Elevating Quantum Well Precision with APT

Correlation between Si QW compositional details and spin qubit properties

Creating an isolated quantum system in condensed matter and making it reliably controllable increasingly requires quantitative understanding of material properties on the atomistic scale. Decisive device performance parameters such as quantum sensor sensitivities or quantum bit (qubit) fidelities are strongly tied to properties at the nanoscale.

In our recent study [1], atom probe tomography (APT) reveals unique quantitative insights into atomistic scale characteristics of a semiconductor heterostructure formed by an isotopically purified ^{28}Si quantum well (QW) in $Si_{0.7}Ge_{0.3}$ potential barriers (Figure 1) and how these characteristics correlate with the properties of a single spin qubit implemented in this heterostructure [1, 2, 3].

The major insight from APT is its ability to provide a highly detailed and sensitive profile of the Si-Ge/^{28}Si/SiGe quantum well. This profile, shown by the black line in Figure 2, reveals Ge segregation during the epitaxy of the heterostructure. While previous studies have examined long-range segregation at higher substrate temperatures, APT uniquely identifies short-range segregation in this study. This level of detail is not achievable with high-resolution ToF-SIMS due to the limitations imposed by the heterostructure's topology [4]. Additionally, the profile shape to the left of the minimum in Figure 2 is influenced by a post-growth anneal, which widens the composition profile by about two atomic monolayers.

The subtle details of the profile revealed by APT turn out to significantly enhance the valley splitting in the conduction band, an important parameter for spin qubit operation: the higher the valley splitting, the easier the qubit operation. Here, variations in Ge concentration affect the wave function of the spin qubit (shown by the green line in Figure 2), leading a high valley splitting.

Finally, by orienting the APT tip in the plane of the quantum well, we accurately quantified the isotope purification of the 10 nm thick ^{28}Si quantum well, despite the small analysis volume. We achieved a purification level of 50 ppm of ^{29}Si, which minimizes qubit decoherence due to hyperfine interactions of the nucleus and electron spins. This purification level matches the source crystal used for epitaxy and is significantly better than the approximately 800 ppm found in state-of-the-art spin qubit devices.

Enhancing our understanding of critical parameters such as valley splitting and qubit fidelity, APT plays a pivotal role in advancing the field of quantum computing and material science.

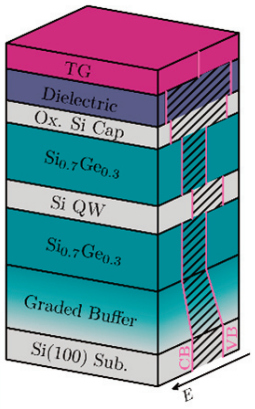


Figure 1:
Schematic of an undoped SiGe/^{28}Si/SiGe quantum well (QW) heterostructure. The band alignment of the conduction (CB) and valence bands (VB) are illustrated across the different layers, with the band gap represented as hatched regions.

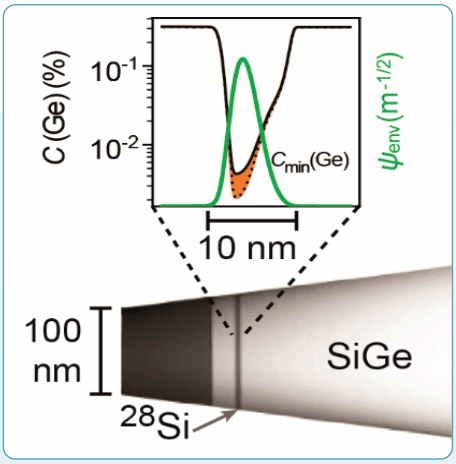


Figure 2:
The lower panel shows a transmission electron micrograph of a needle used for the depth-resolved APT analysis.
The upper panel illustrates the Ge composition profile across the Si-Ge/^{28}Si/SiGe 10 nm QW as determined by APT. The minimum Ge composition $_{cmin}$(Ge) is 0.3%. Dotted line show the extrapolated profile for $_{cmin}$(Ge)=0%. The green line shows the expectation value of the spin qubit wave function.

APT technical details:

The SiGe/Si^{28}/SiGe heterostructure was investigated by APT and compared with the TOF SIMS results. From these comparative studies, we could fit the experimental depth-resolved concentration profiles obtained by APT with an error function model. This could clearly prove that the bottom Si^{28}/SiGe is wider than the top Si-Ge/Si^{28} interface providing further insights in the high-resolution capabilities of APT.

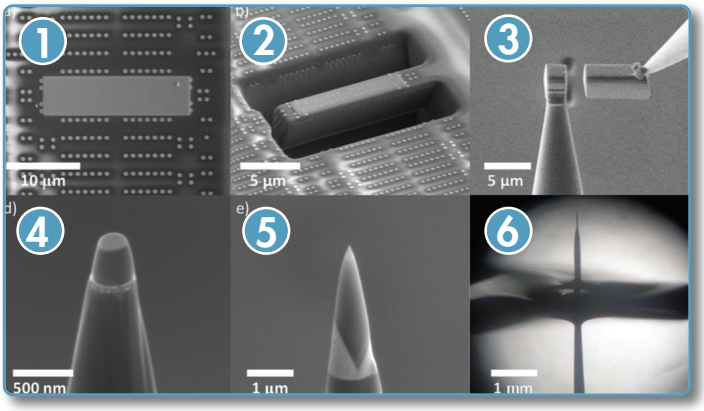
Application note written by Dominique Bougeard (Universität Regensburg, Germany) and Oana Cojocaru-Mirédin (RWTH Aachen University and INATECH, Albert-Ludwigs-Universität Freiburg, Germany).
[1] J. Klos et al. "Atomistic compositional details and their importance for spin qubits in isotope-purified silicon quantum wells", Adv. Sci. 11, 2407442 (2024);
[2] T. Struck et al. "Low-frequency spin qubit energy splitting noise in highly purified ^{28}Si/SiGe", npj Quan-tum Inf. 6, 40 (2020);
[3] A. Hollmann et al. "Large, Tunable Valley Splitting and Single-Spin Relaxation Mechanisms in a Si/Si$_x$Ge$_{1-x}$ Quantum Dot", Phys. Rev. Appl. 13, 034068 (2020);
[4] J. Tröger et al. "Optimizing time-of-flight secondary ion mass spectrometry depth profiles of semiconductor heterostructures", J. Appl. Phys. 137, 025301 (2025).

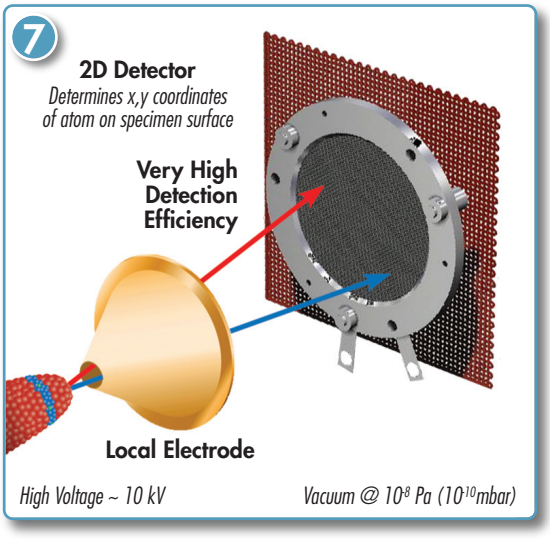
Three Steps to 3D Nanoscale Analysis

An Introduction to Atom Probe Tomography

Step 1: Specimen Preparation

An atom probe specimen usually has a nanoscale region of interest (ROI) requiring both 3D compositional imaging and analysis. The sample is formed into a needle shape containing the ROI. Common APT specimen preparation methods using electropolishing or a Focused Ion Beam system (FIB) are very similar to TEM methods except instead of forming a thin sheet, a needle shaped sample is desired. At the right, standard FIB liftout and mounting of a specimen (figures 1 through 3) and then sharpening the sample with the ROI left at the very apex (4 and 5). In 6, a wire geometry sample is being electropolished.





Step 2: Data Collection

An atom probe produces images by field evaporating atoms from a needle-shaped specimen and projecting the resultant ions onto a detector 7.

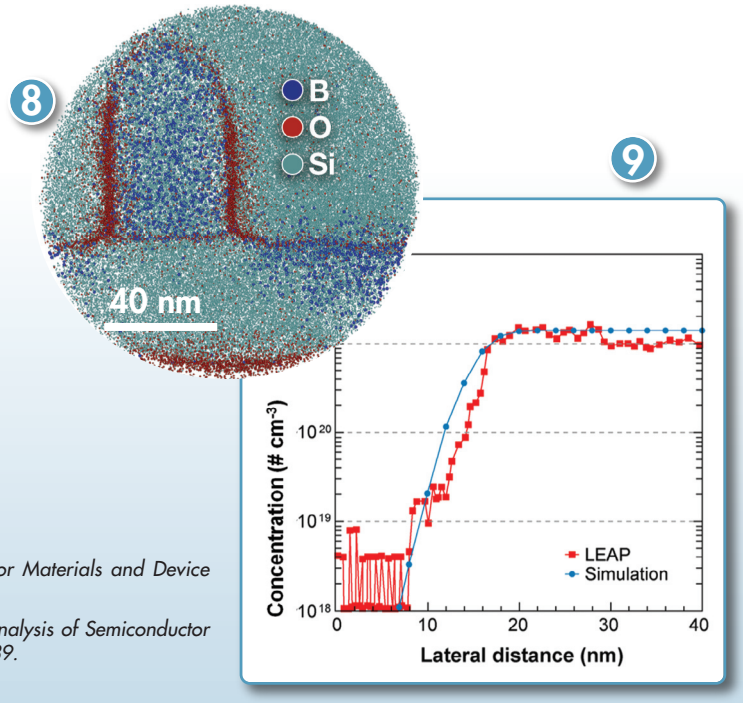
A high magnification results from the ~ 80nm tip being projected onto an 80mm detector resulting in a magnification of approximately 10^6.

An atom probe identifies atoms by their mass-to-charge-state ratio *(m/n)* using time-of-flight mass spectrometry. Charge state, *n*, is typically 1 to 3.

The specimen is held at approximately 50K to reduce surface diffusion during the experiment. The high electric field results in 100% ionization and the high speed detector is capable of measuring up to 80% of the collected ions, independent of ion mass.

Step 3: Data Visualization and Analysis

Examples of data output are illustrated by a slice of a 3D atom map of a transistor† 8, and a dopant composition profile‡ 9. The image shows the positions of individual atoms (oxygen is red and boron is blue) in the transistor with subnanometer resolution. From the reconstructed data set many types of useful analyses are possible. These include 3D visualization, 2D atom mapping 8, 1D depth profiling and line scanning 9, as well as mass spectra and compositional analysis from user-selected volumes.



† *Lauhon, L. J. et al, MRS Bulletin "Atom Probe Tomography of Semiconductor Materials and Device Structures" 34(10) (2009) 738.*

‡ *Moore, J. S.; Jones, K. S.; Kennel, H.; Corcoran, S., Ultramicroscopy "3-D Analysis of Semiconductor Dopant Distributions in a Patterned Structure using LEAP" (2008), 108, 536–539.*

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