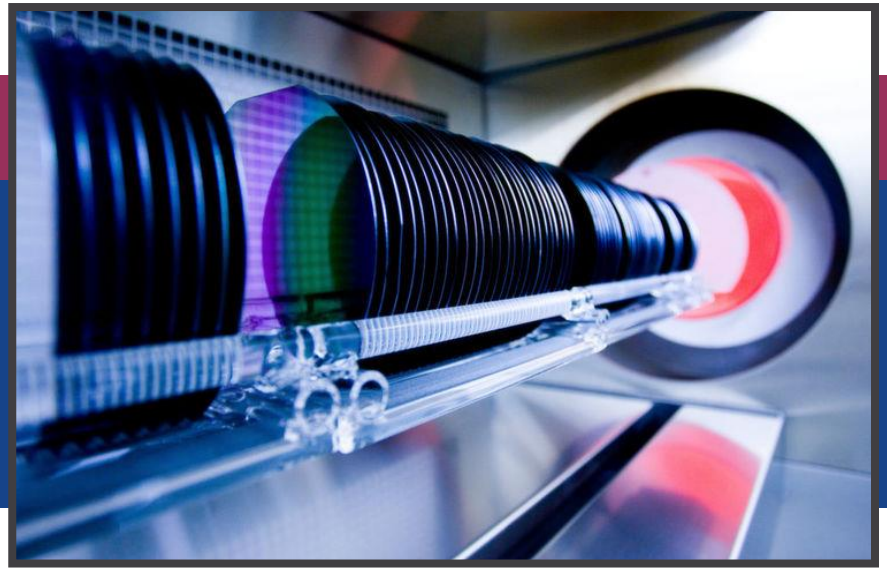
TECHNISCHE UNIVERSITÄT ILMENAU

CiS Forschungsinstitut für Mikrosensorik GmbH



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FORSCHUNG, DIE ANKOMMT.
GRÜNDUNGSMITGLIED

Competence in Silicon

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

30.11.2023

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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_{Si}-Si_i-defect mode
5. Summary
6. Acknowledgement

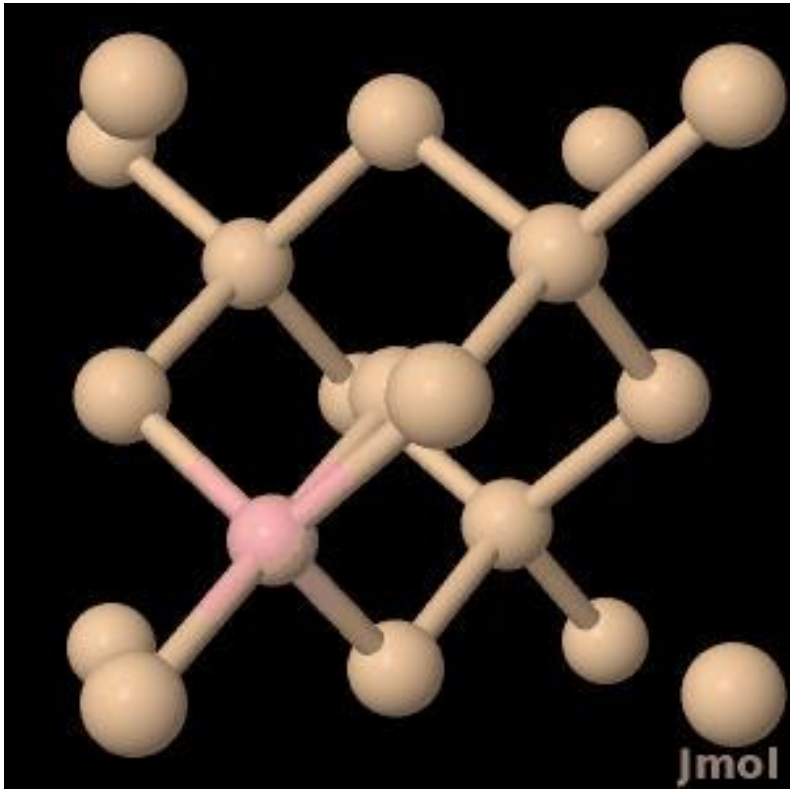
Existing A_{Si}-Si_i-defect model

A_{Si}-Si_i defect model

- A_{Si}: acceptor atom is close to its substitutional position

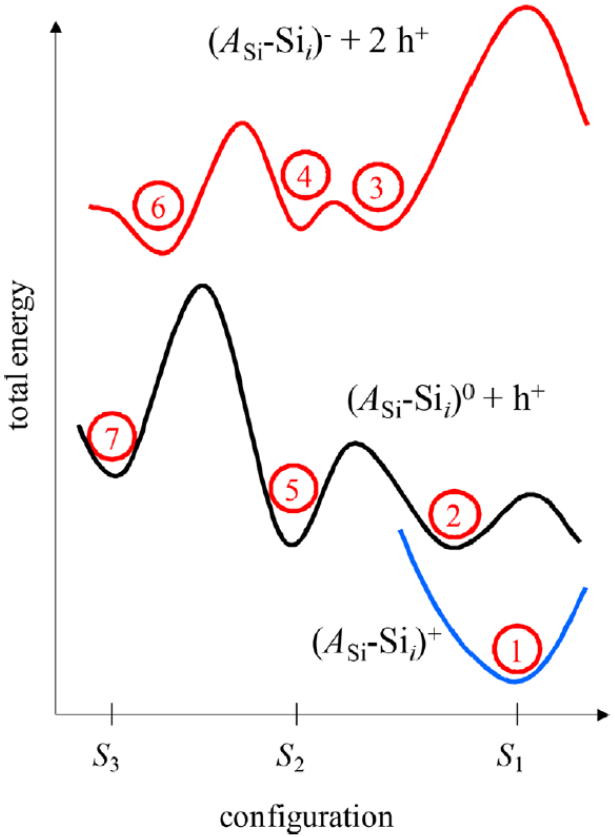
- Silicon interstitial is moving around (tetrahedral, hexagonal and split interstitial position assumed so far)

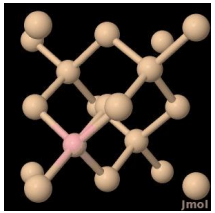
- Model and experimental evidence recently reviewed [1]



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

A_{Si}-Si$_i$ defect model

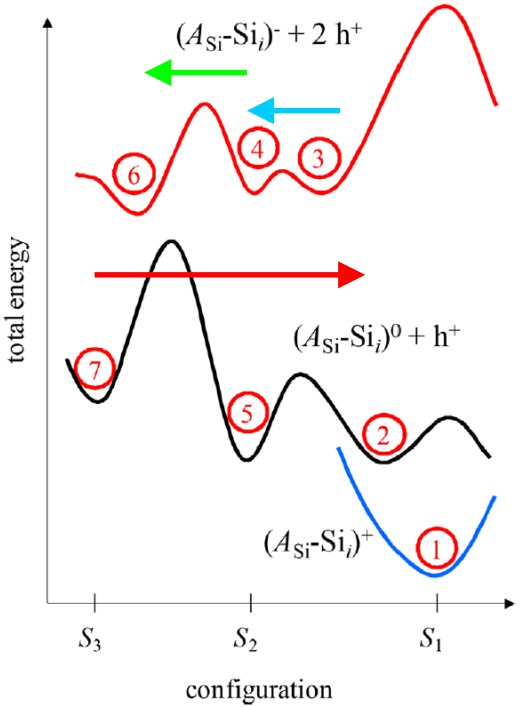


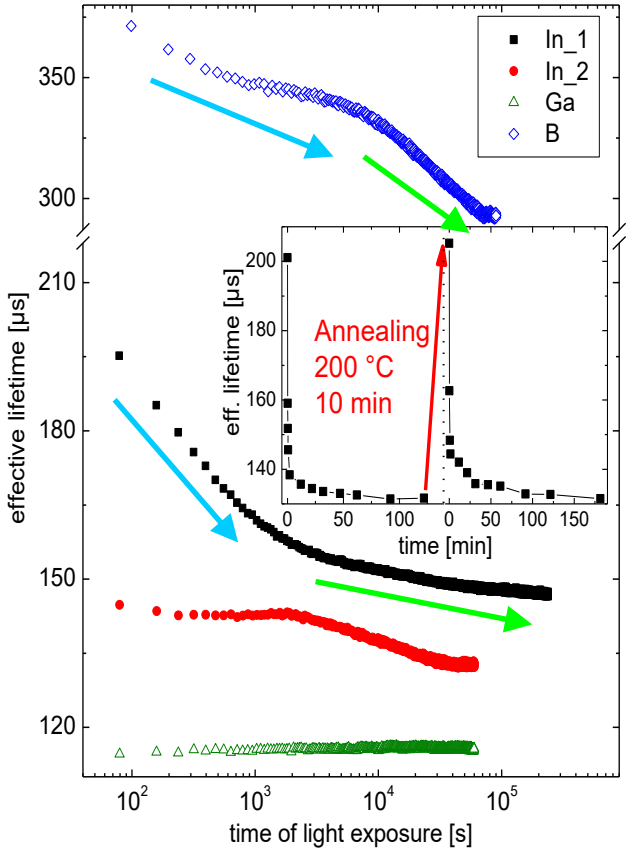


- Configuration coordinate total (electronic + elastic) energy diagram [1] deduced from simulation results of the silicon interstitial [2]
- Three charge states (+, 0, -) and three configurations (S_1, S_2 and S_3) of A_{Si}-Si$_i$ exist within the model
- Energy barriers between configurations (e.g.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





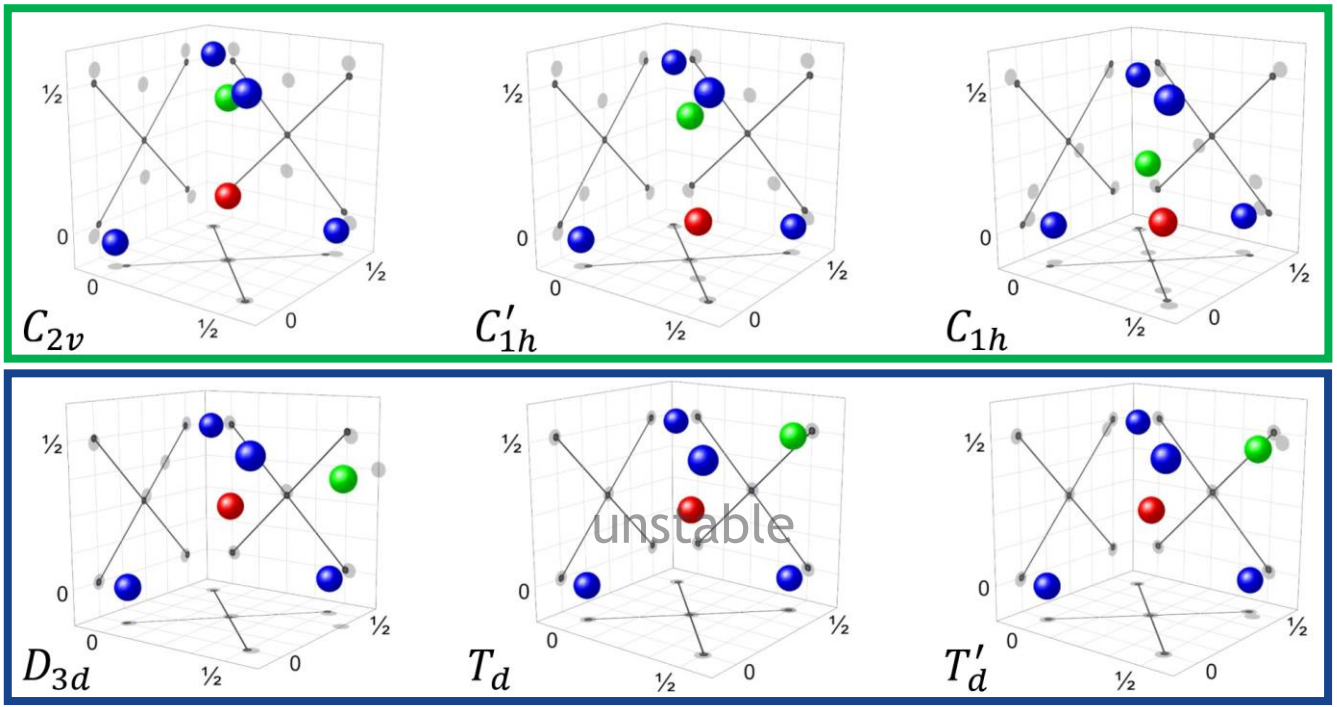
- **LID:** light-induced degradation in silicon solar cells [1]
- **Transition 1 to 3:** defect captures electrons under illumination
- **Transition 3 to 4:** thermally stimulated, fast component of LID (FRC)
- **Transition 4 to 6:** thermally stimulated, slow component of LID (SRC)
- **Transition 7 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

B_iSi_iV $B_{Si}\,Si_i$



- Six different stable configurations found

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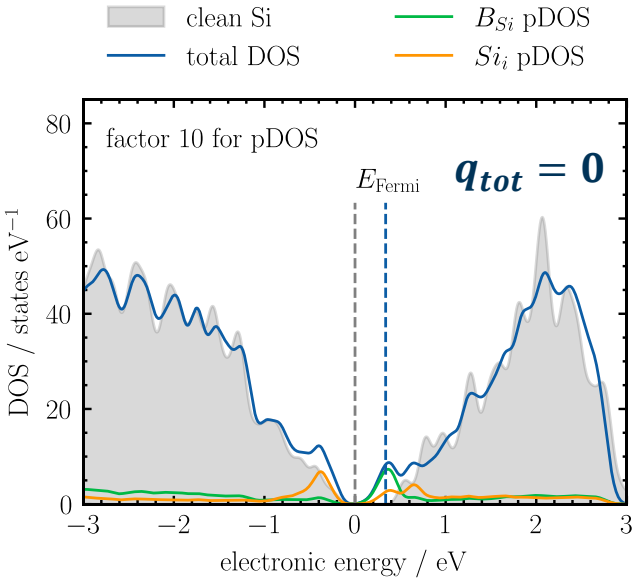
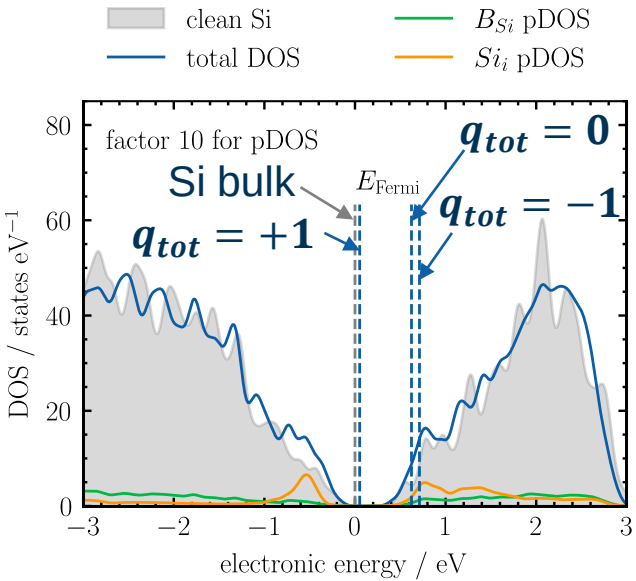
DFT calculation of density of states (DOS)

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

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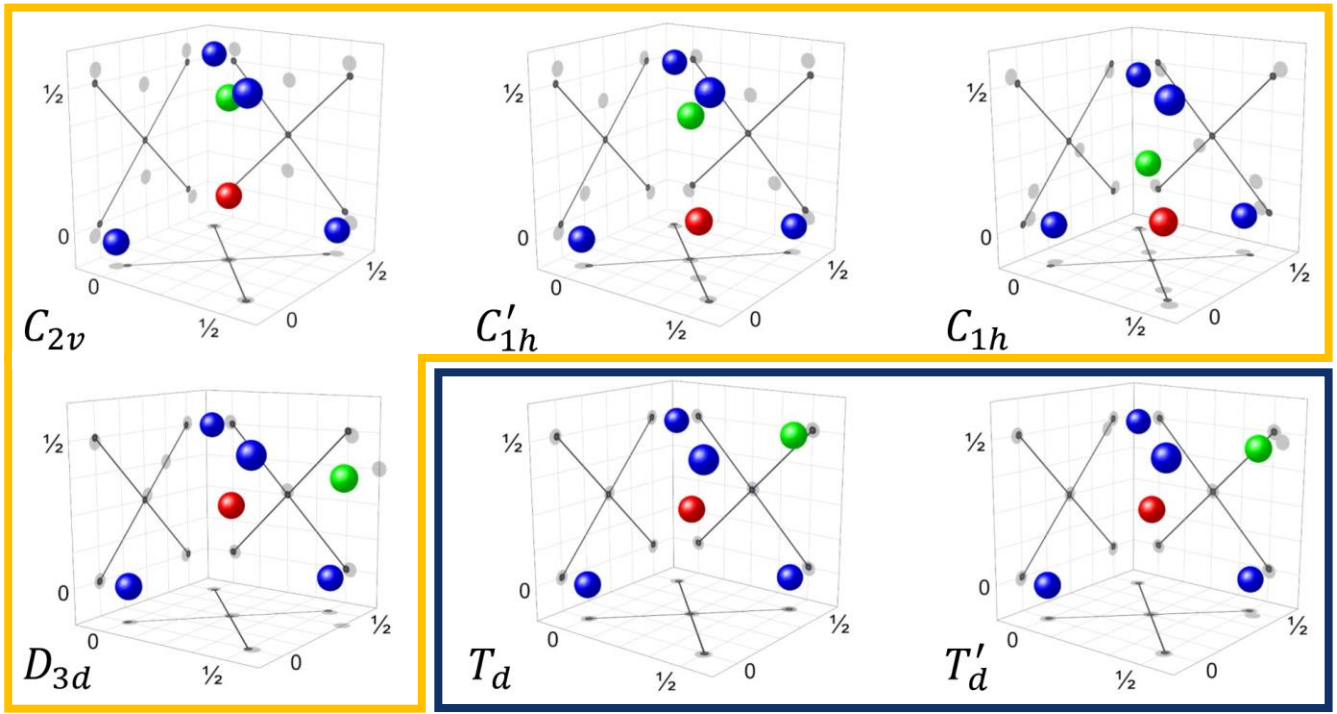
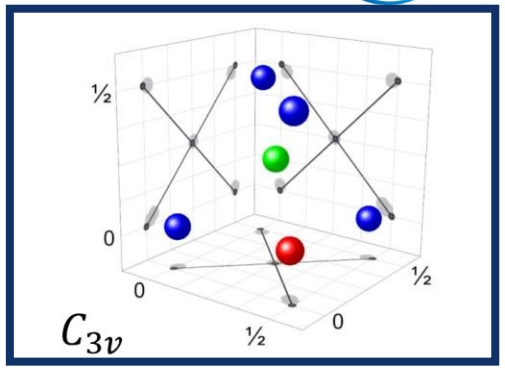
Calculated electronic defect states

deep





shallow

Si Bulk
Si defect
B defect
projection of atoms to {100} planes
projection of lattice sites to {100} planes

- 4 deep and 3 shallow centers found

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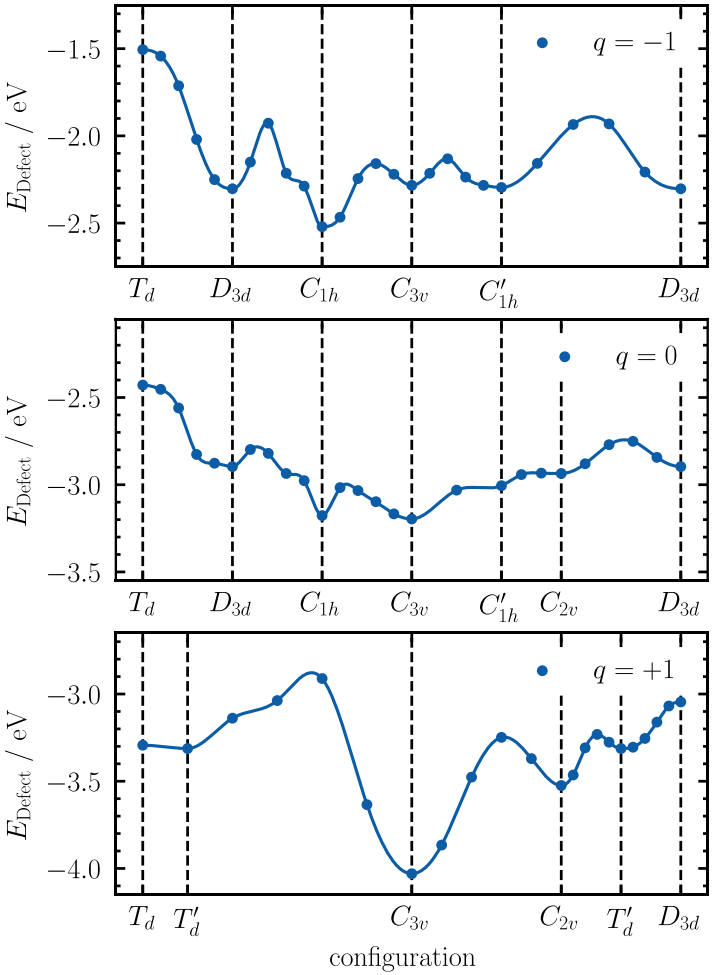
Defect energy landscape

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

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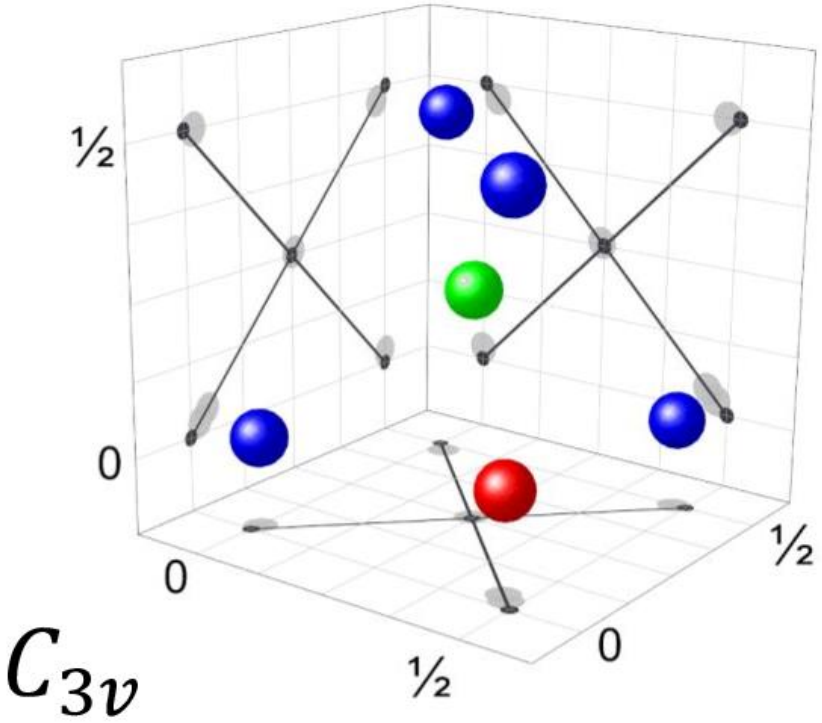
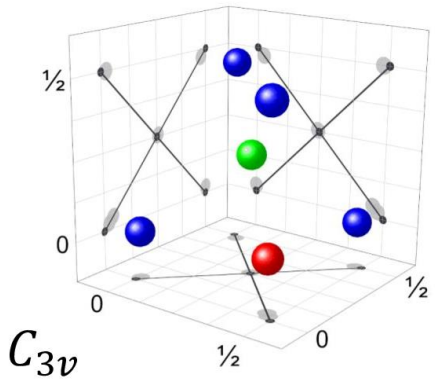


- Irradiation removes silicon atoms from lattice positions
- At low temperatures (~20K) the removed silicon atom moves due to the energy gained by the collision event and is eventually captured by substitutional boron. [1]
- At about room temperature the removed silicon atom might additionally diffuse 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



C_{3v}

- 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

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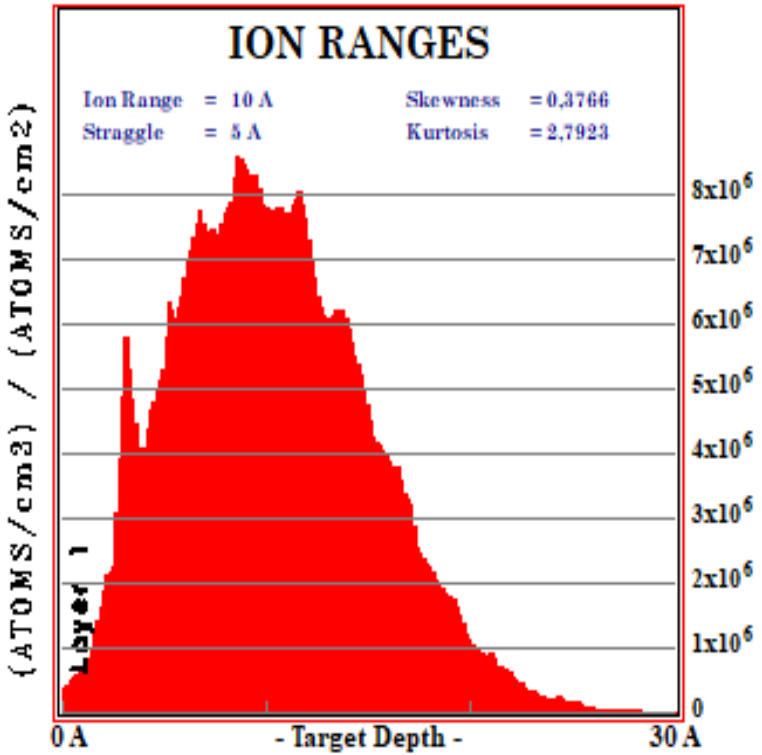
Thanks to RD50 for possibility to present crazy ideas!

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