Project 1 - Quantum Materials

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1   Selected Paper

This report is based on the following.

> **Xue et al.**, "CMOS-based cryogenic control of silicon quantum circuits, " *Nature*, vol. 593, pp. 205–210, 2021.

2   Part (a) : Quantum Materials – How to make them

1.1 *Describe in your own words the basic principles of the associated crystal growth technique.* **Answer:**

The Si/SiGe heterostructure is grown by Reduced-Pressure Chemical Vapor Deposition (RPCVD) in an industrial Epsilon 2000 reactor.

Basic Principles:
1. Gas-Phase precursor decomposition: The technique uses thermal decomposition of gaseous precursors on a heated subtrate:

- $^{28}SiH_4$ (isotopically enriched silane, 1% in H_2) deposits ^{28}Si
- GeH_4 (germane) deposits Ge
- Natural SiH_4 deposits Si for buffer/barrier layers

At substrate temperature 550-650°C, the precursors decompose as:

$$SiH_4(gas) \rightarrow Si(solid) + 2H_2(gas)$$
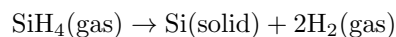
2. Reduced-Pressure operation: The reactor operates at 10-100 Torr (reduced from atmospheric 760 Torr), providing:

- Better uniformity across 100 mm wafers
- Surface-limited reactions (precursors reach substrate before reacting in gas phase)
- Reduced particulate contamination

3. Epitaxial single-crystal growth: Deposited Si/Ge atoms diffuse on the heated surface and incorporate into the crystal lattice, maintaining the single-crystal structure on the substrate. This is critical - the grown layers are not polycrystalline but continue the substrate's crystal orientation.

4. Composition Control: The Ge fraction in $Si_{1-x}Ge_x$ alloys is controlled by adjusting gas flow rates:

$$x = \frac{GeH_4 \text{ flow}}{SiH_4 \text{ flow} + Geh_4 \text{ flow}}$$

By varying flows during growth, composition grading is achieved.

5. Heterostructure Layer Sequence The paper's structure (Extended Data Fig.7a) consists of:

Layer	Composition	Thickness	Purpose
Substrate	n-Si(001)	500 μm	Starting wafer
Graded buffer	$Si_{1-x}Ge_x$ (x: 0 $\rightarrow$ 0.3)	900 nm	Gradual strain relaxation
Relaxed buffer	$Si_{0.7}Ge_{0.3}$	300 nm	Template layer
Quantum well	^{28}Si	**8 nm**	**Electron confinement**
Barrier	$Si_{0.7}Ge_{0.3}$	30 nm	Top confinement
Cap	Si	1 nm	Surface protection

6. Strain Engineering

Si has a smaller lattice constant (5.431 Å) than $Si_{0.7}Ge_{0.3}$ (5.50 Å). When the 8 nm Si quantum well grows on relaxed $Si_{0.7}Ge_{0.3}$, it adopts the substrate's in-plane lattice constant, creating **biaxial tensile strain** in the Si layer.

This strain:

- Modifies the Si band structure
- Reduces electron effective mass
- Enhances mobility (paper reports $> 10^5$ cm^{2}V^{-1}s^{-1} at 55 mK)

7. Isotopic Enrichment for Quantum Coherence

Natural Si contains 4.67% ^{29}Si (nuclear spin $I = \frac{1}{2}$), which causes hyperfine-induced decoherence. The ^{28}SiH$_4$ precursor (obtained by reducing ^{28}SiF$_4$) has only 0.08% residual ^{29}Si (60× reduction, verified by SIMS in Extended Data Fig. 7b).

This creates a **nuclear-spin-free environment**, enabling:

- Long coherence times: $T_2^{\text{CPMG}} > 100$ μs (Extended Data Fig. 5c)
- High gate fidelities: 99.69% (Fig. 3e)

8. Growth Rate and Control

Typical growth rates are 0.1–1 nm/min, providing **atomic-scale thickness control** (±0.5 nm), essential for precise quantum well confinement energies.

1.2 *Name the characterisation technique used for assessing the chemical composition in Si/SiGe heterostructures and describe its basic working principles.* **Answer: Technique: Secondary Ion**

MASS Spectometry (SIMS) The paper uses SIMS to characterize the heterostructure, as shown

in **Extended Data Figure 7b**, which displays depth profiles of ^{28}Si, ^{29}Si, ^{30}Si, Ge, C and 0 concentrations.

Basic working principles:
1. Primary ion bombardment A focused beam of Cs$^+$ ions (energy: 0.5–20 keV, current: 10–100 nA) bombards the sample surface. These energetic ions transfer momentum to surface atoms through collision cascades.

2. Sputtering Process The collision cascades cause surface atoms to be ejected from the sample:

- Sputtering yield: typically 1–10 atoms per incident ion
- Sputtering rate: 0.1–1 nm/s - controllable
- About 0.1–1% of sputtered atoms are ionized as they leave the surface

3. Mass Spectrometry The ionized secondary particles are extracted into a mass spectrometer, which separates them by their mass to charge ratio (m/z) using:

- Magnetic sector analyzer (high resolution)
- Quadrupole filter (fast switching)
- Time of flight (simultaneous full spectrum)

Each element and isotope has a unique (m/z), enabling precise identification.

4. Depth Profiling As sputtering continues, deeper layers are exposed and analyzed. The ion intensity is recorded vs. sputtering time:

- After analysis, crater depth is measured by profilometry
- Time depth conversion provides composition vs depth
- Depth resolution: 2–5 nm for Si-based materials

5. Quantification Raw ion intensities are converted to concentrations using:

- Relative Sensitivity Factors (RSF) from calibrated standards
- Accounts for matrix effects (ionization probability depends on chemical environment)

From **Extended Data Fig. 7b**, SIMS reveals:

1. Isotopic Purity (Critical for Qubit Coherence):

- ^{29}Si concentration: **0.08%** in ^{28}Si quantum well vs. 3.29% in natural Si$_{0.7}$Ge$_{0.3}$ layers
- This **60×** **reduction** in nuclear spins minimizes hyperfine decoherence
- Directly enables $T_2^{\mathrm{CPMG}} > 100$ μs

2. Ge Concentration Profile:

- Shows Ge-free region (8 nm) corresponding to ^{28}Si quantum well

- Constant $\sim 30\%$ Ge in $Si_{0.7}Ge_{0.3}$ barrier/buffer layers
- Verifies composition control during growth

3. Contamination Levels:

- **Carbon:** $< 3 \times 10^{16}$ cm^{-3} (below detection limit)
- **Oxygen:** $< 1 \times 10^{17}$ cm^{-3} (below detection limit)
- Low contamination reduces charge noise sources

1.3 *Name one key feature that SIMS and APT share..* **Answer:** Both SIMS and APT are destructive,

depth-resolved techniques that provide three dimensional composition information with isotopic sensitivity by sequentially removing and analyzing the sample layer by layer.

Shared features:

1. Destructive Layer by layer analysis

- SIMS: Sputters material with ion beam, progressively eroding deeper layers
- APT: Field-evaporates atoms from a needle-shaped specimen tip, atom by atom
- Result: Both techniques consume the sample during analysis
- Consequence: Cannot be used for non-destructive quality control
- Advantage: Enables true 3D compositional mapping

2. Isotopic Sensitivity

- SIMS: Mass spectrometer distinguishes ^{28}Si, ^{29}Si, ^{30}Si
- APT: Time-of-flight mass spectrometry distinguishes isotopes
- Application: Both can verify isotopic enrichment in ^{28}Si quantum wells
- Importance: Essential for characterizing nuclear-spin-free materials for long qubit coherence

1.4 *Which of TEM, SIMS, and APT may be used to provide chemical information of the material stack?* **Answer:** All three techniques (TEM, SIMS and APT) can provide chemical information

about the Si/SiGe heterostructure stack, but they have complementary strengths and are used for different purposes.

1. SIMS (Secondary Ion Mass Spectrometry) - primary choice for chemical composition, because it provides:

- Quantitative elemental concentrations vs depth through entire stack
- Isotopic composition(^{28}Si, ^{29}Si, ^{30}Si) - important for quantum materials

- Ge concentration profile - verifies Si_xGe_{1-x} composition in each layer
- Trace contaminant detection - C, O, H at ppb levels

It is used in the paper for the same reasons as in 1.2.
Advantages for Quantum Heterostructures:

- Large sampling area
- Fast analysis suitable for process optimization
- Direct isotope measurement to verify nuclear-spin-free environment
- High sensitivity detects charge noise sources (O, C)

Limitations:

- Moderate depth resolution (2-5 nm)
- Destructive
- Poor lateral resolution
- Requires calibration standards

2. APT (Atom Probe Tomography) Research tool for atomic scale compositional mapping, not routine quality control

- 3D atomic-scale reconstruction
- Sub-nanometer spatial resolution (0.3 nm in 3D)
- Single-atom detection
- Quantitative - directly counts atoms
- Isotope sensitive - can map ^{28}Si vs. ^{29}Si distribution in 3D

It is not used in the paper, because sample preparation is very difficult and it is expensive and slow
Advantages:

- Unmatched 3D spatial resolution
- True atomic-scale imaging
- Quantitative for all elements

Limitations:

- Very small field of view
- Complex sample preparation
- Destructive
- Not suitable for routine characterization

3. TEM (Transmission Electron Microscopy) Combines structural and chemical information Advantages:

- Correlates structure with chemistry

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- High spatial resolution (0.1–1 nm)
- Non-destructive imaging (though sample prep is destructive)
- Visualizes defects and interfaces directly

Limitations:

- Cannot distinguish isotopes (^{28}Si vs. ^{29}Si) - all Si looks identical
- This is critical for quantum materials characterization
- Only SIMS or APT can verify isotopic enrichment
- Cannot detect ppb-level C, O contamination like SIMS

Conclusion:

All three techniques provide chemical information, but:

SIMS is the primary technique for chemical characterization because:

- Quantifies isotopic enrichment (^{28}Si purity)
- Measures Ge concentration profile
- Detects trace contaminants at ppb levels
- Fast and suitable for process control
- Used in the paper (Extended Data Fig. 7b)

TEM (with EDS/EELS) is complementary because:

- Correlates chemistry with structure
- Verifies layer thicknesses and interfaces
- Detects crystal defects
- Limitation: Cannot distinguish ^{28}Si from ^{29}Si

APT is specialized for:

- Atomic-scale 3D compositional mapping
- Research on interface phenomena and segregation
- Rarely used routinely due to complexity and cost

3 Project 1 (b): Quantum Materials – How to Validate Them in the Lab

2.1 *What cryogenic system would you use to quickly screen the electrical transport properties of charge carriers in a quantum well channel at a temperature of 4.2 Kelvin? What is the basic principle of such system?*

Answer:

To quickly screen the electrical transport properties of charge carriers in a quantum well channel at a temperature of 4.2 K, we would use a liquid-helium dip-stick system. This setup is ideal for fast electrical screening because it provides rapid cooldowns (within minutes) and minimal vibrations, making it perfect for testing electrical transport properties.

By contrast, a variable-temperature insert (VTI) offers a tunable temperature range, which is unnecessary for simple 4.2 K measurements. A closed-cycle cryostat, as discussed in *Article 2*, removes the need for liquid helium but introduces more mechanical vibrations and slower cooldown times, which can disturb sensitive transport measurements. Finally, a dilution refrigerator, described in *Article 3*, is indispensable for measurements at millikelvin (mK) temperatures but is impractical for quick material screening due to its long cooldown time and high cost.

A dip-stick system consists of a probe with electrical feedthroughs, on which the sample is mounted, that is immersed in a liquid-helium (LHe) bath. At atmospheric pressure, liquid helium boils at 4.2 K, providing a stable and vibration-free cryogenic environment. When the probe is inserted, the sample and wiring quickly cool to 4.2 K, enabling immediate low-temperature transport measurements such as the longitudinal resistance (R_{xx}) and the Hall voltage (V_{xy}). From these, the carrier density and mobility of the two-dimensional electron gas (2DEG) can be extracted.

2.2 *What is limiting high-throughput validation of quantum materials at milliKelvin temperatures and what is a possible solution?*

Answer:

Measurements at millikelvin temperatures require a dilution refrigerator (DR), which cools the sample by continuously circulating a mixture of the two stable isotopes of helium: ^{3}He and ^{4}He. At very low temperatures, this mixture separates into two liquid phases, and as ^{3}He atoms cross from the concentrated phase into the dilute phase, they absorb heat from the system, creating a continuous endothermic cooling process.

Although dilution refrigerators are essential for reaching millikelvin temperatures, they are low-throughput systems, as shown in *Articles 2* and *3*. Their main limitations include:

- Very long cooldown and warm-up times (24–48 hours), limiting how many devices can be tested per week.
- Each additional measurement line adds both heat and physical crowding, so only a few dozen devices can be wired simultaneously.
- Replacing or rewiring samples requires warming up the entire system, further increasing downtime.
- High cost, typically €0.5–1 million per system.

Article 1 describes the need to screen devices at 4.2 K before sending only selected samples to mK tests. *Article 2* mentions that wiring and cooling limitations restrict measurement capacity at mK. *Article 3* then introduces an effective solution through the integration of cryogenic multiplexers (cryo-mux) and cryo-CMOS electronics inside the dilution refrigerator.

Cryogenic multiplexers are low-power electronic switches operating at 4 K or 100 mK that allow many quantum devices to share a few measurement lines. The multiplexer locally selects which device is active, meaning that only a small number of control lines enter the fridge. Operating at cryogenic temperatures, these switches dissipate only nanowatts to microwatts, minimizing both heat load and electrical noise. This setup enables parallel or sequential measurements of many devices during a single cooldown.

Cryo-CMOS electronics are specially designed, low-power CMOS circuits that operate at 4 K. They perform local routing, amplification, and control, reducing both cable count and heat.

2.3 *Considering a mobility–density curve, name two metrics that can be extracted to validate the disorder levels in the system. Which metric characterizes disorder at low density and why is it relevant for semiconductor quantum qubits?*

Answer:

A mobility–density curve provides insight into the electronic quality and disorder landscape of a two-dimensional semiconductor system. Two important metrics extracted from such a curve are the **maximum mobility** ($\mu_{\max}$) and the **percolation density** (n_p).

The maximum mobility represents the peak mobility reached at moderate or high carrier densities. It reflects the overall material quality, influenced by factors such as interface roughness, alloy disorder, and background impurity concentration. High values of $\mu_{\max}$ indicate clean epitaxy and smooth interfaces, confirming that the material is suitable for high-performance quantum devices.

The percolation density n_p is the minimum carrier density at which the material begins to conduct electricity. At very low densities, electrons or holes become trapped in small puddles created by disorder, and conduction begins only when these puddles connect. This parameter directly indicates the amount of low-density disorder in the system, such as charge inhomogeneity or interface roughness. A low n_p means that the potential landscape is smooth and carriers remain mobile even at low densities.

This metric is especially important for semiconductor spin qubits, which operate with only a few charge carriers confined by gate voltages. In this regime, disorder determines whether quantum dots can be formed, tuned, and coupled in a stable and repeatable way. A high n_p leads to unstable or unpredictable dots, while a low n_p ensures reliable and uniform qubit performance across a wafer.

As shown in *Lecture 3* and in the three *Articles*, these two parameters together provide a complete picture of the disorder environment and form the essential link between material growth quality, transport properties, and quantum device reliability.

2.4 *Charge is induced in a quantum well channel by applying fixed bias to a top-gate. In a Hall bar geometry with channel length L = 10 um and channel width W = 2 um, a constant source drain is applied. At zero magnetic field, a longitudinal current Ixx=200 nA and a longitudinal voltage*

Vxx = 25 uV are measured. As the magnetic field is increased, a finite transverse voltage drop Vxy builds up across the Hall bar according to the following measurements of [B (Tesla),Vxy (uV)] : [0, 0] [0.1, 25] [0.2, 50] [0.3, 75] [0.4, 100] [0.5, 125]. Assume the current Ixx doesn't change with magnetic field and the electronic charge e = 1.6E-19 C. Calculate charge density (in units of cm-2) and mobility (in units of cm2/Vs) of the two-dimensional channel. **Answer:** At zero magnetic

field, the longitudinal resistance is:

$$R_{xx} = \frac{V_{xx}}{I_{xx}} = \frac{25 \times 10^{-6}}{200 \times 10^{-9}} = 125 \ \Omega.$$

The sheet resistance (per square) is then

$$\rho = R_{xx}\frac{W}{L} = 125 \, \Omega \cdot \frac{2}{10} = 25 \ \Omega,$$

so the sheet conductivity is

$$\sigma = \frac{1}{\rho} = \frac{1}{25} = 0.04 \text{ S}.$$

From the Hall data, the transverse voltage increases linearly with magnetic field:

$$\frac{dV_{xy}}{dB} = \frac{125 \ \mu\text{V}}{0.5 \text{ T}} = 250 \ \mu\text{V/T}.$$

The corresponding Hall resistance slope is

$$\frac{dR_{xy}}{dB} = \frac{1}{I_{xx}}\frac{dV_{xy}}{dB} = \frac{250 \times 10^{-6}}{200 \times 10^{-9}} = 1250 \ \Omega/\text{T}.$$

Using the classical Hall relation

$$\frac{dR_{xy}}{dB} = \frac{1}{ne},$$

the carrier density is

$$n = \frac{1}{e\,\frac{dR_{xy}}{dB}} = \frac{1}{(1.6 \times 10^{-19})(1250)} = 5.0 \times 10^{15} \text{ m}^{-2} = \boxed{5.0 \times 10^{11} \text{ cm}^{-2}.}$$

The mobility is obtained from the relation

$$\mu = \frac{\sigma}{ne} = \frac{0.04}{(5.0 \times 10^{15})(1.6 \times 10^{-19})} = 50 \text{ m}^2/\text{V s} = \boxed{5.0 \times 10^5 \text{ cm}^2/\text{V s}}.$$