



Investigation of defect meta-stabilities in silicon doped with thallium by low temperature photoluminescence spectroscopy

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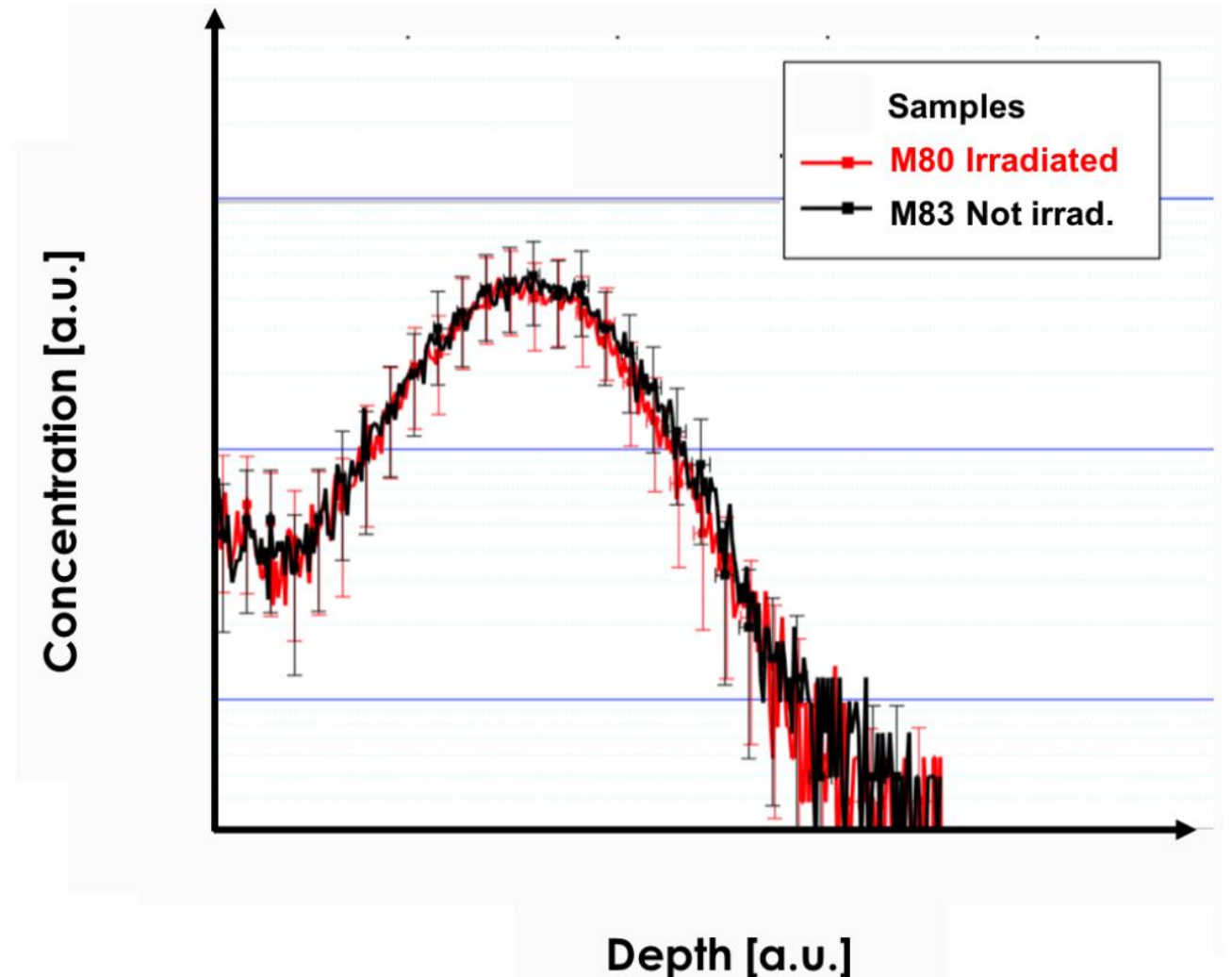
Overview

- Motivation / Background
- Sample preparation
- Photoluminescence (PL) measurements in Si:Tl
- Meta-stabilities of PL in Si:Tl (A and P lines)
- PL measurements in Si:B
- Summary

Motivation/ Background

Motivation/ Background

- Low gain avalanche detectors (LGAD) are hampered by acceptor removal phenomenon (ARP) during irradiation.
- Internal gain of detectors disappears
- Acceptor properties (of e.g. boron) lost, while dopant atoms remain at their positions as observed by SIMS. [1]
- Microscopic understanding of responsible defects is not sufficient to provide solutions for ARP.
- Indications of meta-stabilities of ARP reported [2]



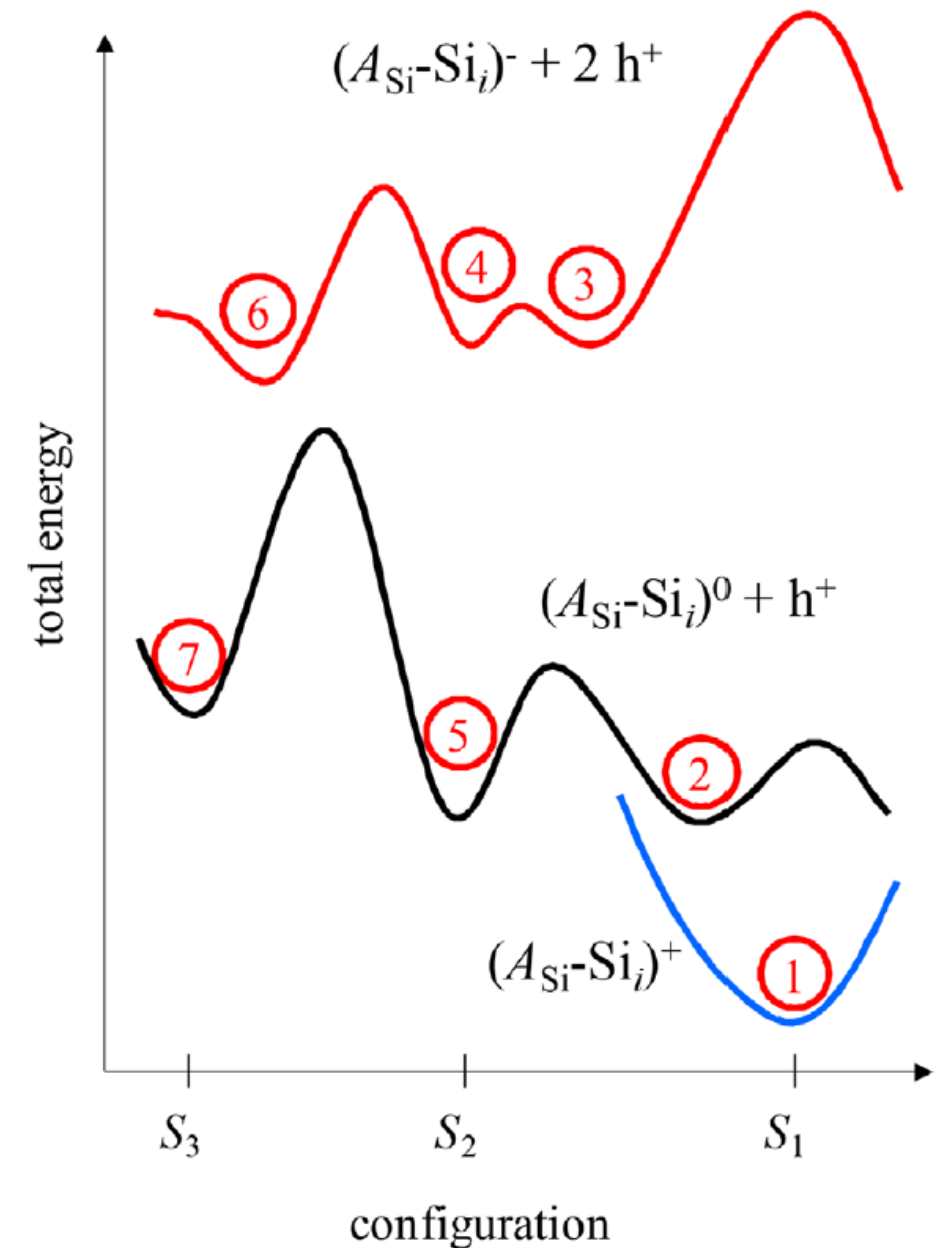
[1] M. Ferrero et al., 'Radiation resistant LGAD design', Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, vol. 919, pp. 16-26, Mar. 2019.

[2] A. Nitescu, C. Besleaga, G.A. Nemnes, and I. Pintilie, "Bistable Boron-Related Defect Associated with the Acceptor Removal Process in Irradiated p-Type Silicon—Electronic Properties of Configurational Transformations," Sensors 23(12), 5725 (2023).

Motivation/ Background

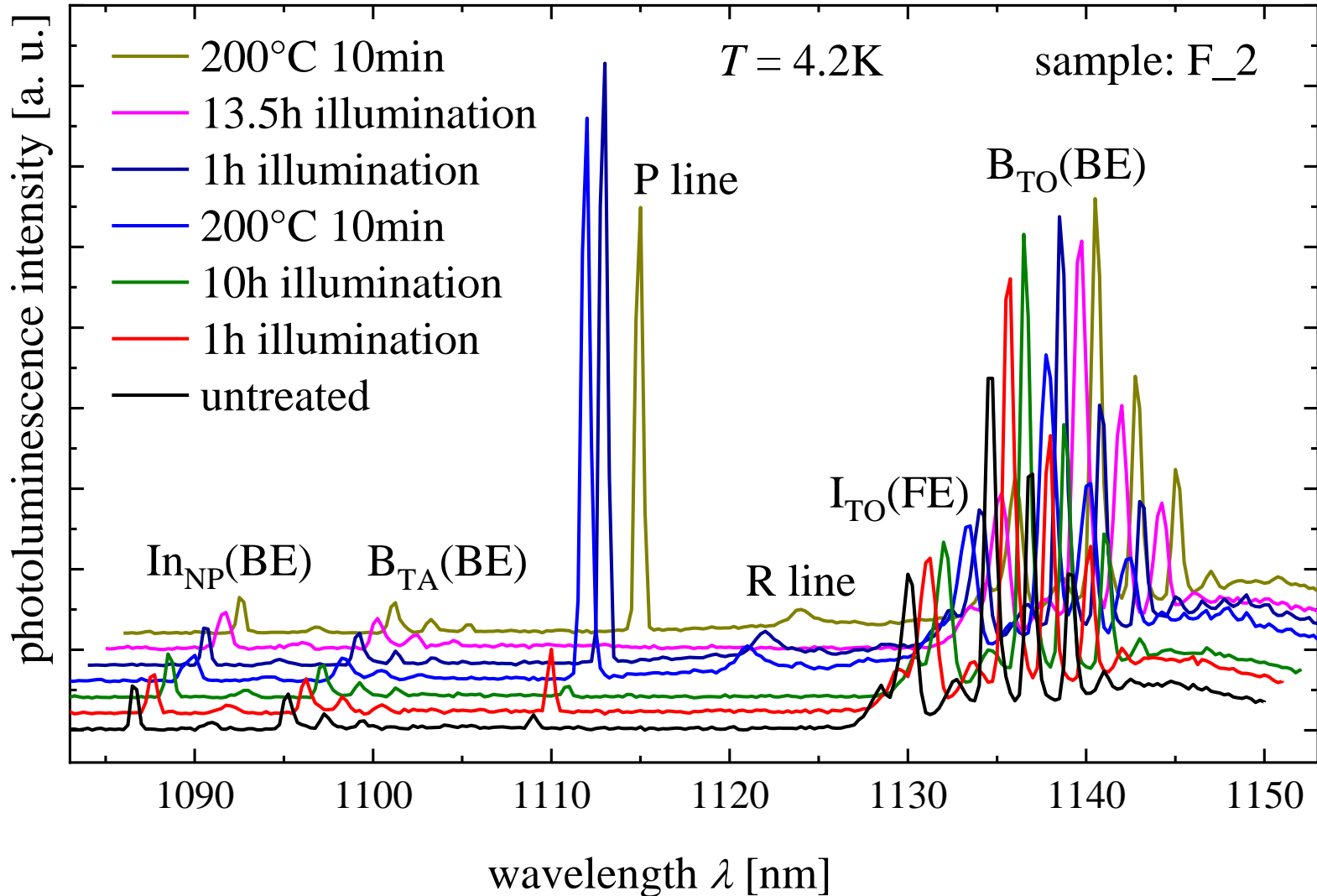
- Explanation for ARP proposed on basis of $A_{Si}-Si_i$ defect model [1,2]
- $B_{Si}-Si_i$ defect is in ground state configuration found to be a donor [3]
- $A_{Si}-Si_i$ defects exhibit meta-stable behavior as exemplified e.g. for the light-induced degradation (LID)
- Aim: learning from different members of the defect category (e.g. acceptors B, In, Tl) using the low temperature photoluminescence spectroscopy (LTPL) method

[1] K. Lauer, K. Peh, D. Schulze, T. Ortlev, E. Runge, and S. Krischok, 'The ASi-Sii Defect Model of Light-Induced Degradation (LID) in Silicon: A Discussion and Review', physica status solidi (a), vol. 219, no. 19, p. 2200099.
[2] K. Lauer, S. Reiß, A. Flötotto, K. Peh, D. Bratek, R. Müller, D. Schulze, W. Beenken, E. Hiller, T. Ortlev, and S. Krischok, "Effect of inelastic ion collisions on low-gain avalanche detectors explained by an A_Si-Si_i-defect mode," [Preprint](#) submitted to NIMB (2023).
[3] E. Tarnow, "Theory of the B interstitial related defect in Si," EPL (Europhysics Letters) 16(5), 449 (1991).



Motivation/ Background

- Case of acceptor indium
- PL signal called P line found to follow LID meta-stability [1]
- Similar meta-stabilities observable for case of acceptor thallium?
- Two PL signals called A and P line known [2]
- → Investigation of thallium doped silicon by LTPL



[1] K. Lauer, C. Möller, D. Schulze, and C. Ahrens, 'Identification of photoluminescence P line in indium doped silicon as InSi-Sii defect', AIP Advances, vol. 5, no. 1, p. 017101, Jan. 2015.

[2] H. Conzelmann, A. Hangleiter, and J. Weber, "Thallium-related isoelectronic bound excitons in silicon. A bistable defect at low temperatures," Physica Status Solidi (b) 133(2), 655-668 (1986).

Motivation/ Background

- A bit off topic: usage of $A_{Si}-Si_i$ defects as qubit in silicon based quantum technology possible?
- These defects have comparable promising properties [1]
- High excited state lifetime
- $In_{Si}-Si_i$ detectable by conventional Si-APD
- Splitting in magnetic field
- High nuclear spin for $In_{Si}-Si_i$

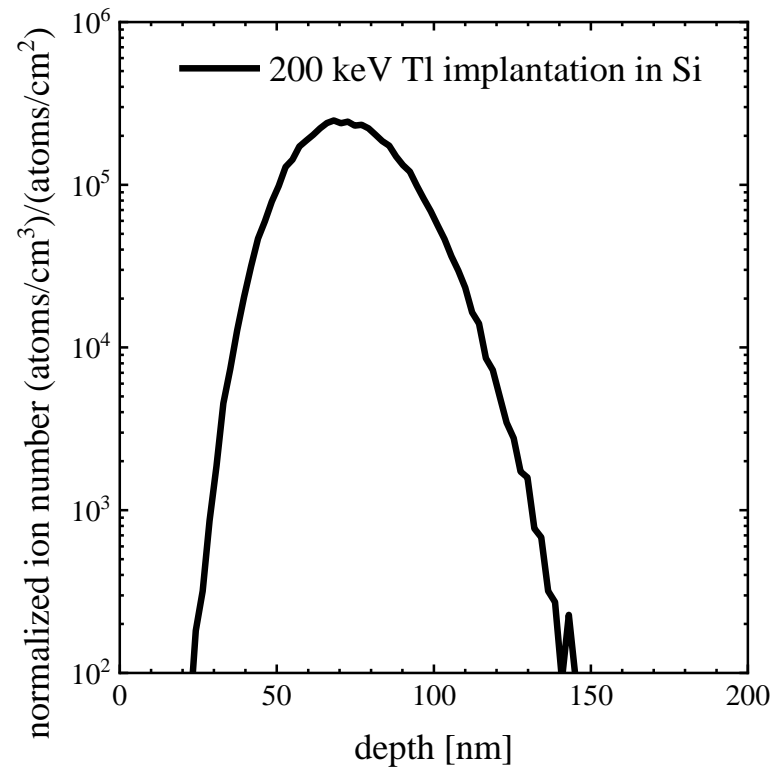
	G center	T center	P donor	Se donor	Er center	$Tl_{Si}-Si_i$ (A)	$Tl_{Si}-Si_i$ (P)	$In_{Si}-Si_i$ (P)
PL line position [nm]	1279	1326	1135	2901	1530	1140	1180	1109
PL intensity (subjective)	high	medium	low	medium	low	high	high	high
lifetime of PL line [μ s]	0.036	0.94		0.0077	1000	53	25	196
split lines (early)	no	5				2	3	3
split lines (recent)	no	44			12			
nuclear spin			1/2	1/2	7/2	1/2	1/2	9/2

[1] K. Lauer, K. Peh, R. Müller, D. Schulze, R. Schmidt-Grund, S. Krischok, A. Flötotto, W. Beenken, E. Runge, A. Reinhardt, M. Bähr, S. Reiß, A. Frank, T. Ortlepp, I. Crowe, R. Sumathi, J. Murphy, A. Gali, A. Pershin, and M. Moll, 'Examining the Properties of the As_i-Si_i -Defects for Their Potential as Qubits', [Preprint](#) submitted (2024).

Sample preparation

Sample preparation

- Thallium implantation into silicon [1]
- Modelled using SRIM [2]
- Rapid thermal process (1000°C, 10s) after implantation
- SIMS and 4pp measurements
- Hole concentrations show weak dependence on implantation dose



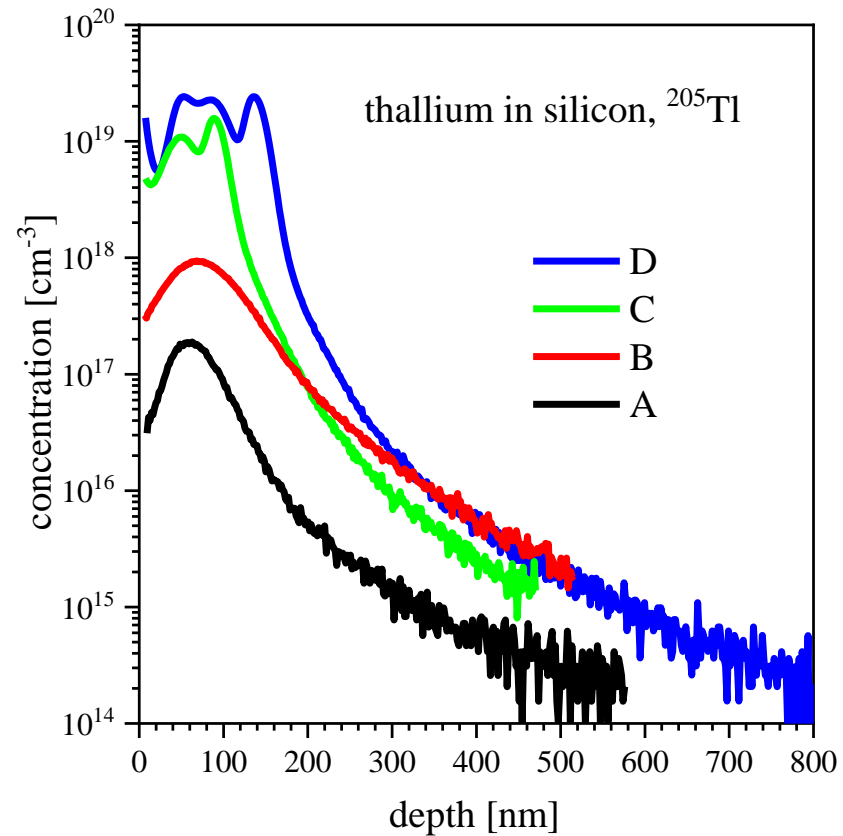
[1] K. Lauer, Robin Müller, Katharina Peh, Dirk Schulze, Stefan Krischok, Stephanie Reiß, Andreas Frank and Thomas Ortlepp, 'Investigation of Tl-doped silicon by low temperature photoluminescence during LID treatments', accepted physica status solidi A (2024)

[2] J.F. Ziegler, M.D. Ziegler, and J.P. Biersack, "SRIM - The stopping and range of ions in matter (2010)," Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms 268(11-12), 1818-1823 (2010).

#	implant energy [keV]	thallium dose [cm ⁻²]	simulated (SRIM) peak thallium concentration [cm ⁻³]	measured (SIMS) peak thallium concentration [cm ⁻³]	measured (4pp) hole concentration [cm ⁻³]	thickness for uniform doping [nm]
A	200	1.5E+12	3.6E+17	1.8E+17	1.7E+15	100
B	200	1.5E+13	3.6E+18	9.2E+17	3.3E+15	150
C	200	1.5E+14	3.6E+19	1.5E+19	2.5E+15	200
D	200	1.5E+15	3.6E+20	2.5E+19	2.2E+15	200

Sample preparation

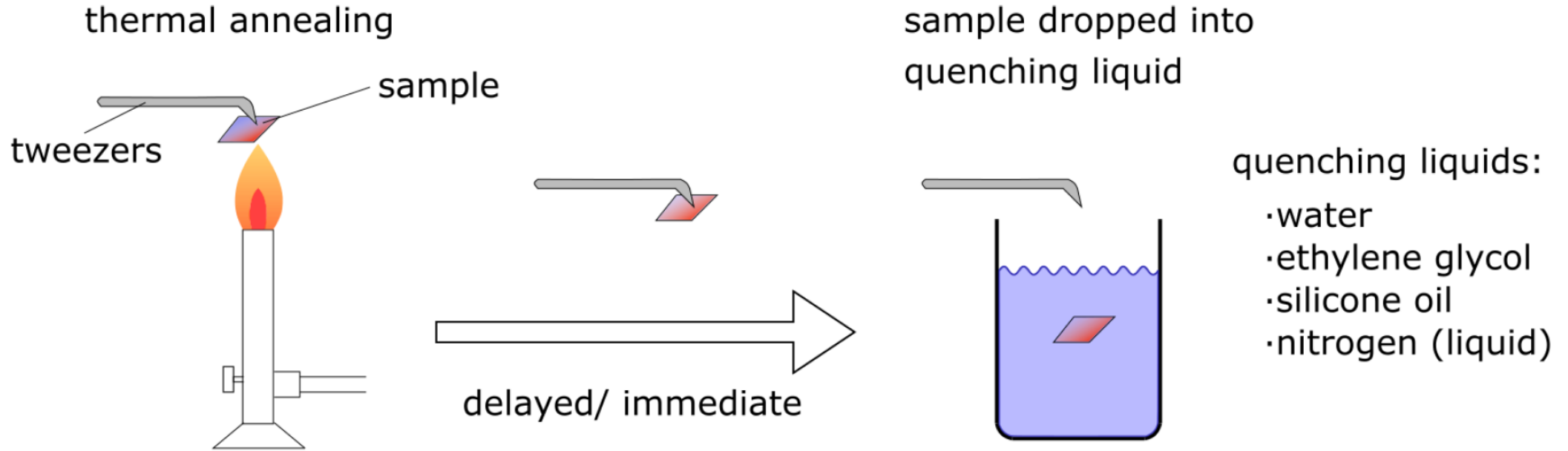
- SIMS measurements done at CiS [1]
- Dose dependence of profiles visible
- Multiple peaks for highest doses not explainable so far



[1] K. Lauer, Robin Müller, Katharina Peh, Dirk Schulze, Stefan Krischok, Stephanie Reiß, Andreas Frank and Thomas Ortlepp, 'Investigation of Tl-doped silicon by low temperature photoluminescence during LID treatments', accepted physica status solidi A (2024)

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B	200	1.5E+13	3.6E+18	9.2E+17	3.3E+15	150
C	200	1.5E+14	3.6E+19	1.5E+19	2.5E+15	200
D	200	1.5E+15	3.6E+20	2.5E+19	2.2E+15	200

Sample preparation



- Defect generation by quenching procedure [1,2]
- Highest cooling rate without sample destruction leads to largest PL signals

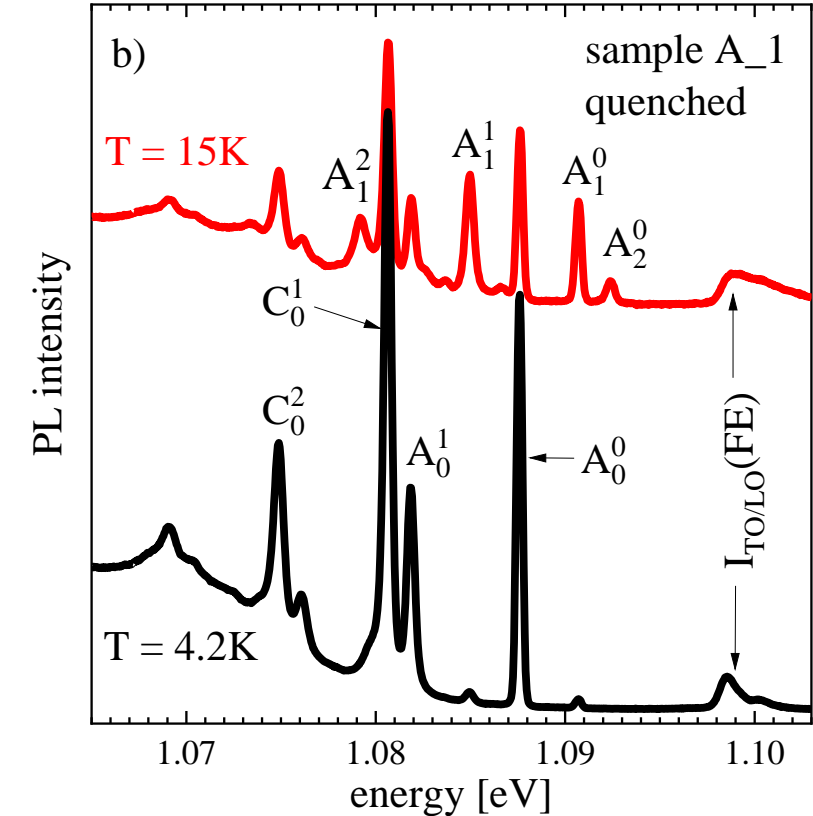
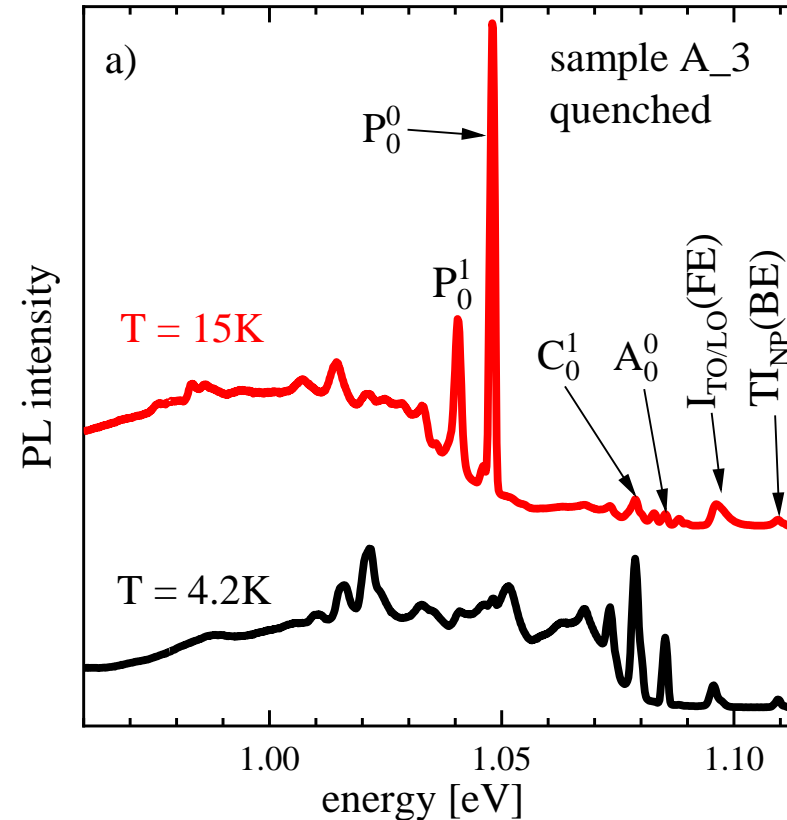
[1] M.L.W. Thewalt, U.O. Ziemelis, and P.R. Parsons, "Enhancement of long lifetime lines in photoluminescence from Si:In," *Solid State Communications* 39(1), 27-30 (1981).

[2] D. Bratek, "Investigation of properties of the P-line with respect to the ASiSii-defect," (2023).

Photoluminescence measurements in Si:Tl

Photoluminescence measurements in Si:TI

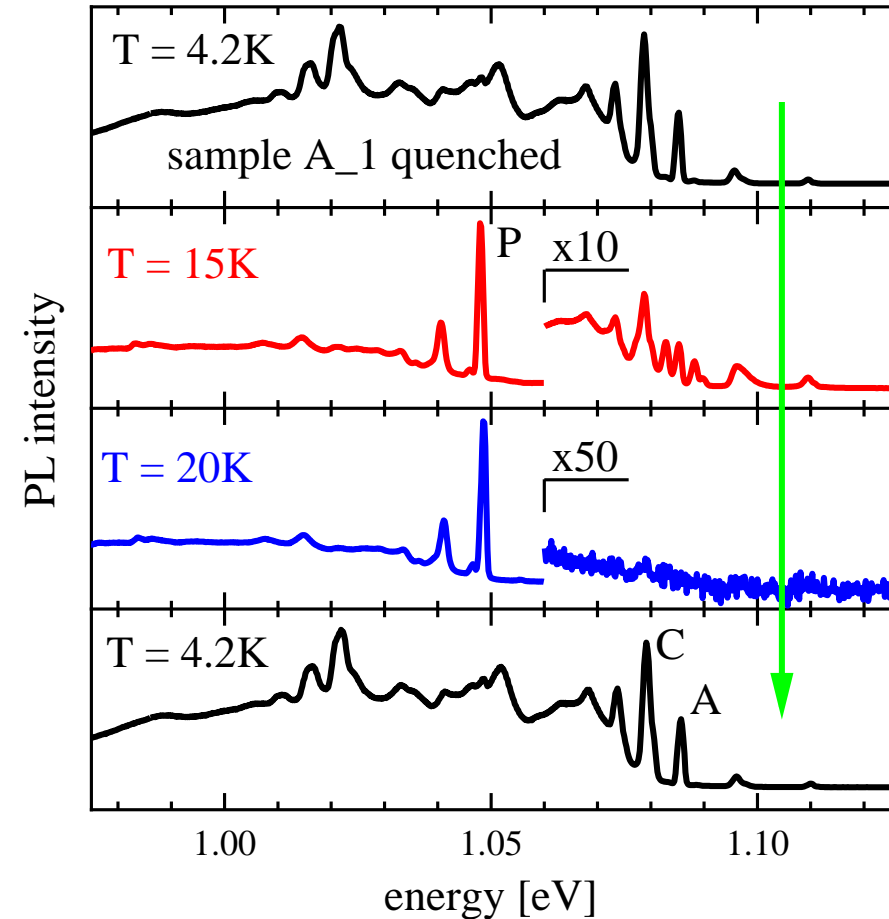
- Known PL lines [1] could be detected. [2]
- Main PL lines A_0^0 and P_0^0 denoted by A and P
- PL spectrum of defect appearing after quenching of Si:TI so far not understood.



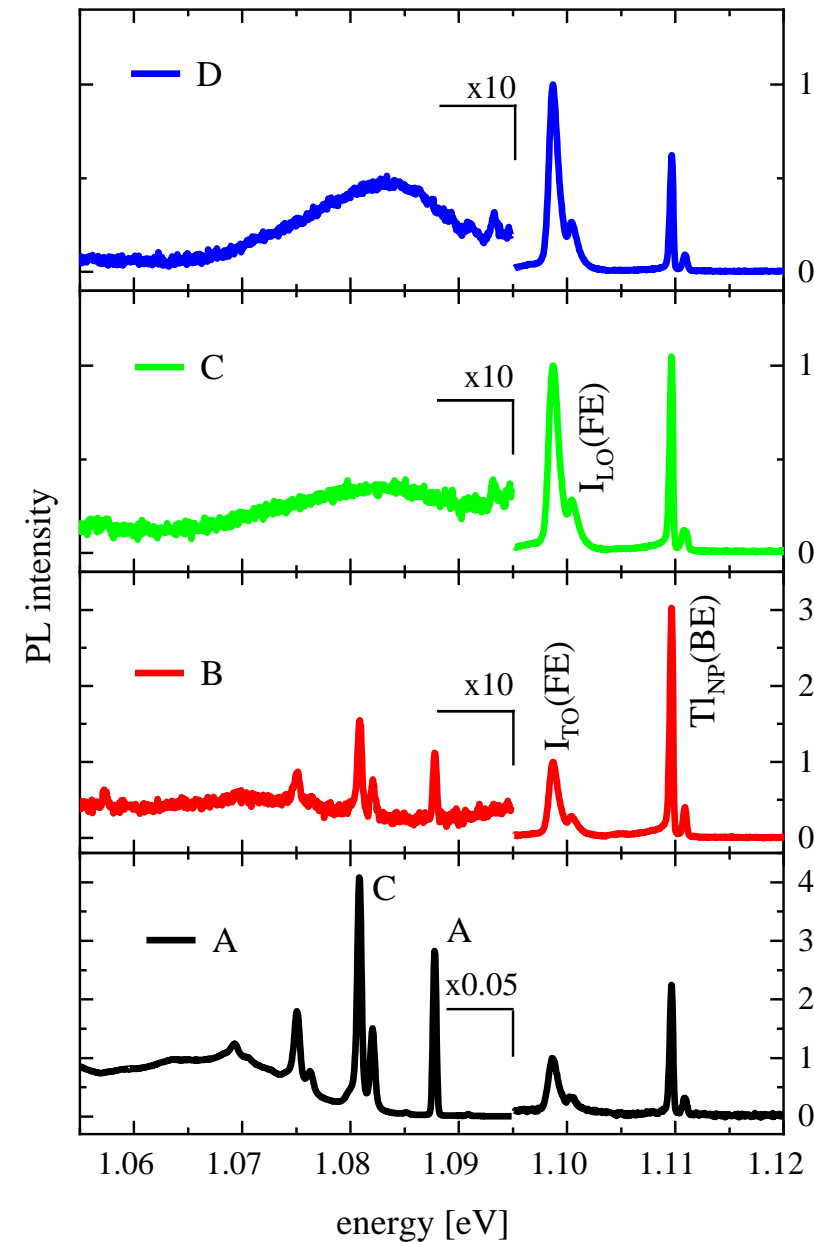
[1] H. Conzelmann, A. Hangleiter, and J. Weber, "Thallium-related isoelectronic bound excitons in silicon. A bistable defect at low temperatures," *Physica Status Solidi (b)* 133(2), 655-668 (1986).

[2] K. Lauer, Robin Müller, Katharina Peh, Dirk Schulze, Stefan Krischok, Stephanie Reiß, Andreas Frank and Thomas Ortlepp, 'Investigation of TI-doped silicon by low temperature photoluminescence during LID treatments', accepted *physica status solidi A* (2024).

Photoluminescence measurements in Si:TI



- Left: reversible interchange between luminescence from A and P line during variation of temperature in the cryostat
- For higher temperatures the defect resides in the configuration responsible for the P line
- Right: implantation dose dependence of the PL spectra
- PL line intensity decreases with increasing thallium implantation dose

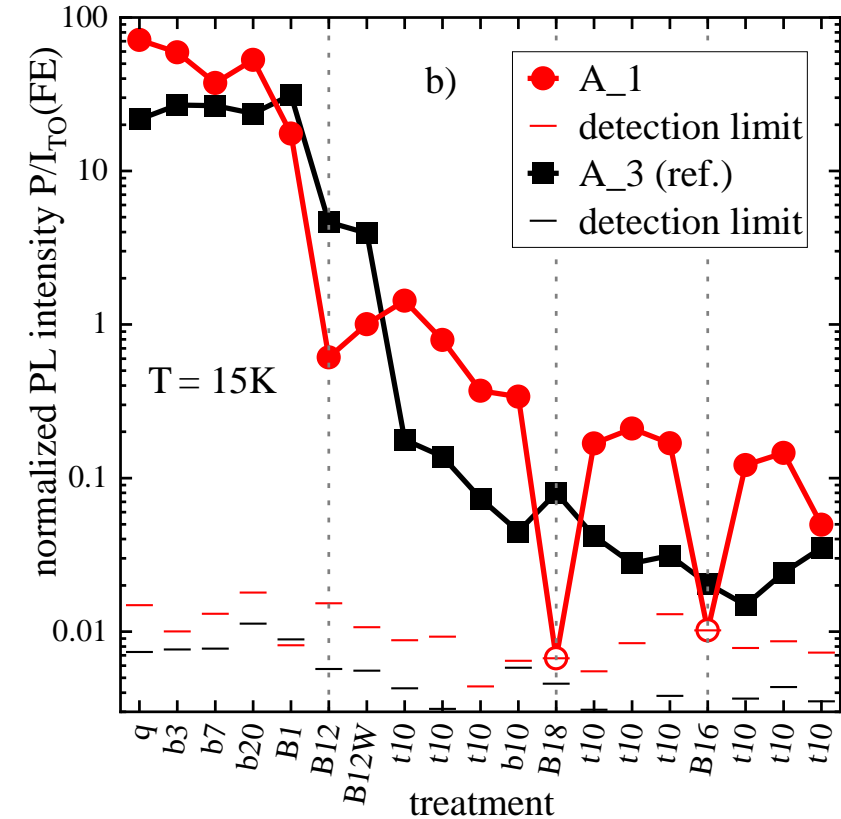
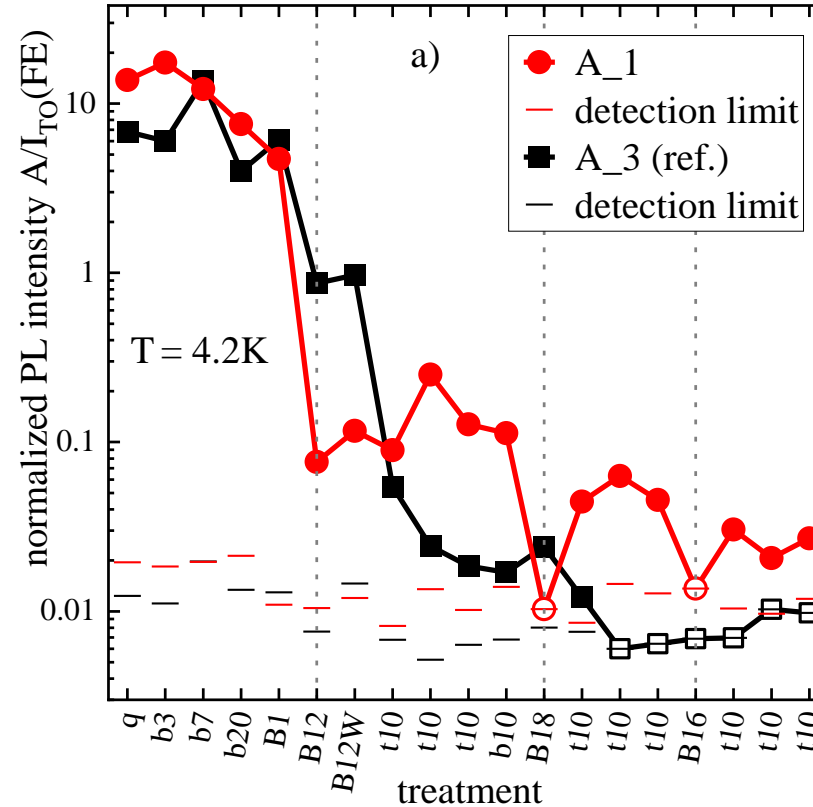


K. Lauer, Robin Müller, Katharina Peh, Dirk Schulze, Stefan Krischok, Stephanie Reiß, Andreas Frank and Thomas Ortlepp, 'Investigation of TI-doped silicon by low temperature photoluminescence during LID treatments', accepted physica status solidi A (2024).

Meta-stabilities of PL in Si:Tl (A and P lines)

Meta-stabilities of PL in Si:TL (A and P lines)

- Response on LID treatments in Si:In found for the P line [1]
- Similar results now found for Si:TL as well [2]
- Investigation of two identical Si:TL samples A_1 and A_3
- No carrier injection by illumination into reference sample A_3
- Irreversible and reversible changes visible
- After long illumination (B18 and B16) A and P line disappear
- Annealing for 10 min at 200° C restores both lines

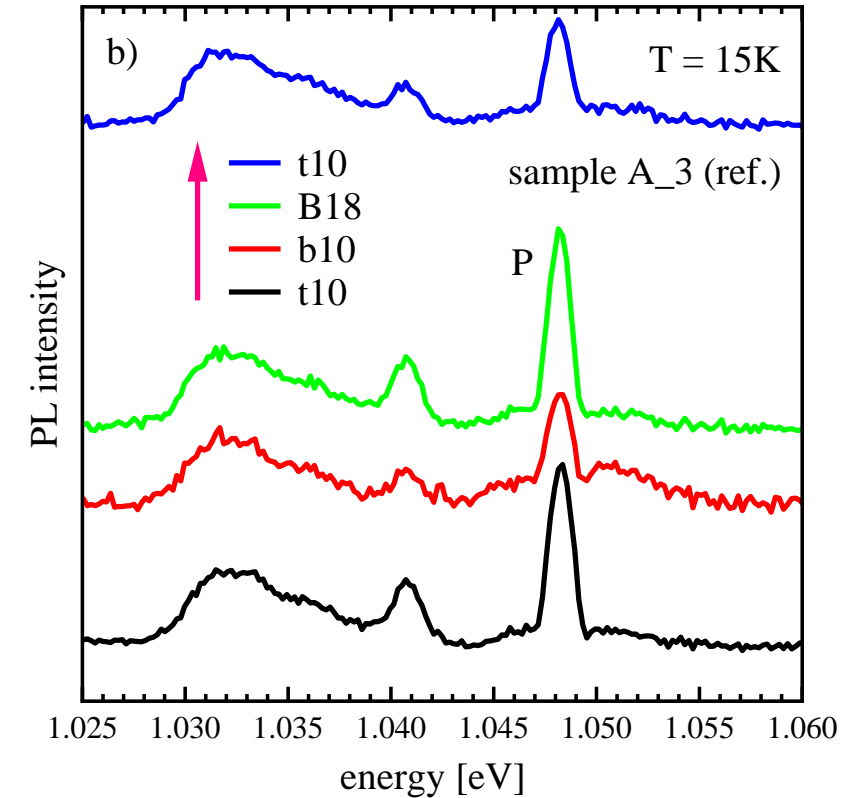
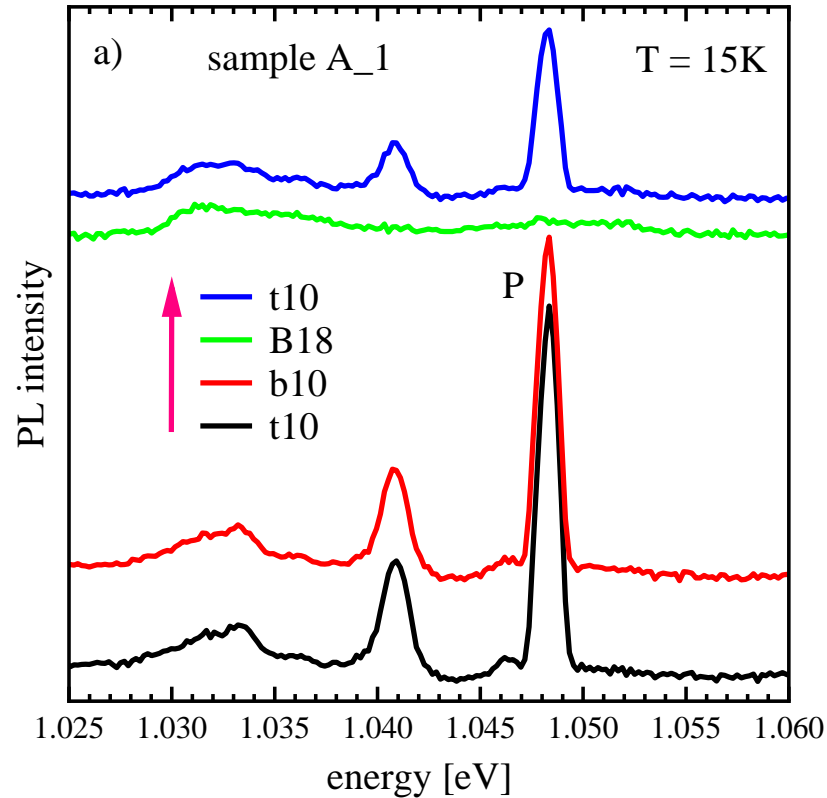


[1] K. Lauer, C. Möller, D. Schulze, and C. Ahrens, 'Identification of photoluminescence P line in indium doped silicon as InSi-Sii defect', AIP Advances, vol. 5, no. 1, p. 017101, Jan. 2015.

[2] K. Lauer, Robin Müller, Katharina Peh, Dirk Schulze, Stefan Krischok, Stephanie Reiß, Andreas Frank and Thomas Ortlepp, 'Investigation of TL-doped silicon by low temperature photoluminescence during LID treatments', accepted physica status solidi A (2024).

Meta-stabilities of PL in Si:Tl (P line)

- Detailed view on one LID cycle [1]
- P line in Si:Tl disappears reversibly after illumination (green spectra of sample A_1)
- Due to similarity to observations in Si:In, a $Tl_{Si}-Si_i$ defect could be proposed as origin for A and P lines in Si:Tl
- Different configurations of $Tl_{Si}-Si_i$ could cause A and P line luminescence

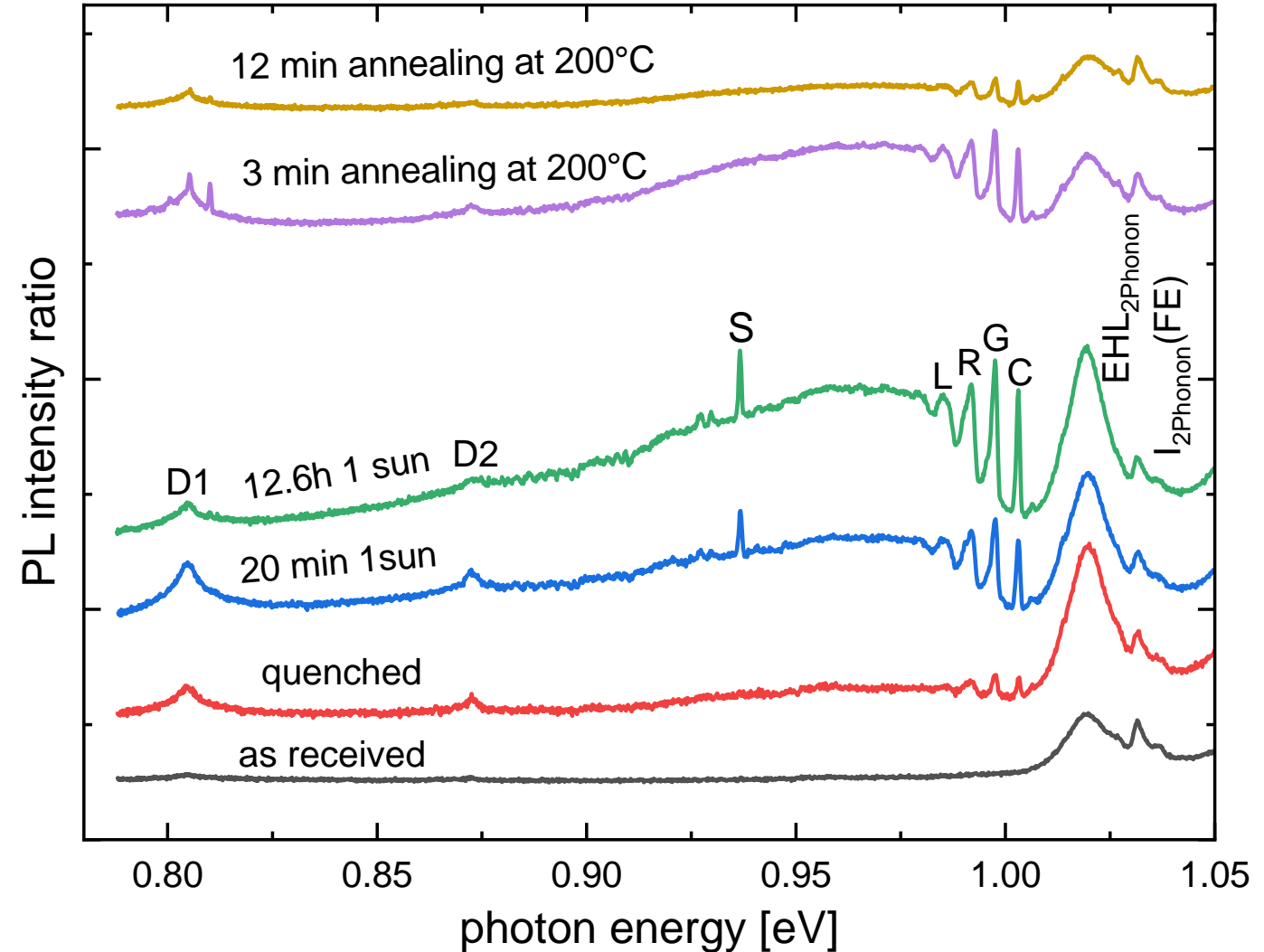


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Photoluminescence measurements in Si:B

Photoluminescence measurements in Si:B

- Implantation, quenching and LID treatments also applied for case of acceptor boron [1]
- New PL line called S line in Si:B found
- S line is also impacted by LID treatments, but in a different way compared to Si:In or Si:Tl
- Interesting: S line and the T center luminescence [2] lie in frame of our measurement accuracy at the same energy
- More investigations needed



[1] K. Lauer, S. Reiß, A. Flötotto, K. Peh, D. Bratek, R. Müller, D. Schulze, W. Beenken, E. Hiller, T. Ortlepp, and S. Krischok, "Effect of inelastic ion collisions on low-gain avalanche detectors explained by an A_{Si-Si_i}-defect mode," [Preprint](#) submitted to NIMB (2023).

[2] D.B. Higginbottom, A.T.K. Kurkjian, C. Chartrand, M. Kazemi, N.A. Brunelle, E.R. MacQuarrie, J.R. Klein, N.R. Lee-Hone, J. Stacho, M. Ruether, C. Bowness, L. Bergeron, A. DeAbreu, S.R. Harrigan, J. Kanaganayagam, D.W. Marsden, T.S. Richards, L.A. Stott, S. Roorda, K.J. Morse, M.L.W. Thewalt, and S. Simmons, "Optical observation of single spins in silicon," *Nature* 607(7918), 266-270 (2022).

Summary

- LGAD suffer from a not well understood acceptor removal phenomenon (ARP)
- One explanation approach is the $A_{Si}-Si_i$ defect model
- → Learning on defect properties by exploiting defect similarities of this defect family
- Photoluminescence signals of silicon doped with acceptors indium and thallium are known
- Similar response on LID treatments found for Si:In and Si:Tl
- Luminescence signal in Si:Tl (A and P line) probably caused by a $Tl_{Si}-Si_i$ defect
- Luminescence signal in Si:B found, which is prone to changes after LID treatments
- Further investigations necessary

- Interesting $A_{Si}-Si_i$ defect properties recognized for application in silicon based quantum technology



Thank you for your kind attention!

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