

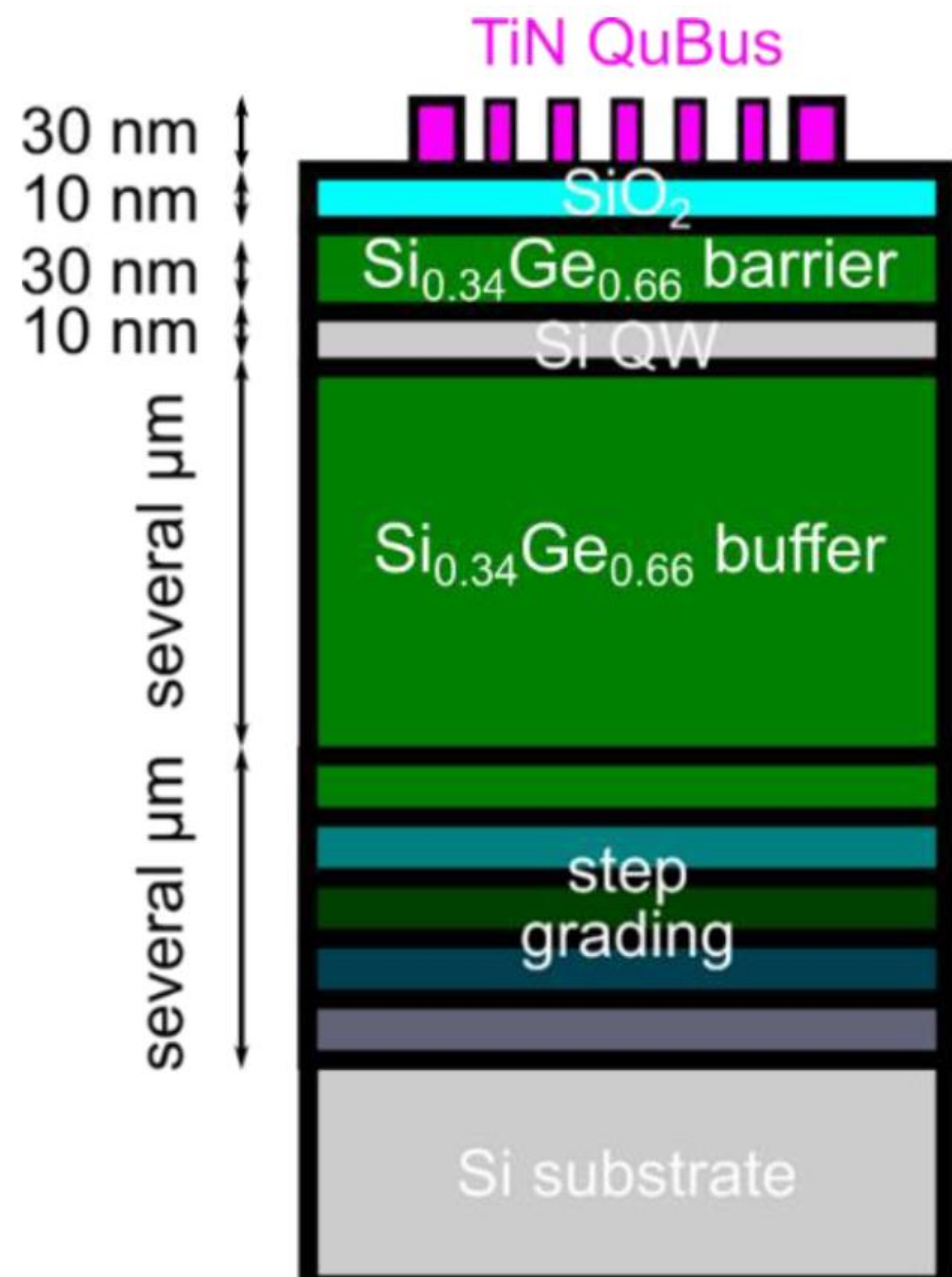
# Simulation of elastic strain in electron shuttling devices

I. Zaitsev

IHP – Leibniz-Institut für innovative Mikroelektronik



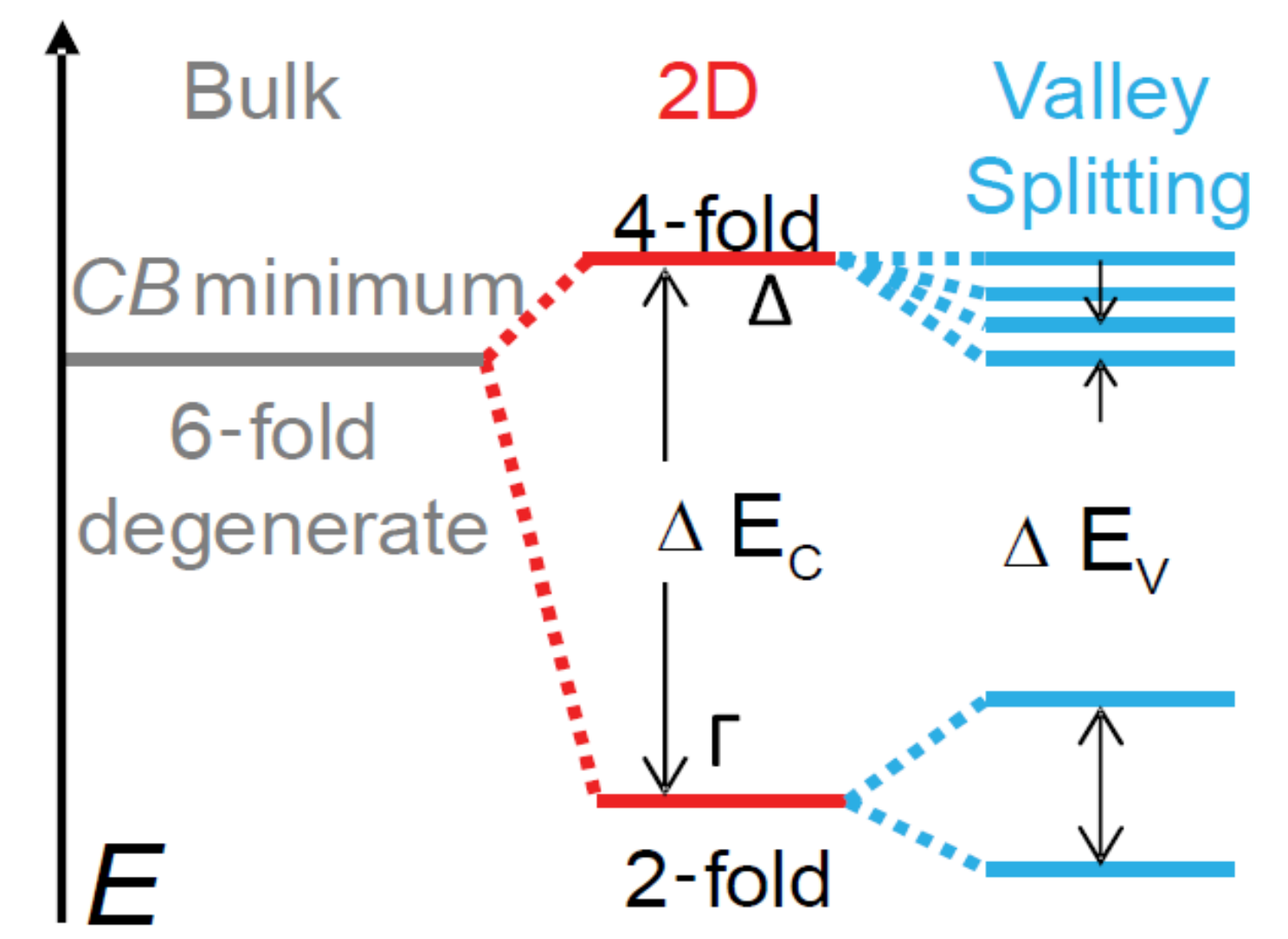
## Si/SiGe BASED SPIN QUBITS



Schematic of the measured microstructure

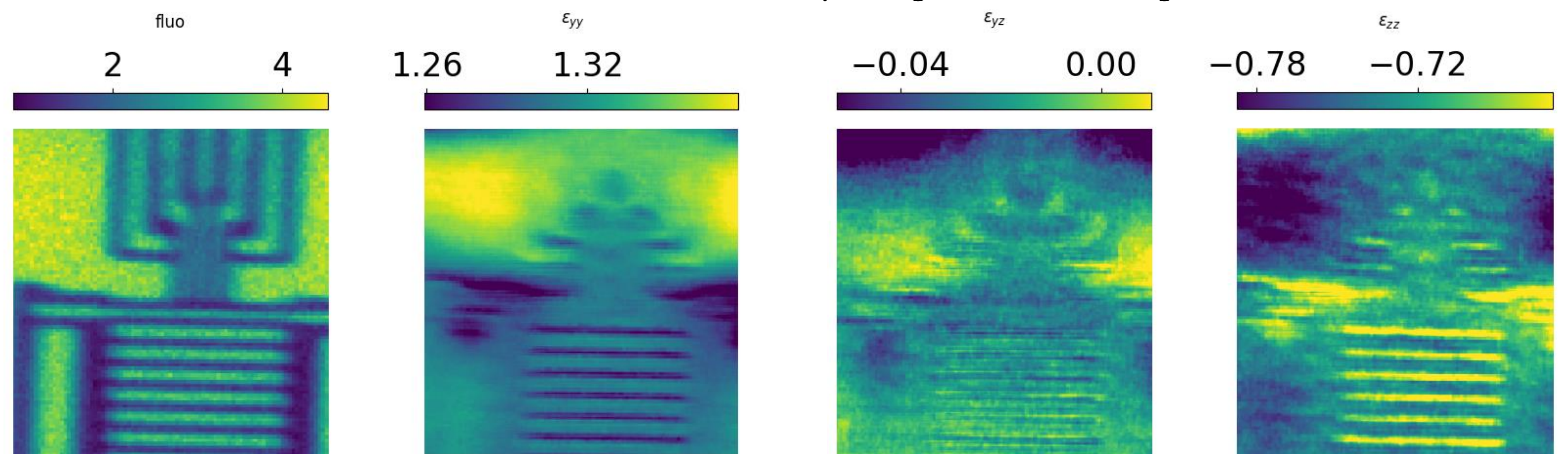
The realization of error-corrected quantum processors will require interconnected arrays of  $> 10^4$  qubits.

- Communication between qubits must be established by e.g. coherent electron shuttling [1], that can be realized with the quantum bus architecture [2].
- Gate operation voltages and shuttling are affected by the local band energy level, which, in turn, depends on the lattice strain in the quantum well (QW) layer [3].



L.R. Schreiber, 2019

Splitting of the band edges in strained silicon.

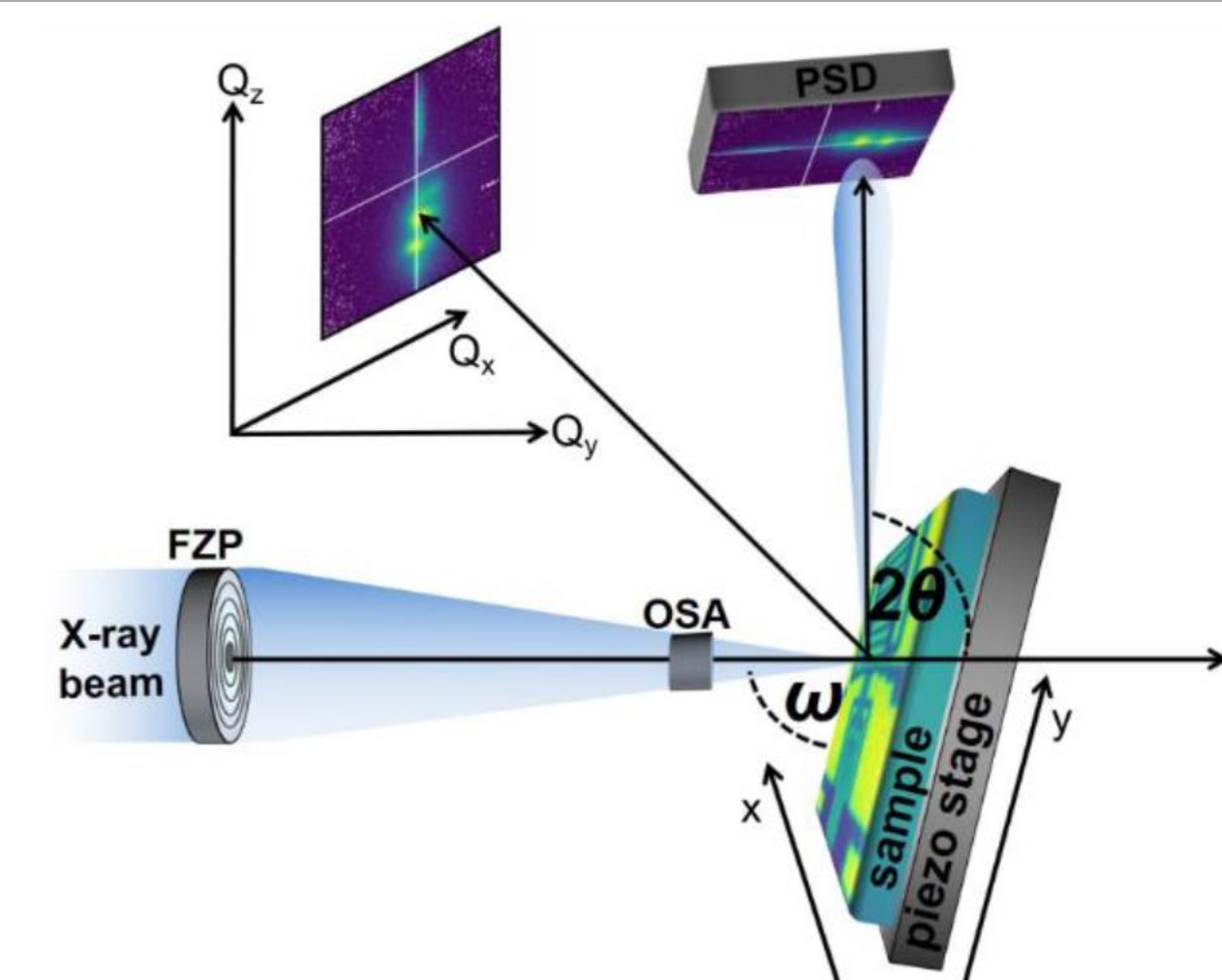


Maps of the TiN K-edge fluorescence and the strain tensor components in the quantum well

## METHODS

### SXDM

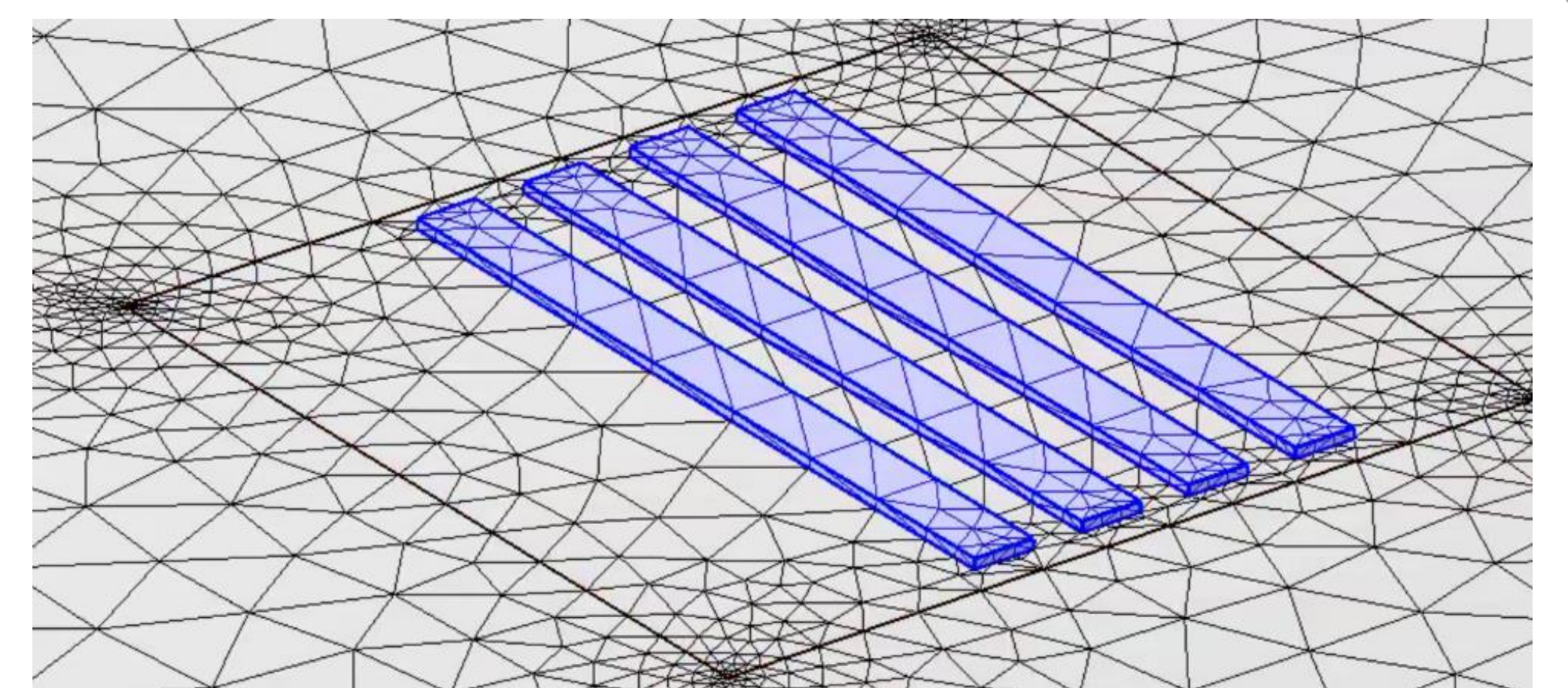
- X-ray nanoprobe beamline ID01/ESRF [1] produces microscopic maps of the lattice strains induced by TiN electrodes deposited on the top surface of two Si/SiGe quantum well samples grown on Si(001) substrates.



Experimental setup of the SXDM measurement [2].

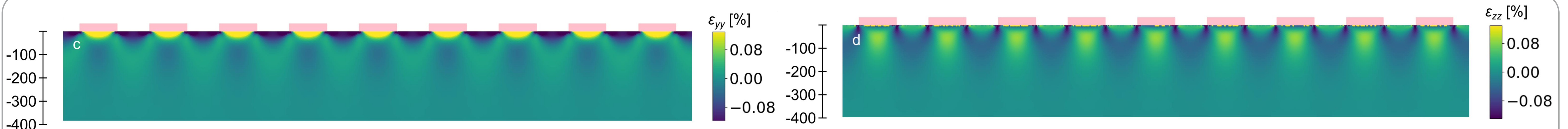
### FEM modeling

- Analysis of mechanical deformations by means of Hooke's law ( $\sigma_{ij} = C_{ijkl}\epsilon_{kl}$ ) in Si/SiGe qubit devices stressed by TiN electrodes.
- Calculation of the changes in the band structure using the k-p method.

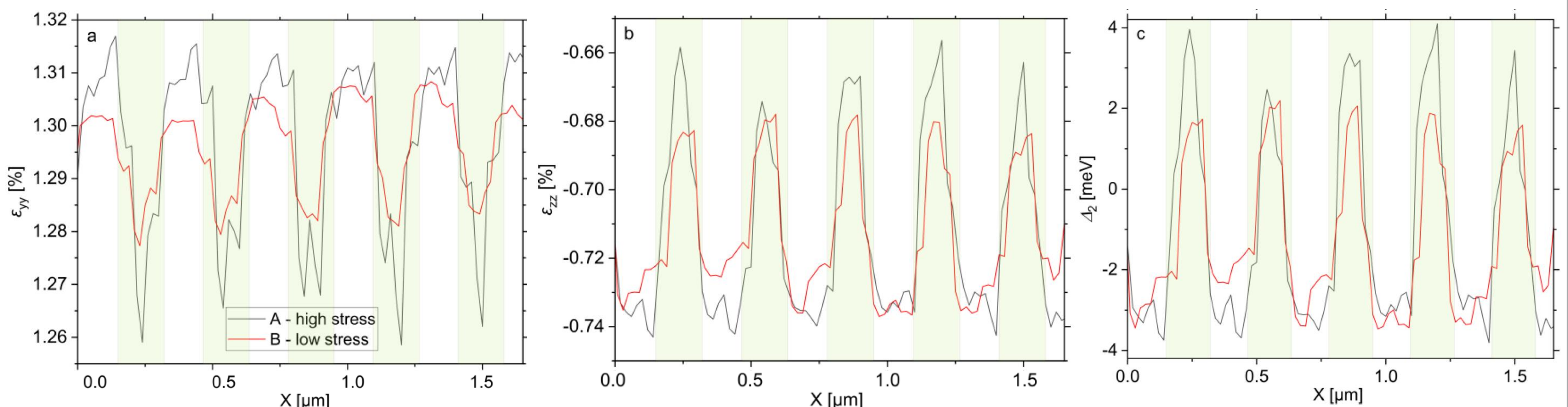


The reproduction of the periodic TiN electrodes on the Si/Si<sub>0.7</sub>Ge<sub>0.3</sub> heterostructure.

## FEM SIMULATIONS AND COMPARISON WITH SXDM



Profiles of the most prominent strain tensor components simulated throughout the layered structure.



Comparison of the measured strain components and the conduction band edge calculated from them. The areas directly under the electrodes are marked green. The electrode-driven strain fluctuations can be seen to be roughly two times greater for the sample with stronger initial stress in TiN.

### Conclusions and outlook

- For the Si quantum well, the calculated strain variation  $\Delta a/a$  due to TiN electrodes of several  $10^{-4}$  is confirmed by XRD measurements.
- Open question: what is the strain landscape at cryogenic quantum operation temperature?
- Conduction band calculations are expected to be within several meV (comparable to quantum dot charging energy).
- Agreement with variation expected from Park *et al.* (1.4 meV per  $10^{-4}$ ) [6].
- After benchmarking, our model can be utilized for strain engineering tailored towards functional quantum devices (Qubits, QuBus)

### References

- [1] Langrock et al. <https://arxiv.org/abs/2202.11793> 2022  
 [3] Bir, Pikus, & Louvish. Symmetry and strain-induced effects in semiconductors. 1974, New York: Wiley  
 [5] Corley-Wiciak et al., ACS Appl. Mater. Interfaces. 2023, 15(2), 3119–3130

- [2] Seidler et al. Npj Quantum Inf. 2022, 8, 1-7  
 [4] Leake et al. J Synchrotron Radiat. 2019, 26, 571-584  
 [6] J. Park, Y. Ahn, J. A. Tilka and et al, APL Materials, vol. 4, p. 066102, 2016.

