SAND2019-8697C

Sandia National Laboratories

Tracking atomic-scale interface disorder in Si/SiGe qubit materials

Luis F. Peña, Justin C. Koepke & Ezra Bussmann (ebussma@sandia.gov)
Center for Integrated Nanotechnologies, Sandia National Laboratories New Mexico USA

Introduction

- SiGe heterostructures are host material for ongoing quantum electronics discovery & SiGe qubits have good key traits for larger QC in Si [1-4]
- Challenge/opportunity: theory indicates critical interplay between material & quantum electronic properties may impact qubit performance[3]
- Our goal: first, measure materials properties, and then connect structure with quantum electronic properties
- **Approach: Grow SiGe heterostructure via molecular beam epitaxy & track evolution *in vacuo* via scanning tunneling microscopy (STM)**

Background

- Six degenerate conduction band minima (valleys) in Si
- For spin qubits, must remove (split) valley degeneracy [1]
- Strain + interface confinement splits valleys
- But theory indicates valley splitting in 2D e- gas, quantum dots, suppressed by atomic-scale disorder at interfaces [1-4]
- For SiGe qubits, this may underpin interdevice variability, decoherence thru degeneracy [3, 4]

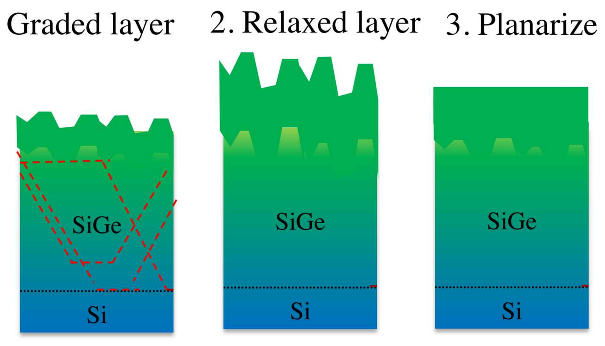
Materials & methods

- Prior studies [5-9] showed general principles driving interface disorder, we focus on specific methods & materials for contemporary qubits [4]
- Buried interface challenging to measure in 3D
- Common method of cross-sectional TEM provides 2D slice thru structure & extrapolations must be made to 3D
- Our approach: image growth surfaces that become buried interfaces as layered structure is deposited

Substrate

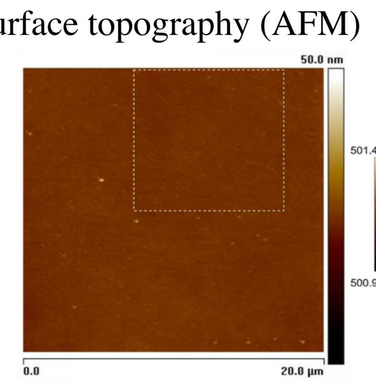
- Commercial virtual substrate (LSRL, Inc)
- Virtual substrate characteristics (as-received)

1. Graded layer 2. Relaxed layer 3. Planarize



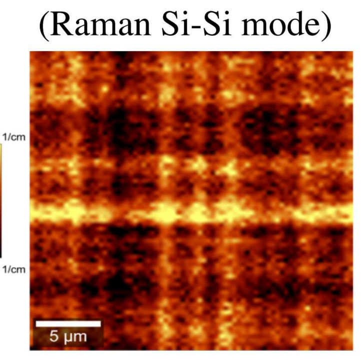
- **$Si_{0.7}Ge_{0.3}$**
- **Linear graded Ge at ~10% /μm**
- **Relaxed layer 600 nm thick**
- **C, O ≤ 10^{17} cm^{-3}**
- **Residual strain variation, Δ strain ~0.1%**
- **Roughness < 1 nm RMS**

Surface topography (AFM)



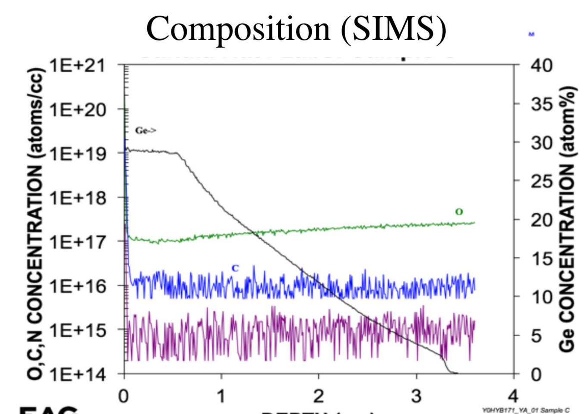
Roughness: 0.5 nm

Strain variation (Raman Si-Si mode)

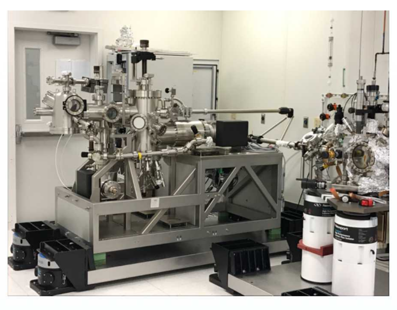


Δ strain ~0.1%

Composition (SIMS)



Toolset MBE+STM



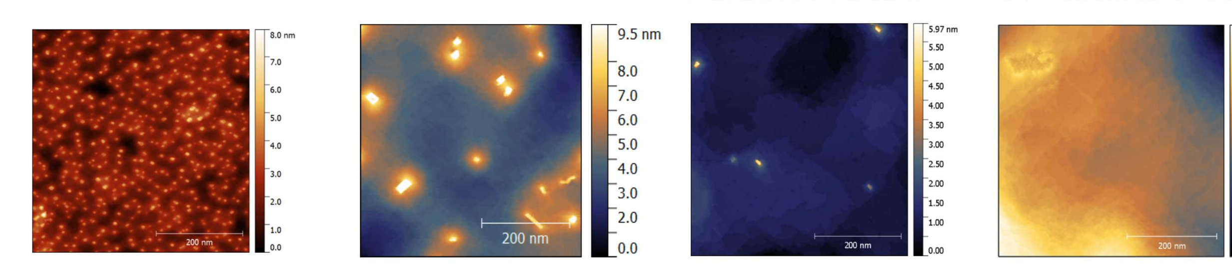
- Coupled MBE+STM (*Omicron*), vacuum 2x10^{-10} Torr
- Si source e-beam heated rod-fed (*Thermionics Inc*)
- Ge source Knudsen cell (*MBE Komponenten*)
- RHEED (*Staib*) to monitor surface during growth
- Band edge thermometer for T measurement

Heterostructure growth tracked by *in vacuo* STM

1. Clean substrate – reduce C, O, H via wet chem + annealing in vacuum

diminishing C contamination

HF dip– H desorption | Oxide desorption | Oxide desorption + atomic H clean | Oxide desorption UV+ atomic H clean

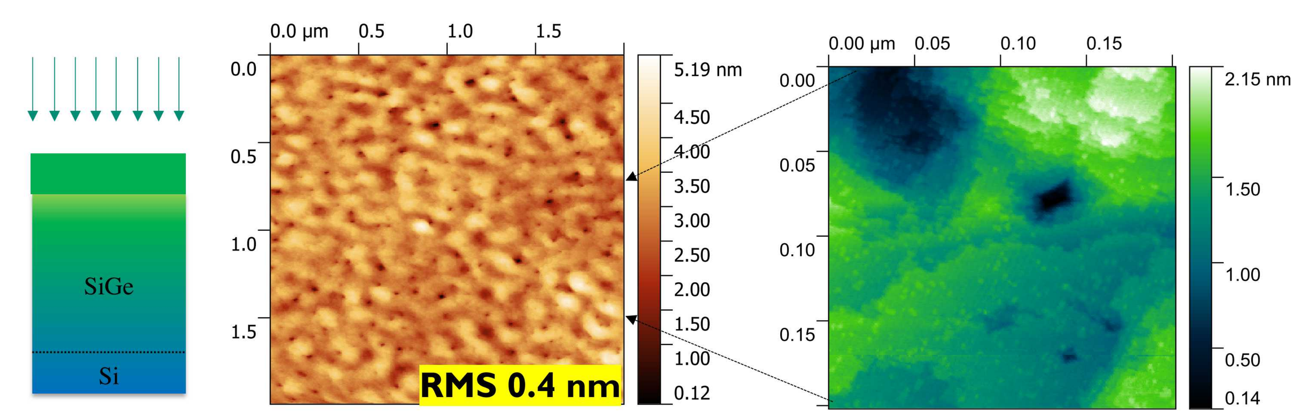


carbon mound density: 2×10^{11} cm^{-2}. | carbon mound density: ~3-6×10^{9} cm^{-2}. | carbon mound density ~1×10^{9} cm^{-2}.

T~550°C | T~800°C

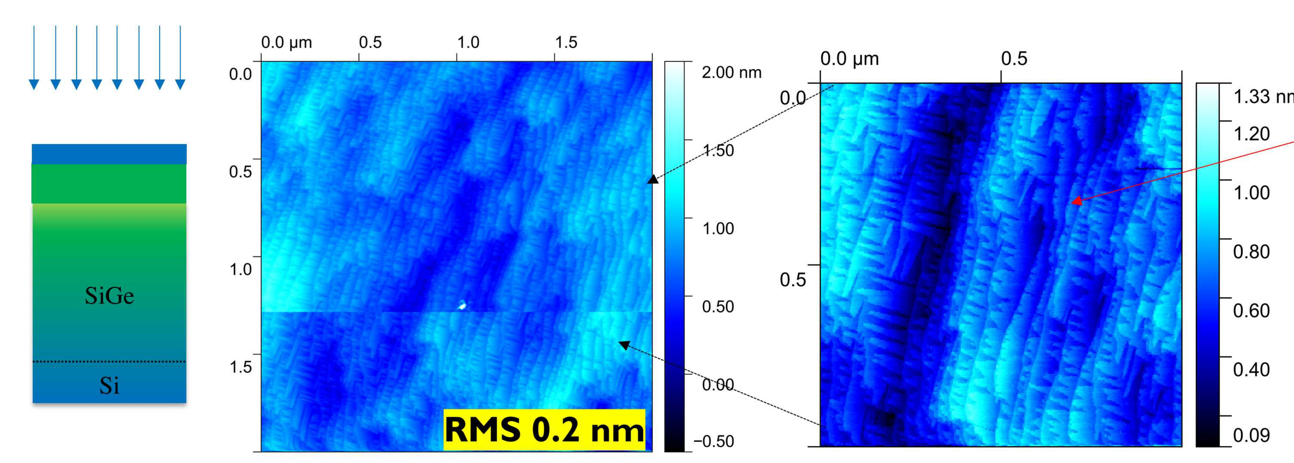
- Compared a few cleans
- Chemical oxide, H annealing, & UV ozone yielded reasonably clean but rougher surface

2. After relaxed SiGe buffer layer deposition



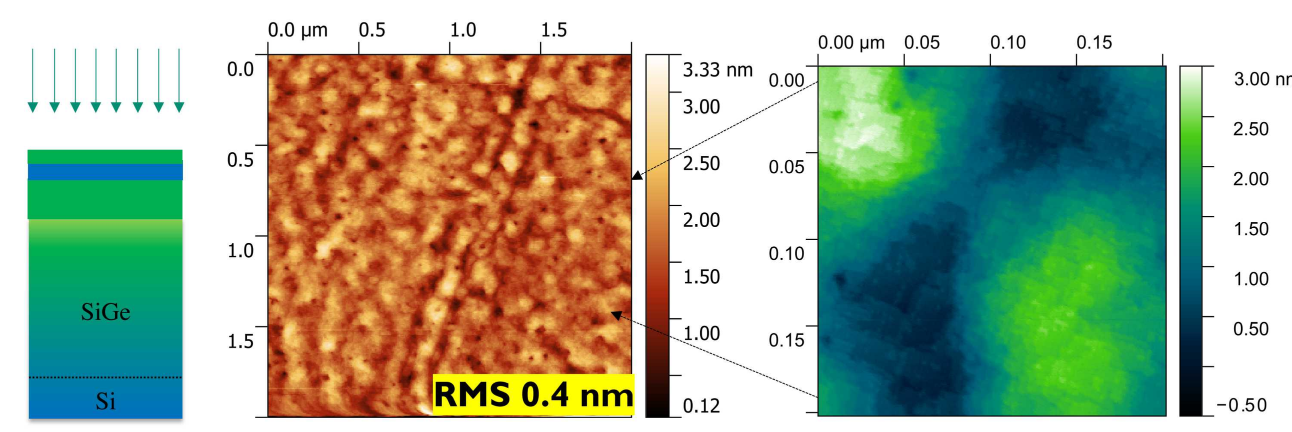
- Composition $Si_{0.7}Ge_{0.3}$
- Isolate subsequent quantum well from disorder at initial surface
- **Roughness can be introduced in this layer**
- 80 nm thick, 2.1 nm/min growth rate, T=550°C

3. After strained-Si quantum well



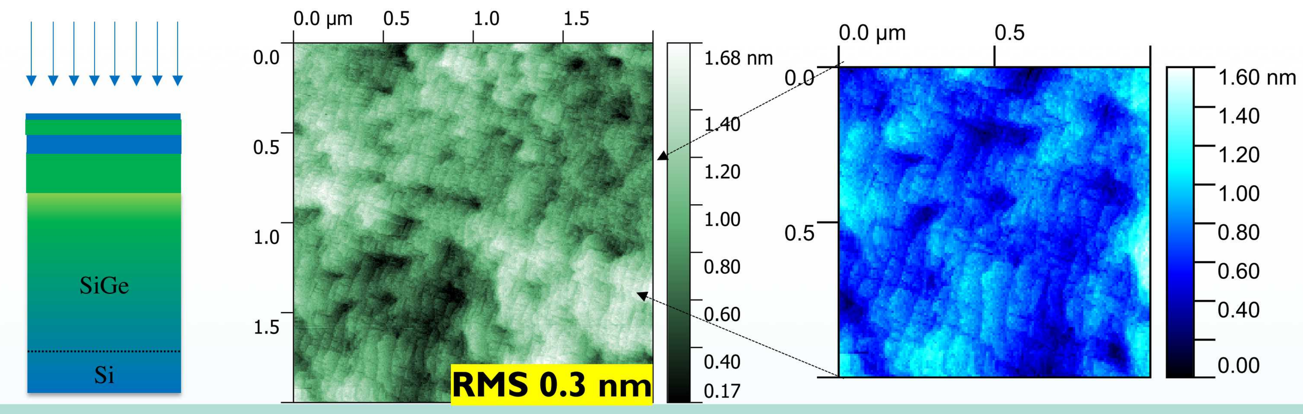
- Smoothing in this step
- **Dense atomic steps with nonuniform distribution**
- Likely owing to tensile strain, higher surface energy, and pure composition
- 10 nm thick, 1.5 nm/min growth rate, T=550°C

4. After relaxed SiGe top layer



- Isolate s-Si quantum well from disorder at finished top surface and subsequent gate stack
- **Roughness can be introduced in this layer**
- Composition $Si_{0.7}Ge0_{.3}$
- 50 nm thick/ 2.1 nm/min growth rate, T=550°C

5. After strained-Si cap – finished heterostructure surface



- Smoothing in this step
- Likely owing to tensile strain, higher surface energy, and pure composition
- 3 nm thick, T=550°C/ 1.5 nm/min growth rate

Conclusions & outlook

- Variable step density across surface following each stage of growth process
- Steps do not follow miscut, but rather local growth kinetics & strain fields
- STM at stage 3 and 5 above point to correlation between well & top-surface roughness
- Next work: correlate atomic disorder & quantum electronic properties, in collaboration with M. Eriksson UW-Madison

References
[1] S. F. Neyens *et al.*, The critical role of substrate disorder in valley splitting in Si quantum wells, *Appl. Phys. Lett.* **112**, 243107 (2018)
[2] S. Goswami *et al.*, Controllable valley splitting in silicon quantum devices, *Nature Physics* **3**, 41 (2007)
[3] M. Friesen, S. Chutia, C. Tahan, and S. N. Coppersmith, Valley splitting theory of SiGe quantum wells, *Phys. Rev. B* **75**, 115318
[4] F. A. Zwanenburg *et al.*, Silicon quantum electronics, *RMP* ***85**, 961* (2013)
[5] F. Schäffler, High Mobility Si and Ge structures, *Semicon. Sci. & Tech.* **12**, 1515 (1997)
[6] J. W. P. Hsu, E. A. Fitzgerald, Y. H. Xie, P. J. Silverman, and M. J. Cardillo, Surface morphology of related Ge_xSi_{1-x} films, *Appl. Phys. Lett.* **61**, 1293 (1992)
[7] M. A. Lutz, R. M. Feenstra, F. K. LeGoues, P. M. Mooney, and J. O. Chu, Influence of misfit dislocations on the surface morphology of $Si_{1-x}Ge_x$ films, *Appl. Phys. Lett.* **66**, 724 (1995)
[8] M. Albrecht, S. Christiansen, J. Michler, W. Dorsch, and H. P. Strunk , P. O. Hansson, E . Bauser, Surface ripples, crosshatch pattern, and dislocation formation: Cooperating mechanisms in lattice mismatch relaxation, *Appl. Phys. Lett.* **67**, 1232 (1995)
[9] K. Sawano, N. Usami, K. Arimoto, K. Nakagawa, Y. Shiraki, Strain field and related roughness formation in SiGe relaxed buffer layers, *Thin Solid Films* **508**, 117 (2006)

This work was performed, in part, at the Center for Integrated Nanotechnologies, an Office of Science User Facility operated for the U.S. Department of Energy (DOE) Office of Science. Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. DOE's National Nuclear Security Administration under contract DE-NA-0003525. The views expressed in the article do not necessarily represent the views of the U.S. DOE or the United States Government.
SAND No. SAND2018-8224 D