Atomic structure description of interface disorder in Si/SiGe thin-film heterostructures

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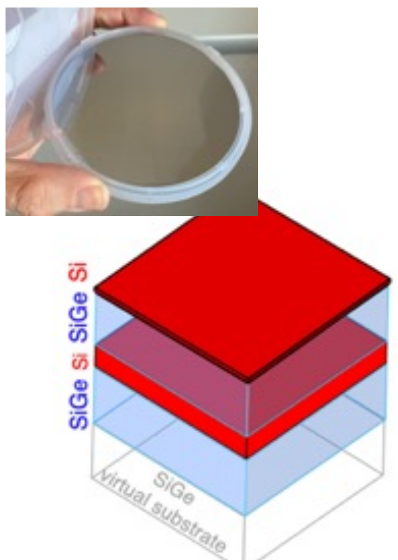
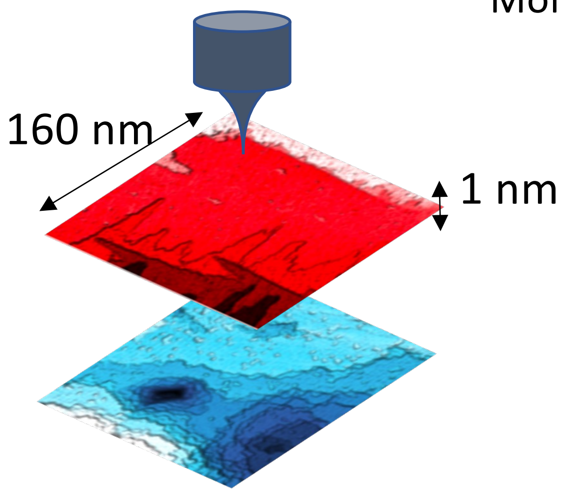
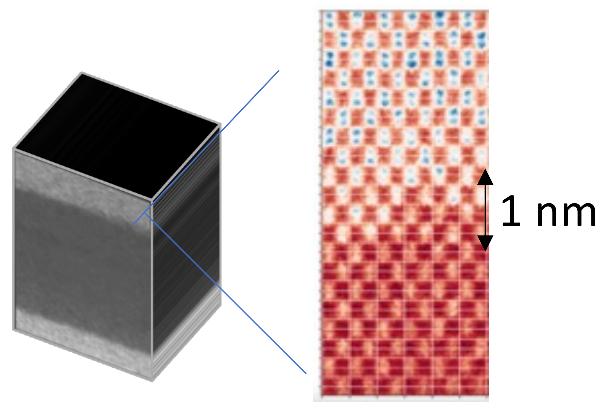
&

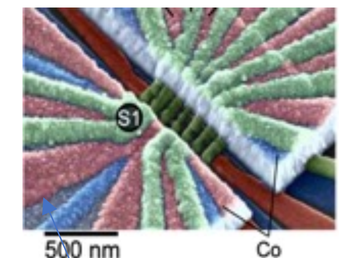
μATOMS Energy Frontier Research Center

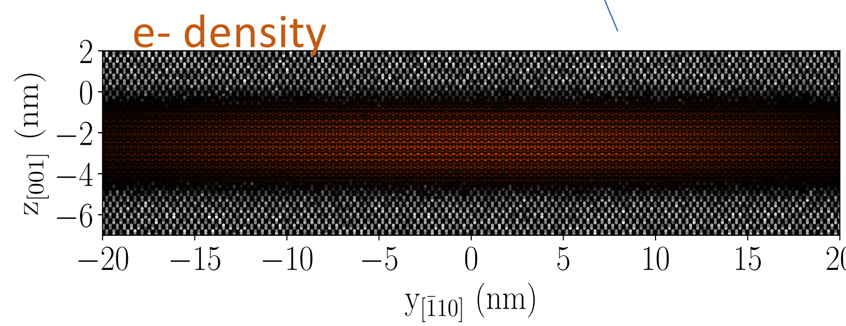
Monday, January 30, 2023









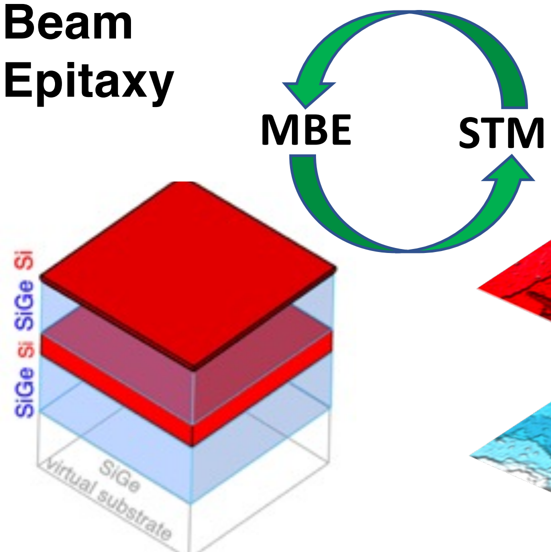


Talk overview

Part 1 Interface structure description

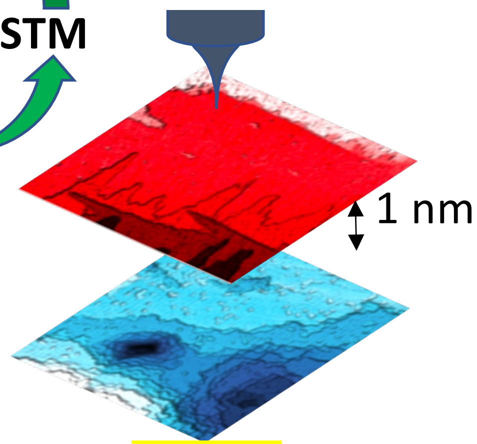
- Interface structure descriptions key to model electronic phenomena – transport scattering, Schottky barriers, all sorts of quantum effects…
- Interface 3D atomic structure notoriously difficult to measure/visualize – need for tools to clearly resolve

Molecular Beam Epitaxy



Strained-Si & $Si_{0.7}Ge_{0.3}$ quantum well MBE

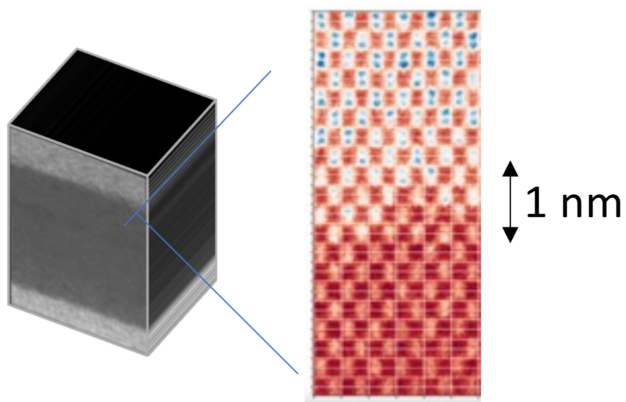
Scanning Tunneling Microscopy



Surface roughness

Cross-sectional high-angle annular dark field Scanning transmission electron microscopy

HAADF cross section



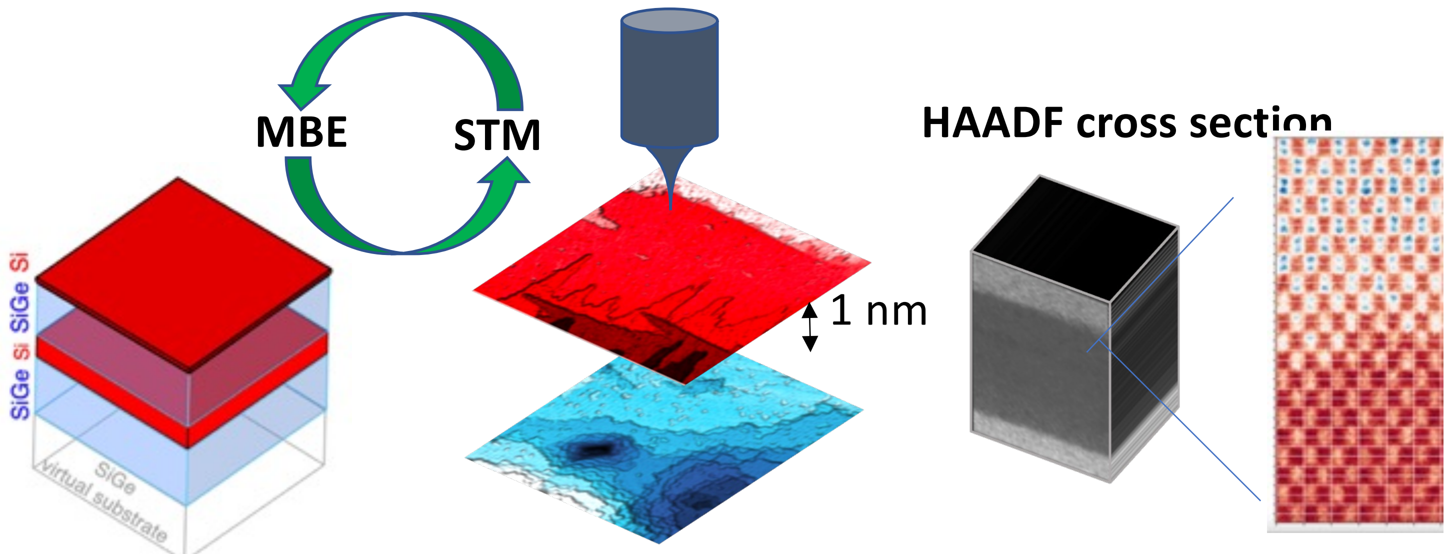
Intermixing

Talk overview

Part 2 model: atomistic multivalley effective mass theory utilizing structure

- Predict structure-properties variability for Si/SiGe quantum dot qubit exemplar
- STM indicates roughness → orbital state level variability over dot ensembles
- HAADF indicates Intermixing → conduction band valley splitting (VS) variability in dot ensembles

Part 1 Interface structure description



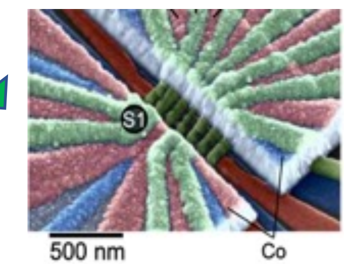
Strained-Si & $Si_{0.7}Ge_{0.3}$ quantum well MBE

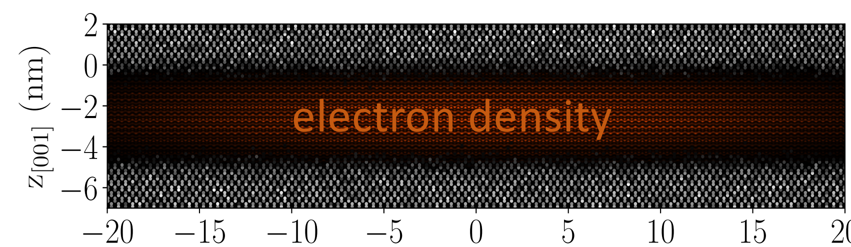
Surface roughness

Intermixing

Structure description

Quantum dot qubit spectra forecasting

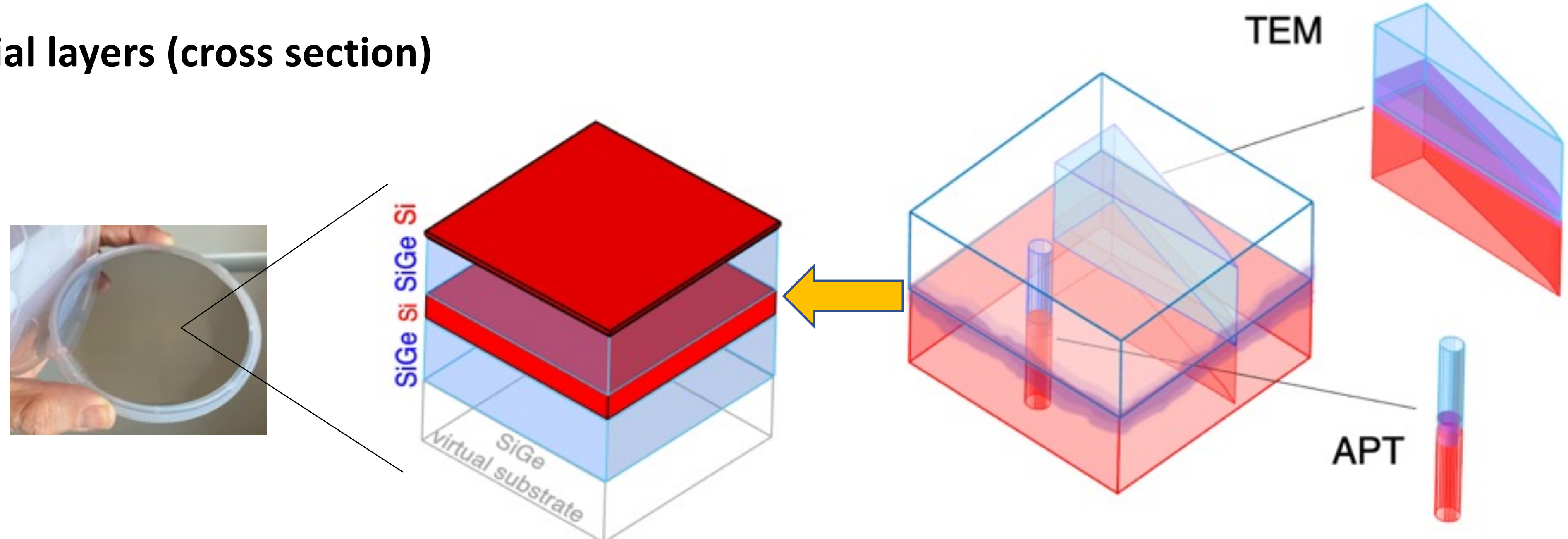




Atomic structure model
Multivalley effective mass theory

Part 1: Interface atomic structure measurement

Wafer + epitaxial layers (cross section)



Dominant atomic-to-nano resolution interface resolving techniques

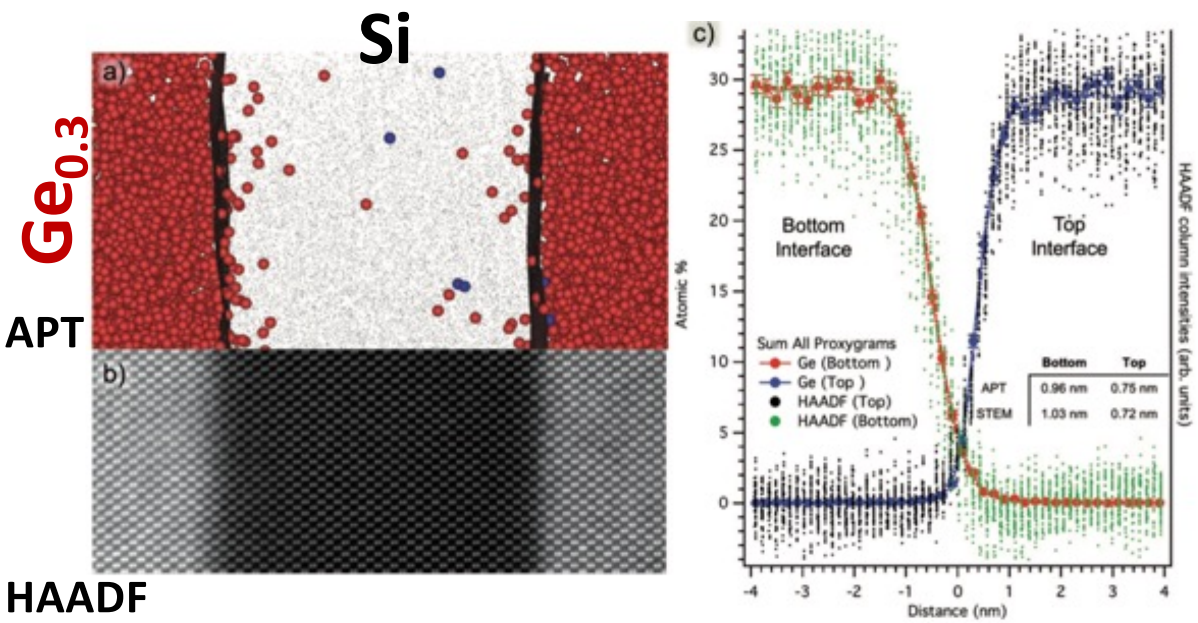
X-rays or neutrons
scattering or absorption
smaller volume (~10 nm)
hard x-ray nanoprobes

Electron microscopy

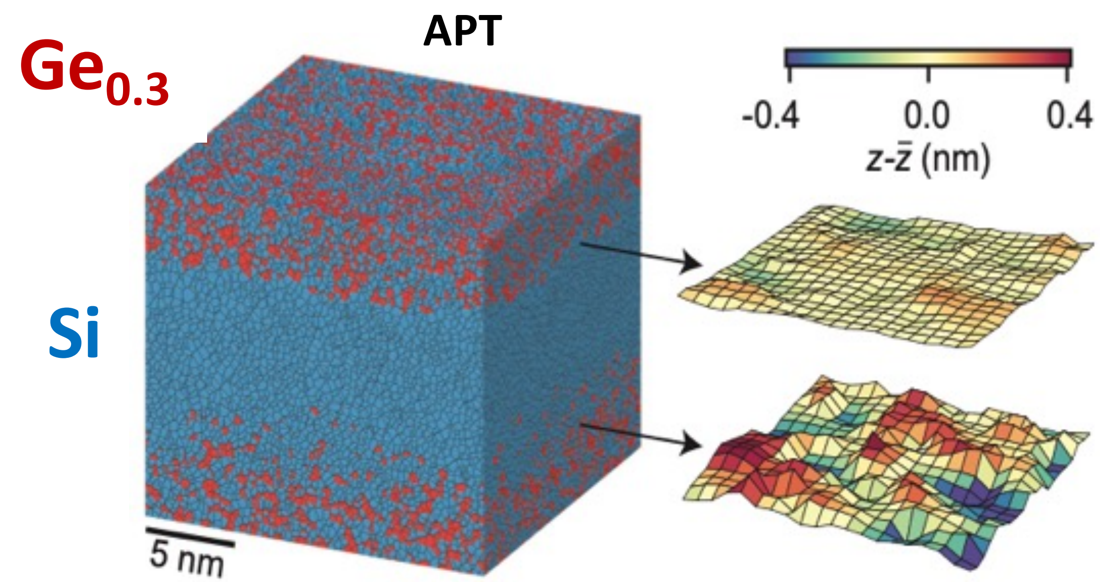
Atom probe Tomography (APT)

3D atomic structure measurement Si/SiGe interface

- Post growth interface data using APT and HAADF STEM
- Si/SiGe for quantum dot app - commercial CVD material



[Dyck, et al. Adv. Mat. Interfaces 4, 1700622 (2017)]



[Wuetz, et al. arXiv:2112.09606 (2021)]

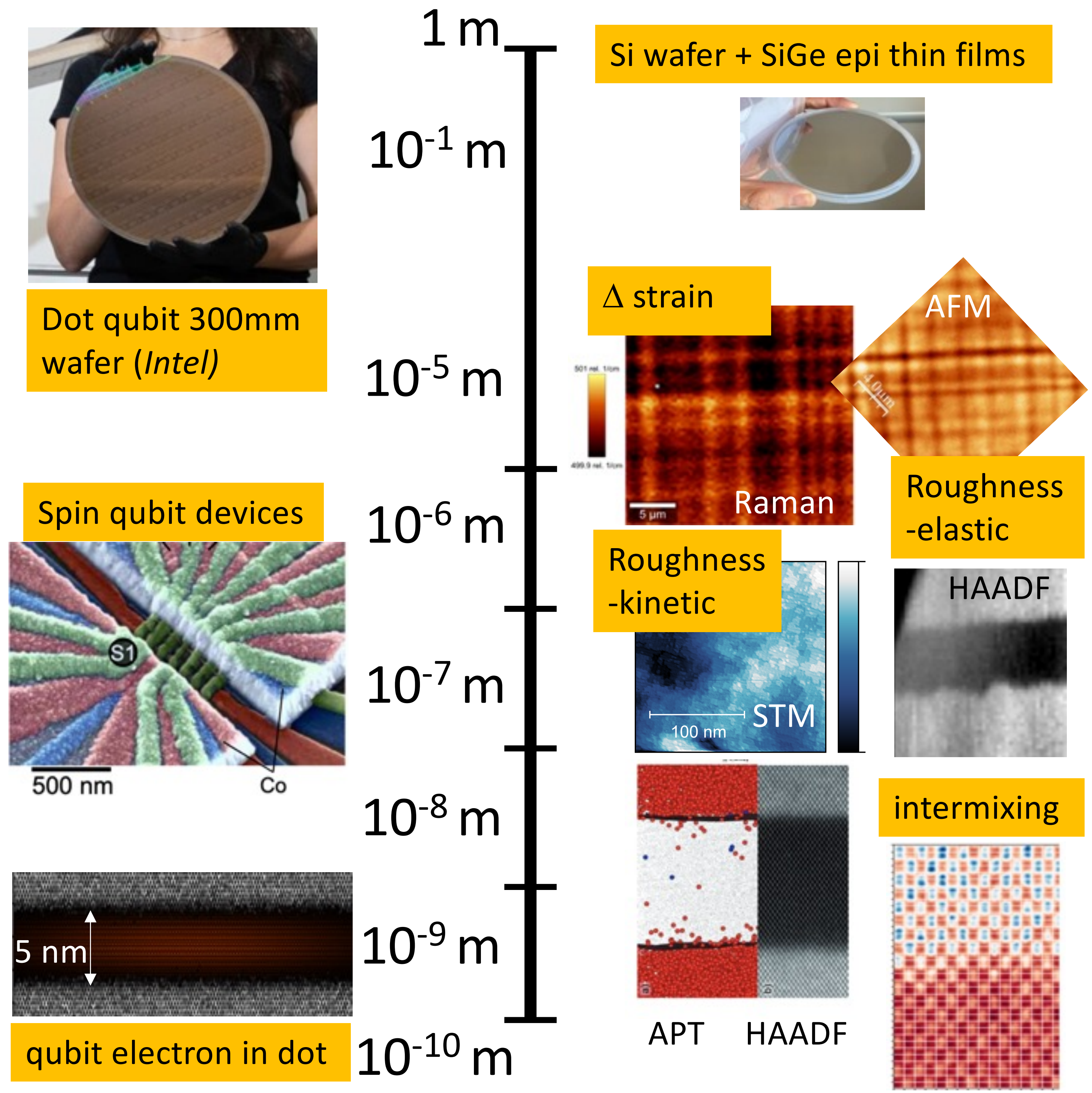
- **Si-Ge intermixing dominates broadened interface ~ sigmoidal, width 0.7-1.0 nm (5-9 layers)**
- **APT and HAADF capture intermixing (miscibility) but we want longer-range structure too**

Challenge of scale and complexity

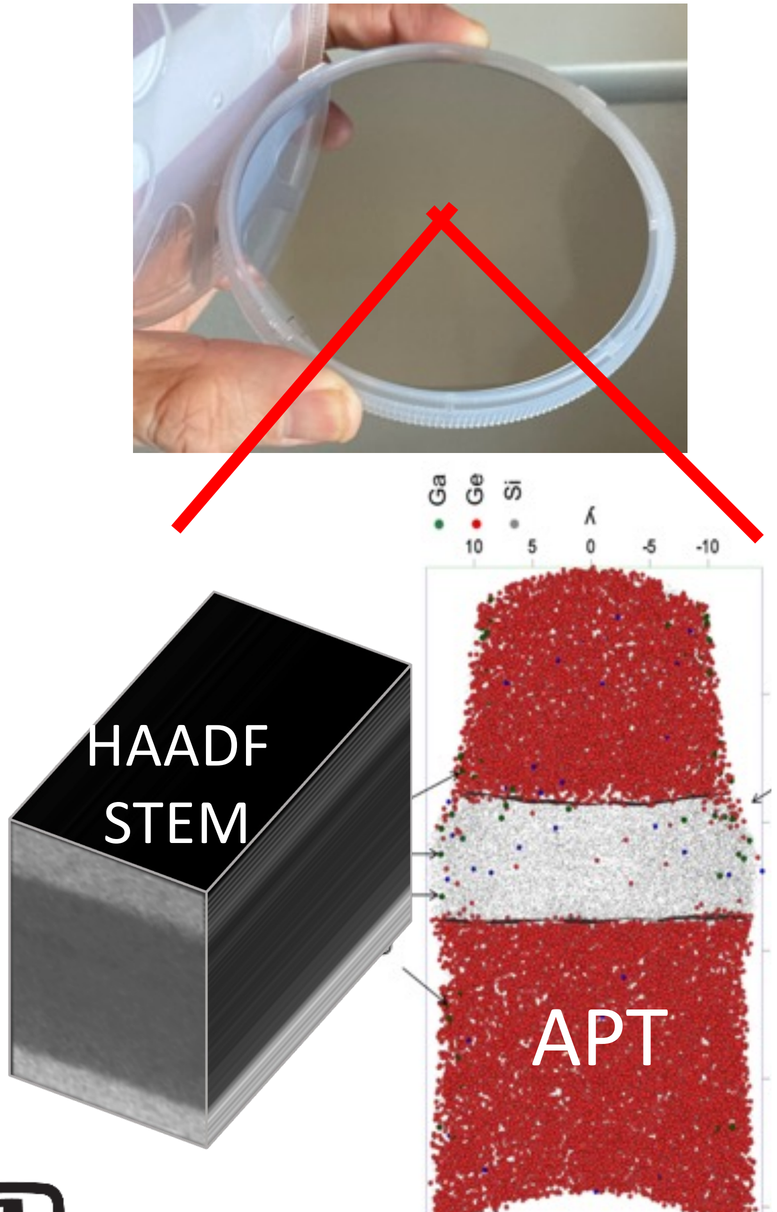
App future goal : make & understand/control many similar qubits covering distances up here

Various sorts of materials complexity & variability over entire scale influence each qubit: Roughness, intermixing (miscibility), Δstrain

Qubits & atomistic materials measurement/description/ models are down here



Analogy relating size of various things



EAG- Dycus

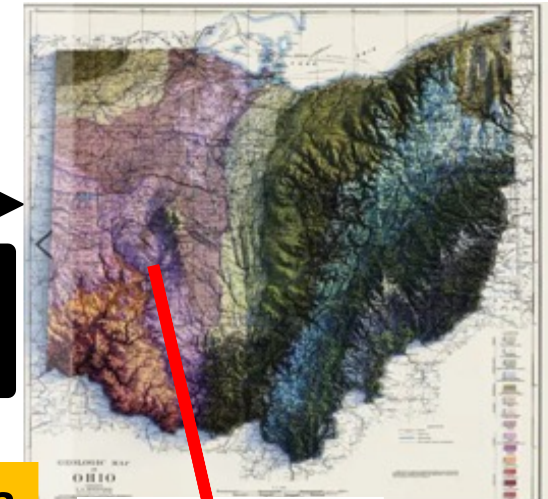
Oak Ridge - Dyck

Epi wafer

10^{-1} m

Ohio

10^{5} m



- **Probe volume limitations → additional data sources would be a good idea**
- **Compare/contrast/combine various 2D/3D data at various scales**

10^{-8} m

10^{-10}m

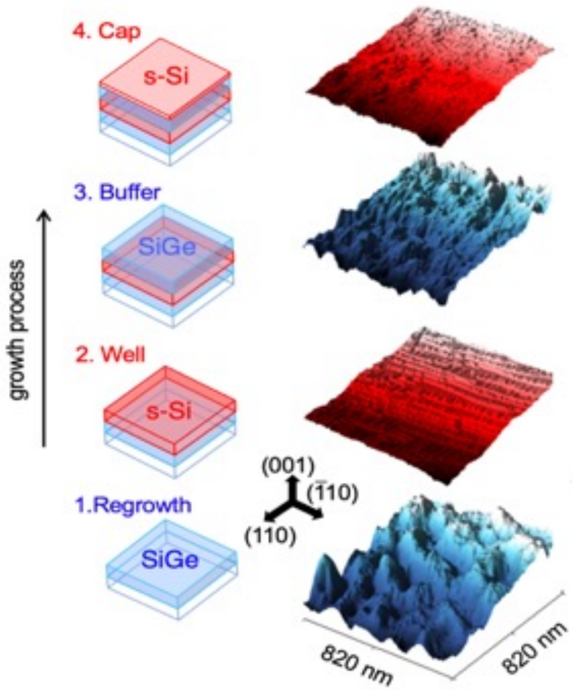
10^{-1} m

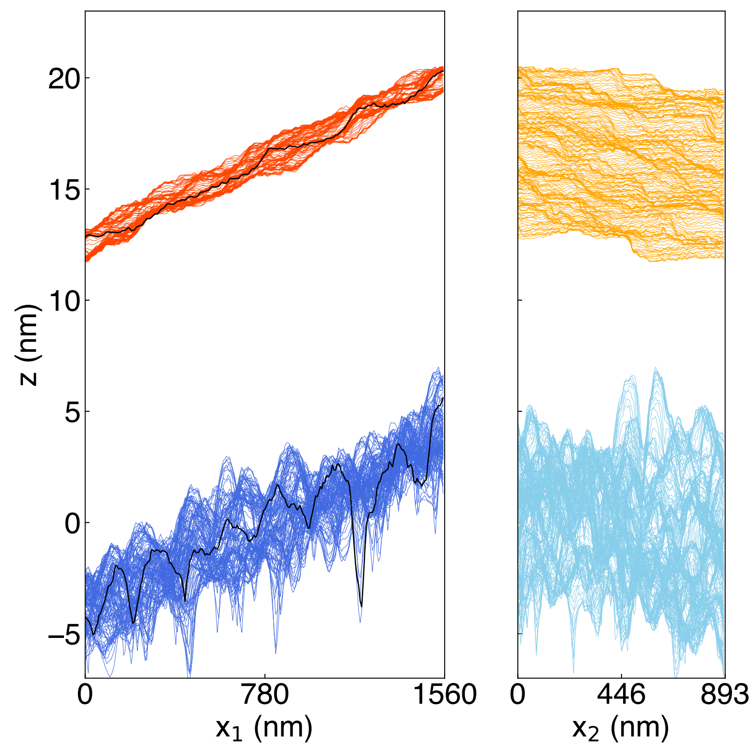
Rock Sample

https://ohiodnr.gov/

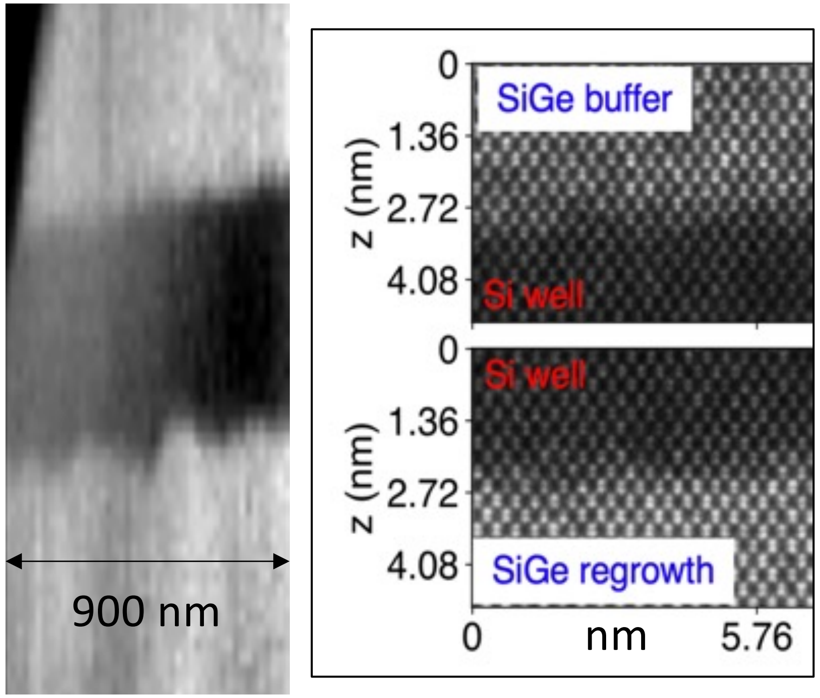
Overview of our approach to interface measurement/description spanning atomic-to-micron

(1) Track growth surface atomic resolution STM → surface roughness





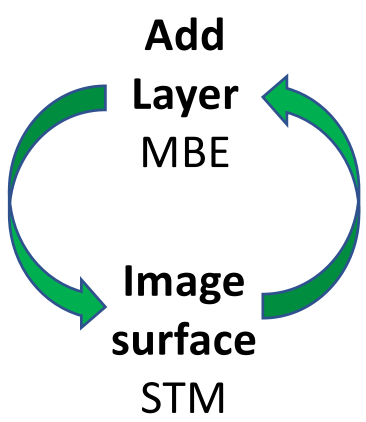
(2) What survives burial? Post growth HAADF STEM → local intermixing



(3) Analysis: compare/contrast STM+HAADF → final structure description

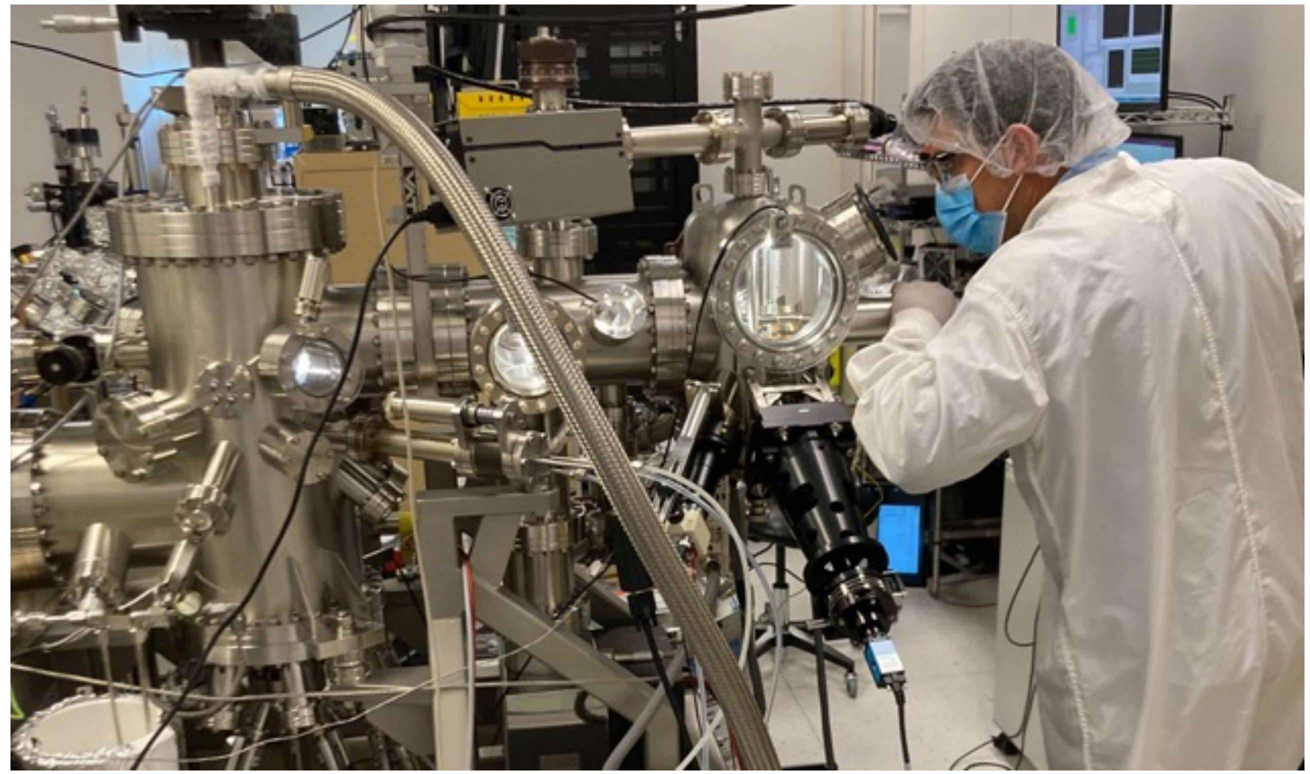
Track growth surface evolution

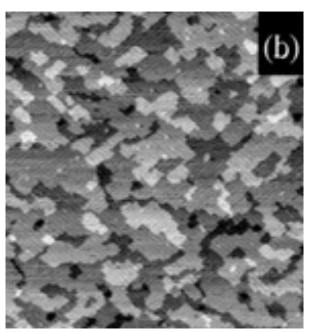
Process:



- Replicate qubit-relevant stack
- Typical conditions (T, thickness,…)

Small MBE **Scanning tunneling microscope (STM)** **postdoc**

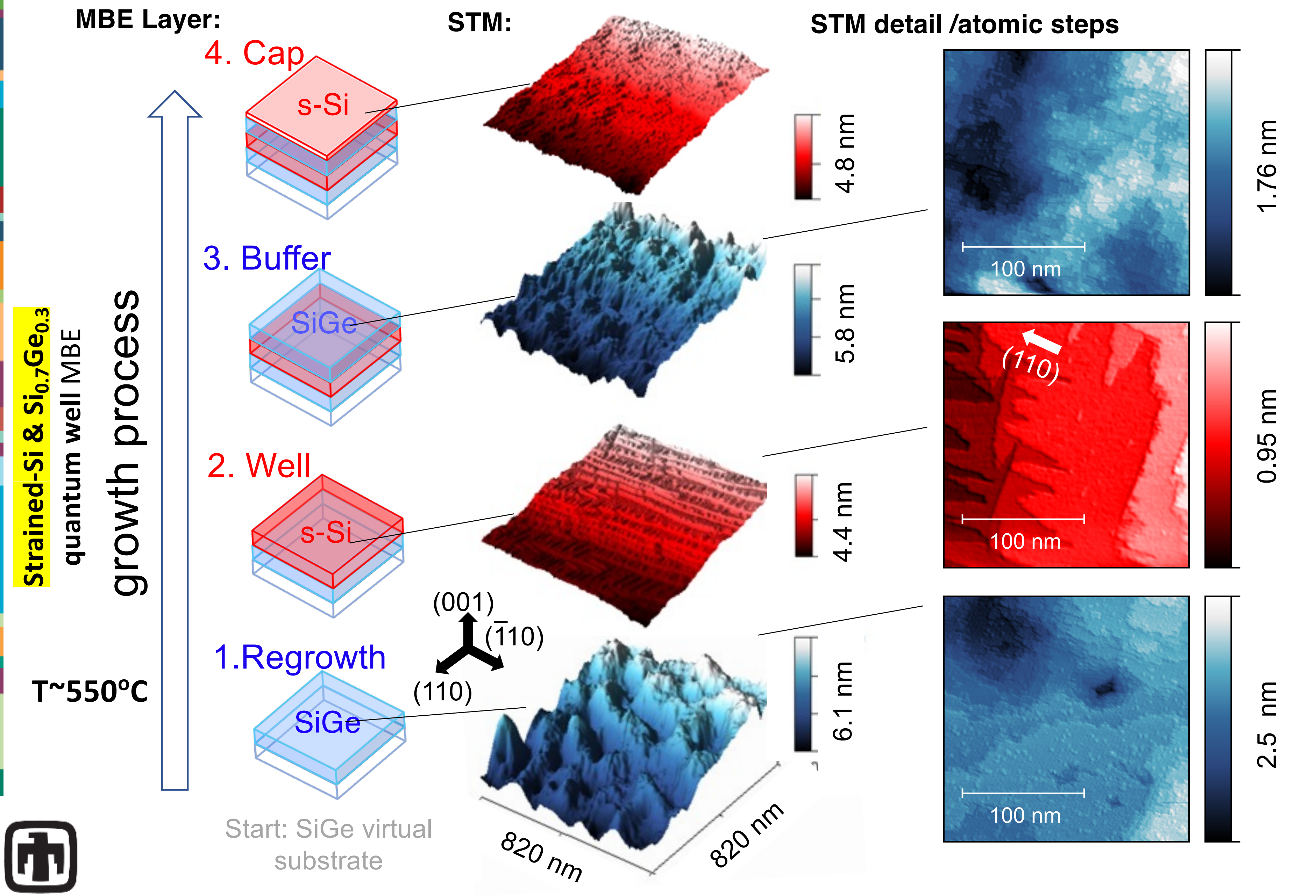




[G. G. Jernigan & P. E. Thompson, Surface Science 516 (2002) 207–215]

*Earlier look SiGe alloy MBE with STM - reveals general trends, considerably different compositions/scales

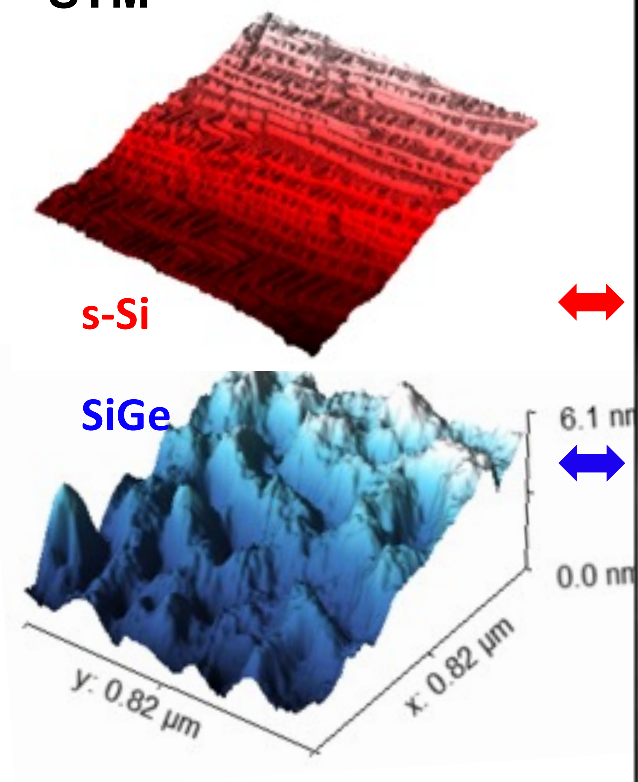
Track growth surface evolution



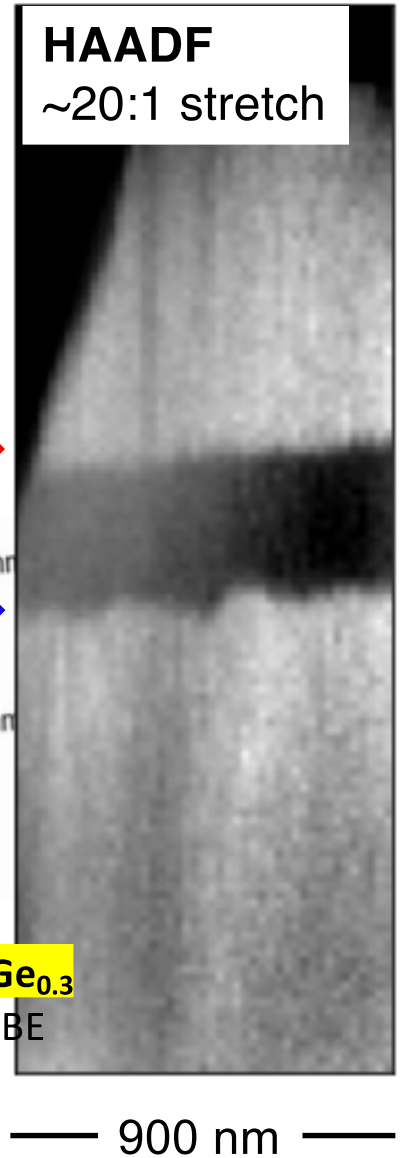
- **Nanosized undulation SiGe surface**
- **Å-sized atomic steps apparent on Si & SiGe**
- **No correlation of features between interfaces**

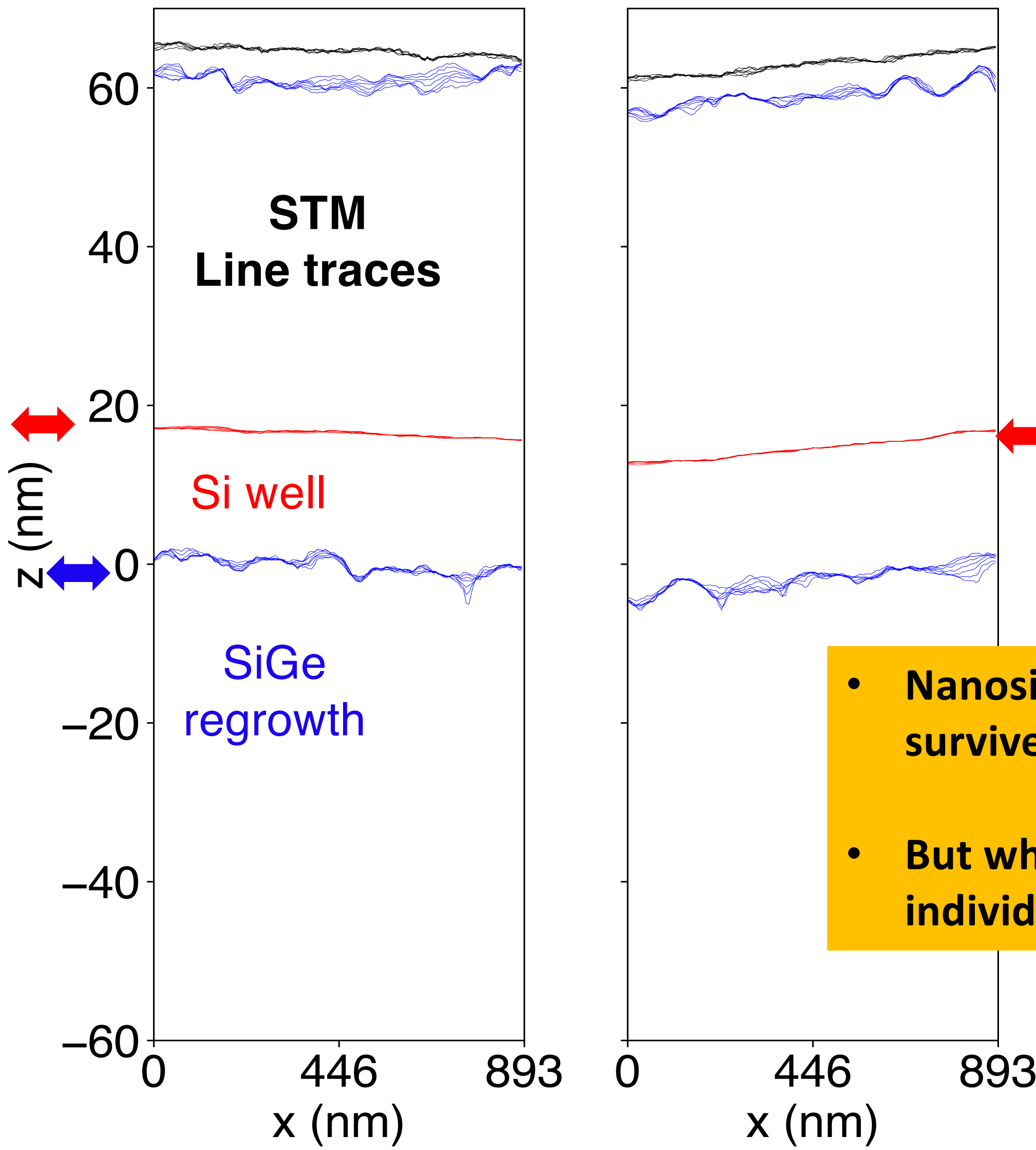
What survives burial?

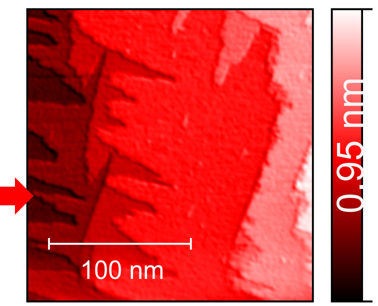
STM



strained-Si & $Si_{0.7}Ge_{0.3}$
quantum well MBE
T=550°C

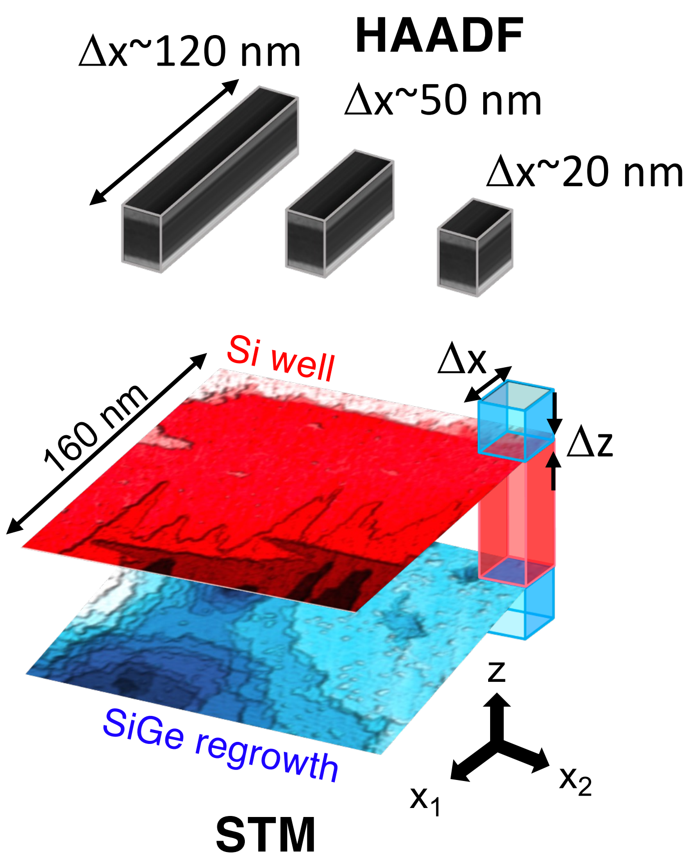


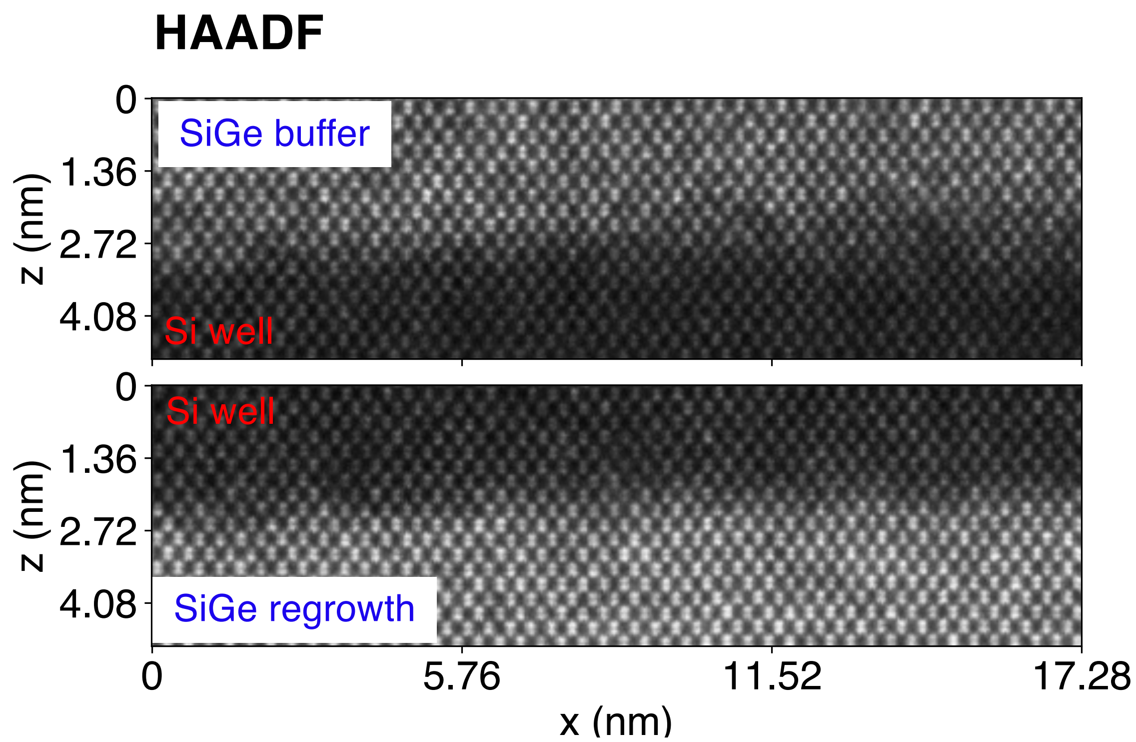




- **Nanosized undulation survives growth**
- **But what about atomic individual atomic steps?**

No atomic steps apparent in interface anywhere, rather intermixing at several-layer (~1 nm) scale:





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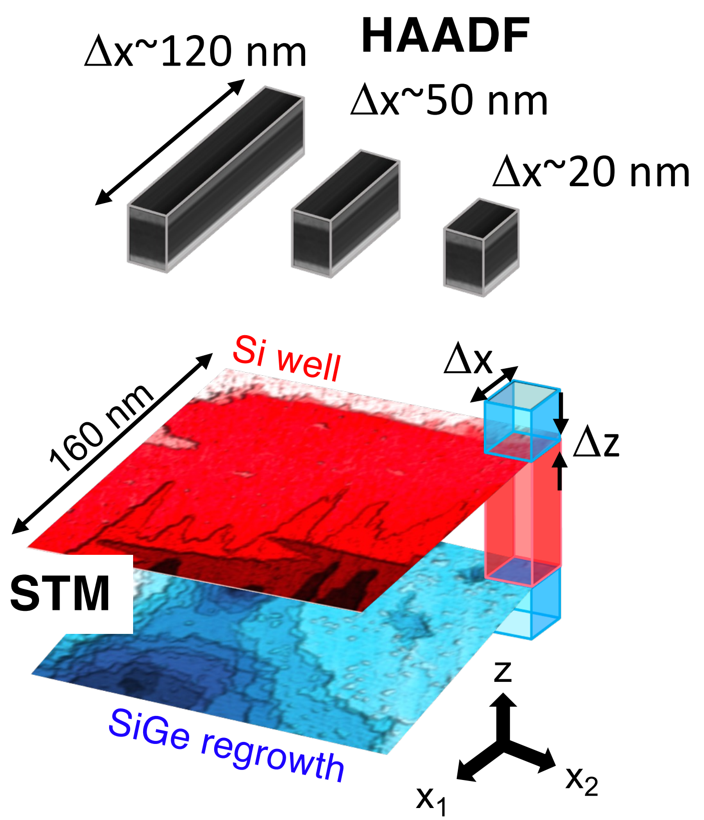
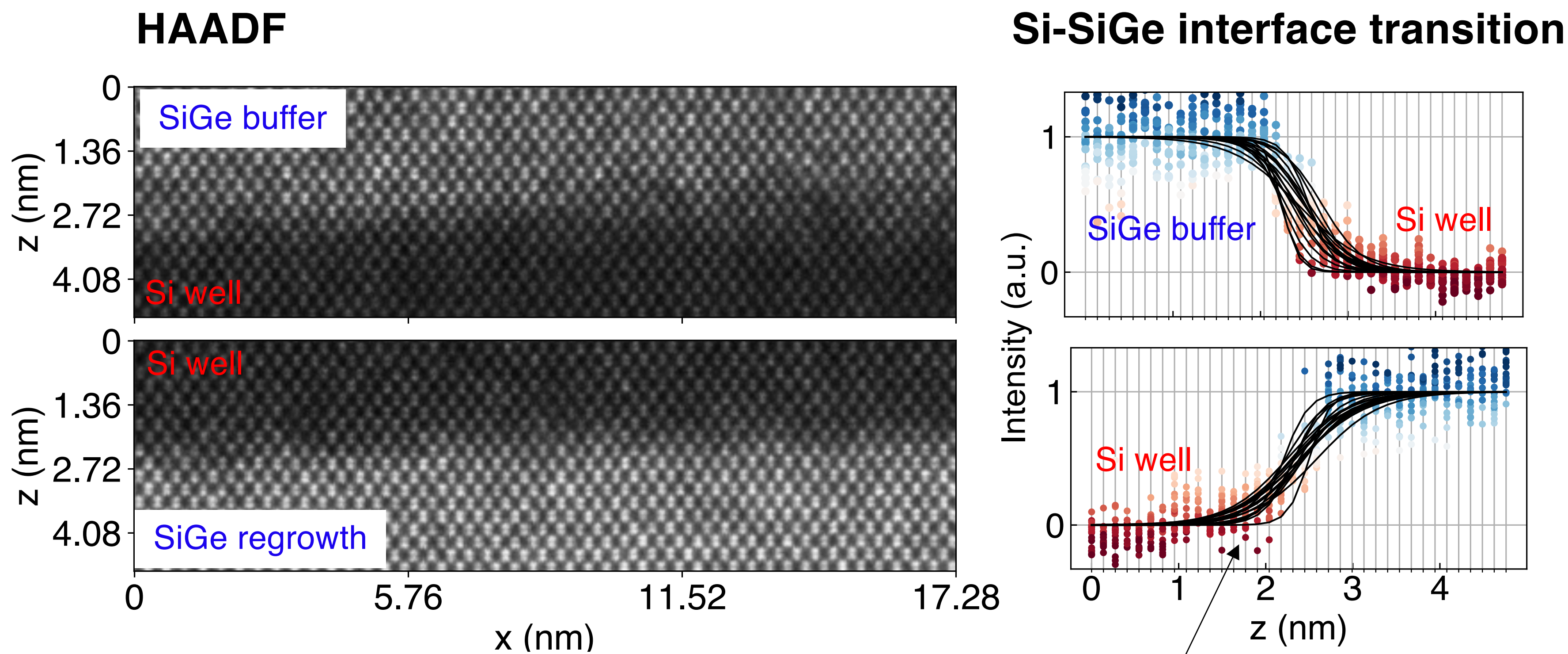
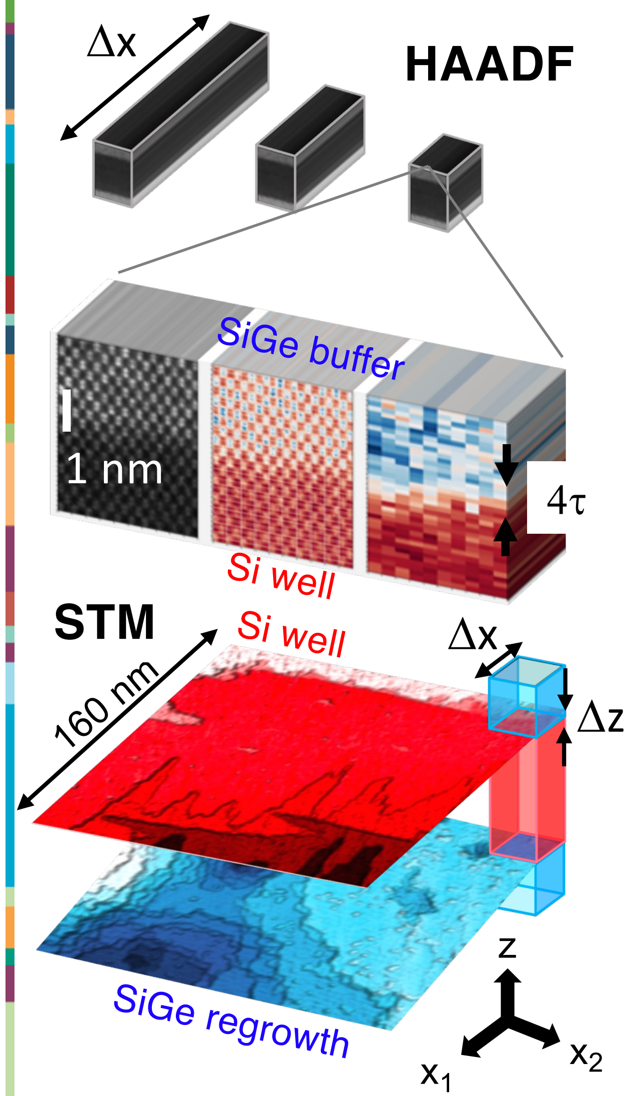




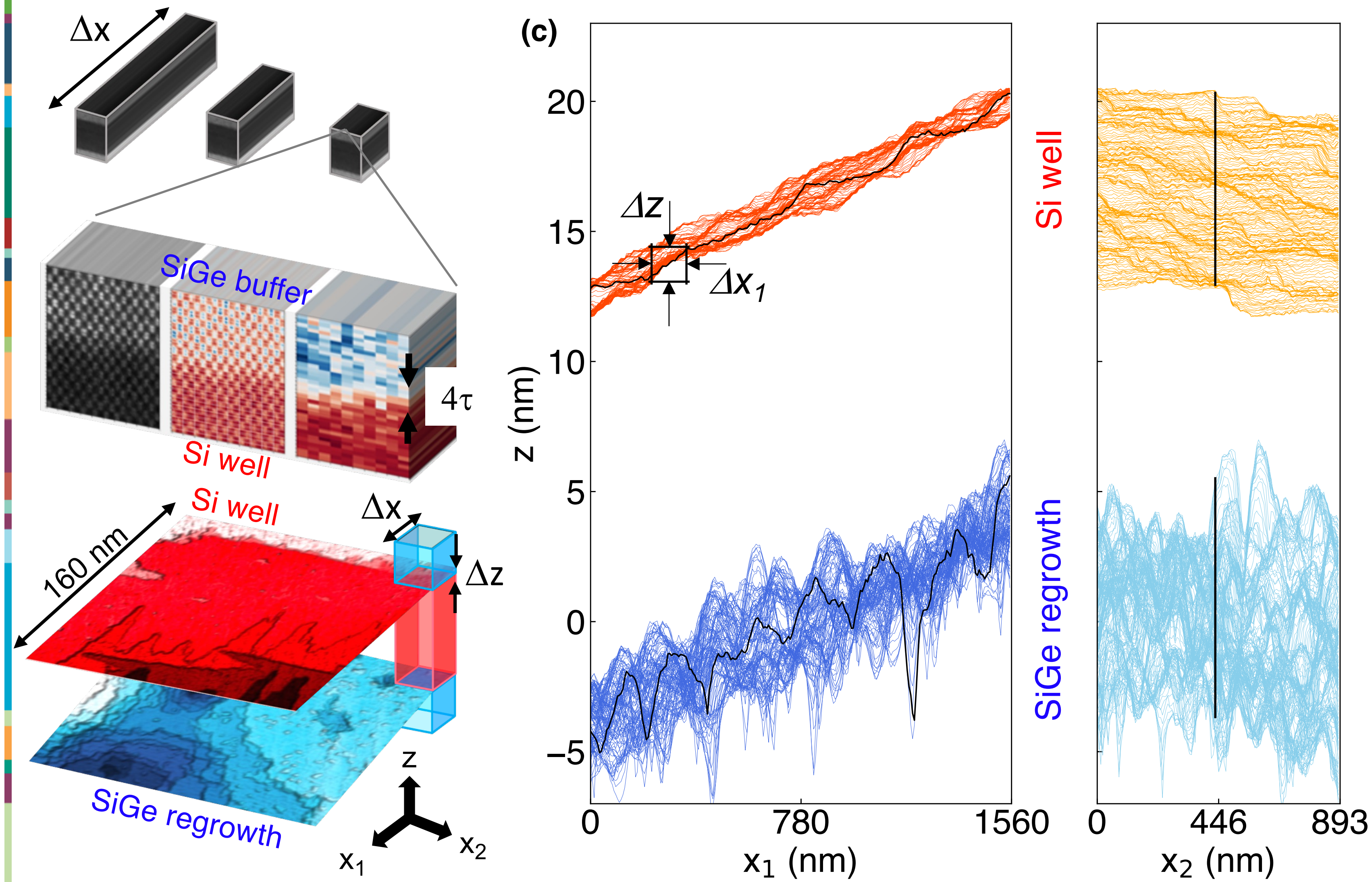
- Sigmoid fits: $I(z,\tau) = [1+\exp((z-z_o)/\tau)]^{-1}$
- 4τ measures 0.12-0.88 distance

- HAADF intensity proportional to element (Si, Ge) composition $I \sim Z^{1.8}$
- Interface width estimate: $\langle 4\tau \rangle = 1.0 \pm 0.4$ nm (all HAADF data)

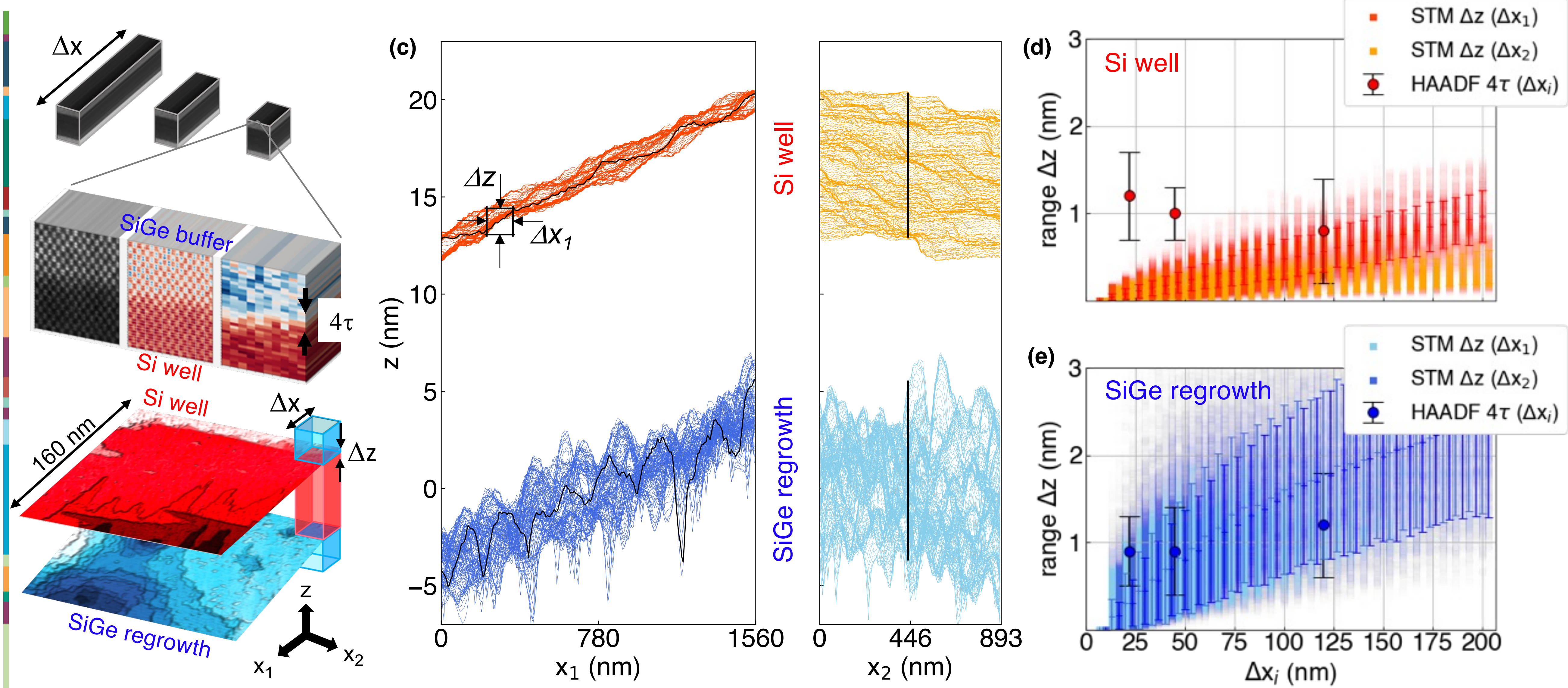
Resolve roughness *vs* intermixing width contribution



Resolve roughness *vs* intermixing width contribution



Resolve roughness *vs* intermixing width contribution



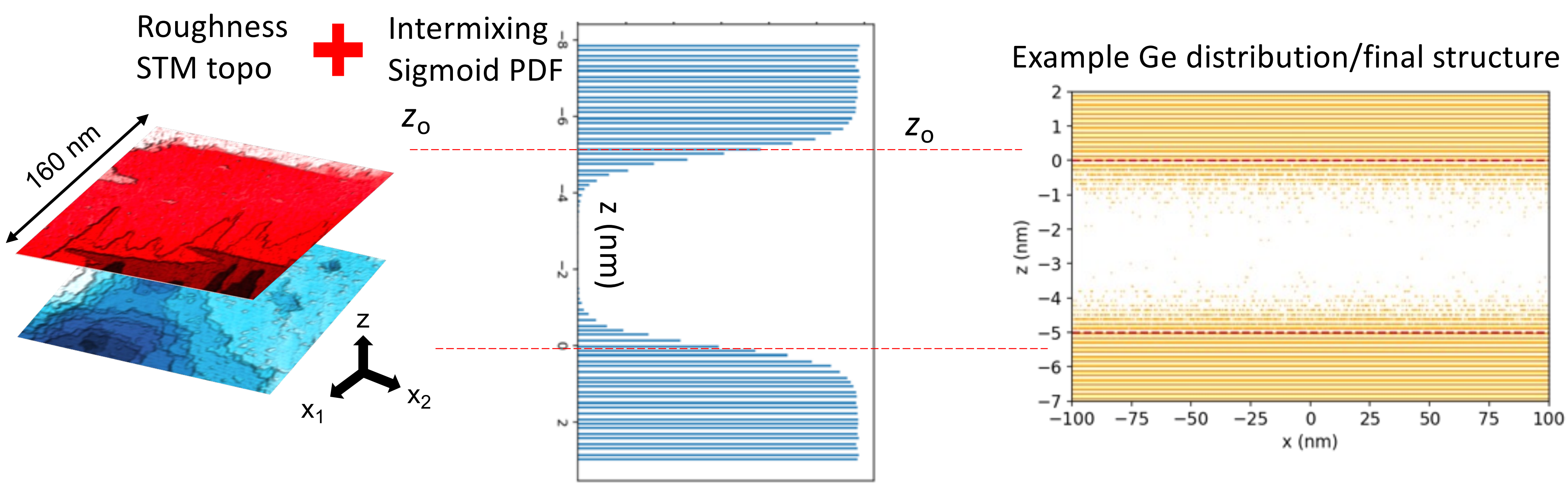
- STM surface roughness does not entirely account for HAADF interface width
- Intermixing is more likely scenario, supported by other recent reports from APT work (Dyck, Wuetz)

Our interface atomic structure model

1. Roughness: Interface mean position = STM height (z_o)
2. Intermixing: Lattice site occupants across transition $Si_{1.0}$ to $Si_{0.7}Ge_{0.3}$ follow sigmoid PDF width τ (4τ from HAADF or APT) along growth axis (z) across interface
3. Sigmoid center location = z_o

Sigmoid intermixing distribution [Dyck, et al. (2017)]:

$$I(z,\tau) \sim 1/[1+\exp((z-z_o)/\tau)]$$



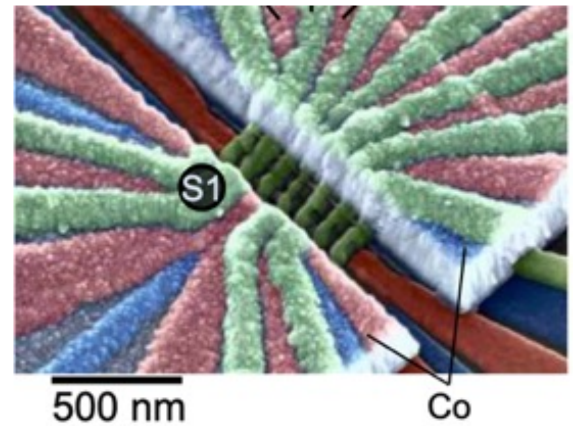
Example Ge fraction histogram

Part 2 : theory/model: predict quantum electronic structure-properties variability

- **App: spectra predictions for Si/SiGe dot e- spin qubits**
  - Good qubits & high-quality logic gates
  - Scalable Si foundry processing, e.g. *Intel*
  - Rapid maturation: steadily increasing number of working & interacting qubits on-die

Two spin qubit device

Petta Group Princeton/UCLA



[Mills et al., Sci. Adv.8, eabn5130 (2022)]

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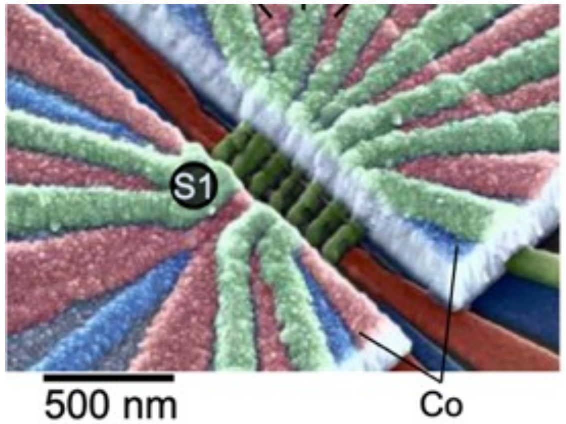


[Mills et al., Sci. Adv.8, eabn5130 (2022)]

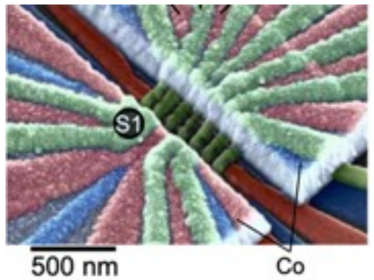
Materials structure-properties interaction is salient hurdle:

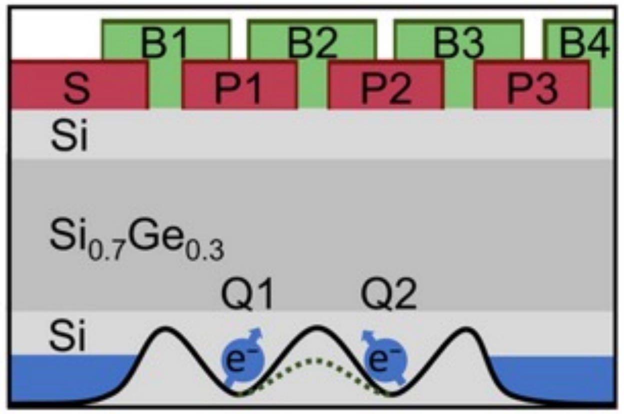
- Complex dot e- interaction with Si-SiGe interfaces causes dot spectral variability

Next, we describe how:

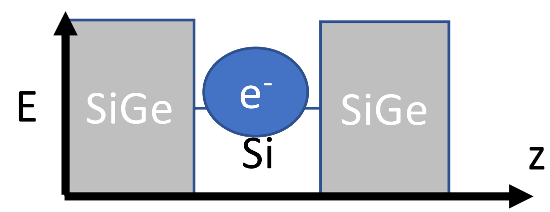
- Roughness → energy bias variability across dot-ensembles
- Intermixing → valley state splitting (VS) variability across ensembles

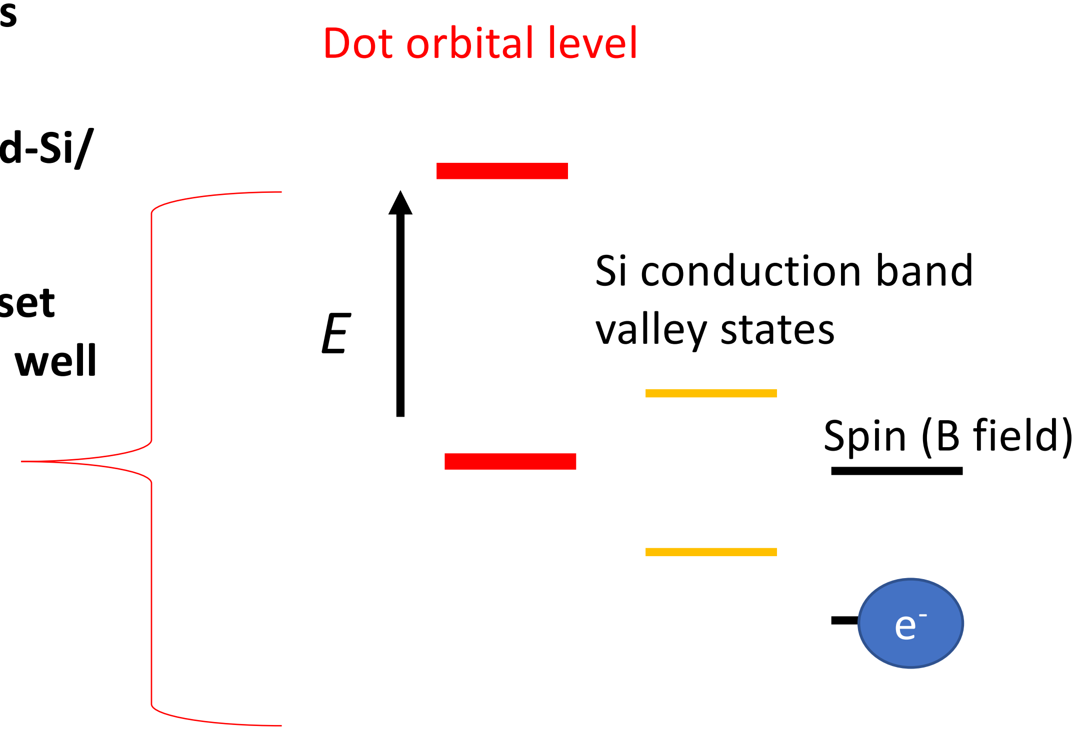
Brief intro to app: Si/SiGe quantum dot e- spin qubit





- **Gate-defined quantum dots in Si well**
- **Metal gate layer on Strained-Si/ $Si_{0.7}Ge_{0.3}$**
- **Si QW conduction band offset (Type II) – gates pull e- in Si well**





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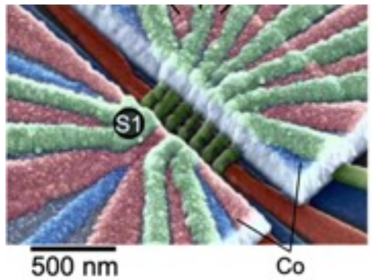

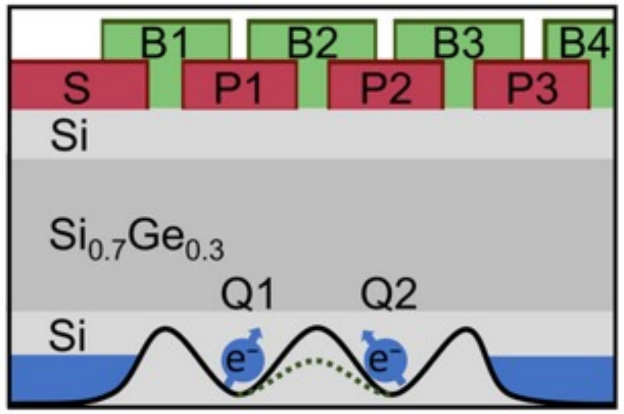

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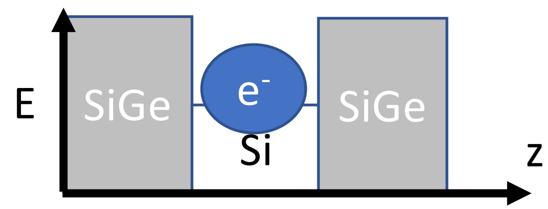
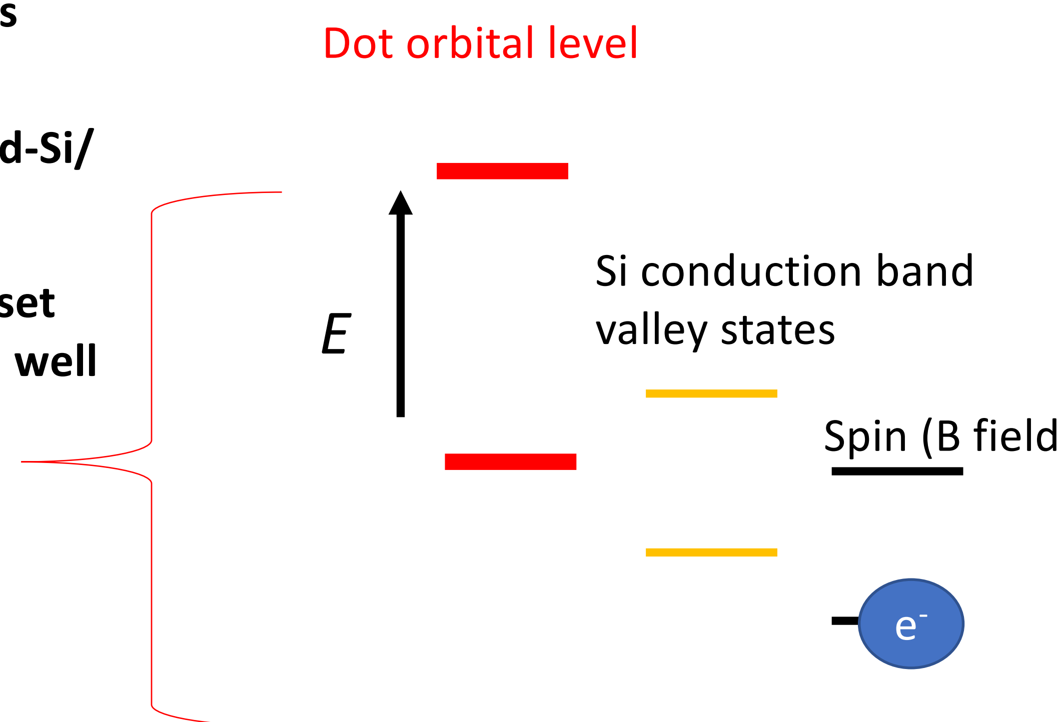
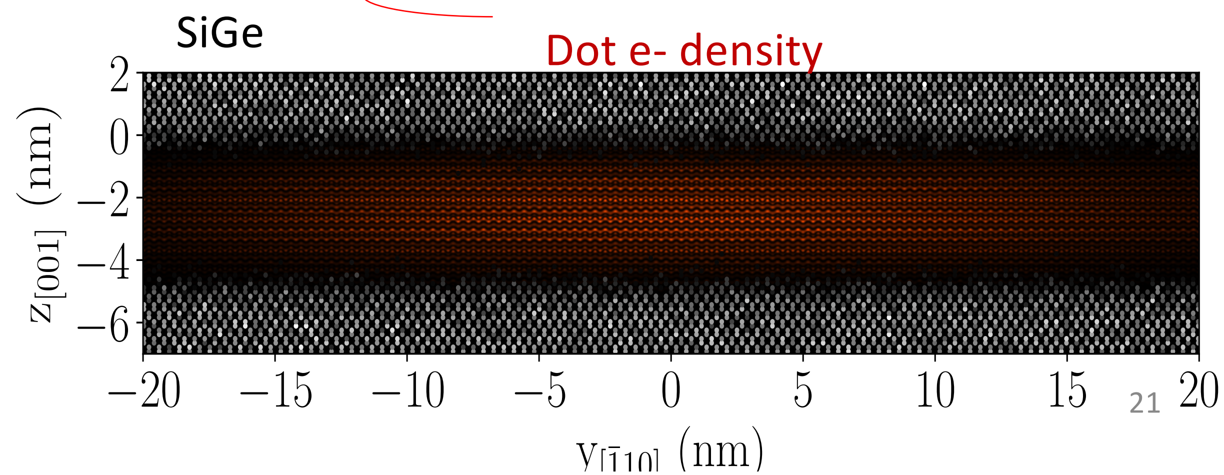


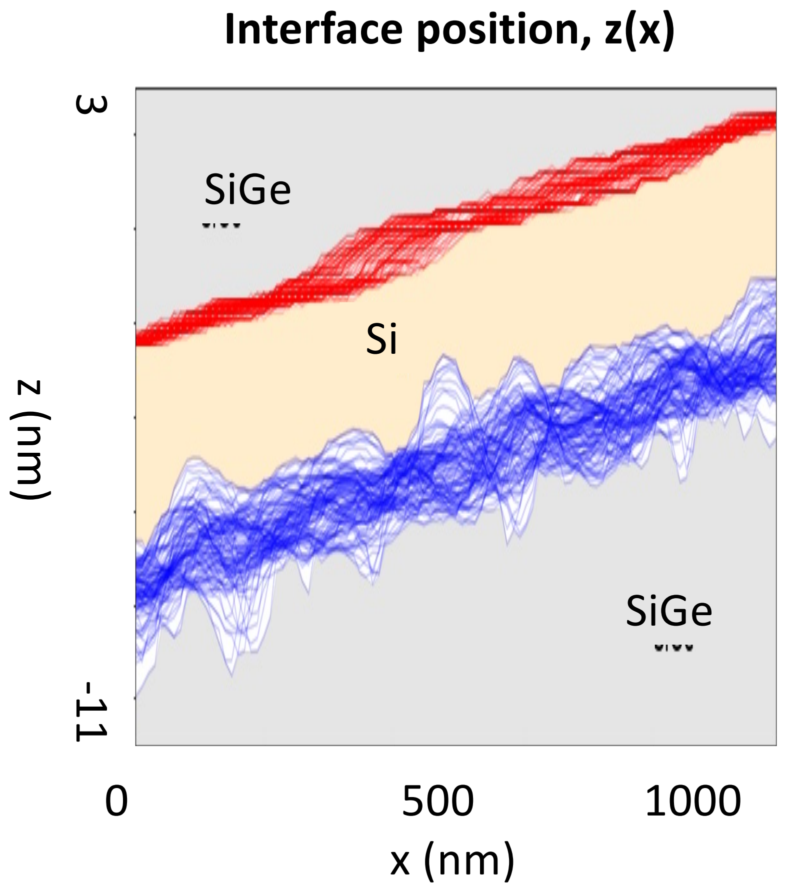


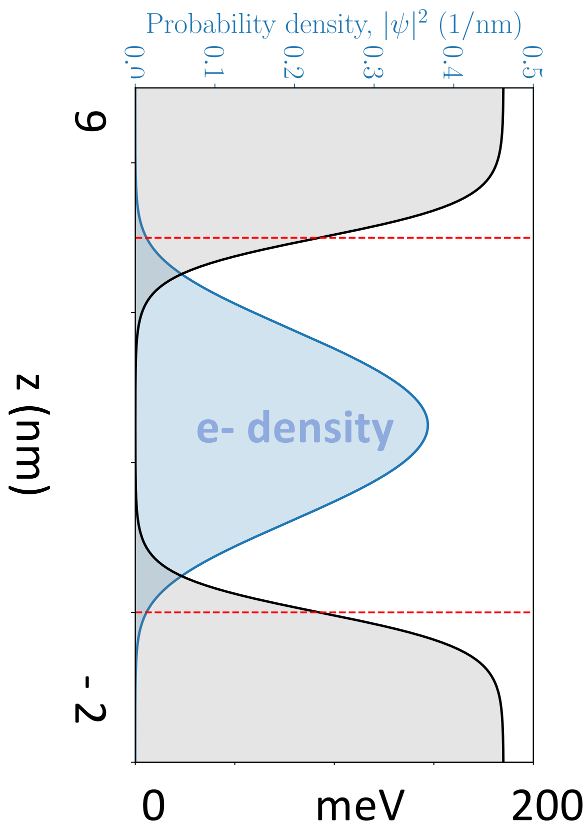


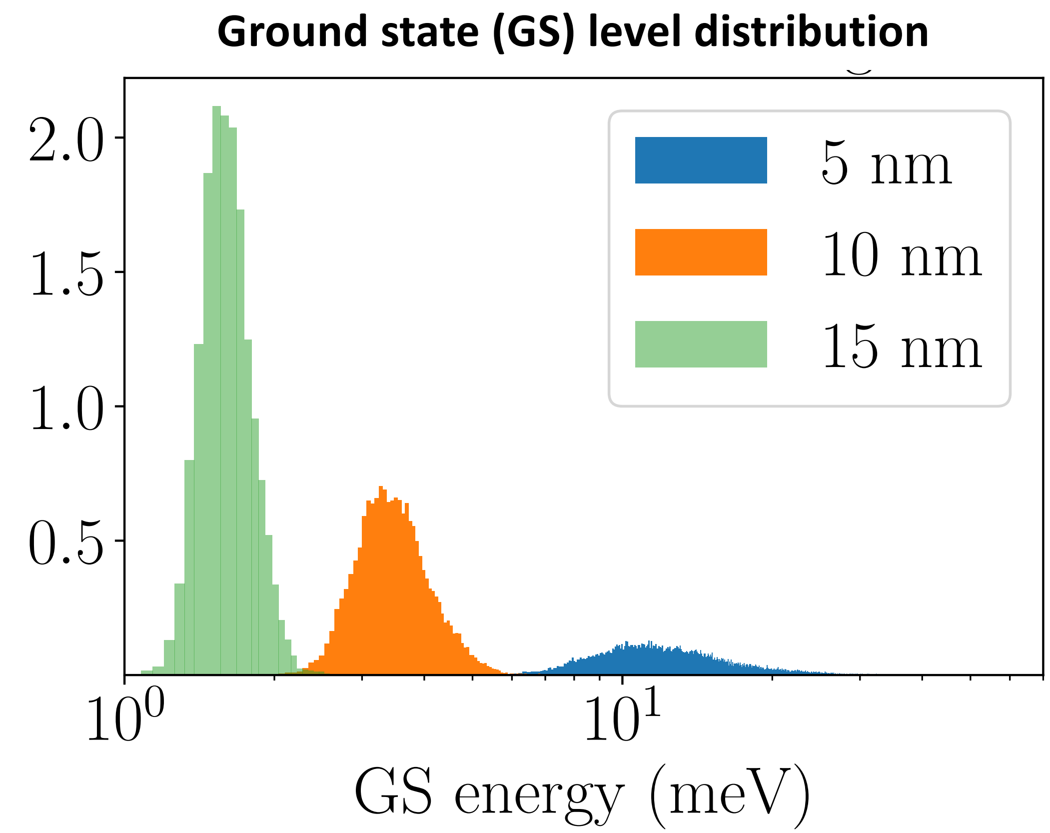
"Given many measured realizations of dot interface structure & disorder, what can we expect of dot qubit spectra variability?"

[Mills, Sci. Adv. 8, eabn5130 (2022)]

Roughness (Δwell thickness) → orbital level variability





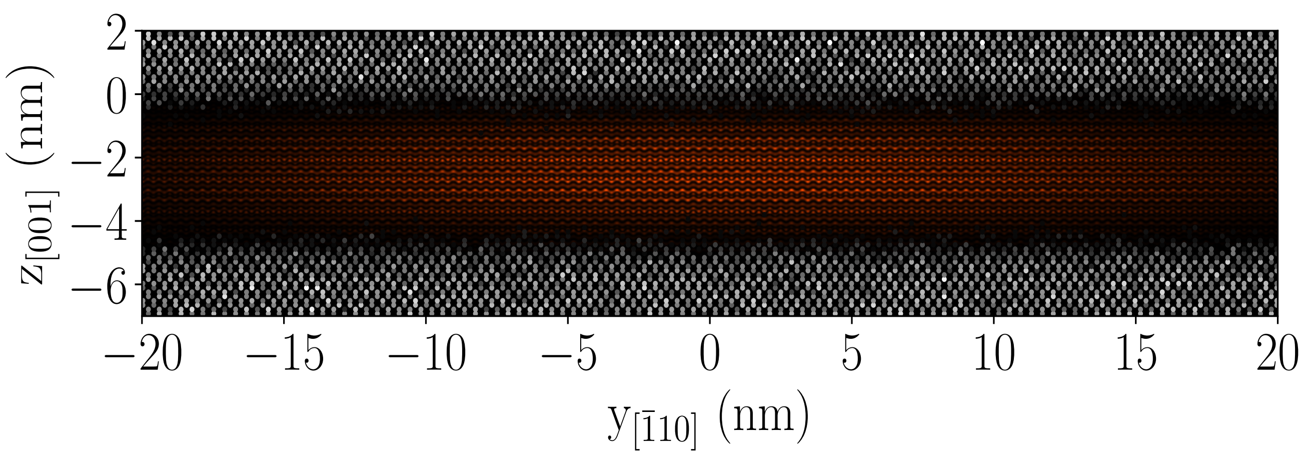


- Estimate growth-axis confinement energy via 1D Schrödinger solve
- **Confinement energy variance is considerable for thinner wells needed for larger valley splitting, i.e. mean ~ standard deviation (note x-logscale)**
- Impact: GS 1e-dot formation, gate operations, & e- manipulation e.g. shuttling –
- Variability → each dot is uniquely tuned

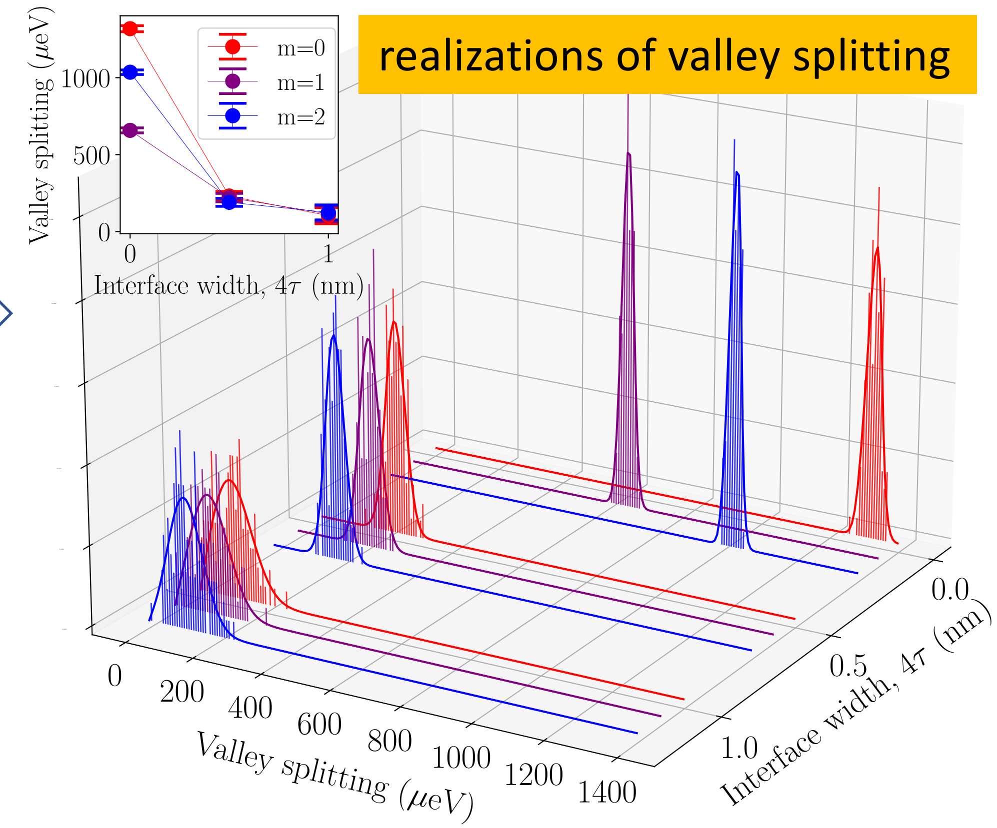
Intermixing → valley splitting variability

- Dot e- states: conduction band valley Bloch functions, 2 ~degenerate CB valleys on z[001]
- Abrupt interface potential → asymmetry that lifts valley state degeneracy - *energy gap-protected qubit states*
- Intermixing softens interface potential → significant valley splitting variability

realizations of atomic coordinates



realizations of valley splitting



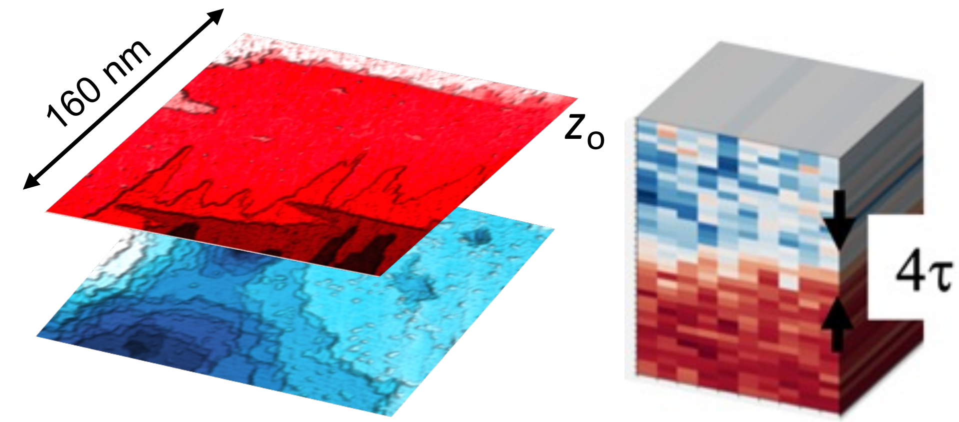
m= # of atomic steps in well

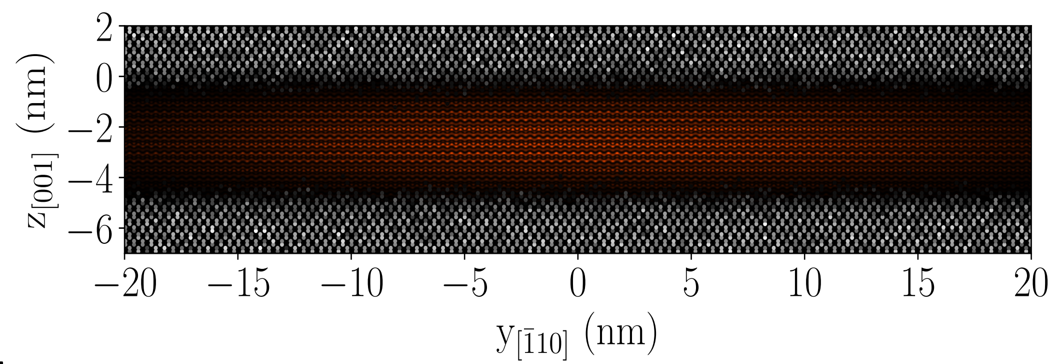
- **Calculation: Atomistic multi-valley effective mass theory (Toby Jacobson, Sandia)**

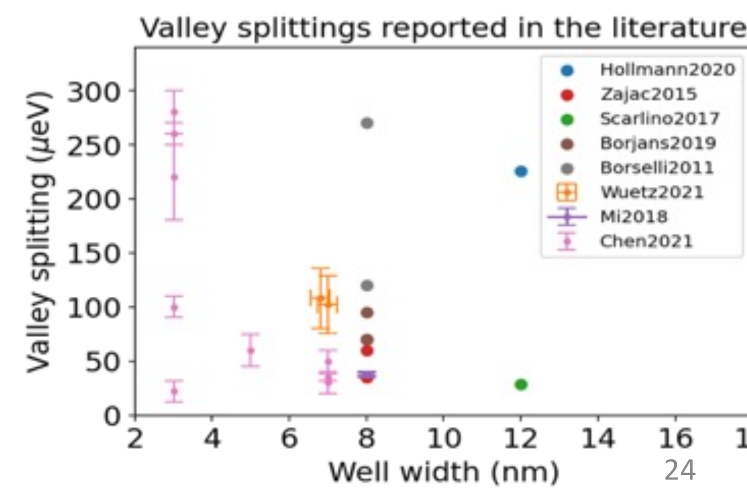
- **Variability of valley states energy ~0.01-0.2 meV (mean~spread)**
- Impact: qubits with varying spectra and spin/valley/orbit interaction, difficult to engineer

Summary & commentary

- **Atomistic structure description to micron scale** including roughness & intermixing during growth (using STM&HAADF)
- Utilize atomistic structure description to calculate spectral variability of e- states in dot qubits
- Orbital state variability ~ 1 meV scale (potentially challenging tune-up/control issue)
- **Atomistic effective mass theory:** Valley splitting measured in numerous experiments: 0.01-0.3 meV, our results cover similar range (0.01-0.2 meV)
- Owing to larger volume/area description, we will look to longer-range issues, e.g. simulation of dot couplings via tunneling for shuttling electron along interfaces







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