



Si Quantum Dots via Rapid Ge Diffusion During High Temperature Oxidation of Si/SiGe Nanostructures

Emily Turner¹

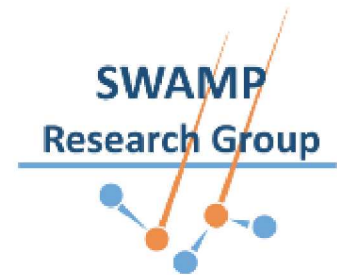
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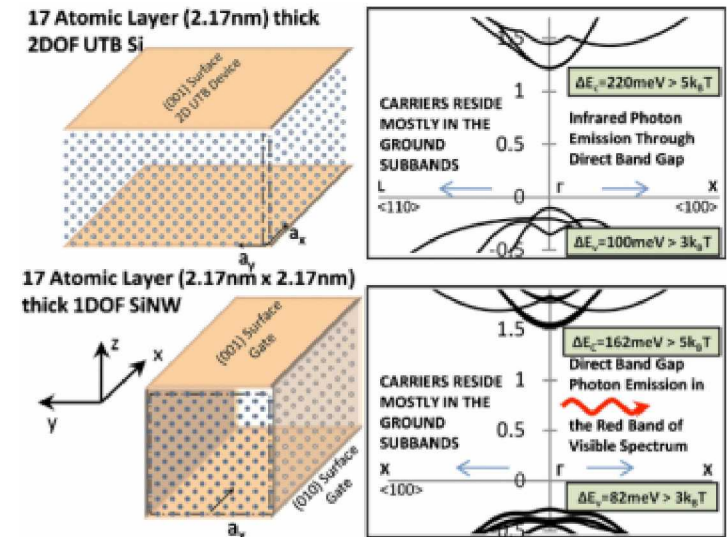


Outline

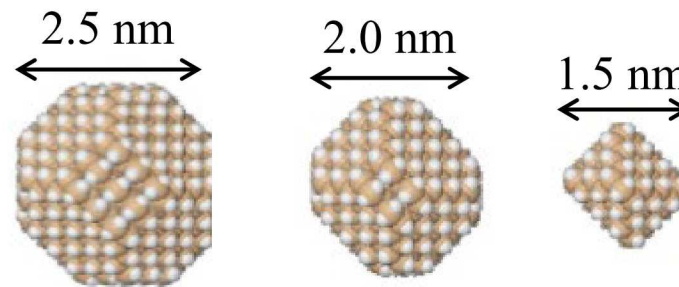
- Introduction
 - *Si and SiGe for quantum applications*
 - *Enhanced diffusion of Ge along Si/SiO₂ interface*
- Oxidation of Si/SiGe fin structures
- Oxidation of Si/SiGe pillar structures
 - *Method for FIB cross section fabrication of 3-D nanostructures*
 - *Si dot formation during oxidation*
- Conclusions

Si and SiGe for quantum applications

- Si/SiGe quantum structures have potential as on-chip optical sources, microelectronics, & quantum computing
- Interesting material property changes as dimensions decrease to quantum sizes
- Fabricating on-chip quantum structures challenging



Theoretical calculations suggesting Si may transition from having indirect to direct bandgap properties when spatially confined ²

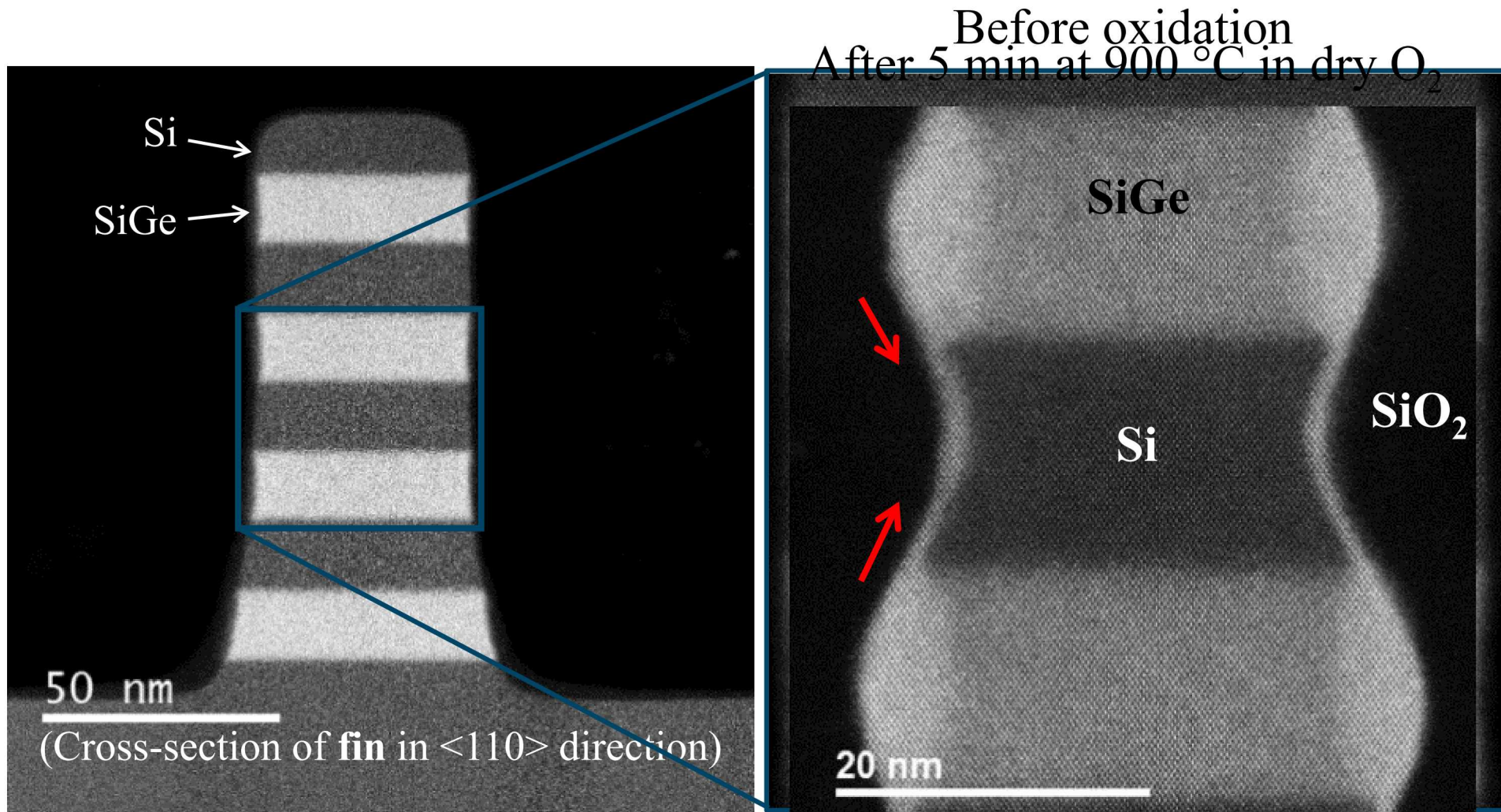


DFT analysis of Si-H QDs for electronic structure information ¹

¹Hapala, P. *et al.* Theoretical analysis of electronic band structure of 2- to 3-nm Si nanocrystals. *Phys. Rev. B - Condens. Matter Mater. Phys.* **87**, 1–13 (2013).

²M. O. Baykan, S. E. Thompson, and T. Nishida, "Strain effects on three-dimensional, two-dimensional, and one-dimensional silicon logic devices..," *J. Appl. Phys.*, **108**, 1–24, (2010).

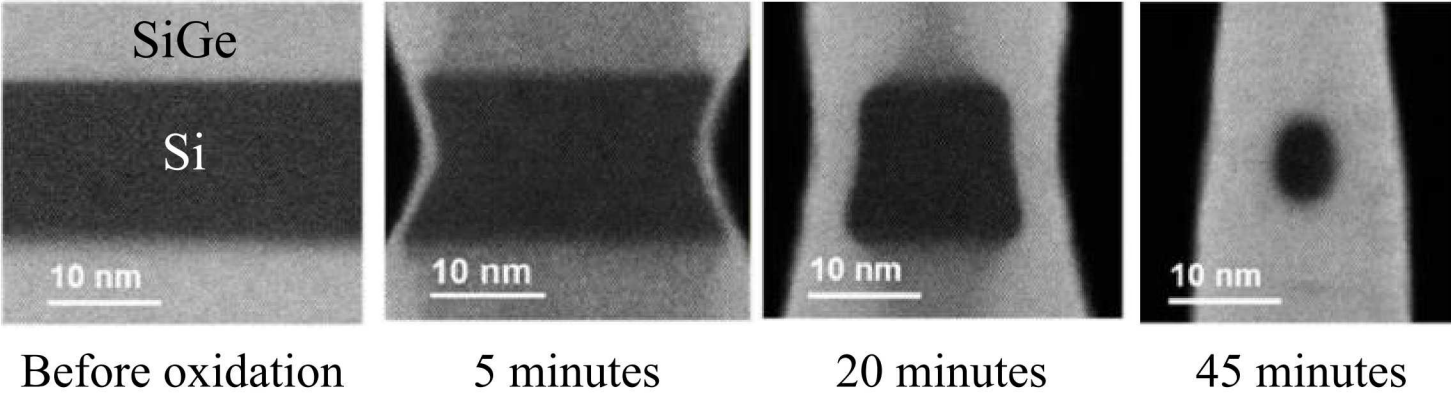
Enhanced diffusion of Ge along Si/SiO₂ interface



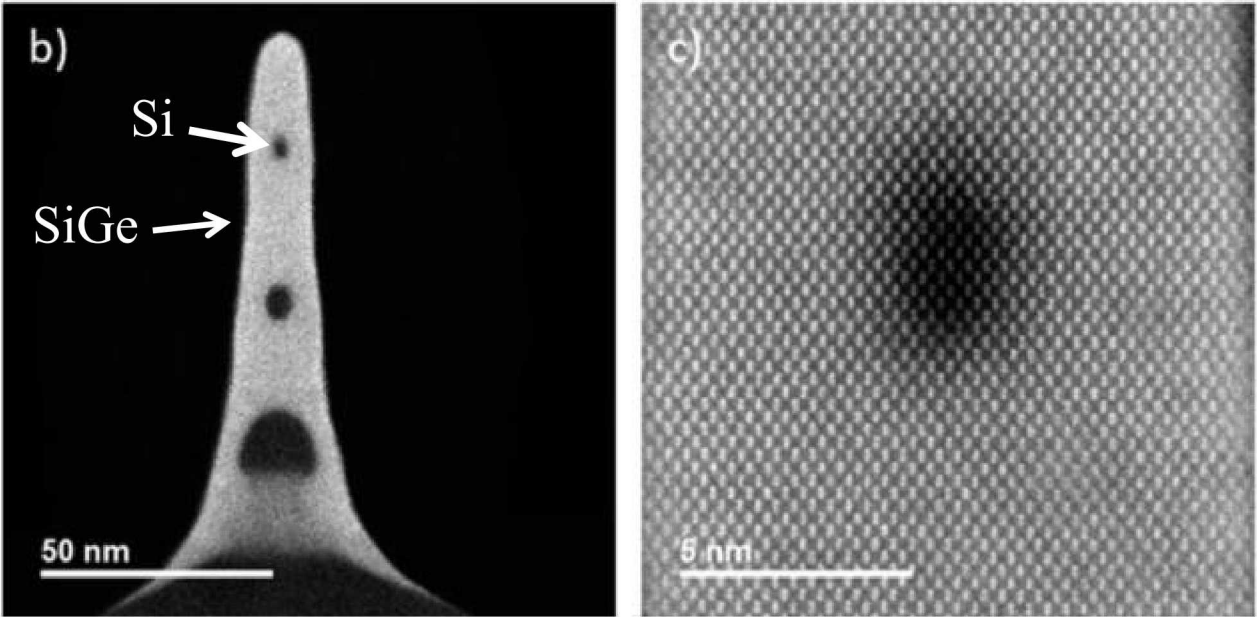
Brewer, W. M. *et al.* Lateral Ge Diffusion During Oxidation of Si/SiGe Fins. *Nano Lett.* **17**, 2159–2164 (2017).

Si nanowire formation during 900 °C oxidizing anneal

- Fin cross section during oxidation at 900 °C in O₂



- Unexpected formation of lateral Si nanowires down to 2 nm in diameter!

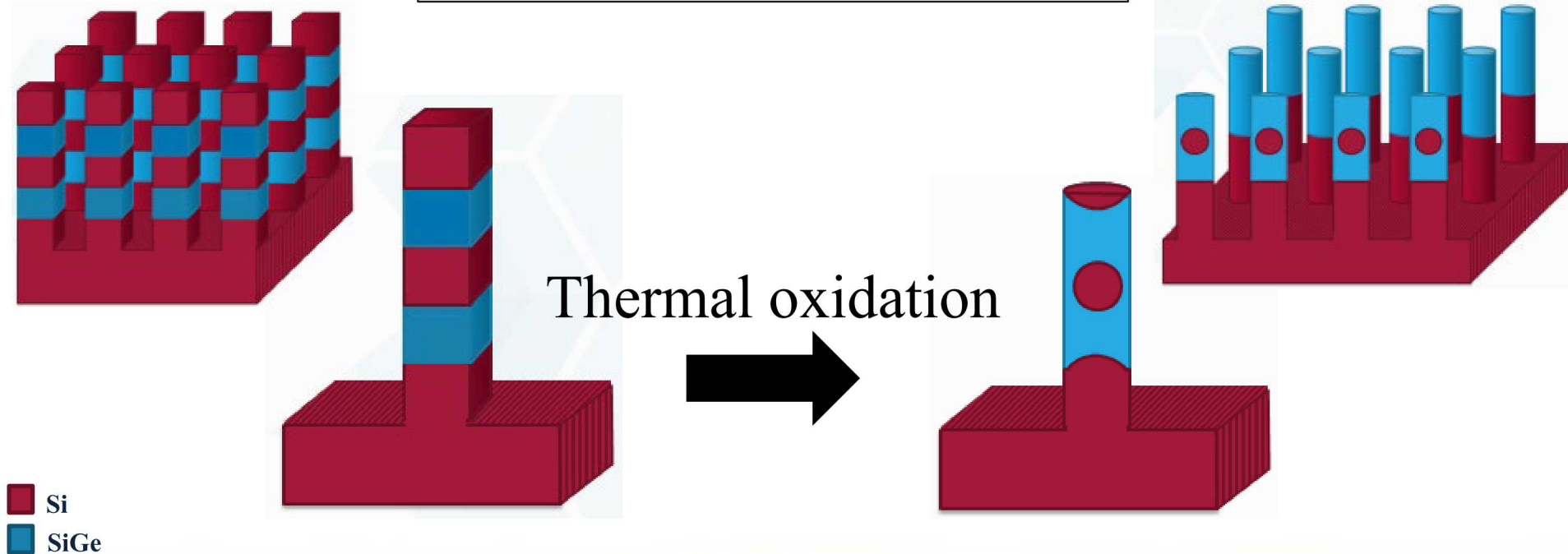


Brewer, W. M. *et al.* Lateral Ge Diffusion During Oxidation of Si/SiGe Fins. *Nano Lett.* **17**, 2159–2164 (2017).

Enhanced Ge diffusion for novel fabrication method

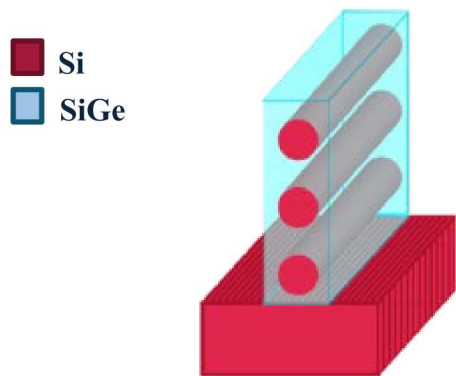
- Need scalable methods for on-chip Si nanostructures with dimensions $< 10\text{nm}$
- Can we extend the use of this enhanced Ge diffusion process to create 0D structures (quantum dots) in addition to lateral 1D nanowires?

Next step: Si/SiGe pillars

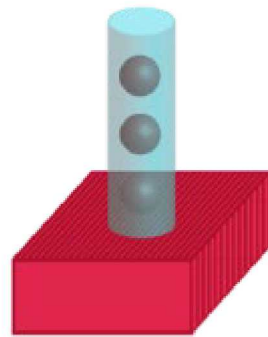


FIB Cross Sectioning of 3-D nanostructures

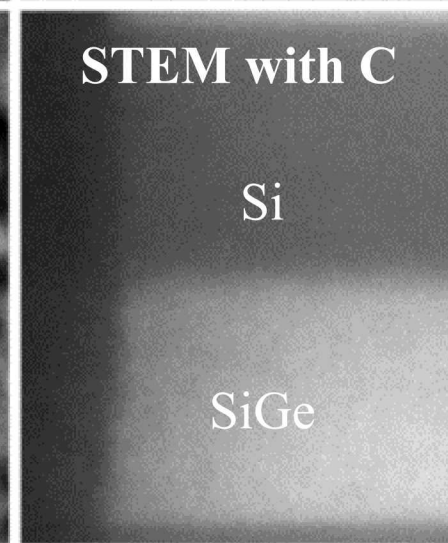
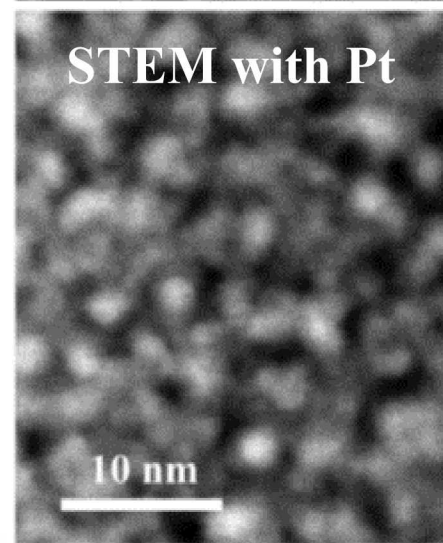
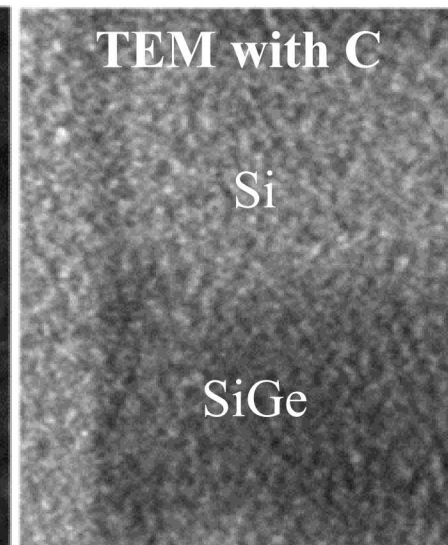
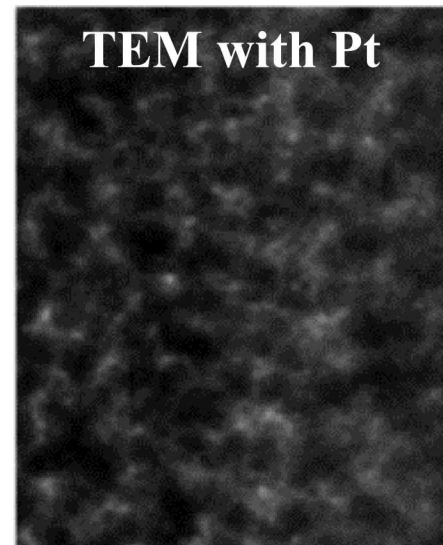
- Typically use a protective material like C and/or Pt to avoid ion beam damage during preparation
- Works very well for bulk and 2-D nanostructures (e.g. fins)
- Causes obstruction of 3-D nanostructures (e.g. nanopillars, vertical nanowires, QDs) during TEM analysis



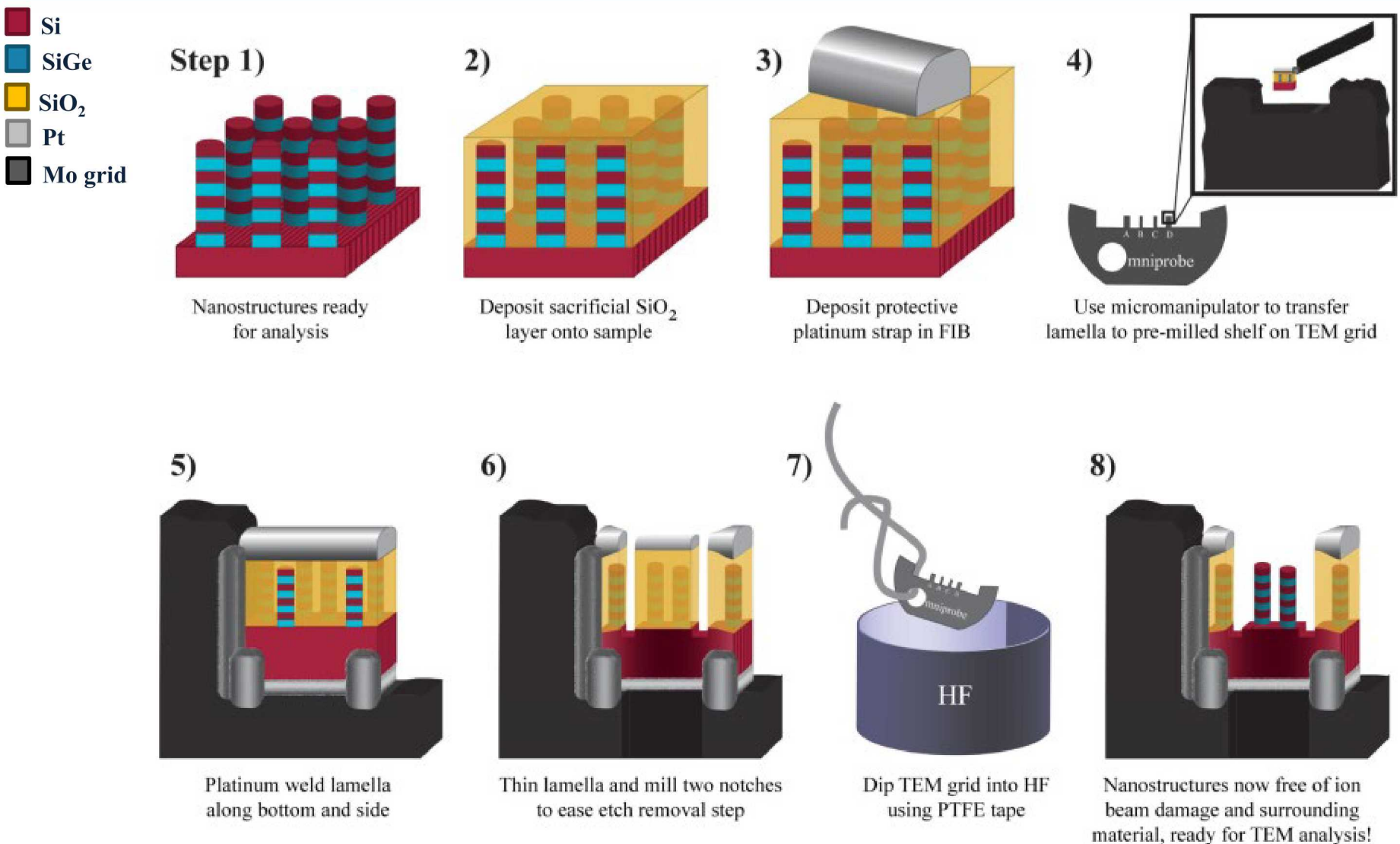
Fin



Pillar

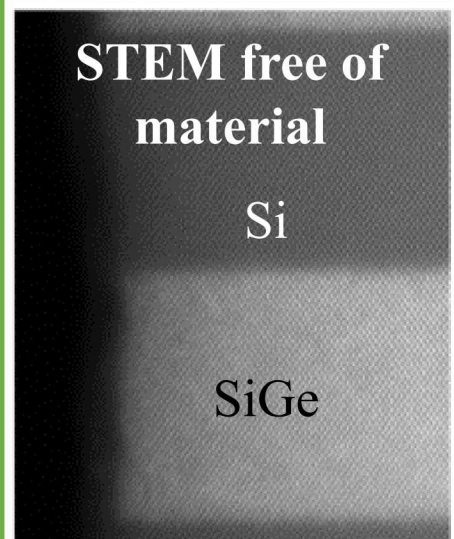
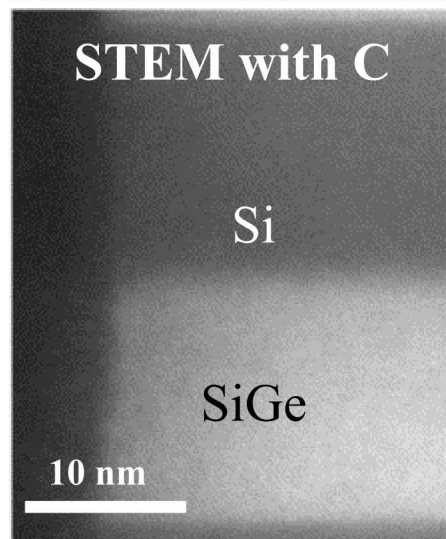
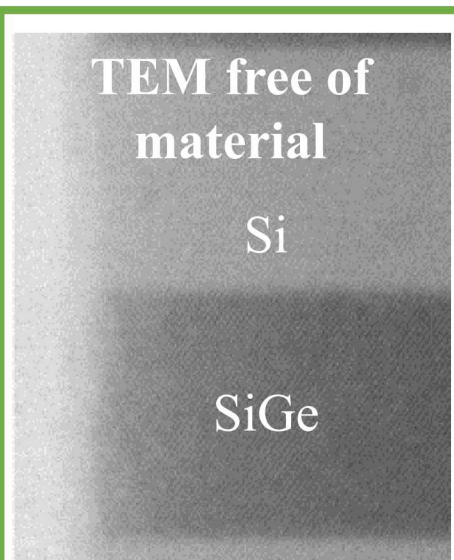
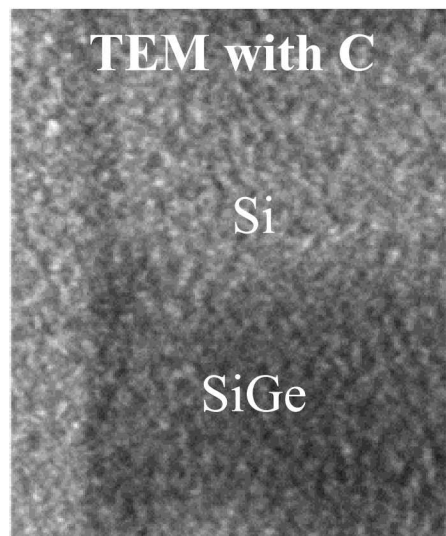


Method for 3-D nanostructure characterization

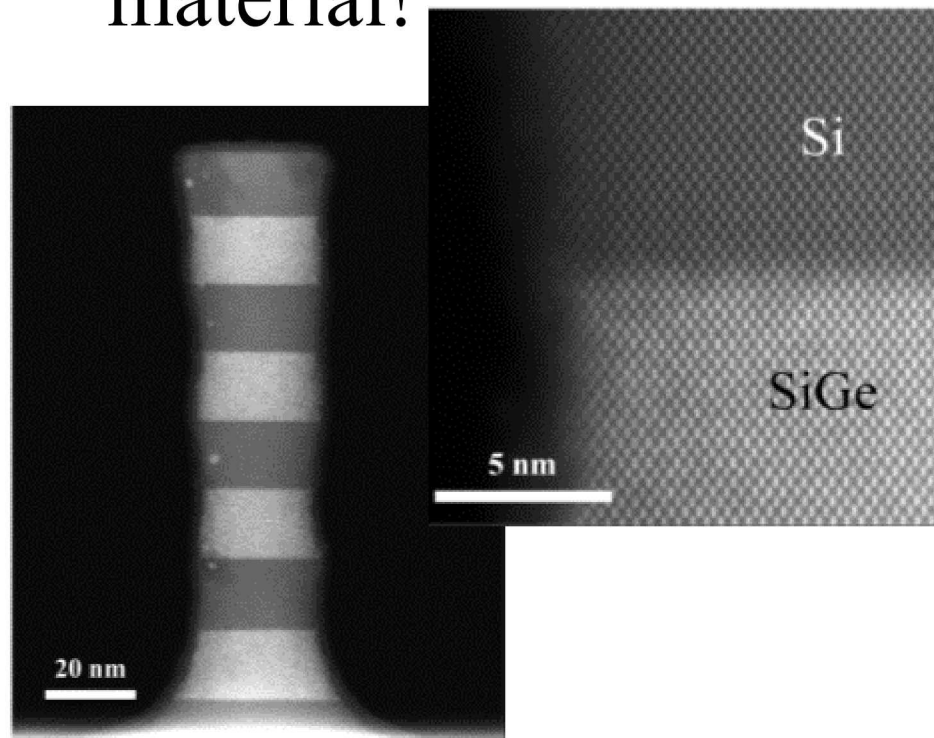


Turner, E. M. *et al.* Wet-chemical Etching of FIB Lift-out TEM Lamellae for Damage-free Analysis of 3-D Nanostructures *Ultramicroscopy*. (2020).

Results of new wet etch method



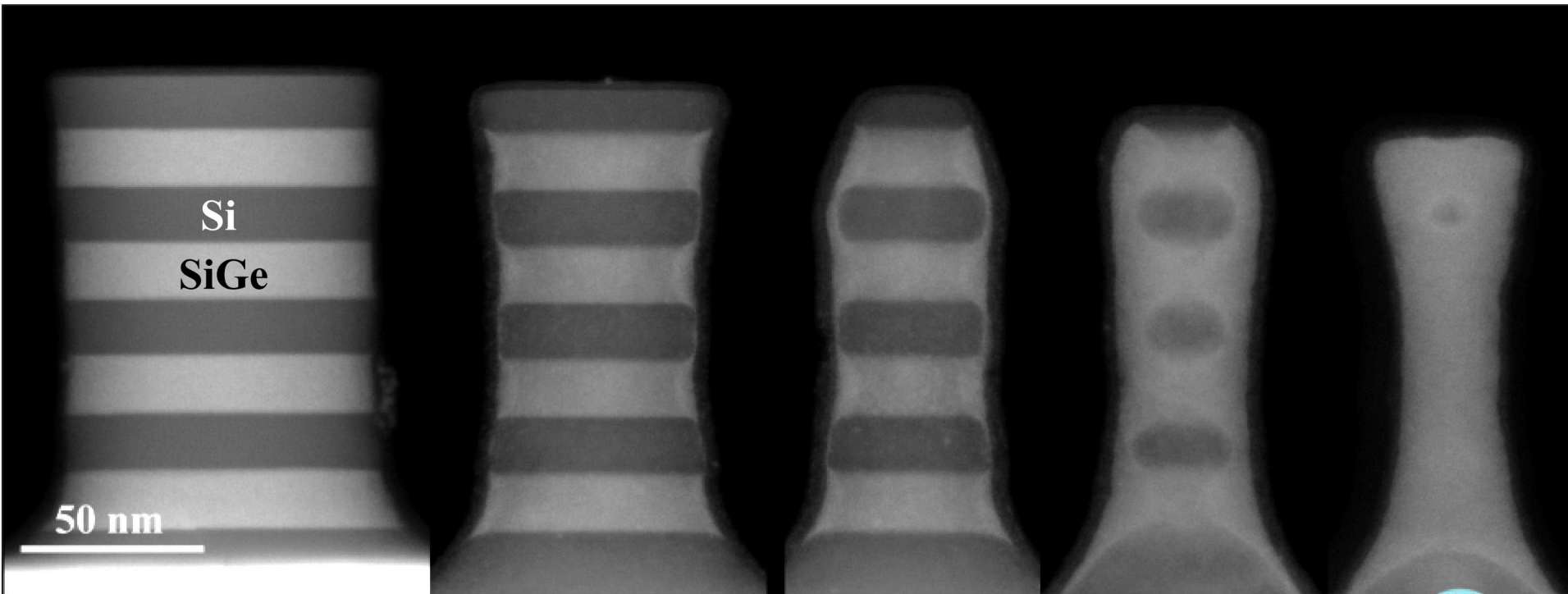
- Now able to image 3-D nanostructures without damage or obstructing material!



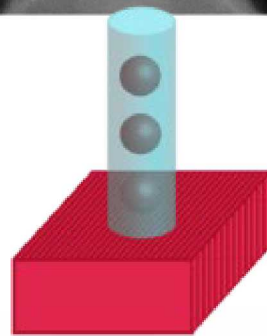
30 nm diameter Si/SiGe pillar

Evolution of Si/SiGe pillar during oxidation

Unoxidized pillar 5 min ox 10 min ox 20 min ox 35 min ox

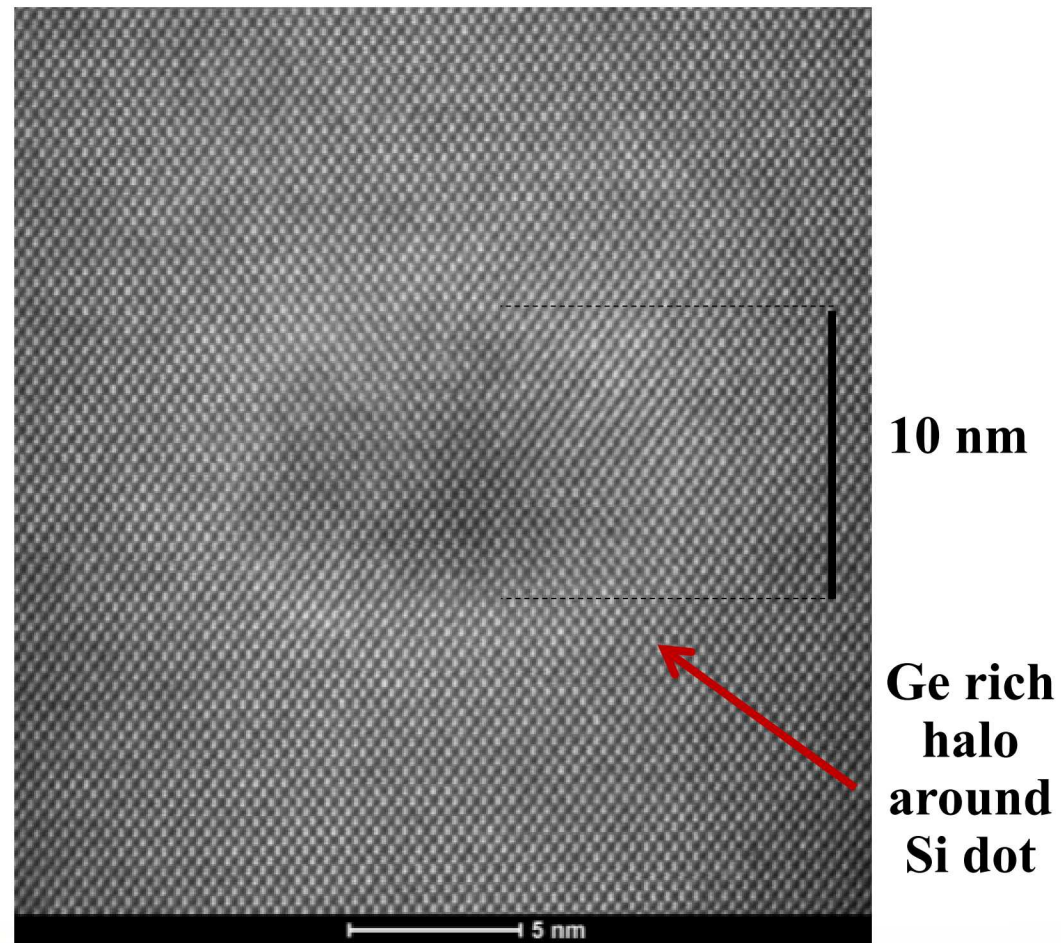
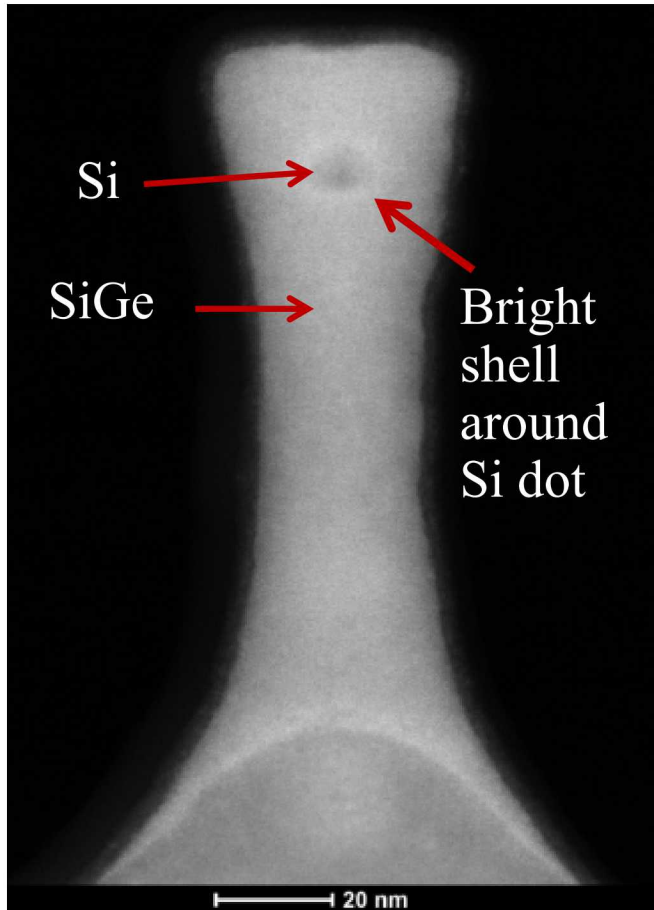


- HAADF STEM images of Si/SiGe pillars after oxidation at 900 °C in dry O₂ for a range of oxidation times
- Ge diffusion results in **Si dots encapsulated in SiGe pillars!**

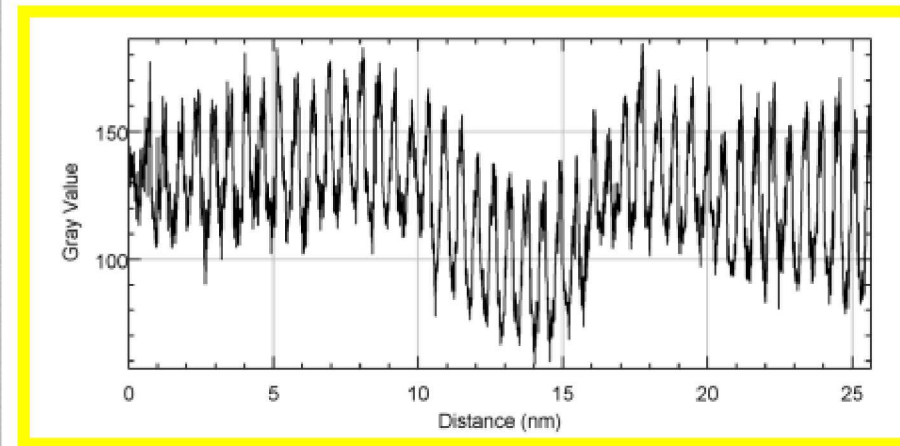
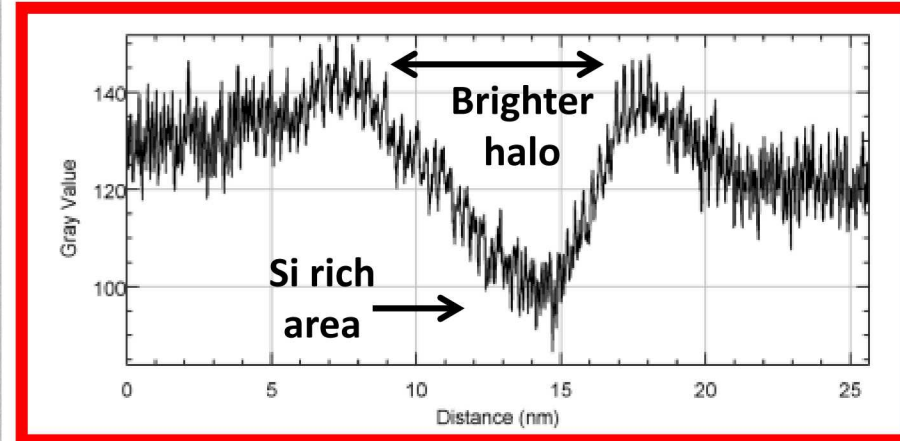
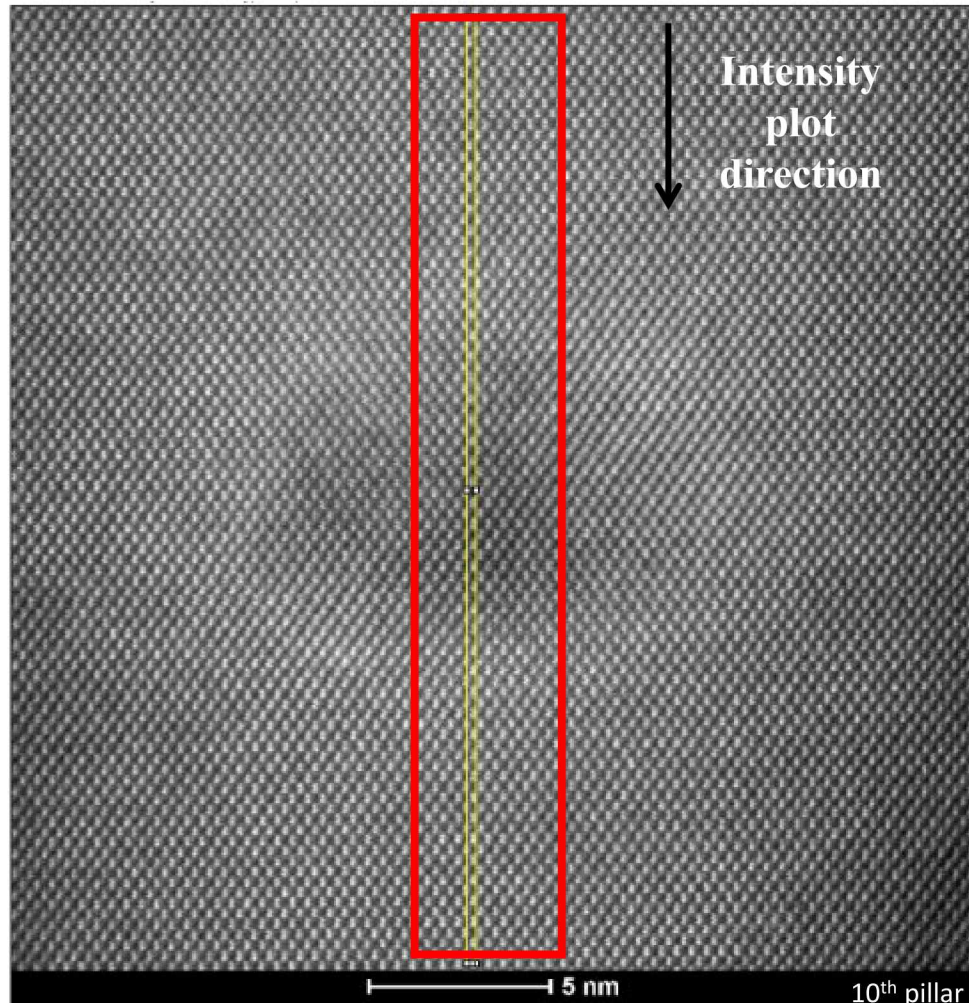


STEM of encapsulated Si dot in SiGe

- Si layers fully encapsulated by single crystal SiGe
- **Unexpected Ge rich halo around Si dot**



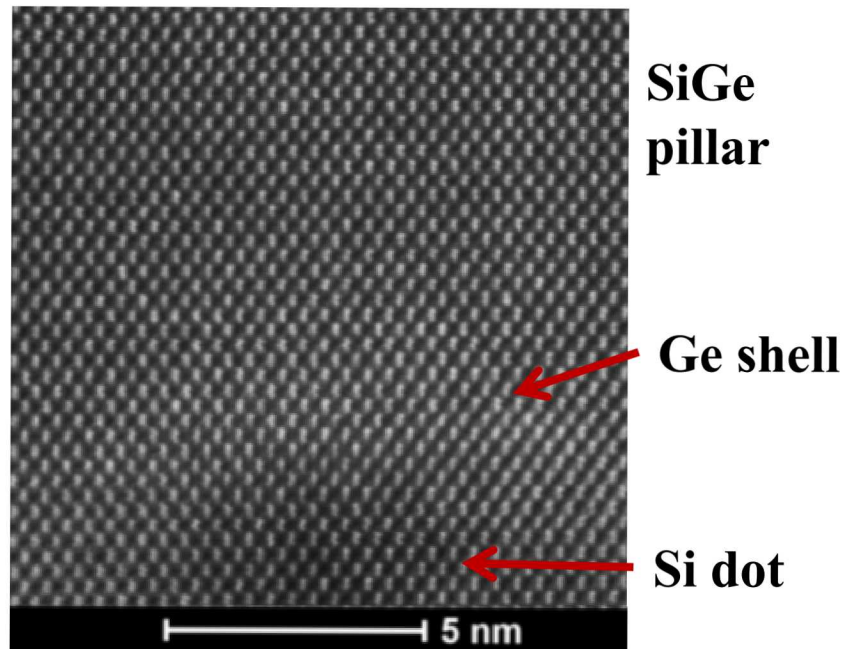
STEM of encapsulated Si dot in SiGe



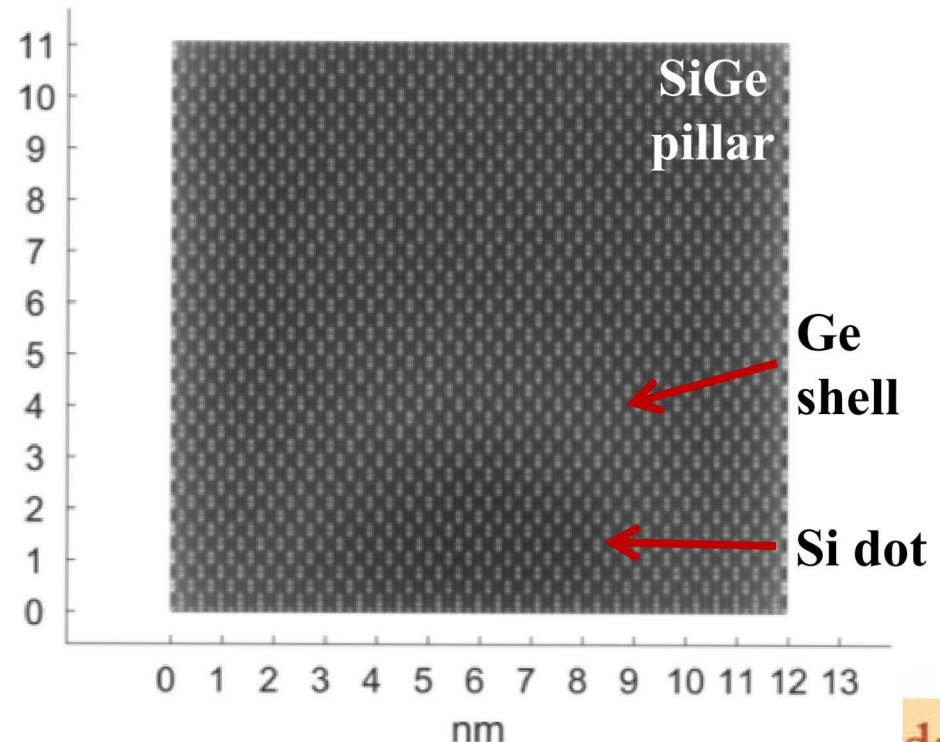
STEM modeling of Si dot and Ge shell

- Is the bright region around the Si dot due to strain or composition?
- If we are able to match a simulated STEM image with the experimental data, can have some confidence about compositional makeup of Si/SiGe pillar

Experimental STEM image



Simulated STEM image



Conclusions

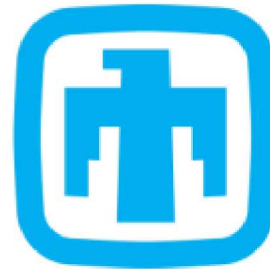
- New method developed for damage free cross sectioning of 3-D nanostructures free of surrounding material
- Novel Ge diffusion also observed in Si/SiGe pillar structures
- Continued oxidation forms encapsulated Si QDs!
- Next steps include investigating electronic structure of QDs
- Enhanced Ge diffusion could pave the way to formation of novel Si (and SiGe) structures for future electronics applications



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expected graduation FA2020

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 - CINT
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**Sandia
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FLORIDA

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