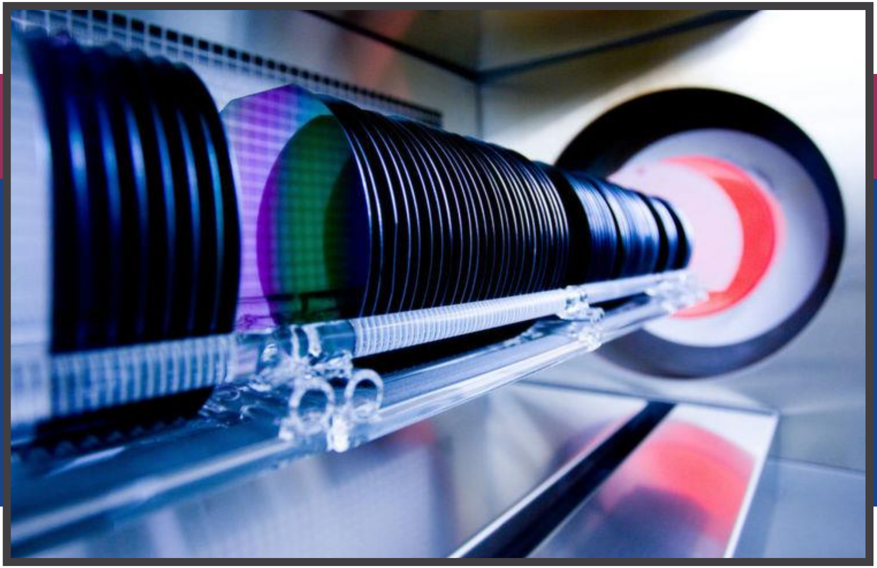
TECHNISCHE UNIVERSITÄT
ILMENAU

CiS Forschungsinstitut für
Mikrosensorik GmbH



Competence in Silicon

The numerous configurations of „interstitial boron“ and their involvement in ARP of LGADs

30.11.2023

Kevin Lauer, Aaron Flötotto, Katharina Peh,
Robin Müller, Wichard Beenken, Erich Runge,
Dirk Schulze, Stefan Krischok, Thomas Ortlepp

ZUSE-GEMEINSCHAFT
FORSCHUNG, DIE ANKOMMT.
GRÜNDUNGSMITGLIED

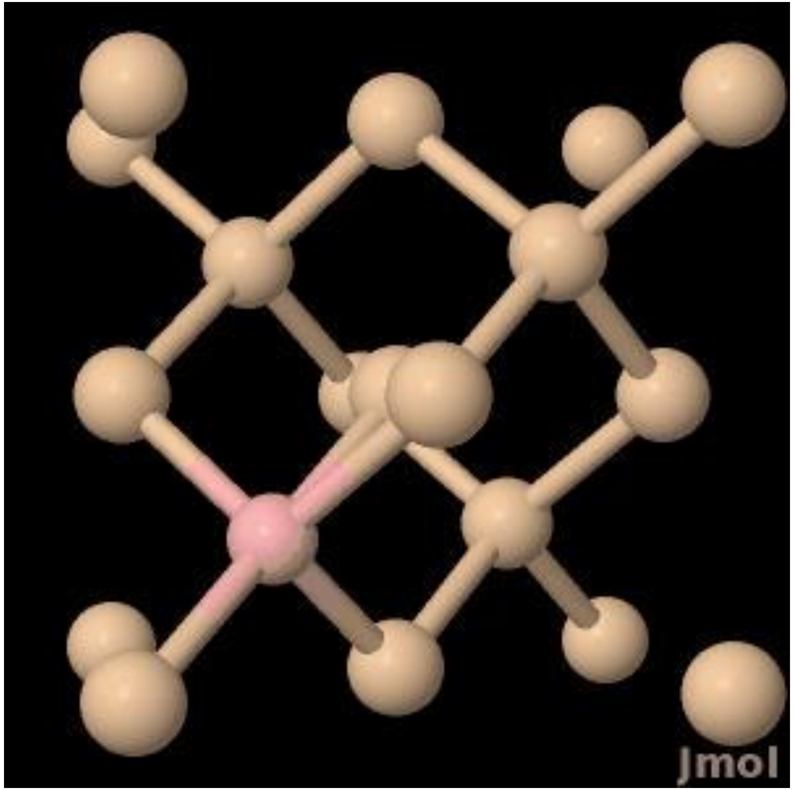
Overview

1. Existing A_{Si}-Si$_i$-defect model
2. Configurations of “interstitial boron” obtained by DFT calculations
3. Defect energy landscape
4. Explanation of ARP in LGADs by the B$_{\mathrm{Si}}$-Si$_i$-defect mode
5. Summary
6. Acknowledgement

Existing A_{Si}-Si_i-defect model

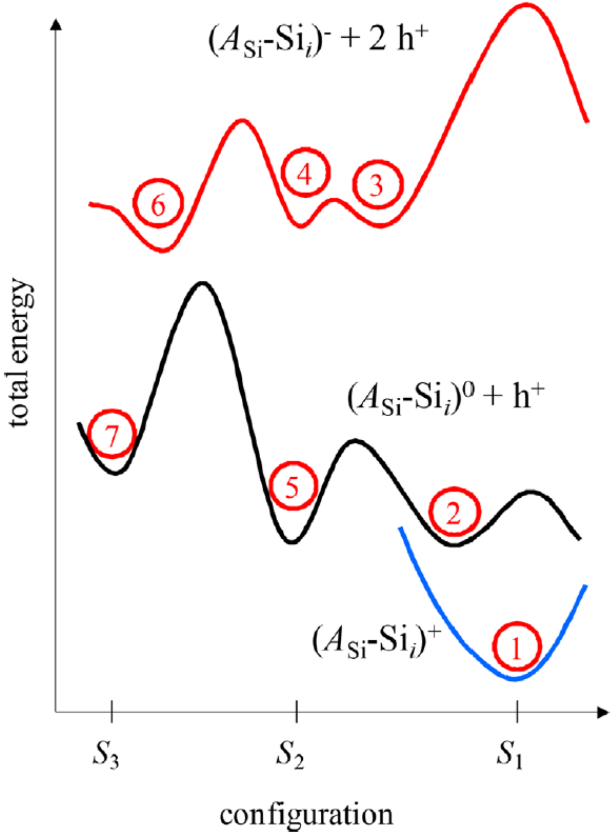
A_{Si}-Si_i defect model

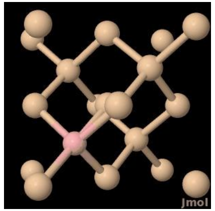
- A_{Si}: acceptor atom is close to its substitutional position
- Silicon interstitial is moving around (tetrahedral, hexagonal and split interstitial position assumed so far)
- Model and experimental evidence recently reviewed [1]



[1] K. Lauer et al. In: Phys. Status Solidi A (Aug. 2022), 2200099

A_{Si}-Si_i defect model



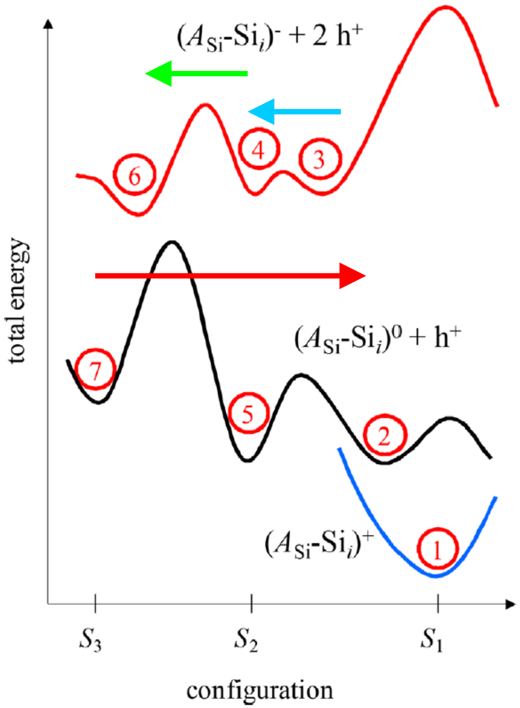


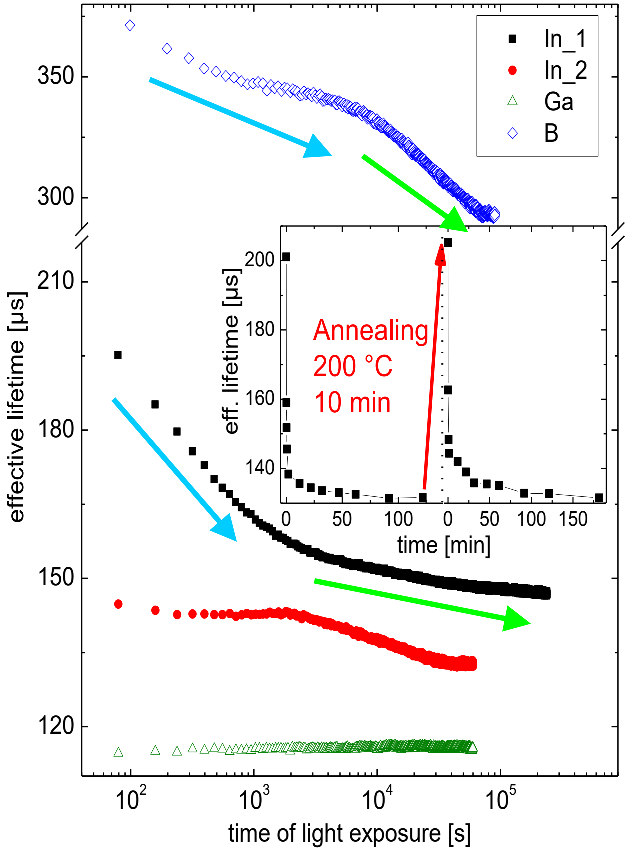
- Configuration coordinate total (electronic + elastic) energy diagram [1] deduced from simulation results of the silicon interstitial [2]
- Three charge states (+, 0, -) and three configurations (S_1, S_2 and S_3) of A_{Si}-Si_i exist within the model
- Energy barriers between configurations (e.g. E_{34}, E_{46})

- Negative charge state: S_3 energetically favored
- Neutral charge state: S_2 and S_1 energetically favored

[1] K. Lauer et al., Physica Status Solidi (c) 14, 1600033 (2017).
[2] R. Jones et al., Materials Science and Engineering: B 159–160, 112 (2009).

Explanation of LID by A_{Si}-Si_i defect model



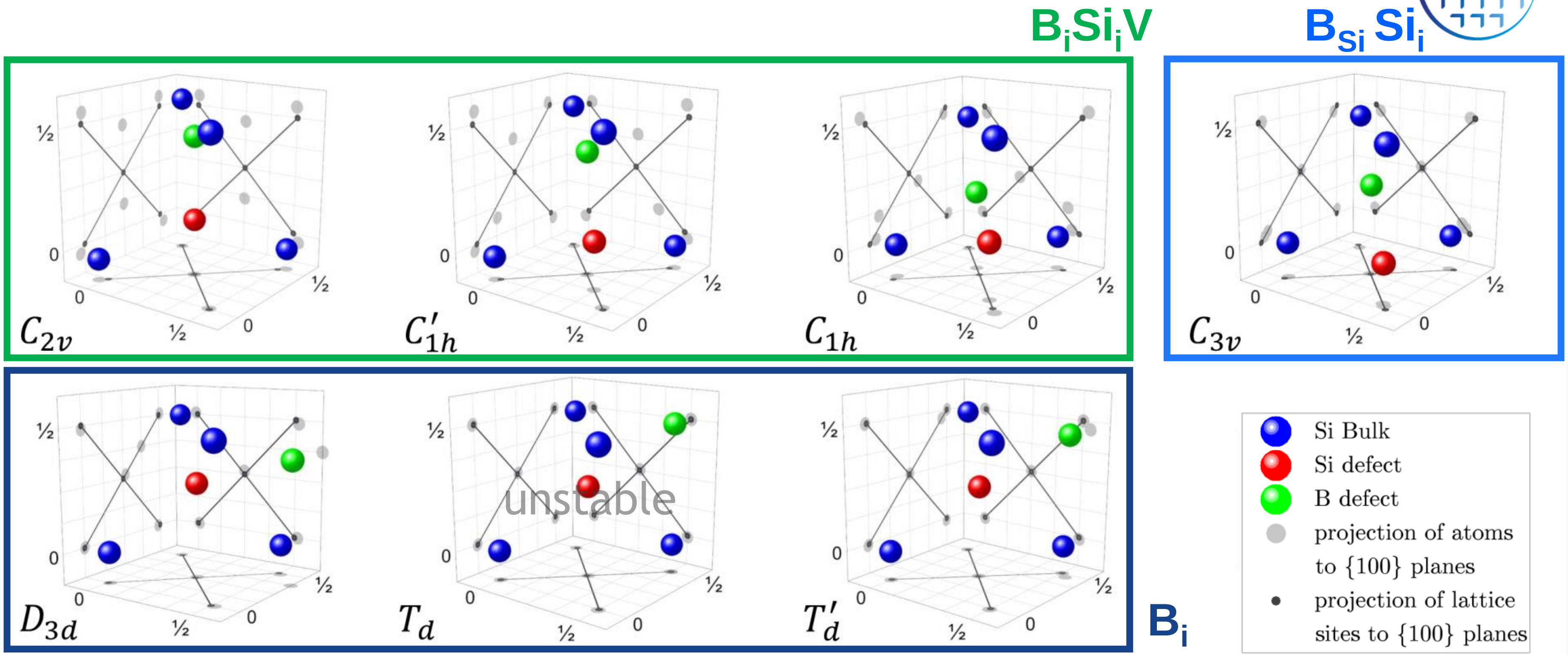


- **LID:** light-induced degradation in silicon solar cells [1]
- **Transition 1 to 3:** defect captures electrons under illumination
- **Transition 3 to 4:** thermally stimulated, fast component of LID (FRC)
- **Transition 4 to 6:** thermally stimulated, slow component of LID (SRC)
- **Transition 7 to 1:** thermally stimulated, recovery of defect, without illumination

[1] C. Möller et al., phys. stat. sol. RRL 7, 461 (2013)

Configurations of “interstitial boron” obtained by DFT calculations

DFT calculation of stable defect configurations

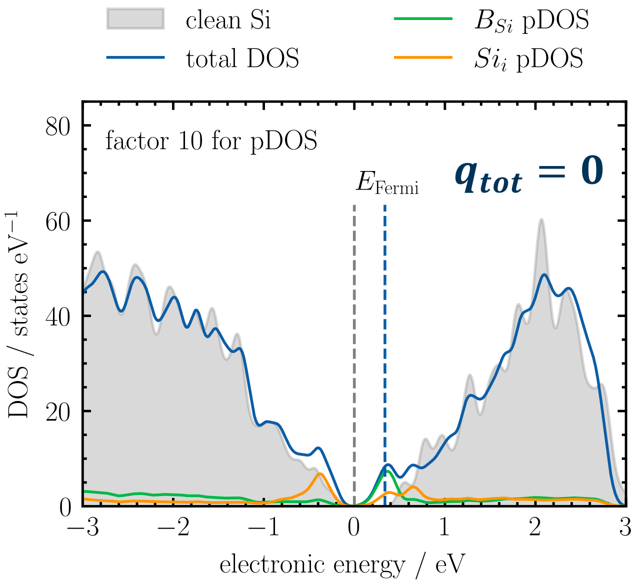


- Six different stable configurations found

To be published A. Flötotto et al. 2024

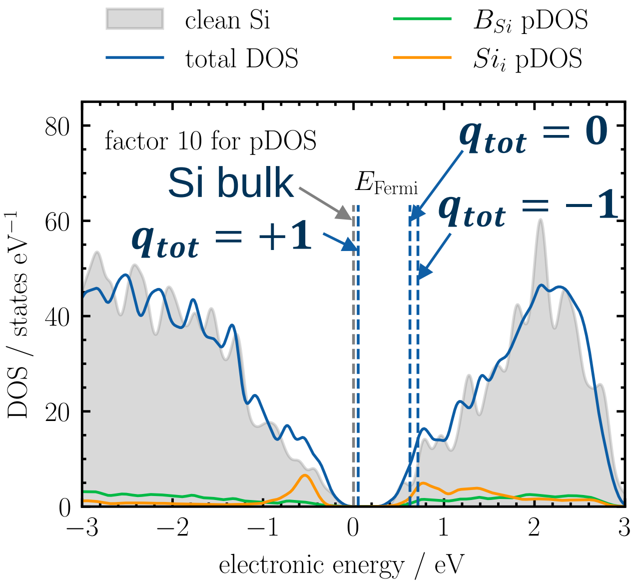
DFT calculation of density of states (DOS)

B_iSi_iV defect (C_{1h})



→ **Deep donor**

$B_{Si}Si_i$ defect (C_{3v})



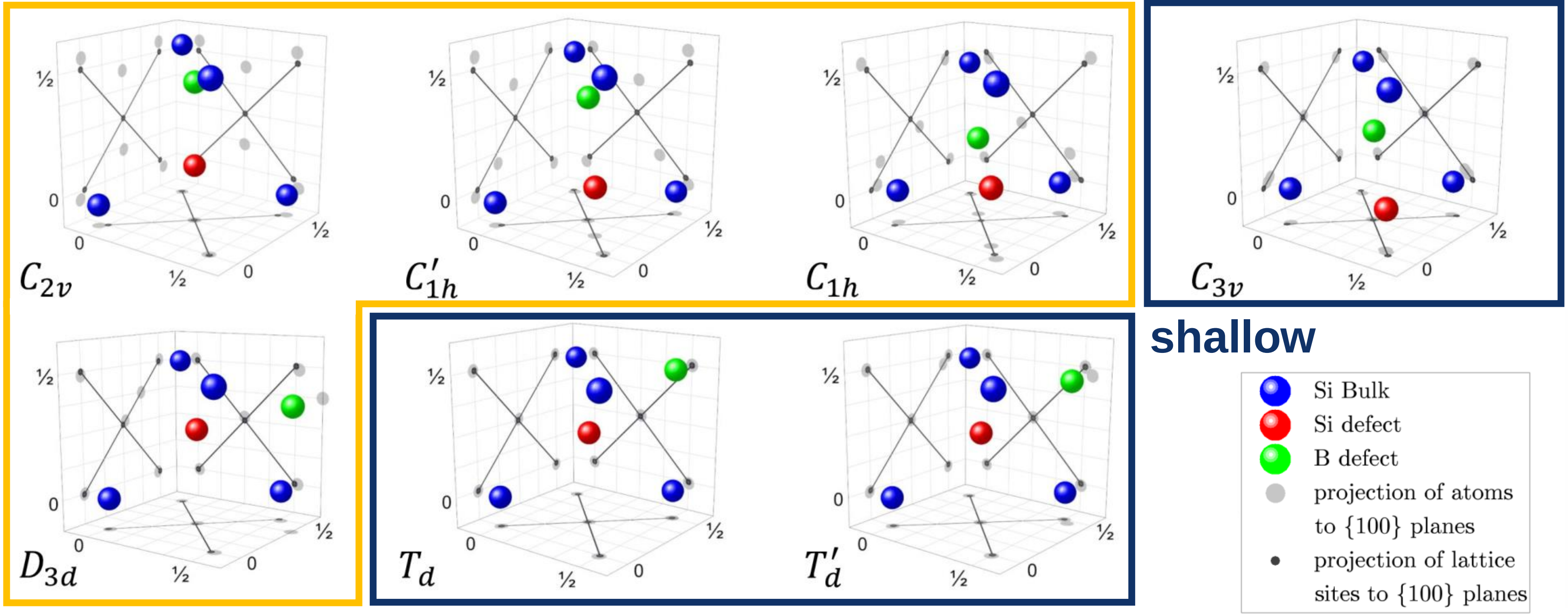
→ **Shallow donor**

- $B_{Si}Si_i$ defect in C_{3v} configuration is shallow donor

To be published A. Flötotto et al. 2024

Calculated electronic defect states

deep



shallow

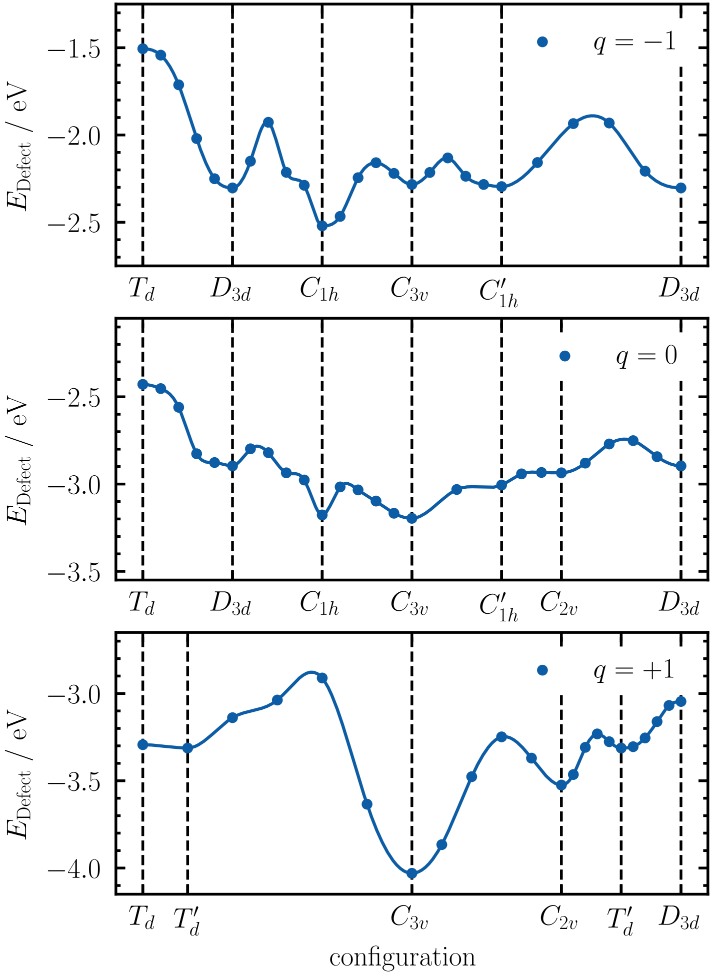
- 4 deep and 3 shallow centers found

To be published A. Flötotto et al. 2024

Defect energy landscape

Calculated defect energy landscape

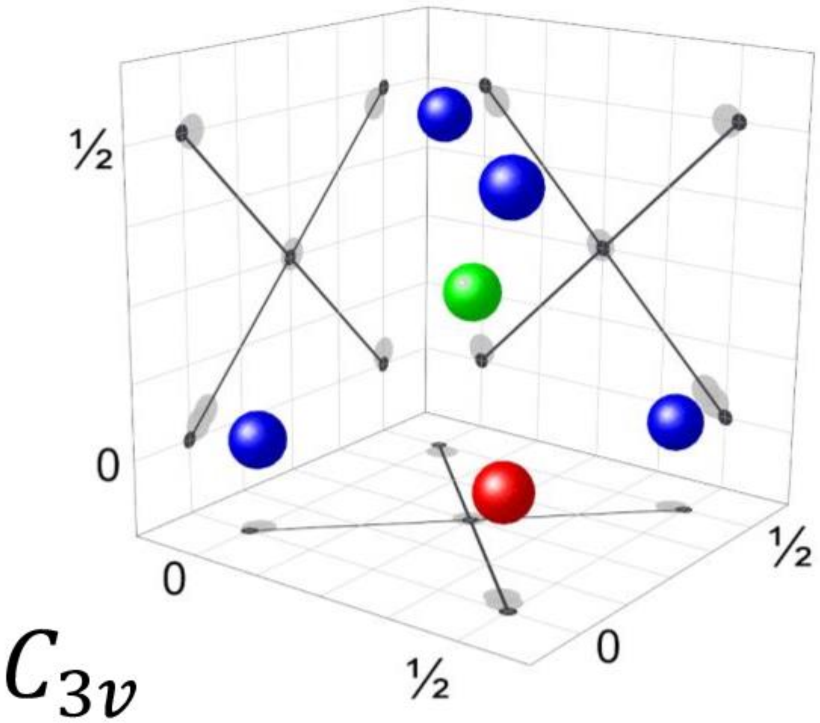
- Calculation of all Minimal Energy Paths (NEB method) between defect configurations for each charge state
- Ground state in positive charge state (p-type silicon) is C_{3v} configuration
- From DFT calculations: no energetical reason for the substitutional boron to follow the Watkins replacement reaction!



To be published A. Flötotto et al. 2024

Explanation of ARP in LGADs by the B_{Si}-Si_{i}-defect mode

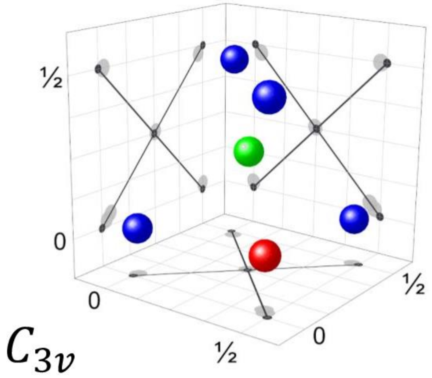
Explanation of ARP in LGADs by B_{Si}-Si_i-defect mode



- Irradiation removes silicon atoms from lattice positions
- At low temperatures (~20K) the removed silicon atom moves due to the energy gained by the collision event and is eventually captured by substitutional boron. [1]
- At about room temperature the removed silicon atom might additionally diffuse thermally due to its weak mobility. [2]
- Shallow donor mode of the B_{Si}-Si_i-defect (C_{3v}) forms

[1] K. Lauer et al., https://arxiv.org/abs/2311.07280
[2] A.N. Buzynin et al., NIMB, **186**(1), 366–370 (2002).

Summary



- Comprehensive DFT calculations made for “interstitial boron”
- Six different stable configurations found
- Configuration with lowest energy in p-type silicon is C_{3v} with boron residing very close to regular lattice position
- C_{3v} configuration is found to be a shallow donor
- Explanation of acceptor removal phenomenon (ARP) in low-gain avalanche detectors (LGAD):
  - Substitutional boron acceptor captures silicon atom, which was removed from a lattice position by irradiation.
  - The resulting defect is a shallow donor.
  - Amplification property of the boron gain layer in LGADs gets lost by irradiation.

Thank you for your kind attention!

DFG Project SimASiSii:
DFG KR 2228/11-1, LA 4623/1-1, RU 1383/6-1

BMWI Project eLGAD (49MF220095)

DFG Deutsche Forschungsgemeinschaft
German Research Foundation

Federal Ministry
for Economic Affairs
and Climate Action

CiS Forschungsinstitut für
Mikrosensorik GmbH

TECHNISCHE UNIVERSITÄT
ILMENAU

Titular Saint
Franz of Assisi

Konrad-Zuse-Str. 14
99099 Erfurt, Germany
www.cismst.de

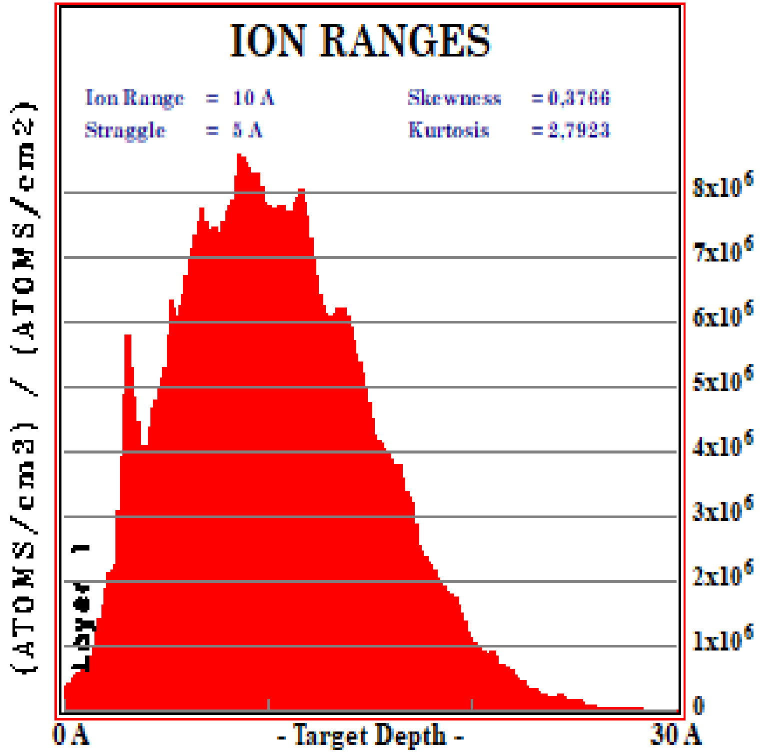
Telefon: +49 361 6631211
Telefax: +49 361 6631413
E-Mail: klauer@cismst.de

Thanks to RD50 for possibility to present crazy ideas!

Back-up

Possibility for silicon recoils to reach B atoms

- 1 MeV electron irradiation of silicon generates silicon recoils exhibiting kinetic energy
- ~10% of these recoils have more than 80eV
- ~50% of these 10% travel more than 1nm (SRIM)
- For 10^{16}cm^{-3} boron density every 23th of these left recoils is able to reach a boron atom
- If 10% of the silicon recoils reaching boron to form the B_{Si}-Si_i-defect, a B_{Si}-Si_i-defect density of about 10^{15}cm^{-3} is under typical conditions (electron current and duration) possible.
- => Sufficient to explain EPR signals [1] without assumption of fast defect diffusion [2]



[1] G.D. Watkins, Physical Review B 12(12), 5824 (1975).
[2] K. Lauer et al., https://arxiv.org/abs/2311.07280