD) and *Machine Learning* (ML) techniques for by-passing numerically intensive simulations in the context of annealing schedules.

Milestones, deliverables and timeline (in form of a table shown below)

Summary of milestones (M) and deliverables (D):

Number	**Deliverable/Milestone Title**	**WP project #/task**	**Lead Beneficiary** (participants)	**Type**	**Dissemination Level**	**Due Date**
D- task #1	**Report on microscopic and macroscopic investigations in irradiated defect engineered gain layers for Si based LGADs,** fluences up to 10^{17} n_{eq}/cm^2	**WP3.X/1**	**NIMP** (CERN, CiS, NIPNE, INFM Torino, Vilnius, IFCA, JSI, ISS, IHEP)	**Report**	**Conferences and Publications**	**Q4 2026**
M- task #-1.1	Fabrication and testing of as processed defect engineered Si sensors (enrichment with O, C and/or P) mimicking the gain layer in LGADs		CiS	Prototype	DRD3 report	Q2 2025
M- task # 1.2	Irradiation of the fabricated samples		JSI	Report	DRD3 report	Q3 2025
M- task # 1.3	Setting up techniques for assessment of complex defect formation		NIMP	Report	DRD3 report	Q3 2025
D- task #2	**Device modeling of PiN and LGAD devices with radiation induced defects**	**WP3.X/2**	**HH** (NIPNE, NIMP, CERN, JSI, INFN Torino)	**Report**	**Conferences and Publications**	**Q2 2027**
M- task # 2.1	Identify the differences between experimental data and modeling predictions		HH	Report	DRD3 report	Q1 2026
M- task # 2.2	Calibration of models for Si devices implementing new defect reactions		NIPNE	Report	DRD3 report	Q3 2026

D- task #3	**Report on microscopic and macroscopic investigations in irradiated defect engineered optimized LGADs,** fluences up to 10^{17} n_{eq}/cm^2	**WP3.X/3**	**CERN** (NIMP, HH, CiS, IHEP, JSI, NIPNE, ISS, Vilnius, ISS, INFN Torino)	**Report**	**Conferences and Publications**	**Q 2 2028**
M- task # 3.1	Fabrication and testing of as processed defect engineered optimized LGADs		CiS	Prototype	DRD3 report	Q1 2027
M- Task # 3.2	Irradiation of the fabricated LGAD samples		JSI	Report	DRD3 report	Q2 2027
M- Task # 3.3	Identify the differences between experimental data and predictions of the parametrization model		HH	Report	DRD3 report	Q4 2027

Details on Deliverables or Milestone:

Deliverable/Milestone	**Planned Start Month**	**Duration (months)**	**Project WP/task**	**Research Objectives** **Description and expected result**	**Type**	**Lead beneficiary** (participants)
D- task #1 **Report on microscopic and macroscopic investigations in irradiated defect engineered gain layers for Si based LGADs,** fluences up to 10^{17} n_{eq}/cm^2	1	23	3.X/1	*O1) Understand the gain loss in Silicon LGADs exposed to irradiation fluences above 10^{15} n_{eq}/cm^2;* *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 and*	DRD3 report, Conferences and Publications	**NIMP (**CERN, CiS, NIPNE, INFM Torino, VU, IFCA, JSI, ISS, IHEP)

				find ways to improve the Si based devices; *O3) Model the defects formation in Silicon, dynamics and metastabilities in connection with doping and extrinsic impurities;*		

Description:

The most powerful technique for detecting and characterizing electrically active defects is the DLTS method, providing the defect parameters required for any attempt of modelling the device electrical characteristics. However, in structures like LGADs, with layers of different resistivity, DLTS can be applied only for fluences $\Phi_{eq} < 10^{12}$ n_{eq}/cm^2, when the bulk region is not so damaged and the electric field profile remains similar to unirradiated devices. On PiN diodes, comprehensive DLTS defect investigations have been performed so far only on Si with resistivity larger than 50 Ωcm (doping below $3x10^{14}/cm^3$) and so, the defects formed after fluences above $10^{14}/cm^2$ could not be investigated. To reveal the defects generated after larger fluences, PiN diodes with bulk resistivity of 3 Ωcm (A) and 15 Ωcm (B) will be investigated. Such Si diodes, mimicking the gain layer in LGADs, are fabricated on standard float-zone (FZ) and oxygenated FZ (DOFZ) Si and Co-doped with C (different implantation doses), labeled as G-FZ/DOFZ-A/B or simply G-type. They will be investigated by DLTS after fluences up to 10^{15} n_{eq}/cm^2 (NIMP, CERN, VU, HH) and with TSC/TSCap (NIMP, CERN, HH) for fluences up to $2x10^{16}$ n_{eq}/cm^2. For larger irradiation fluences these samples will be investigated by FTIR (NIMP). If new defects are detected after irradiations with fluences above 10^{15} n_{eq}/cm^2 annealing studies at elevated temperatures will be performed in order to identify the chemical structure of the defects. Measurements of IV/CV (all participants), CCE (ISS,….), TCT (JSI, IFCA), Carrier lifetime (VU) and Hall mobility (NIMP) will be performed for the full range of irradiation fluences. The fundamental aspects of processes occurring during and after irradiation will be investigated by dedicated software packages. It will start from calculations on initial defect distribution produced by irradiation, e.g. *Geant4&TRIM (ISS, ...)* followed by investigations of their subsequent dynamics by performing Molecular Dynamics (MD) simulations using classical force-fields implemented in LAMMPS (NIPNE, …) to capture defects metastability in the context of doping with impurities and irradiation fluence. The relevant defect configurations will be assigned for further investigations of electronic properties by *ab initio* calculations using density functional theory (DFT) implemented in SIESTA (NIPNE, CiS…). A supercell approach will be considered in order to establish the defect reactions and determine the potential local minima configurations as well as to evaluate the defects formation energies in the context of extrinsic impurities (measured experimentally by SIMS). Neutral and charged defects shall be considered. The donor character of Boron containing defects (BCD) will be investigated in connection with the acceptor removal process. High-throughput calculations will be employed to explore the configurational space. The mapping of energy landscape provides possible pathways between the meta-stable states. Besides the large-scale MD simulations performed with

LAMMPS, which aim at large time-scales, the MD at DFT level provides accurate description of short-time processes. In addition, nudge elastic band (NEB) simulations provide the transition states between metastable configurations. The parameters determined from experiments will be used as reference values or inputs for modeling the defect generation and kinetics.

Expected results:

Experimental:

- *Detection and characterization of new defects induced by irradiation above 10^{15} n_{eq}/cm^2 (e.g. defects formed via 2nd order processes and/or new Boron related defects)*
- *Reveal the role of O, C and P (co-doping) impurities in low resistivity B doped Si in the formation of defects impacting on the device performance and on the corresponding gain layers in LGADs.*
- *Reveal the intrinsic and radiation induced FTIR structural signals of p-type Si*
- *Reveal the structure and concentration of defects induced by irradiation with more than $2x10^{16} n_{eq}/cm^2$*

Theoretical aspects:

- *Determine initial defects distribution, starting from Geant4&TRIM simulations*
- *Determine the defect' configuration and metastabilities by MD using LAMMPS*
- *Determine the electronic properties of irradiated Silicon, by ab initio calculations (SIESTA), in relation with doping and impurity content*
- *Understanding the effect of co-doping with O, C and/or P on the radiation hardness of gain layers in LGADs and develop defect engineered strategies for improving the radiation hardness of Silicon based sensors*

D- task #2 Device modeling of PiN and LGAD devices with radiation induced defects	4	28	3.X/2	*O4) Device modeling and parametrization of radiation effects in Si over a large fluence range and in connection with doping and extrinsic impurities*	DRD3 report, Conferences and Publications	**HH** (NIPNE, NIMP, CERN, JSI, INFN Torino)

Description:

The radiation induced changes in I-Vs/C-Vs will be investigated using customized computer programs and concern the changes established based on MD and ab initio simulations. 3D models provide information about charging and current distribution according to doping profile which will be further refined by including the specific technology details in TCAD. In addition, an evaluation of irradiated electronic devices based on fluence, irradiation type and annealing will be used for developing parametrization models based on Machine Learning tools. By combining both, the theoretical and experimental results with *ML* techniques, efficient predictive models can be developed and used further to identify the technological ways for improving the Silicon material with respect to radiation

<table>
<tr><td colspan="7">hardness/operational conditions. The results obtained with TCAD will be compared to experimental data and further processed in order to establish parametrizations based on Φ_{eq}, irradiation type, impurity content and annealing. This will enable a predictive tool that will by-pass the TCAD time and resource consuming calculations.

Expected results:

- Device modeling of PiN and LGAD devices with radiation induced defectsametrization of radiation damage in PiN and LGAD Silicon devices by ML techniques</td></tr>
<tr><td>D- taskt #3

Report on microscopic and macroscopic investigations in irradiated defect engineered optimized LGADs, fluences up to 10^{17} n_{eq}/cm^2</td><td>24</td><td>12</td><td>3.X/3</td><td>O5) Improve LGAD radiation resistance up to 1 ･ 10^{16} n_{eq}/cm^2</td><td>DRD3 report, Conferences and Publications</td><td>CERN (NIMP, HH, CiS, IHEP, JSI, NIPNE, ISS, VU, ISS, INFN Torino)</td></tr>
<tr><td colspan="7">Description: Based on previous experimental results and developed parametrization models the most promising in terms of radiation hardness defect engineered LGADs will be fabricated and characterized from microscopic and macroscopic point of view.

Expected results:

- Improve the radiation hardness of LGADs up to 1 ･ 10^{16} n_{eq}/cm^2
- The experiments on these defect engineered LGADs will be used to validate and calibrate the previously developed radiation damage parametrization model.</td></tr>
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Collaborative work:

Required WG activities involved for planar and LGAD silicon sensors: WG3-, DLTS, TSC, FTIR, Hall, carrier lifetime, WG4- GEANT4, TCAD, WG5 -TB, TCT. The characterisation of irradiated and non-irradiated devices will be done in collaboration of WG2, WG3 and WG5, modelling of radiation damage will be done in collaboration with WG3 and WG4. Dissemination and outreach will be done in WG8.

Potential synergies with similar projects

RD50-2022-01 – Defect engineering in PAD diodes mimicking the gain layer in LGADs;
RD50-2023-05 – Partial activation of Boron to enhance the radiation tolerance of the gain implant;
RD50-2023-06 – Impact ionization parametrization at extreme fluences;
RD50-2023-07 – PIN sensors for dosimetry & NIEL studies

Participants, contact person, main activities:

1. **NIMP**, Ioana Pintilie ioana@infim.ro, CV/IV, DLTS/TSC/FTIR
2. **CiS**, Kevin Lauer klauer@cismst.de , samples fabrication, CV/IV, PL
3. **CERN**, Michael Moll Michael.Moll@cern.ch , irradiations, CV/IV, DLTS/TSC, TCAD
4. **Hamburg University (HH)**, Joern Schwandt Joern.Schwandt@cern.ch , CV/IV, DLTS/TSC, TCAD
5. **NIPNE,** George Alexandru Nemnes alexnemnes@yahoo.com, *ab initio*, MD, *ML* modeling
6. **Vilnius University (VU),** Tomas Ceponis, tomas.ceponis@cern.ch, CV/IV, DLTS/ lifetime
7. **ISS**, Andrea Danu andrea.Danu@cern.ch , CCE, GEANT modeling
8. **INFN Torino**, Valentina Sola sola.valentina@gmail.com, CV/IV, TCAD
9. **JSI,** Gregor Kramberger Gregor.Kramberger@ijs.si, irradiations, TCT
10. **IFCA-CSIC-UC (IFCA),** Ivan Vila ivan.vila@csic.es, CV/IV, TCT
11. **IHEP,** Mei Zhao mei.zhao@cern.ch , samples fabrication, CV/IV

Resources needed

- Available resources needed for completion of the project

	Deliverable									**Total**		
	Di1			**Di2**			**Di3**					
Institution / Funding Agency	**Material / kCHF**	**Physicists: FTE months**	**Engineers and technicians: FTE months**	**Material / kCHF**	**Physicists: FTE months**	**Engineers and technicians: FTE months**	**Material / kCHF**	**Physicists: FTE months**	**Engineers and technicians: FTE months**	**Material / kCHF**	**Physicists: FTE months**	**Engineers and technicians: FTE months**
Major (e.g. national) Funding Agencies												
NIMP	0	1	0.1		0.1	0	0	0	0	0	1.1	0.1
CiS												
CERN												

HH												
NIPNE		0.1			0.1							0.2
VU	70	1.2								30	1.2	
ISS		0.1										0.1
INFN Torino												
JSI												
IFCA												
IHEP												
Total Major Funding Agencies												

- Missing/Requested resources - asked (key for strategic funding)
  - large equipment needed and missing (e.g. state-of-art oscilloscopes)
  - services cost (e.g. processing runs, SIMS, …)
  - labour cost (FTEs)

	Deliverable									**Total**		
	Di1			**Di2**			**Di3**					
Institution / Funding Agency	**Material / kCHF**	**Physicists: FTE months**	**Engineers and technicians: FTE months**	**Material / kCHF**	**Physicists: FTE months**	**Engineers and technicians: FTE months**	**Material / kCHF**	**Physicists: FTE months**	**Engineers and technicians: FTE months**	**Material / kCHF**	**Physicists: FTE months**	**Engineers and technicians: FTE months**
Major (e.g. national) Funding Agencies												
NIMP	10	3	1		1		50	2	1	5	5	1
CiS												
CERN												
HH												
NIPNE	10	2			1		15	1		25	4	0
VU												

ISS	5	2	1				15	1	0.5	20	3	1.5
INFN Torino												
JSI												
IFCA												
IHEP												
Total Major Funding Agencies												

Project structure

- contact person: Ioana Pintilie
- other roles and responsibilities
  - for reporting:
    - NIMP for D- task #1 and M-task #1.3
    - HH for D-task #2, M-task #2.1 and M-task #3.3
    - CERN for D-task #3
    - CiS for M-task #1.1 and M-task #1.3
    - JSI for M-task #1.2 and M-task #3.2
    - NIPNE for M-task #2.2