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Optical detected magnetic resonance (ODMR) of A_{Si}-Si_i defects: case of acceptor indium

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Overview

- Background / Motivation A_{Si}-Si_i defect
- Explanation of LGAD ARP by B_{Si}-Si_i defect
- Optically detected magnetic resonance (ODMR) of C_{Si}-Si_i defect
- Cooled ODMR setup @ CiS
- ODMR signals of In_{Si}-Si_i defect
- Conclusion

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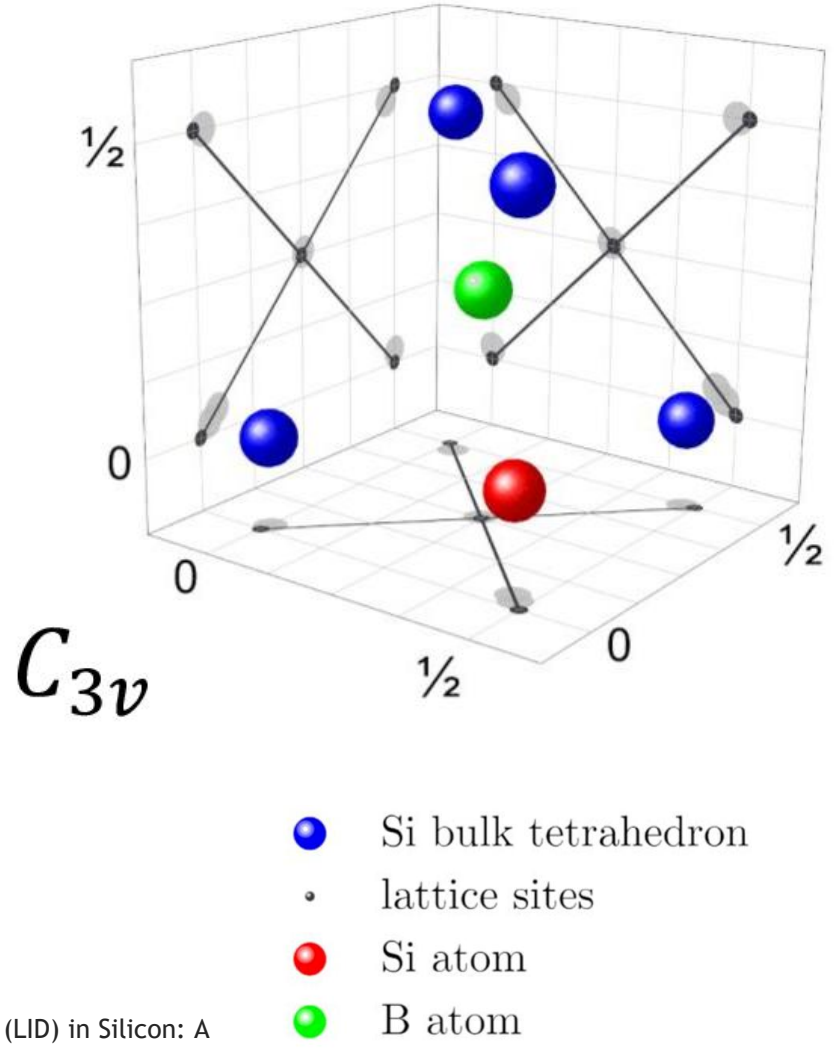
Background

- An acceptor-silicon (A_{Si}-Si_i) defect consist of an acceptor atom (B, Al, Ga, In and Tl) and a silicon atom co-located around a lattice site [1,2]
- Indications exist that these defects are involved in detrimental effects on silicon devices:

  ➔Light-induced degradation (LID) in silicon solar cells

  ➔Acceptor removal phenomenon (ARP) in low-gain avalanche detectors (LGAD)
- Possibly applicable in silicon-based quantum technology [3]



[1] K. Lauer, K. Peh, D. Schulze, T. Ortlepp, E. Runge, and S. Krischok, "The A_{Si}–Si_i Defect Model of Light-Induced Degradation (LID) in Silicon: A Discussion and Review," Physica Status Solidi (a) 219(19), 2200099 (2022), doi: 10.1002/pssa.202200099.
[2] A. Flötotto, W.J.D. Beenken, K. Lauer, S. Krischok, and E. Runge, "Electronic structure and energy landscape of B_{Si}-Si_i related defects," Phys. Rev. Mater. 9(2), 024601 (2025), doi: 10.1103/PhysRevMaterials.9.024601
[3] 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Moll, 'Examining the properties of the A_{Si}–Si_i-defects for their potential as qubits', presented at the GADEST but unpublished, Bad Schandau: ResearchGate, May 2024. doi: 10.13140/RG.2.2.18793.51048.

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Background

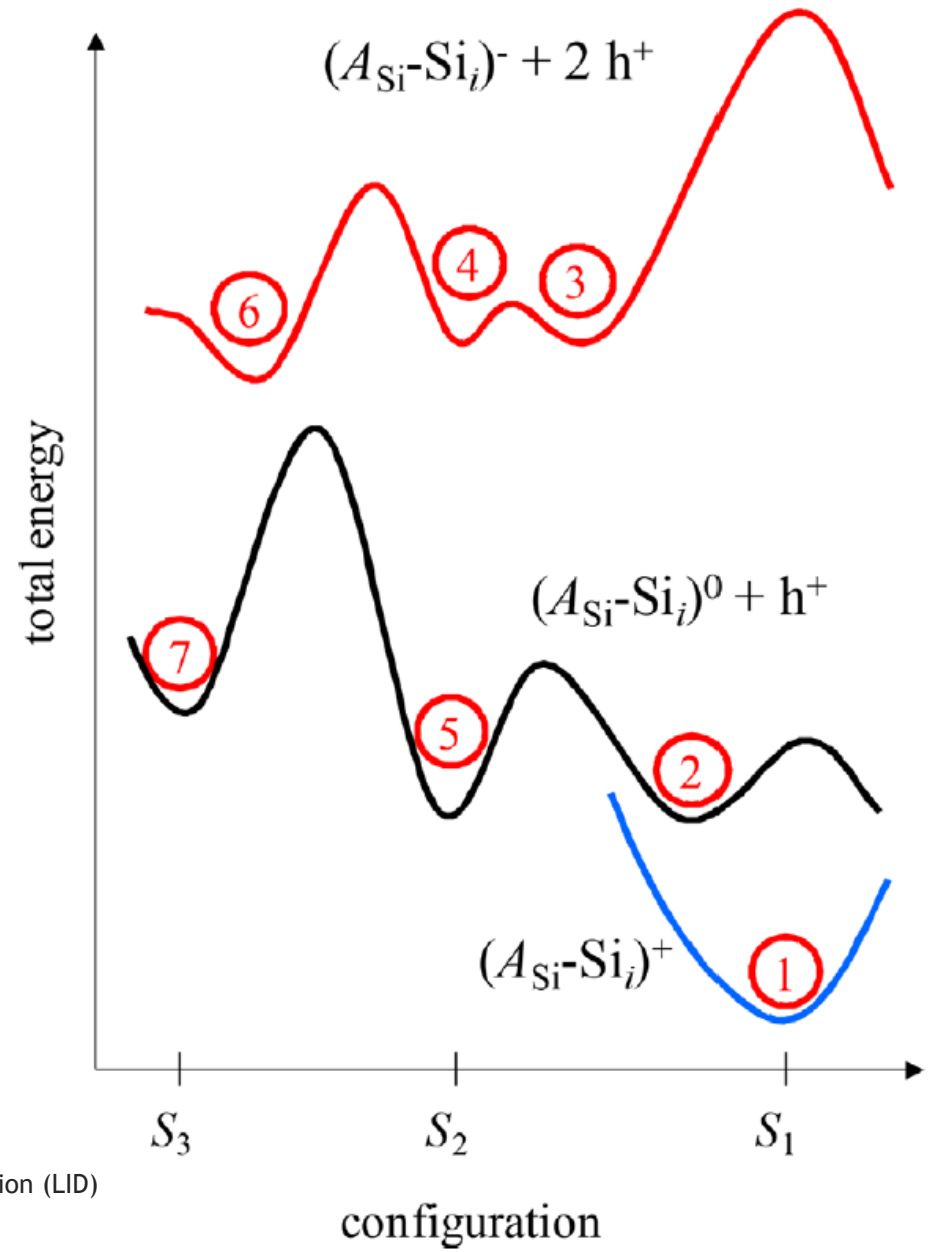
- Comprehensive spectrum of defect properties developed, collected and discussed [1] like cc-diagram, photoluminescence signals, carrier recombination, stability, energy barriers, …
- A_{Si}-Si_i defects exist in several stable configurations (see LID, ARP, PL signals, …)
- But, defect understanding far away from full knowledge
- Interesting points are:

  →Defect configuration changes

  →Luminescence properties

  →Electronic/magnetic resonances

  →Single defect properties



[1] K. Lauer, K. Peh, D. Schulze, T. Ortlepp, 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) 219(19), 2200099 (2022), doi: 10.1002/pssa.202200099.

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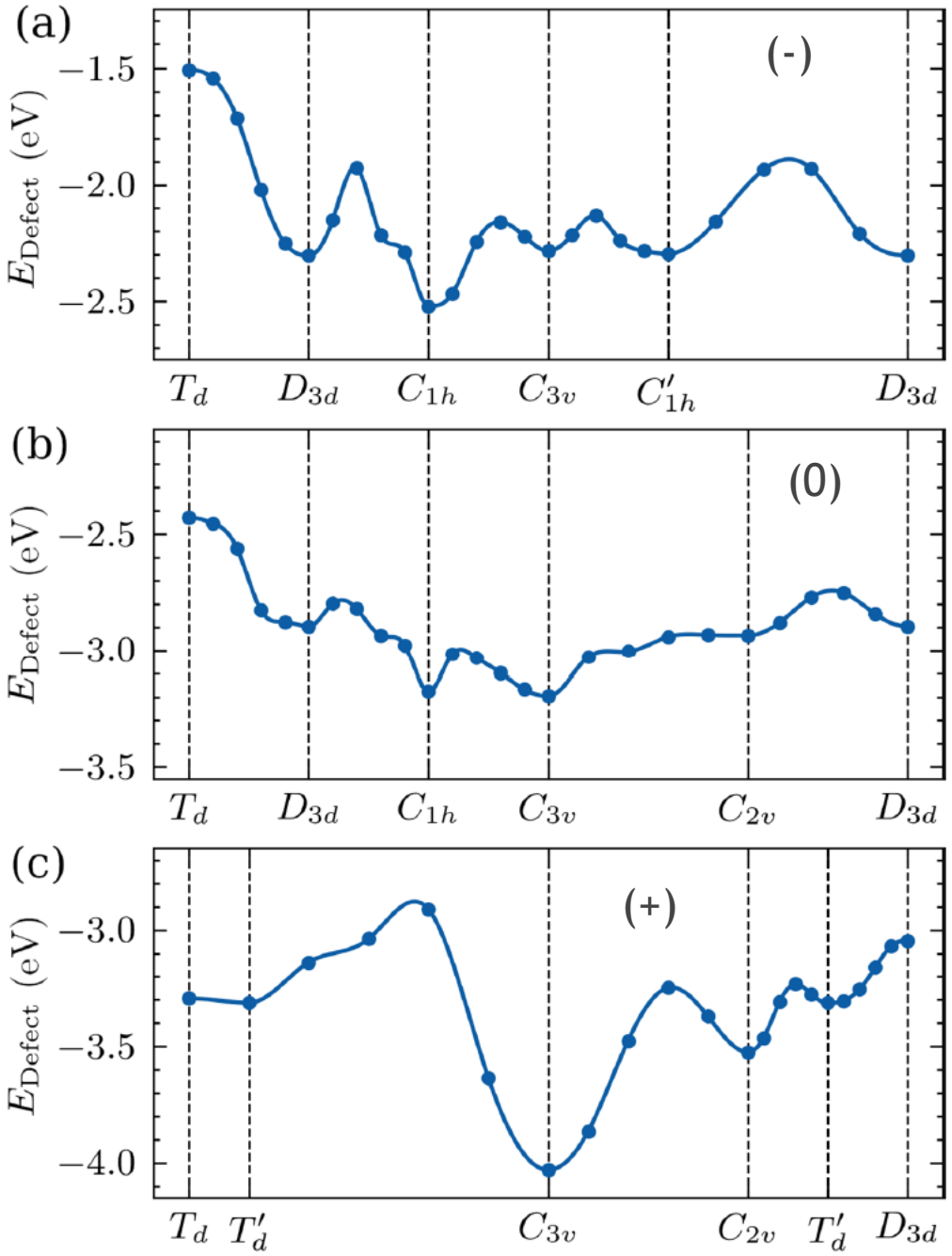
Explanation of LGAD ARP by B_{Si}-Si_i defect

- Defect formation: interstitial silicon (generated by irradiation) is captured by substitutional acceptor boron [1]
- Defect configuration with lowest formation energy (ground state) is C_{3v} (B_{Si}-Si_i) [2]
- B_{Si}-Si_i in ground state is donor (change form acceptor to donor => ARP)
- Other defect configurations are possible depending on treatments like carrier injection (by irradiation or illumination) or low temperature annealing [3]



[1] K. Lauer et al., 'Effect of inelastic ion collisions on low-gain avalanche detectors explained by an A_{Si}-Si_i-defect mode', Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, vol. 555, p. 165472, Oct. 2024, doi: 10.1016/j.nimb.2024.165472.
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[3] K. Lauer et al., 'Modeling the light-induced degradation (LID) in silicon due to A_{Si}-Si_i-defects', Tagungsband 5. Niedersächsisches Symposium Materialtechnik: 23. bis 24. Februar 2023, June 2023, doi: 10.21268/20230628-0.

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Advantages of ARP explanation by B_{Si}-Si_i defect compared to B_iO_i approach

- B_iO_i approach needs the substitutional boron acceptor to be removed from substitutional position (C_{3v}) to an interstitial position (T_d, D_{3d}, …)
- This replacement reaction is from DFT calculation of the energy and energy barriers unlikely [1].
- B_iO_i approach needs the assumption of a fast B_i migration to an O_i
- A fast B_i migration is experimentally not seen e.g. in SIMS measurements [2,3]
- Involvement of oxygen in DLTS E1 level (B_iO_i) unlikely after latest literature [4]

- In B_{Si}-Si_i approach all these 3 unlikely assumption are not needed.
- ARP removal ideas by defect configuration changes or hydrogen involvement???

[1] A. Flötotto, W. J. D. Beenken, K. Lauer, S. Krischok, and E. Runge, 'Electronic structure and energy landscape of B_{Si}-Si_i related defects', Phys. Rev. Mater., vol. 9, no. 2, p. 024601, Feb. 2025, doi: 10.1103/PhysRevMaterials.9.024601.
[2] K. Lauer, K. Peh, D. Schulze, T. Ortlepp, 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, 2022, doi: 10.1002/pssa.202200099.
[3] K. Lauer, K. Peh, S. Krischok, S. Reiß, E. Hiller, and T. Ortlepp, 'Development of Low-Gain Avalanche Detectors in the Frame of the Acceptor Removal Phenomenon', physica status solidi (a), vol. 219, no. 17, p. 2200177, June 2022, doi: 10.1002/pssa.202200177.
[4] L. Vines, E. V. Monakhov, A. Yu. Kuznetsov, R. Kozłowski, P. Kaminski, and B. G. Svensson, 'Formation and origin of the dominating electron trap in irradiated p -type silicon', Physical Review B, vol. 78, no. 8, p. 085205, Aug. 2008, doi: 10.1103/PhysRevB.78.085205.

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Knowledge is key

- Physical understanding of A_{Si}-Si_i defects necessary to develop strategies for e.g. solutions of the ARP
- For example the electronic level scheme of different configurations of In_{Si}-Si_i defect interesting

  →Performing optically detected magnetic resonance (ODMR) measurements

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C_{Si}-Si_i defects in silicon (XG), ODMR

- C_{Si}-Si_i defects proposed by Thunke et al. [1]
- “Comparable” to A_{Si}-Si_i defects
- Acceptor (A) substituted by carbon (C)
- C_{Si}-Si_i defects show ODMR signals [2]
- A_{Si}-Si_i defects may also show ODMR signals

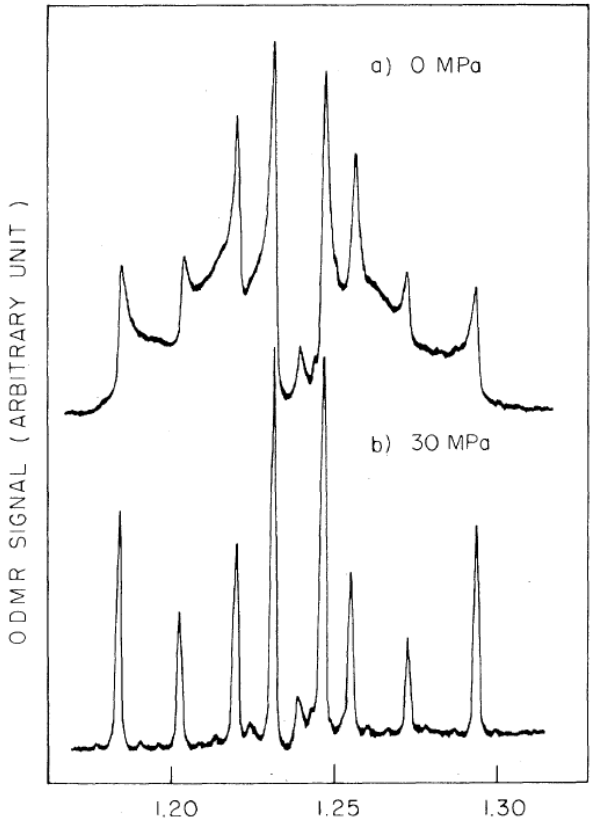

FIG. 1. (a) ODMR spectrum with $\vec{B}\parallel[011]$ at $T \cong 1.7$ K, $\nu = 35.0$ GHz. (b) Spectrum, same orientation, with compressional stress of 30 MPa, $\vec{T}\parallel[0\bar{1}1]$, showing ^{29}Si hyperfine satellites.

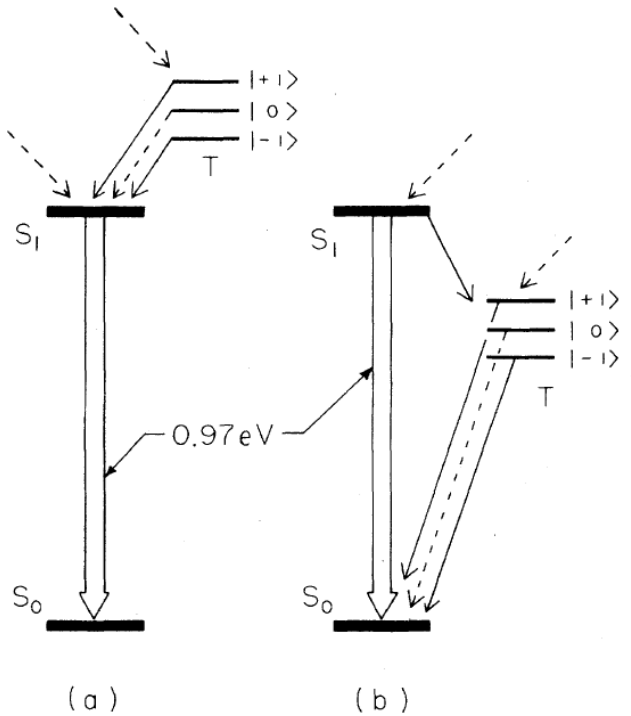

FIG. 3. Two models for triplet ODMR in the singlet-to-singlet luminescence. (a) The triplet state is above the radiative singlet state and ODMR $\Delta M = \pm 1$ transitions enhance the decay to the radiative state by emptying the bottlenecked triplet $|M>$ state. (b) The triplet state is below the radiative state and ODMR enhanced radiationless decay to the ground state provides more defects in the ground state for excitation to the emitting state.

[1] K. Thunke, H. Klemisch, J. Weber, and R. Sauer, “New model of the irradiation-induced 0.97-eV G line in silicon: A C_{Si}-Si* complex,” Phys. Rev. B 24(10), 5874–5886 (1981), doi: 10.1103/PhysRevB.24.5874.
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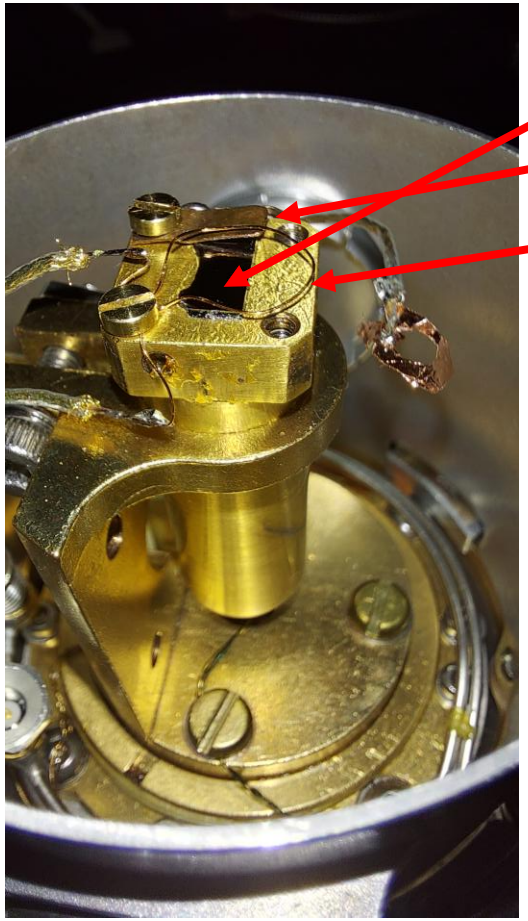
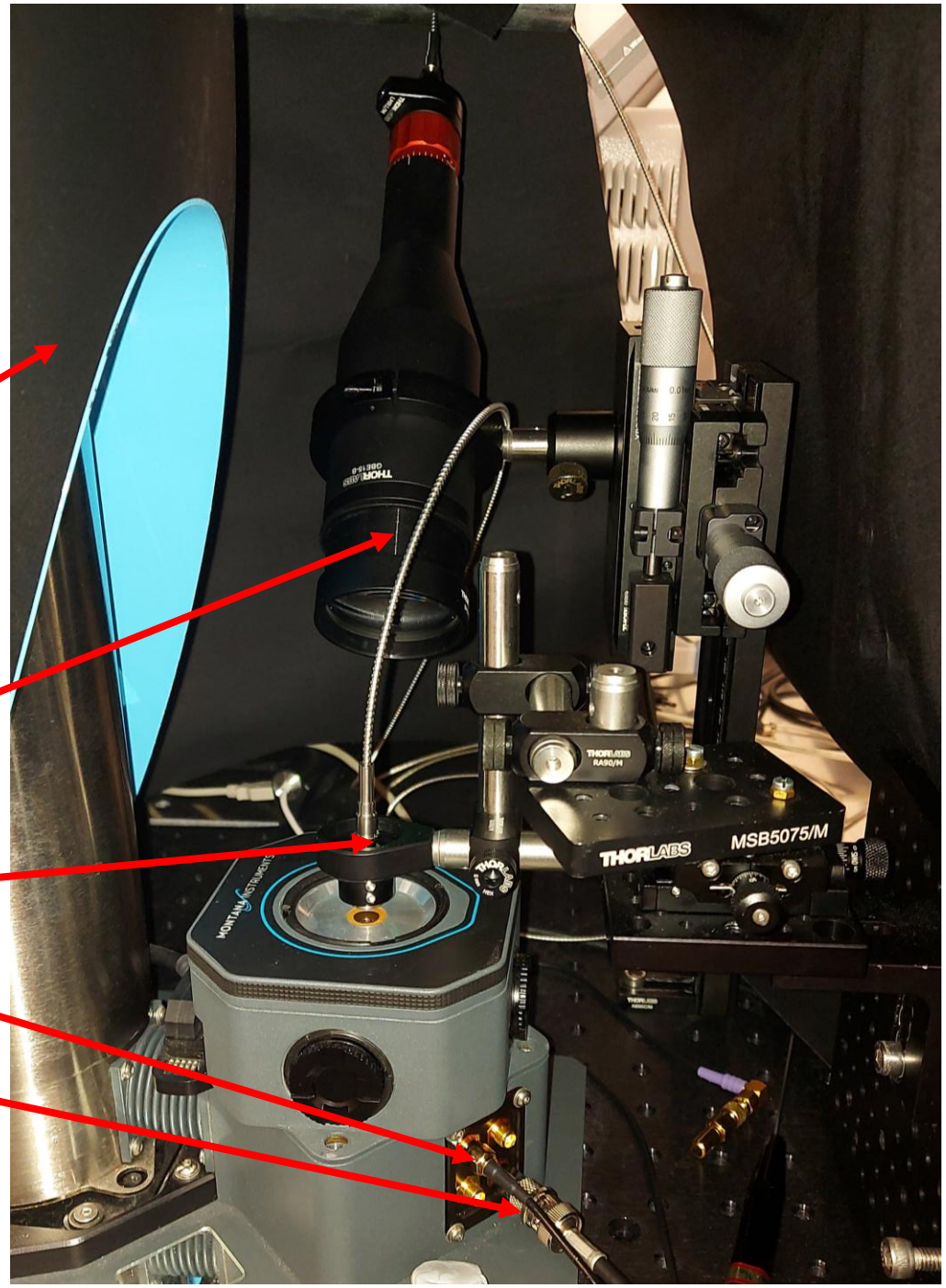
Cooled ODMR setup @ CiS



- Sample
- Thermometer
- Ω-antenna

- Cryostat
- Excitation laser objective
- Fiber to monochromator with InGaAs line detector
- Cable to microwave generator
- Cable to microwave analyser



Sample preparation

- Cz:In silicon from Institute for Crystal Growth Berlin
- Saw damage etch in KOH
- Sample glowing in flame for 10s
- Quenching in distilled water

→In_{Si}-Si_i defects form [1,2]

[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), doi: 10.1016/0038-1098(81)91040-1.
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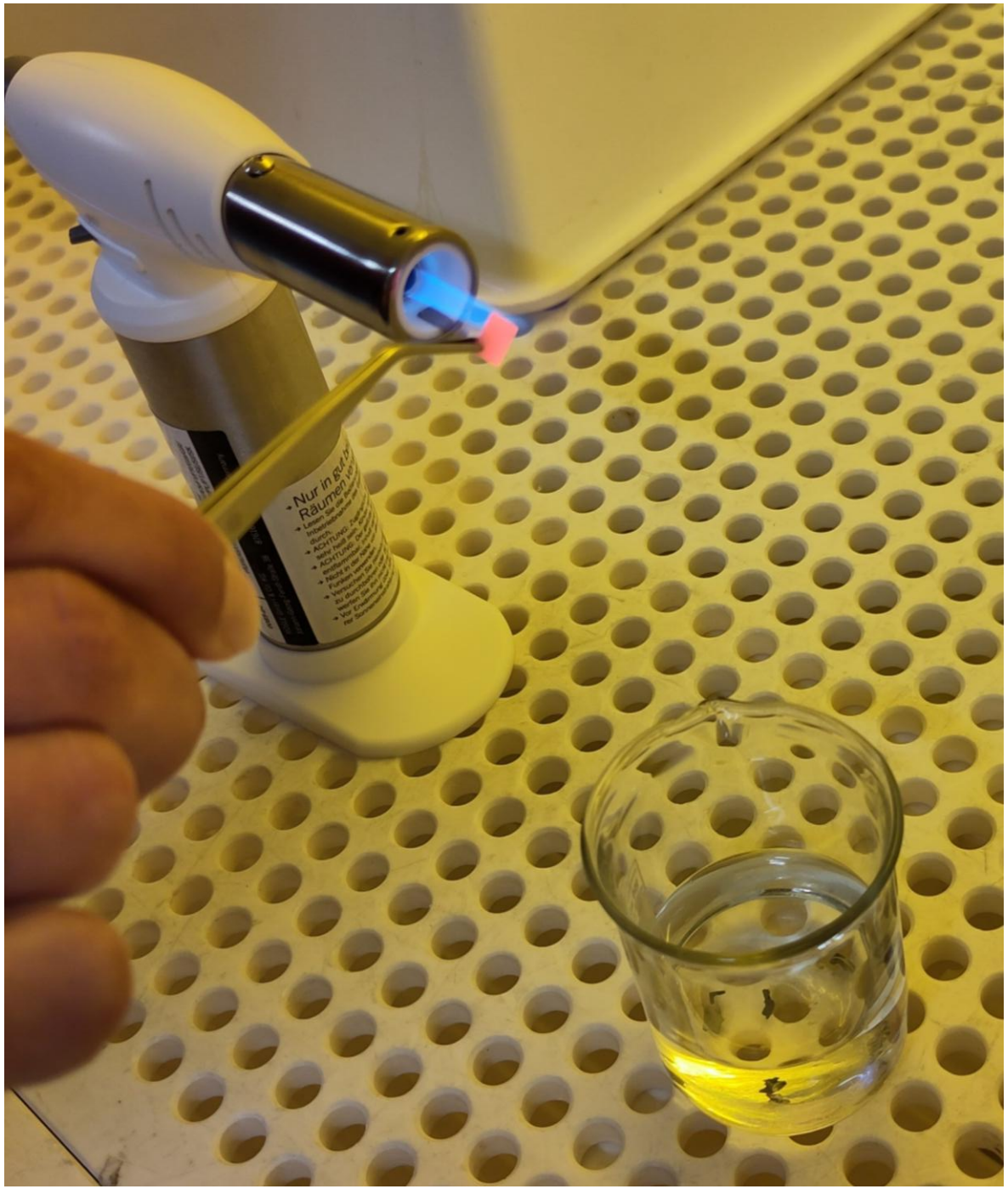
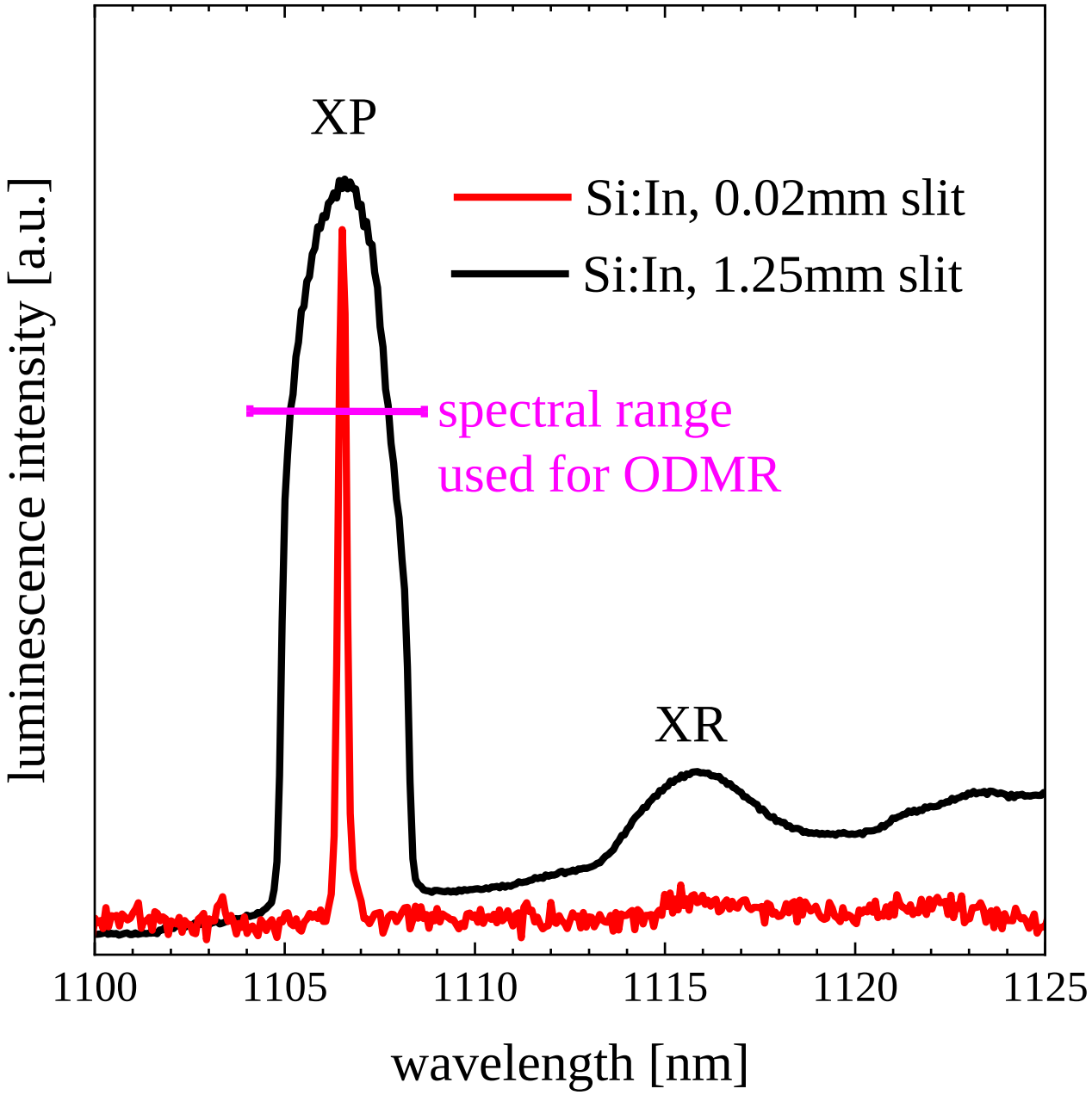


Photoluminescence (PL)

- Excitonic PL by In_{Si}-Si_i defects denoted by XP and XR
- Large PL peaks visible
- To maximize ODMR signal monochromator slit opened widely
- ODMR measurements: XP peak area monitored during microwave sweeps



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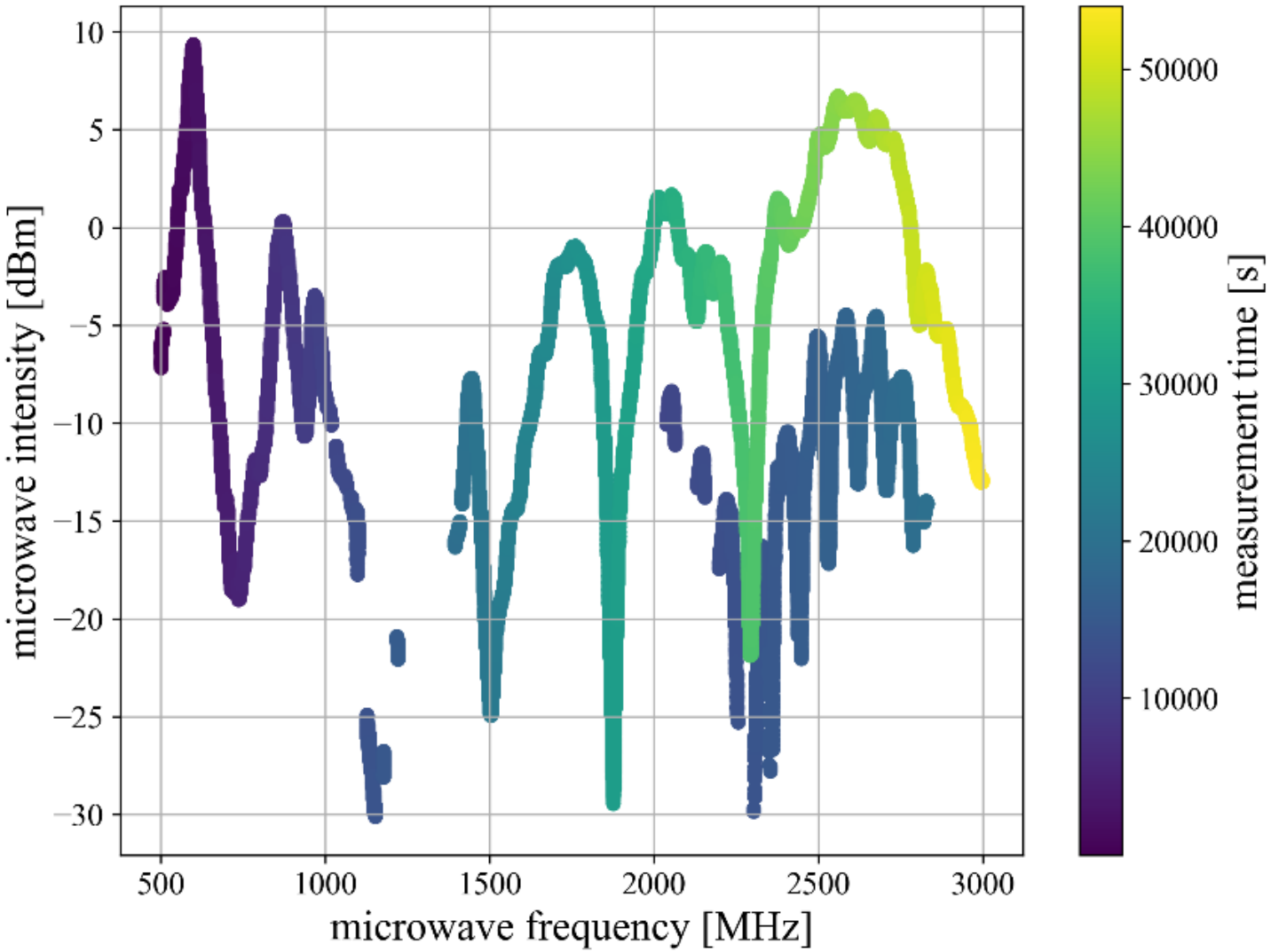
Microwave (MW) signal

- MW generated and amplified
- MW intensity measured by spectrum analyser behind Ω-antenna
- MW sweeps applied
- Intensity of largest peak in MW spectrum recorded
- Largest peak does not always coincide with tuned frequency of MW generator
- MW intensity spectrum strongly depends on Ω-antenna design



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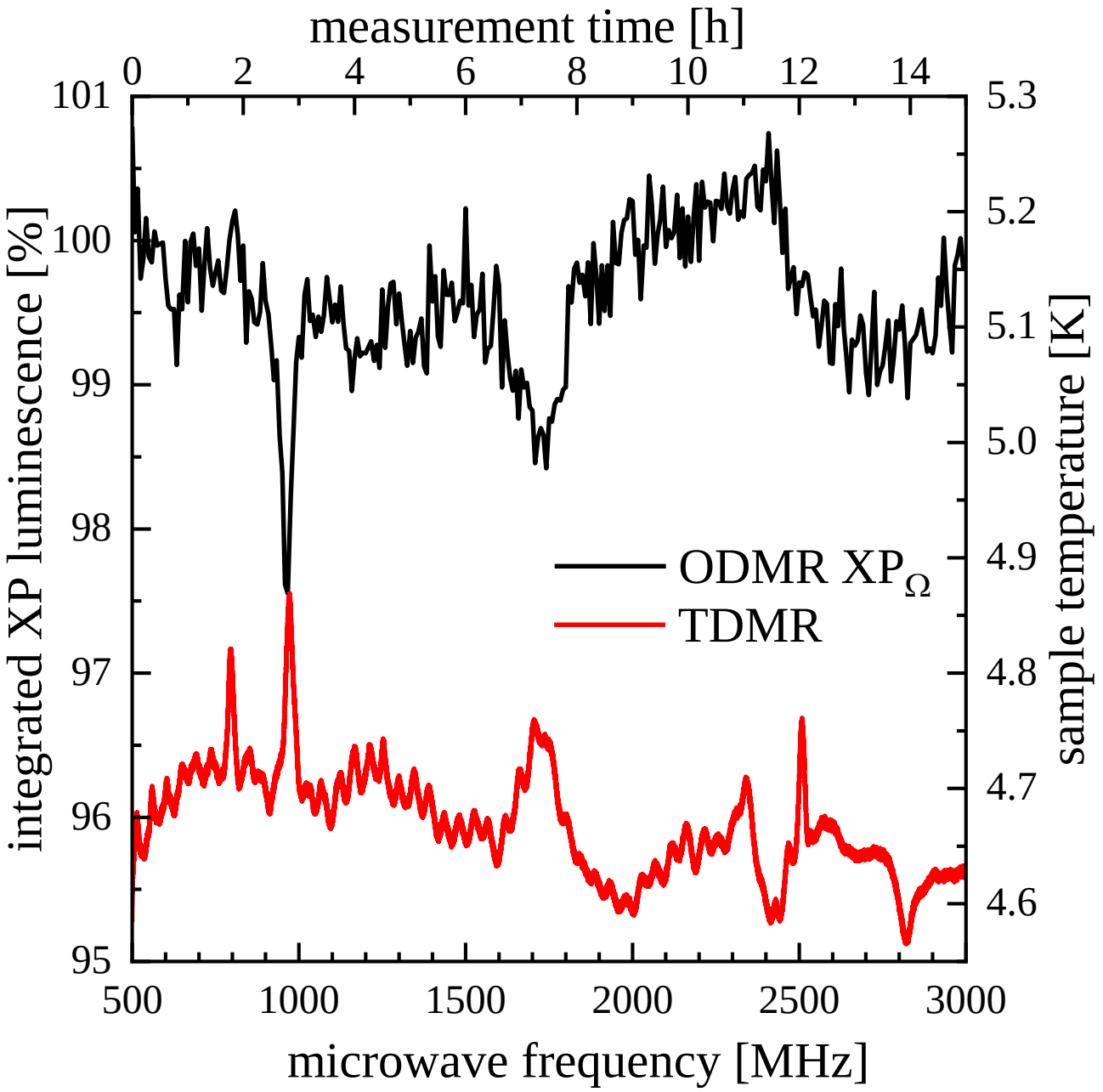
ODMR results

- So far two ODMR signals visible
- ODMR correlates with TDMR (temperature detected magnetic resonance)
- Temperature for TDMR is monitored close to sample during MW sweep
- Not all TDMR signals are visible in the ODMR



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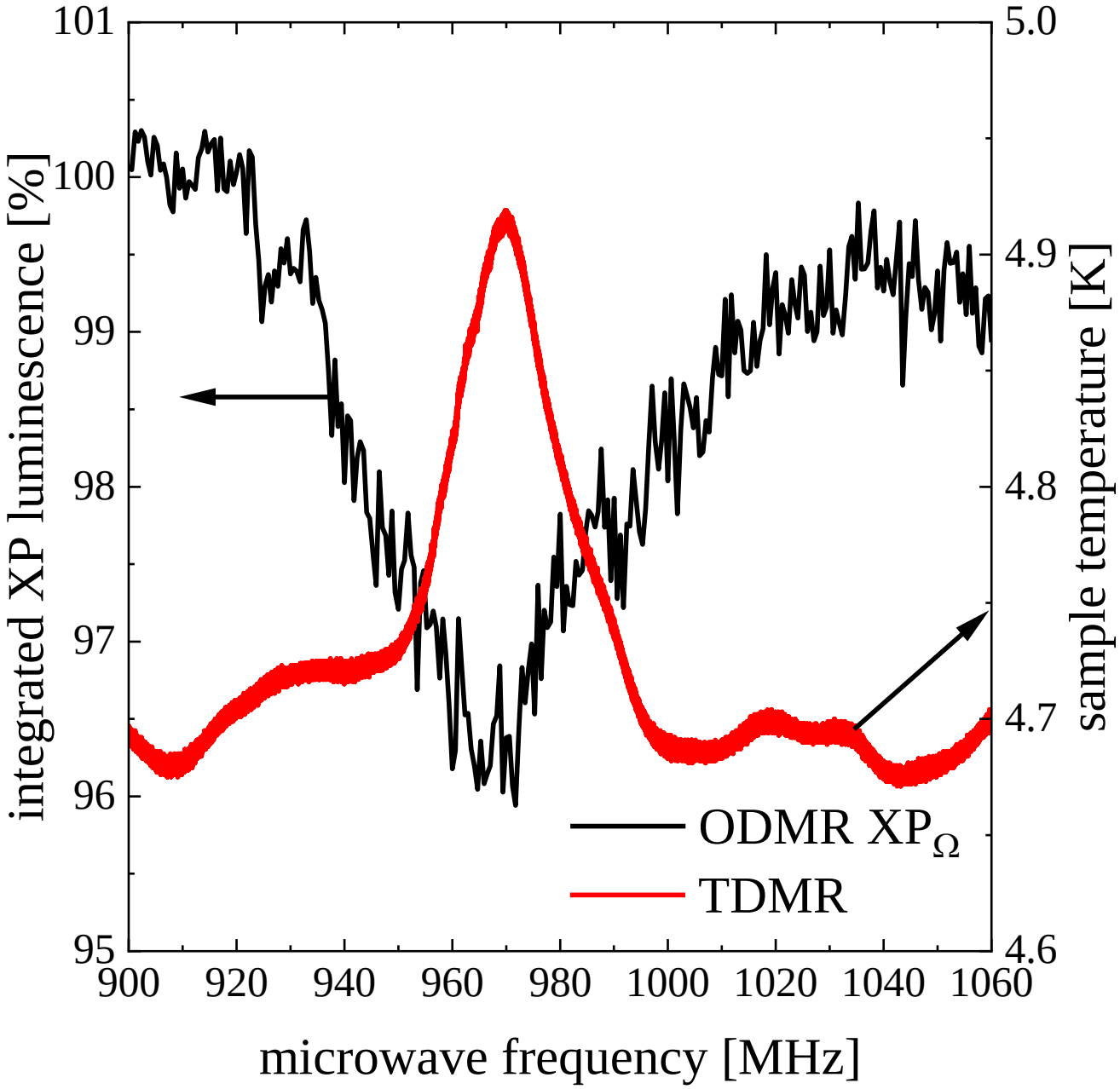
ODMR results

- High resolution measurement of the XP ODMR and TDMR signal caused by In_{Si}-Si_i defects



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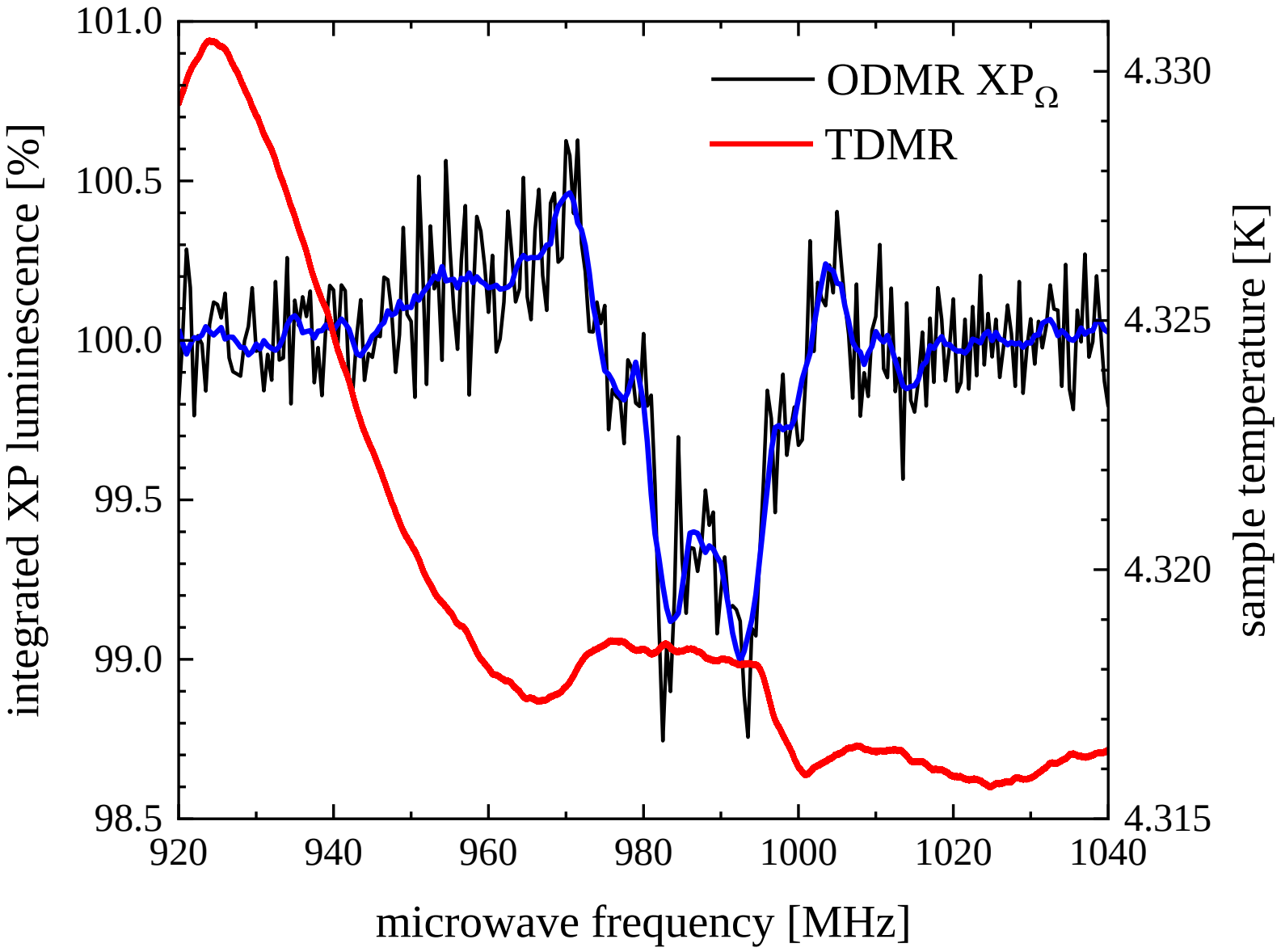
ODMR results

- Best ODMR of XP measured so far
- Fine structure visible

- Due to metastability of A_{Si}-Si_i defects and other problems still no full control over ODMR XP_Ω signal so far



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Conclusion

- A_{Si}-Si_i defects consist of an acceptor atom and a silicon atom co-located around a lattice site
- Case of acceptor boron (B_{Si}-Si_i) can explain ARP of LGADs
- Substitutional boron captures one interstitial silicon, which was generated by irradiation
- B_{Si}-Si_i defect is in ground state a donor (change from acceptor to donor => ARP)

- Further knowledge gain of A_{Si}-Si_i defects necessary e.g. by applying optically detected magnetic resonance (ODMR) measurements
- ODMR setup build at CiS and ODMR measurements done for In_{Si}-Si_i defect
- ODMR and TDMR signals found for XP_{Ω} signal of In_{Si}-Si_i defect

- Much work to be done: interpretation and modelling of electronic levels, application of static magnetic fields, …

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