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WHAT STARTS HERE CHANGES THE WORLD

Raman Spectroscopy and Transmission Electron Microscopy of Si_xGe_{1-x}-Ge-Si Core-Double-Shell Nanowires

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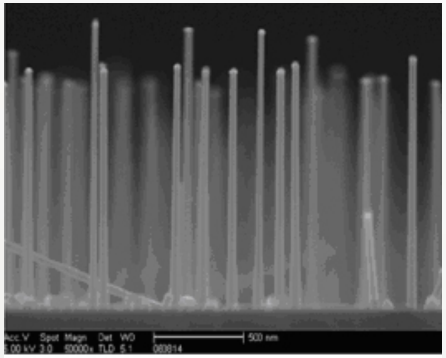
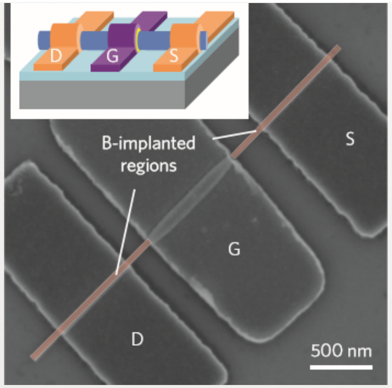
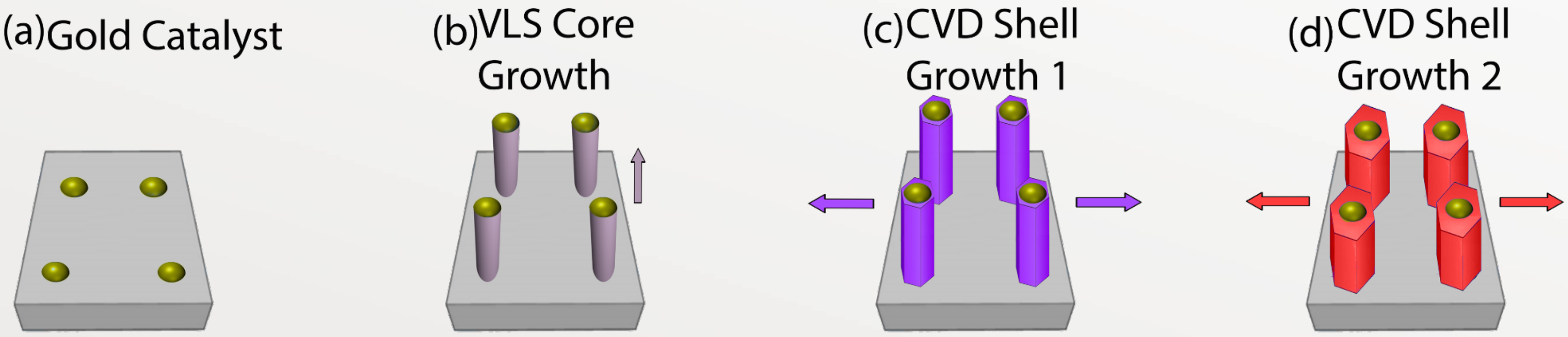
Background

- One-dimensional semiconducting nanowires (NWs)
  - Reduced dimensions and ability to engineer their electronic properties
  - Attractive for nanoscale electronics and photonics
    - Field-effect transistors
    - Solar cells





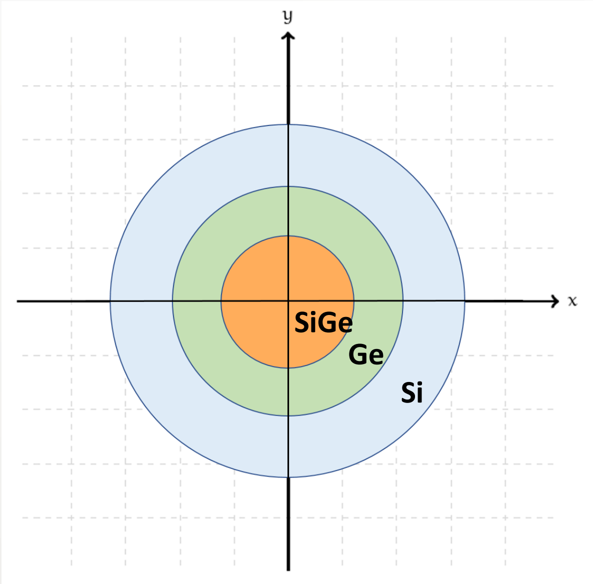
Nanowires Growth Process



Schematic of Si_xGe_{1-x}−Ge−Si core-double-shell nanowire growth. (a) Au catalyst droplets prior to growth. (b) Vapor-liquid-solid Si_xGe_{1-x} core growth. (c) and (d) ultra-high vacuum chemical vapor deposition for the Ge shell growth and Si shell growth, respectively.

Strain

- SiGe core can be used as non-planar substrate for depositing compressively strained Ge layers and tensile strained Si layers



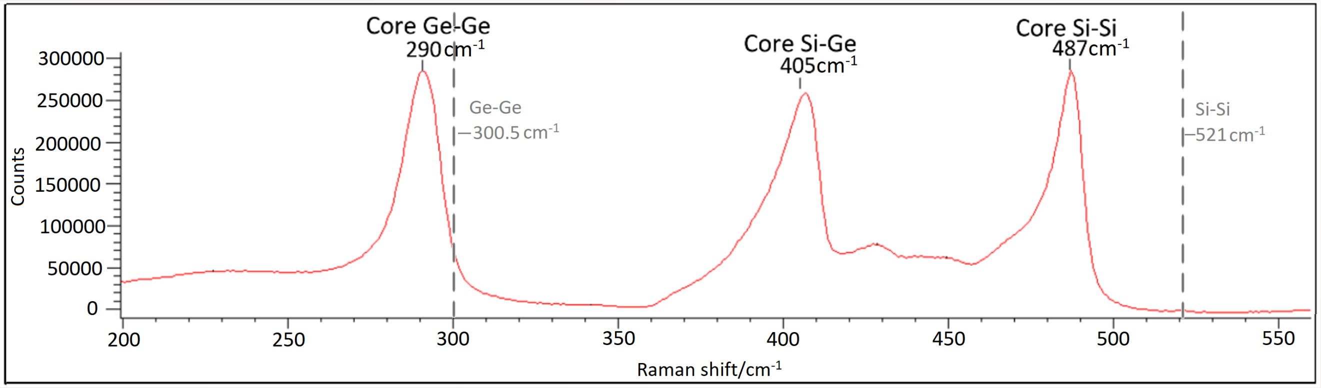
- Strain can change the band structure and optical phonon frequencies
  - Depends on core composition, core diameter, shell thickness, and shell morphology

Raman Spectroscopy

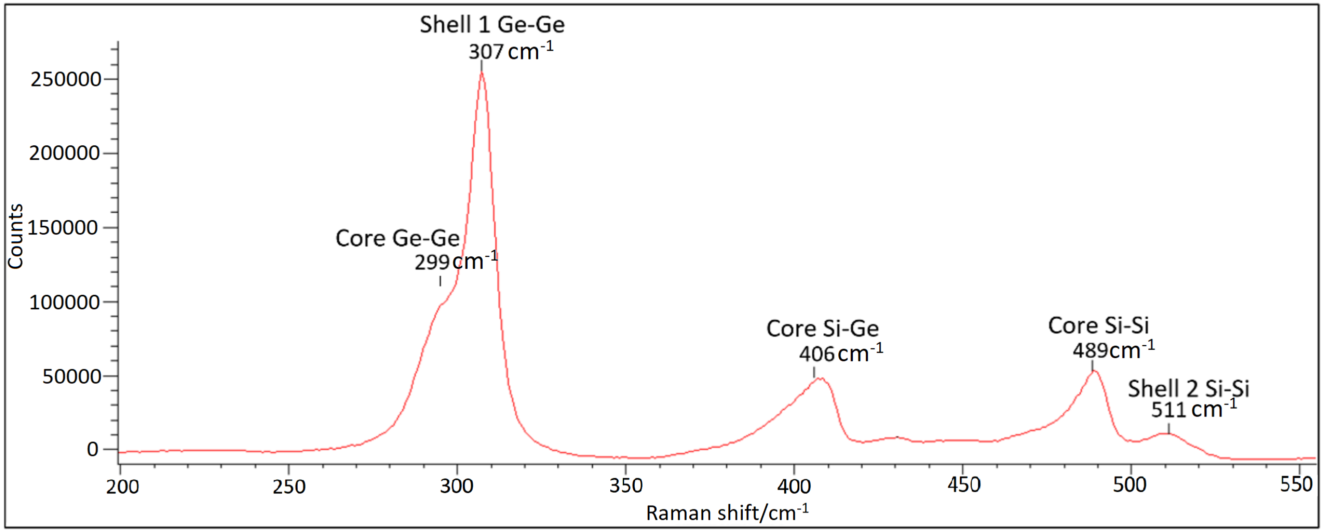
- Vibrational Spectroscopy
- Raman bands arise from specific molecular vibrations
- Used to probe strain and elemental content

- Tensile Strain in Si → red shift of Si-Si mode
- Compressive strain in Ge → blue shift of Ge-Ge mode

Raman Spectroscopy of SiGe and core-double-shell NWs



Raman spectra of Si_xGe_{1-x} NW

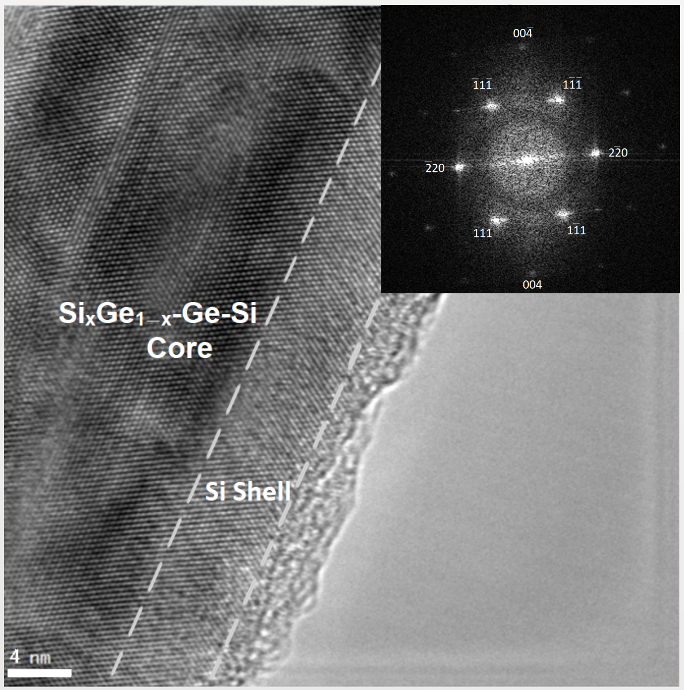


Raman spectra of Si_xGe_{1-x}−Ge−Si core-double-shell NW

Transmission Electron Microscopy (TEM)

- Microscopy technique in which a beam of electrons is transmitted through a specimen to form an image
- Planar and cross-sectional TEM are used to probe the crystal structure and measure the shell thickness.

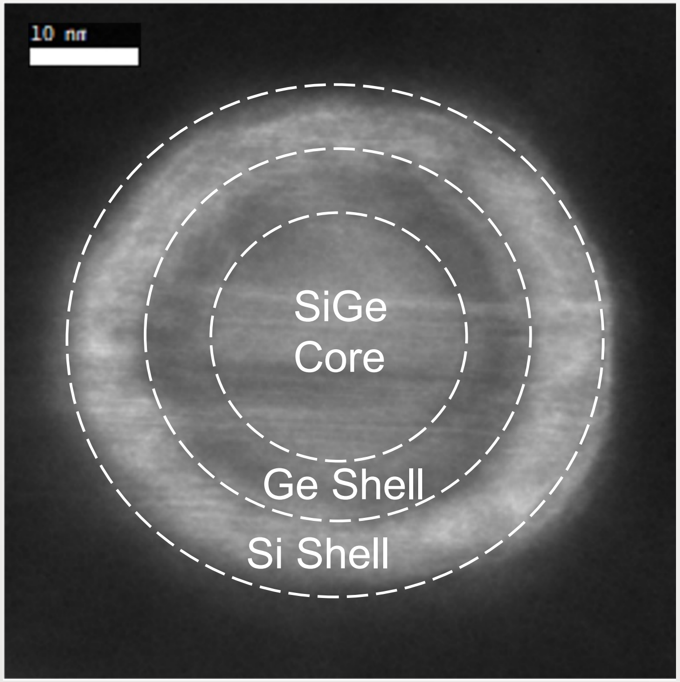
TEM of core-double-shell NWs



Planar view TEM of a Si_xGe_{1-x}−Ge−Si NW. Inset: Fourier Transforms (FFT) of the NW.

- Single crystal structure, epitaxial shell growth
- The FFT is used to determine the nanowire orientation
- The VLS growth yields NWs along the <110> direction

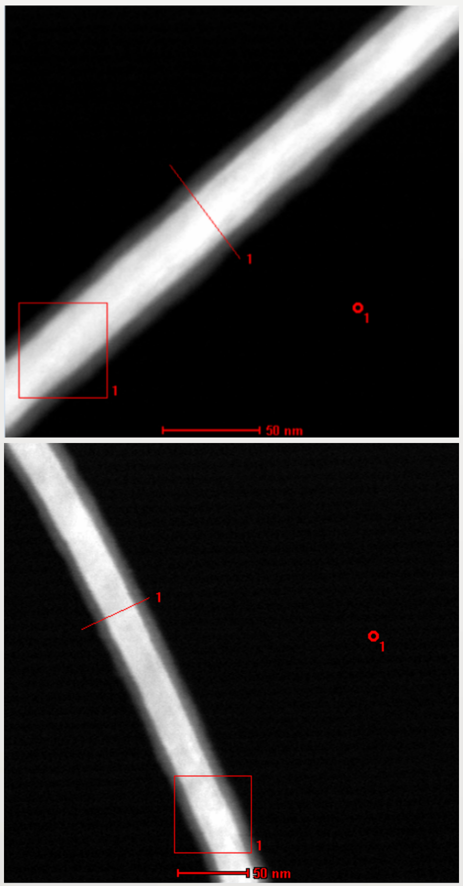
TEM of core-double-shell NWs



Cross-sectional TEM of a Si_xGe_{1-x}−Ge−Si NW.

- Cylindrical core
- Slightly faceted shells
- Core: 10-30 nm
- Ge Shell: ~4 nm
- Si Shell: ~5 nm

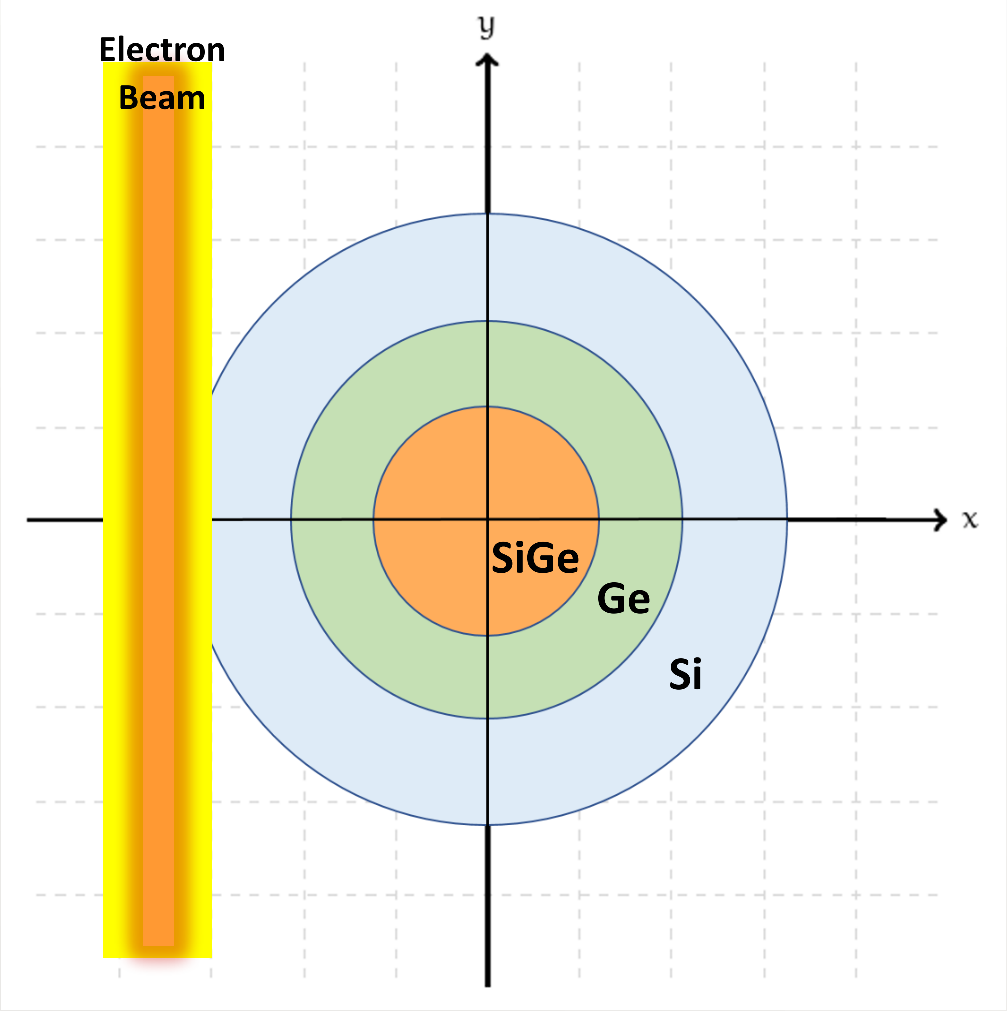
Energy Dispersive X-ray Spectroscopy (EDX)



STEM images of Si_xGe_{1-x}−Ge−Si NWs.

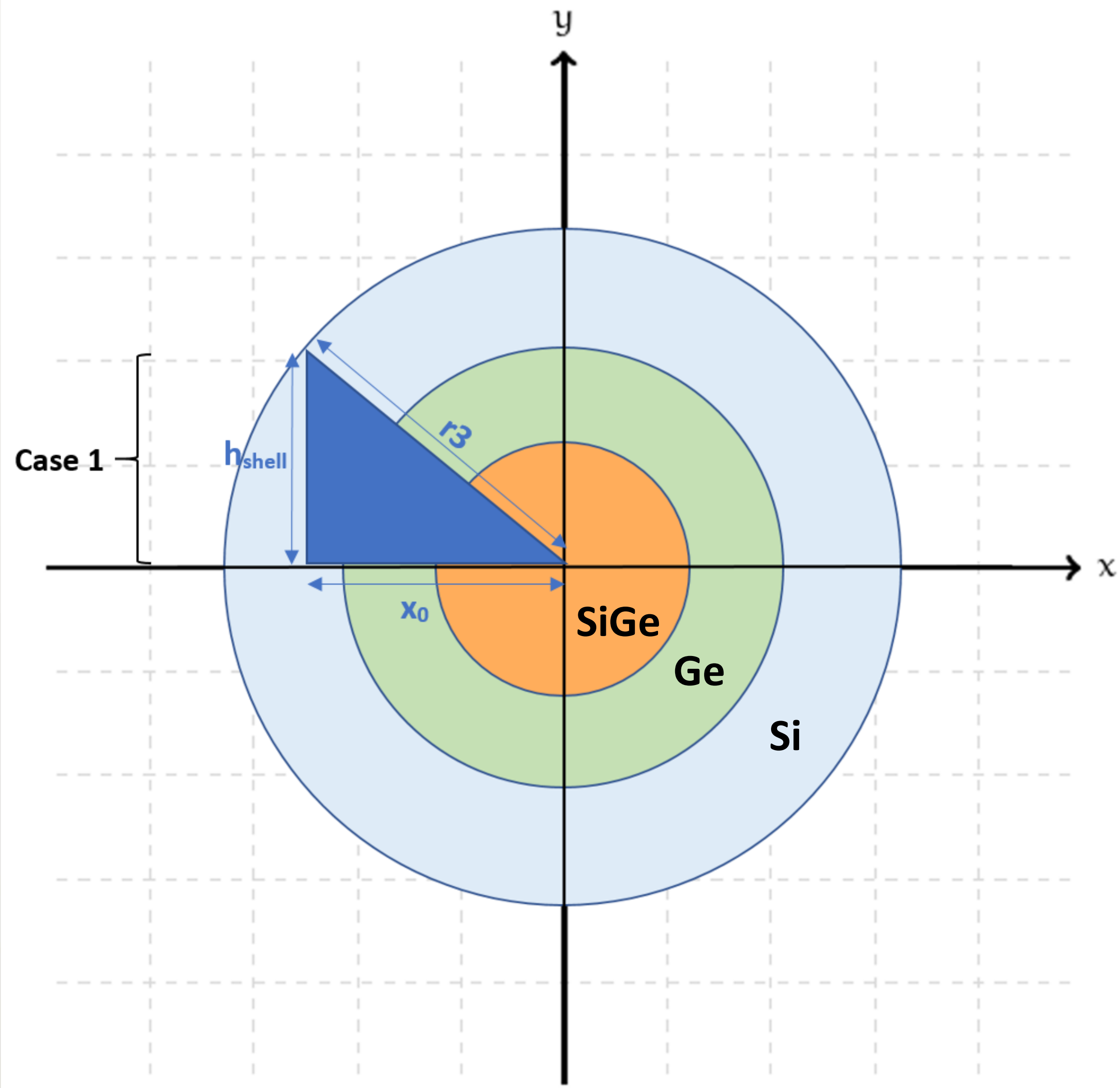
- EDX used to determine the shell thickness and core elemental composition
- Measurements acquired using line scans across the nanowires
- Si and Ge signals are fitted with a model based on the convolution of nanowire geometry and a Gaussian electron beam

EDX Linescan Across NW



Cylindrical morphology was assumed for simplicity

EDX Linescan Across Nanowire



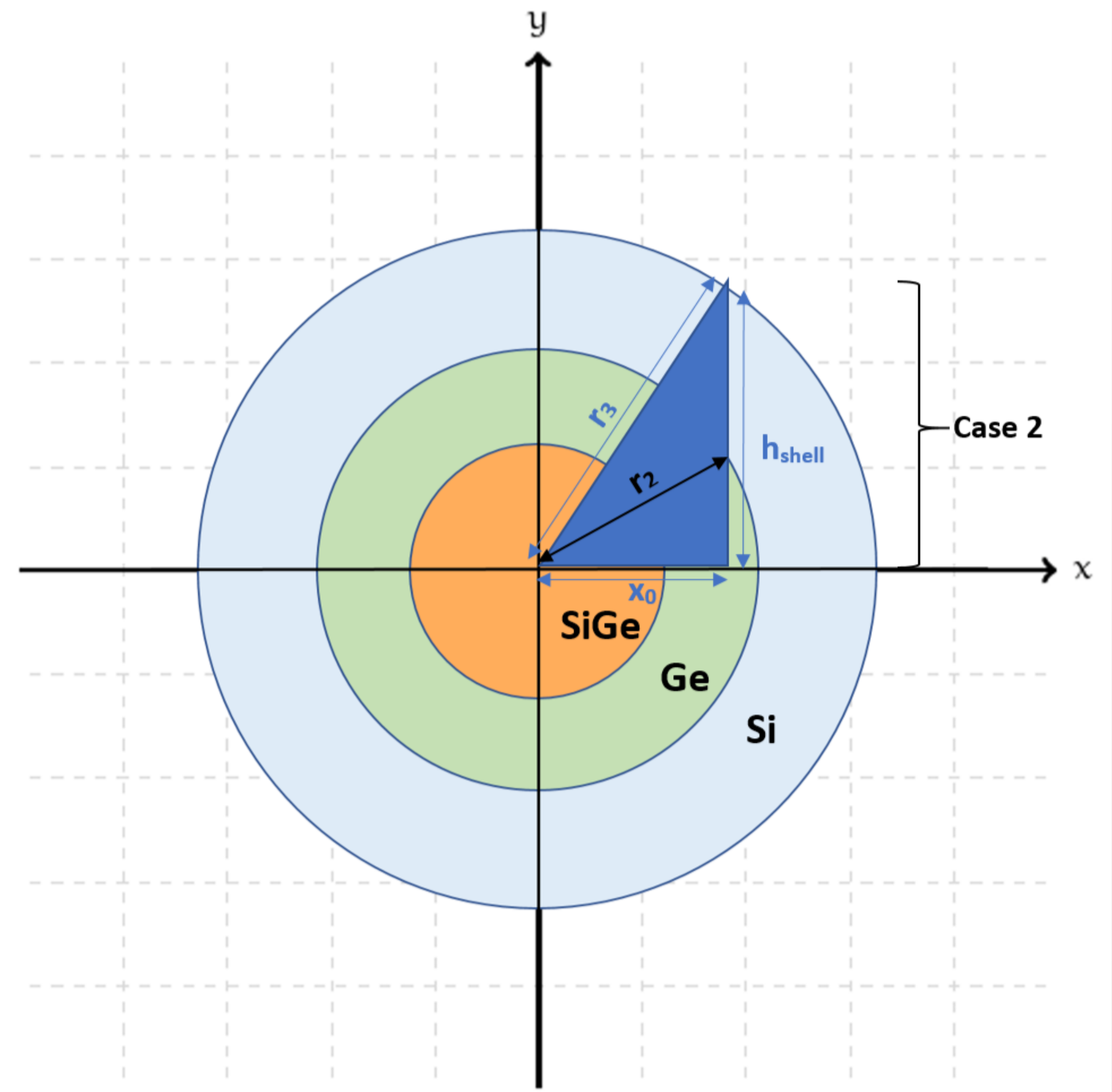
Case 1:

$|x_0| \geq r_2$ & $|x_0| \leq r_3$

$\psi_{Si} = 2 * \sqrt{(r_3^2 - x^2)}$

$\psi_{Ge} = 0$

EDX Linescan Across Nanowire



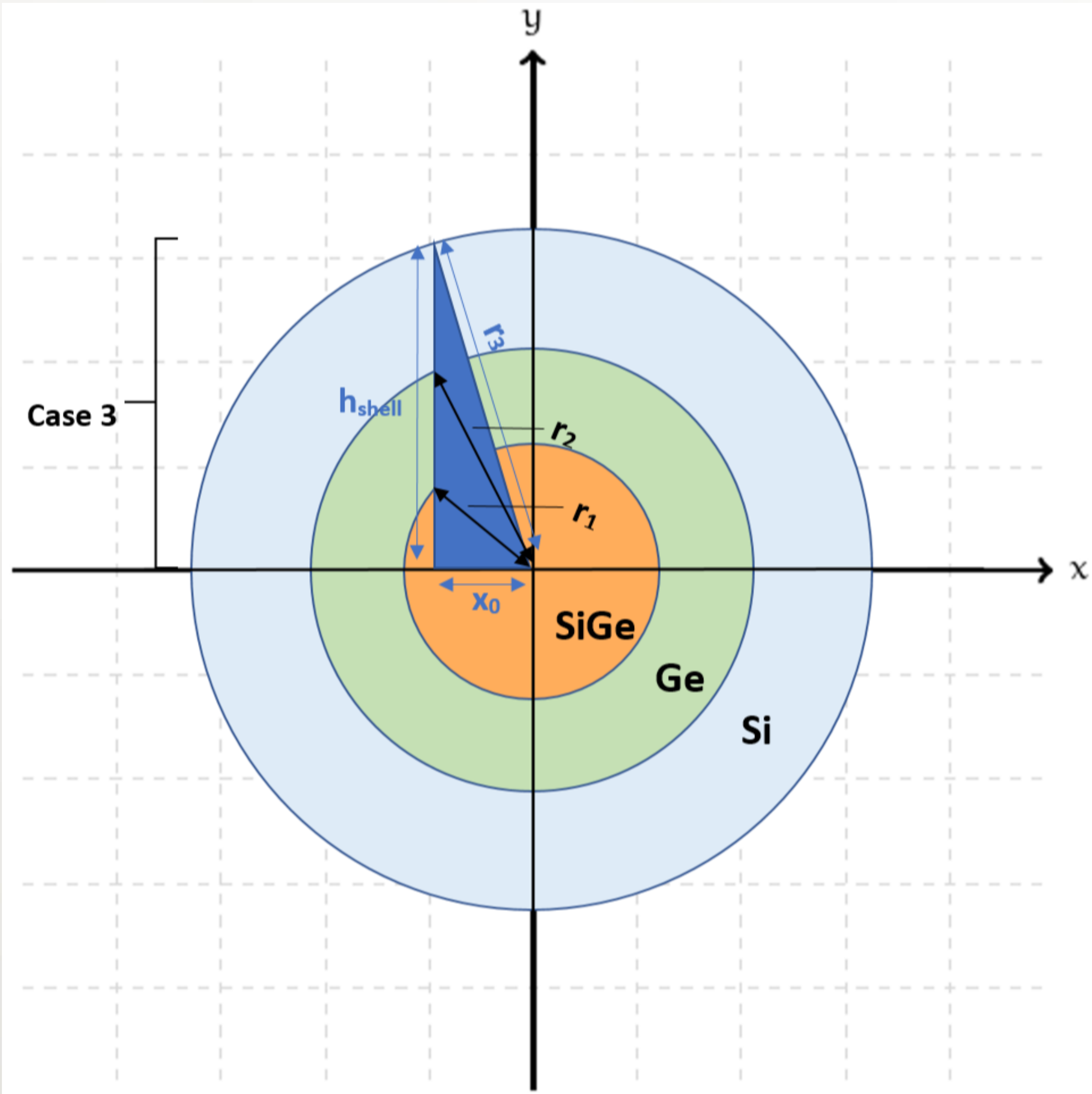
Case 2:

$|x_0| \geq r_1$ & $|x_0| < r_2$

$\psi_{Si} = 2*(\sqrt{(r_3^2 - x^2)} - \sqrt{(r_2^2 - x^2)})$

$\psi_{Ge} = 2*\sqrt{(r_2^2 - x^2)}$

EDX Linescan Across Nanowire



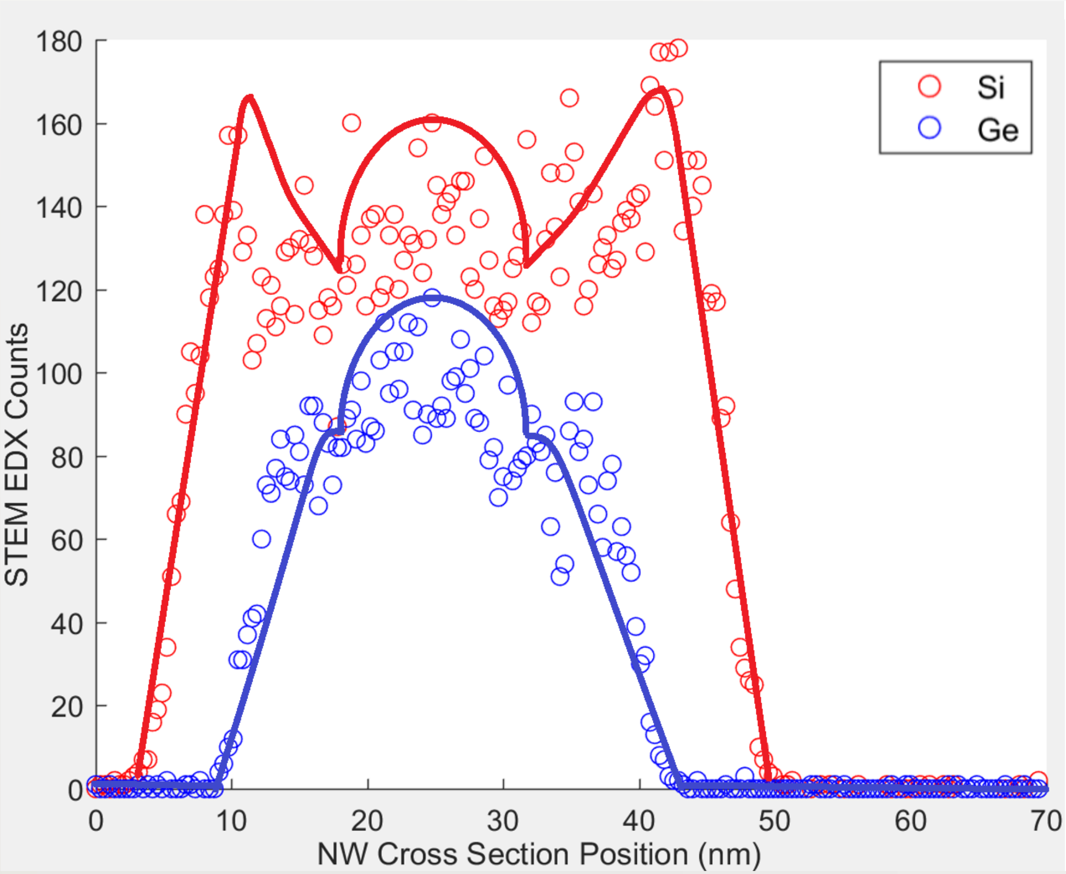
Case 3:

$|x_0|<r_1$

$\psi_{Si}= 2*(X_{Si}*(\sqrt{}(r_1^2-x^2) + (\sqrt{}(r_3^2-x^2) - \sqrt{}(r_2^2-x^2)))$

$\psi_{Ge}= 2*(\sqrt{}(r_2^2-x^2)-(\sqrt{}(r_1^2-x^2)) + (1- X_{Si}) \sqrt{}(r_1^2-x^2)$

EDX Linescan Across Nanowire



- Core radius: 18 nm
- Shell 1 thickness: 4 nm
- Shell 2 thickness: 5 nm
- Concentration of Si vs. Ge in shell: 0.5
- E-beam: 1.5
- Center: 70
- Proportionality coefficient: 0.8

MATLAB simulation of EDX data from both Si and Ge K-alpha signals

Future Work

- Build an accurate mathematical model taking actual morphology and beam incident angle to the nanowire
- Quantify and understand strain in NWs using growth parameters (temperature, pressure, gas flow, etc.) in Raman spectroscopy data

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