Python-Driven Automated Analysis and Machine Learning for Semiconductor Nanowire Characterization

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JSNN Joint School of Nanoscience and Nanoengineering

Why Nanowires? Why GaAsSb?

- Nanowires: 1D crystal structures with a high surface-area-to-volume ratio
- GaAsSb: tunable bandgap suited for near-infrared detection
- Can be grown on non-native substrates despite lattice mismatch — enabling integration with existing platforms

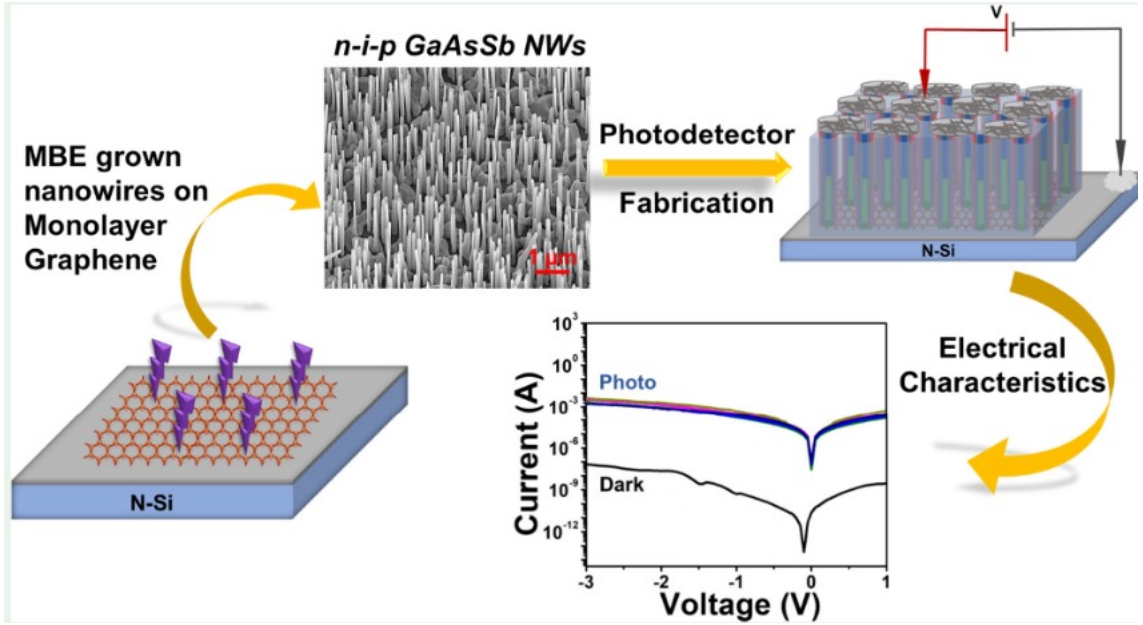
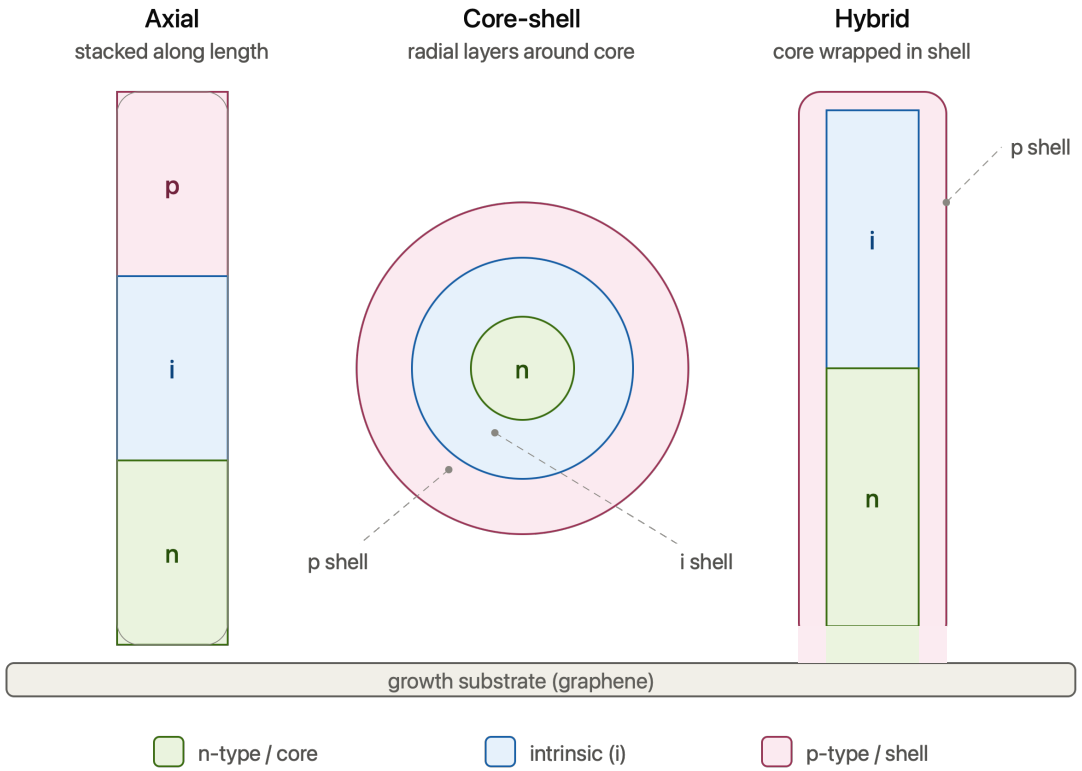


Image curtesy of paper: Study of n−i−p Axial/Core−Shell Hybrid GaAsSb Dense Nanowire-2 Based Near-Infrared Photodetectors on Graphene
https://pubs.acs.org/action/showCitFormats?doi=10.1021/acsanm.4c01241&ref=pdf

Growing the Nanowires: MBE

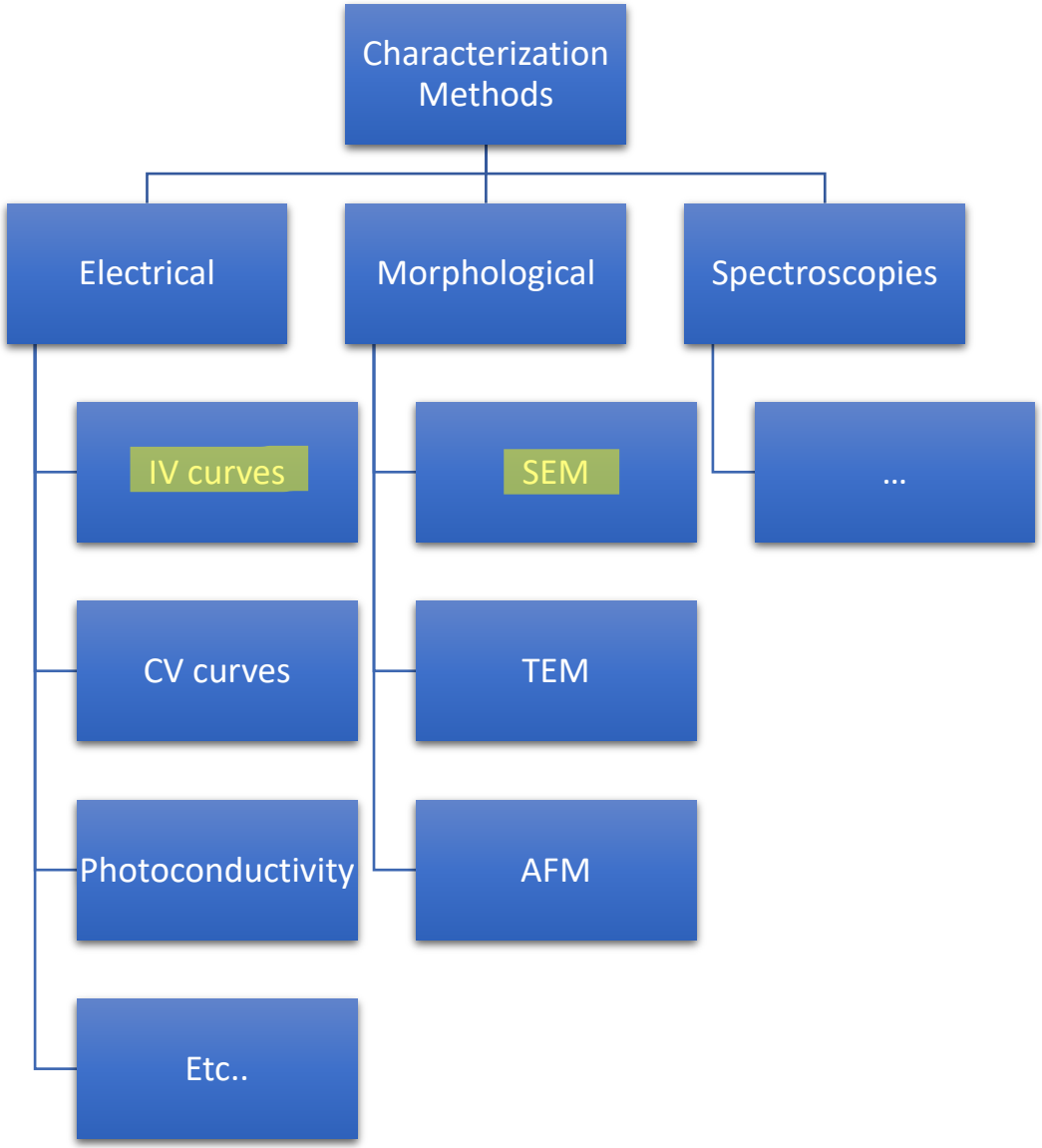
- Grown via Molecular Beam Epitaxy (MBE) on a graphene-coated substrate
- Ga, As, and Sb atoms deposited in ultra-high vacuum, self-assembling into wires
- Three structural variants: axial (segments stacked end-to-end), core-shell (radial layers), and hybrid (stacked core, more layers wrapping around)



* Image is only for conceptual reference only. Actual product may differ *

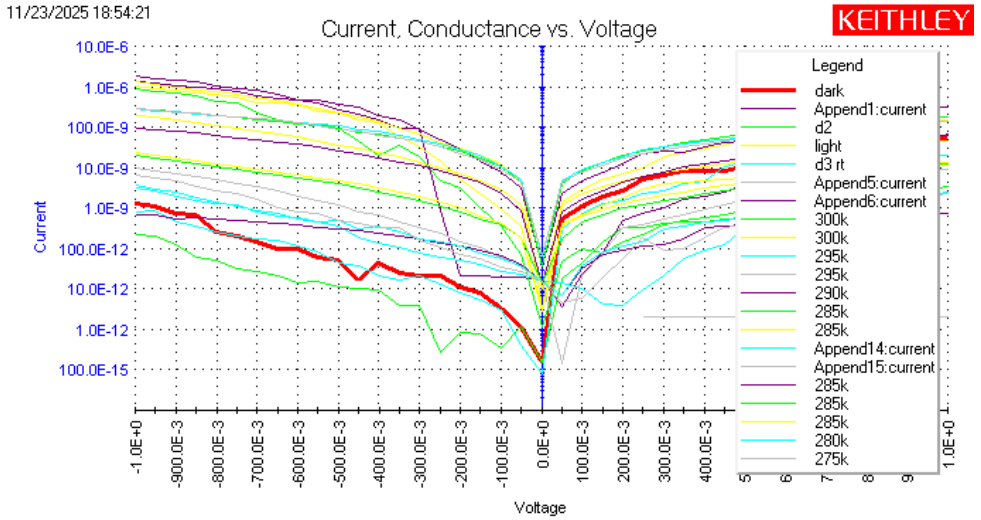
Characterizing Nanowires

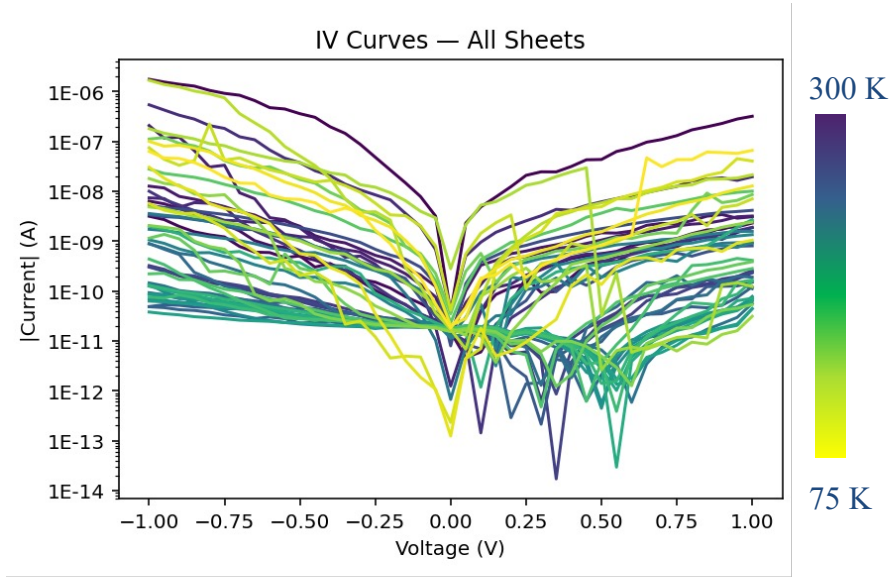
- Electrical characterization — current vs. voltage (I-V) curves & Arrhenius analysis
- Structural characterization — scanning electron microscopy (SEM) imaging & machine learning
- Together: a fuller picture of what makes one nanowire sample perform differently from another



Probing Transport: I-V Curves

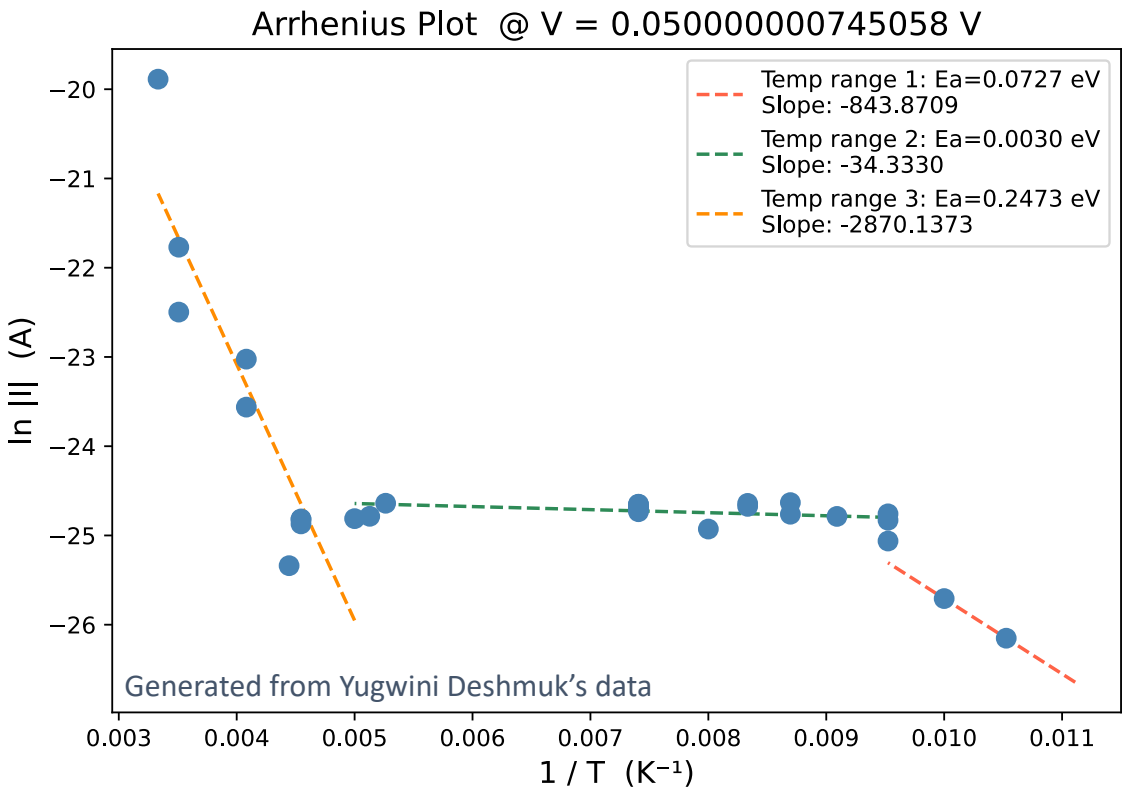
- I-V (current-voltage) curves capture how much current flows through a device at a given bias
- Dark current (no illumination) reveals leakage and baseline transport behavior
- Measured across a range of temperatures — different physical mechanisms dominate in different regimes
- Multiple sweeps are taken at the same temperature to help separate real signal from noise
- Likely cause of noise : the probe needle shifting, misaligning, or not fully settling into contact during measurement

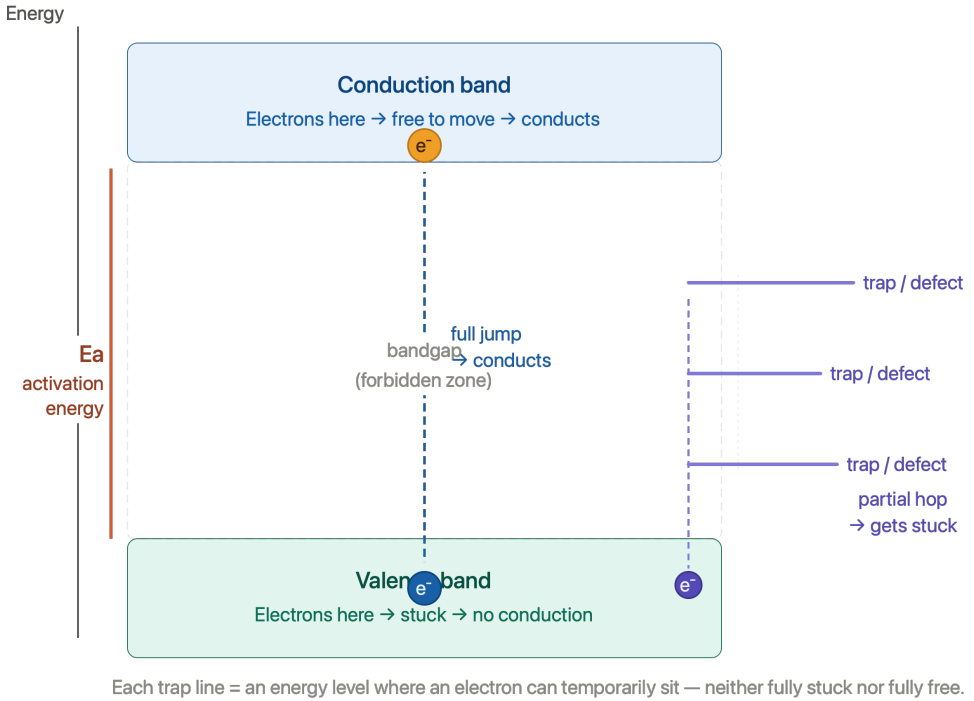




Generated from Yugwini Deshmuk's data

From I-V to Arrhenius





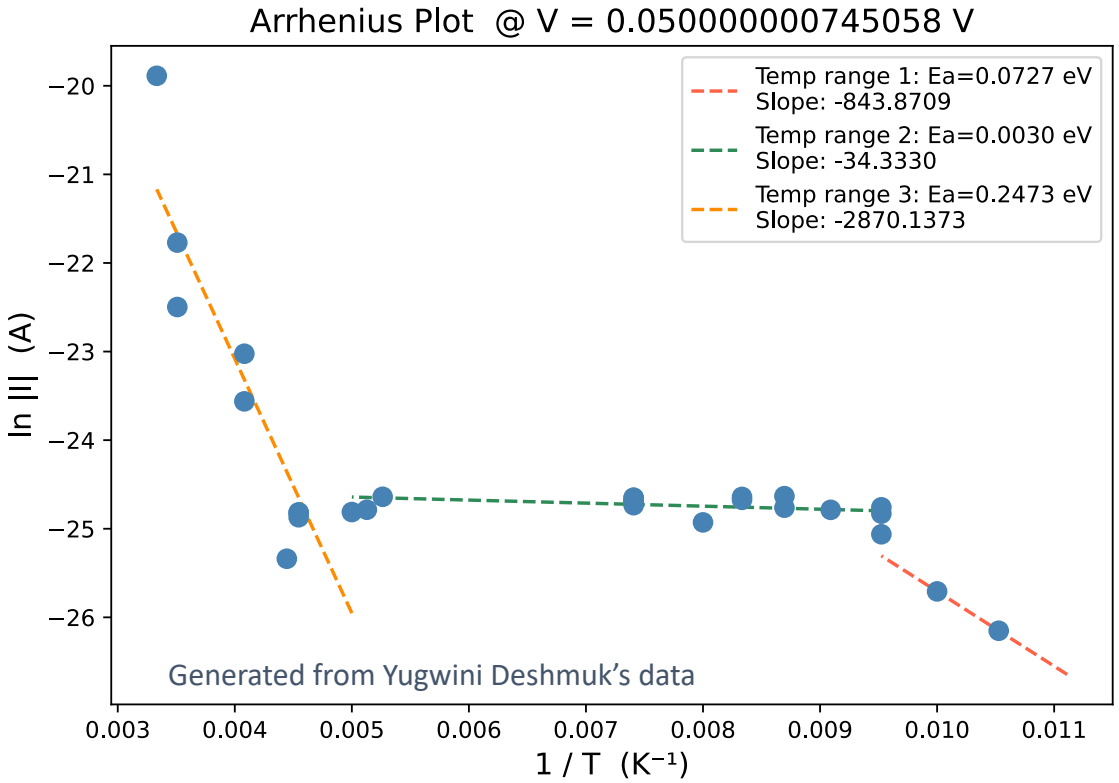
Each trap line = an energy level where an electron can temporarily sit — neither fully stuck nor fully free.

- Arrhenius plot: ln|I| vs. 1/T
- Assumes current is thermally activated: $I \propto \exp(-Ea / kBT)$
- The slope of each linear region gives an activation energy (Ea)

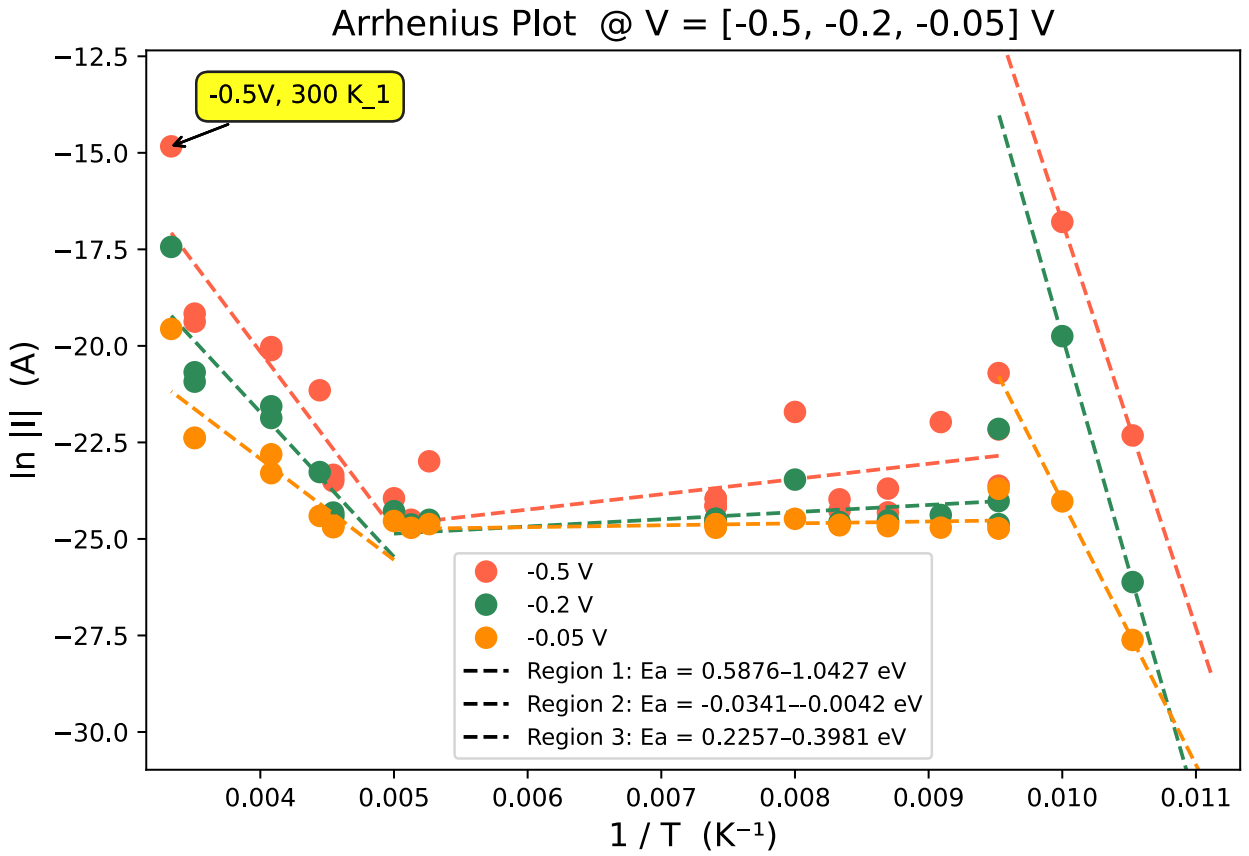
- Activation Energy (Ea): the energy needed to excite an electron from the valence band to the conduction band (or from a trap/defect state)

Activation Energies (Ea)

- Different temperature regimes can be governed by different mechanisms — each with its own Ea
  - High temperature – diffusion current
    - electrons jump the entire bandgap
  - Medium range – Shockley-Read-Hall effect
    - electrons uses defects in the material to move partially up the bandgap
  - Low – possibly surface leakage or dopant freeze-out
    - Dopant on the nanowire did not ionized properly



Superimposed Arrhenius Plots at Chosen Voltages



Generated from Yugwini Deshmuk's data

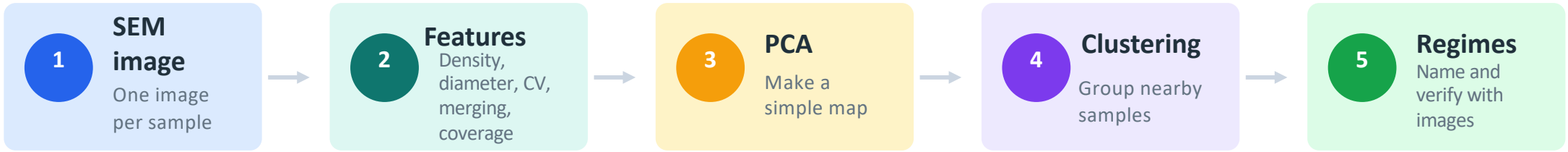
- Ea acts as a fingerprint for the dominant transport/recombination mechanism at a given temperature and bias

Next: Looking at the Nanowires Themselves

Structural characterization — SEM imaging & machine learning

OVERVIEW

Workflow

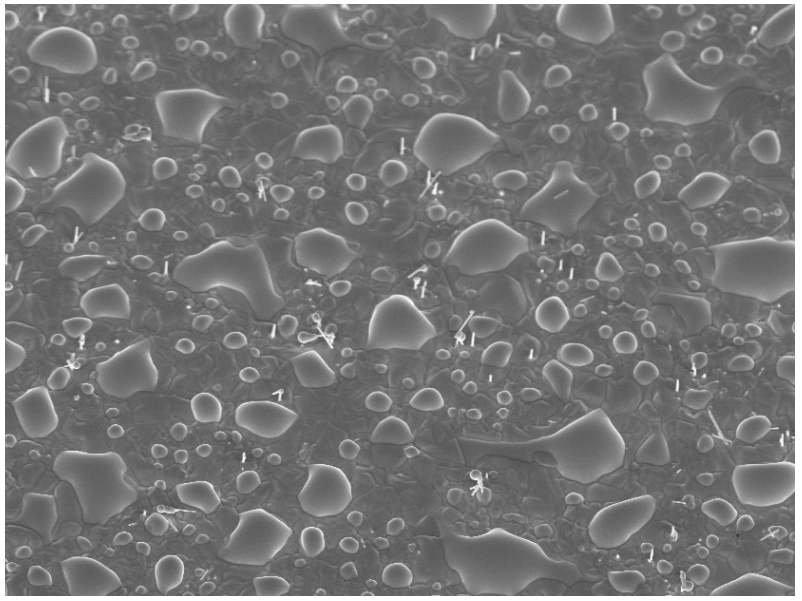


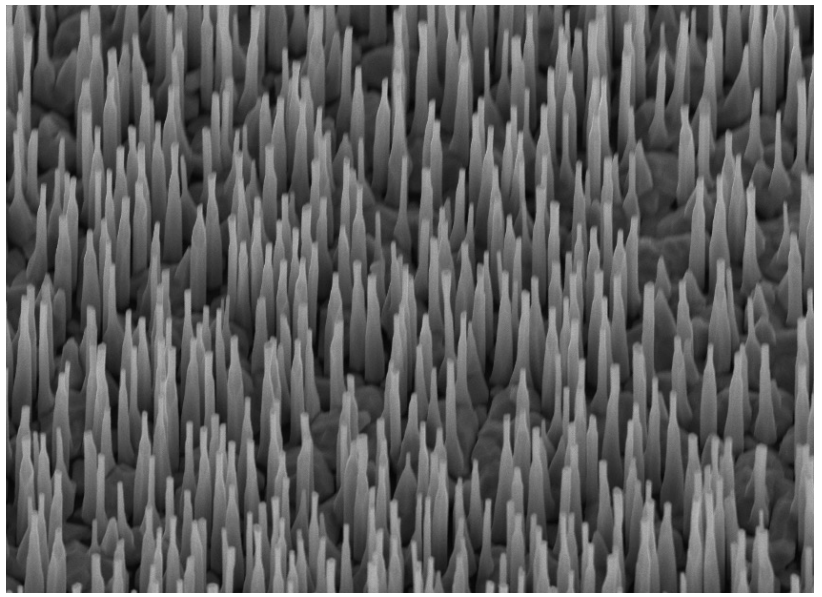
Currently have a candidate grouping. The next scientific step is to confirm each cluster with the original SEM images.

Goal: Use ML to group the SEM images automatically so we can read the features of each group, adjust MBE growth settings, and even automate nanowire growth.

Why Look at Morphology? 1 2

- One SEM image per sample is measured for six quantitative features: density, mean diameter, diameter variability (CV%, uniformity), % merged wires, surface coverage, angle spread

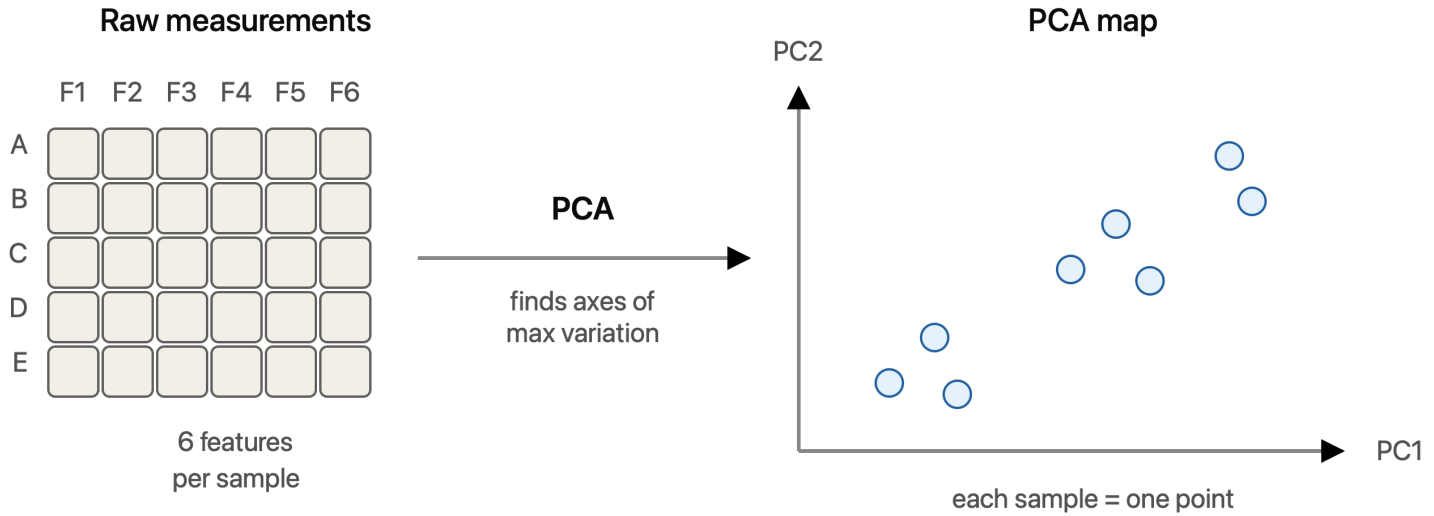




From Images to a Map: PCA + Clustering

3 4

- Principal Component Analysis (PCA) is a technique that reduces the number of features in a dataset while keeping the most important information (aka the principal components).
  - PC1 captures the most spread in the dataset, PC2 captures the most spread in a different (perpendicular) direction, and so on
- K-means clustering: algorithm that groups nearby samples automatically. Unsupervised method (no predefined labels)

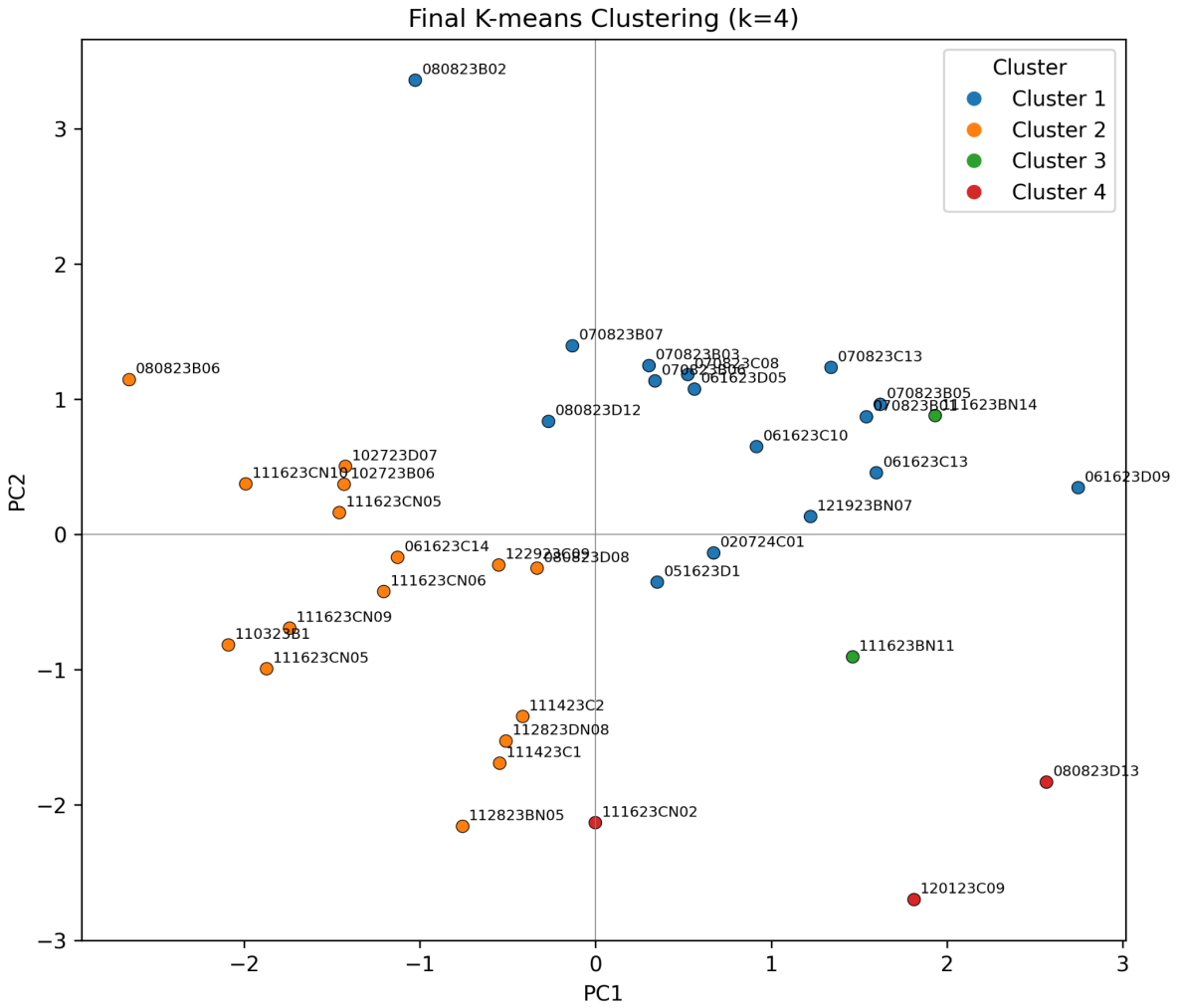


PCA re-expresses many correlated measurements as a few new combined axes that capture the most sample-to-sample variation.

It doesn't group samples — it only makes them easier to compare and visualize.

What We Found

- k = 4 gave the best (though still modest) cluster separation
  - k=4 had the highest silhouette score (~0.34)
  - *Silhouette score (-1 to +1)* : metric to evaluate clustering models. The higher the better.
- Two larger groups (blue, orange) and two small groups (green, red) emerged
- Small clusters need extra scrutiny — could be real morphology types, or outliers



Credit: Arjun Sharma Poudel

What Defines Each Group

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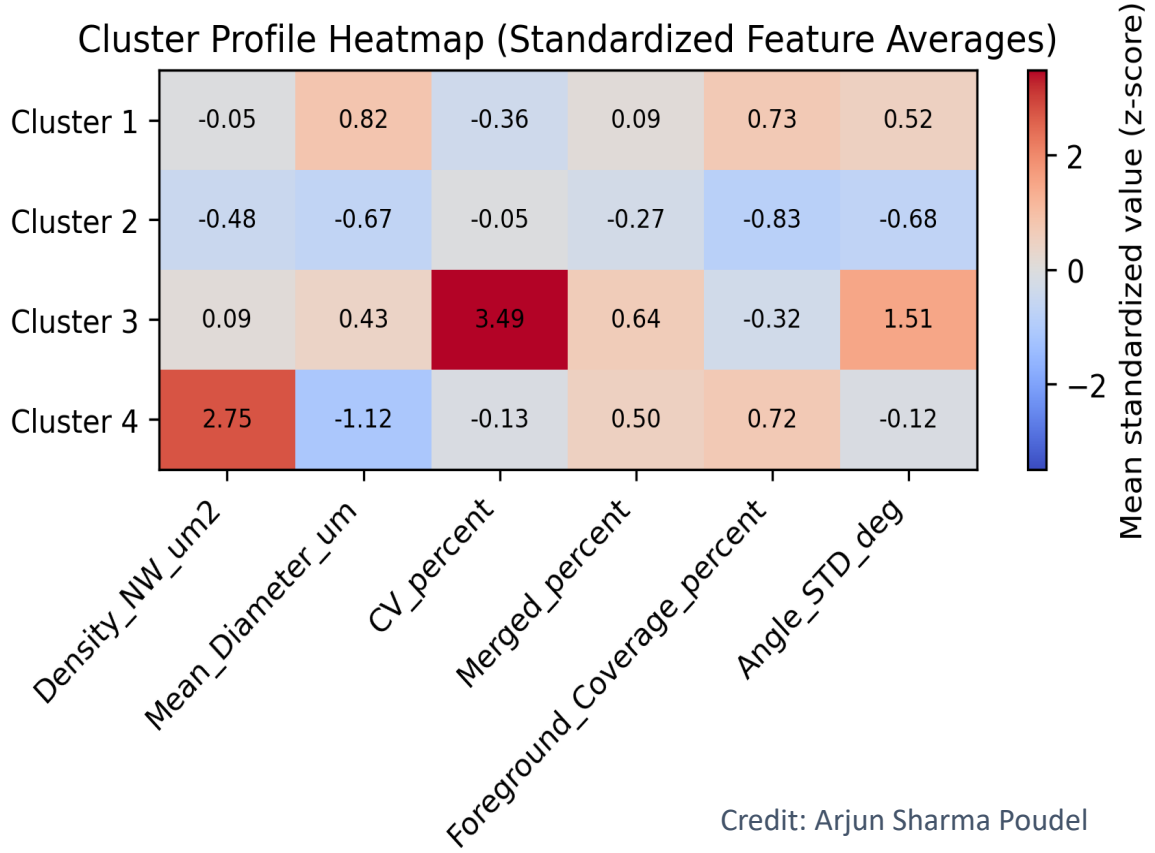
- The heatmap translates cluster assignments back into physical meaning
  - Cluster 1: larger-diameter, high coverage
  - Cluster 2: Sparse / low coverage
  - Cluster 3: Highly nonuniform
  - Cluster 4: High density, small diameter
- These are candidate groupings — next step is verifying against SEM images and MBE growth logs



Credit: Arjun Sharma Poudel

Summary

- Electrical analysis (I-V / Arrhenius) tells us how a device behaves
- Structural analysis (SEM / ML) tells us why, in terms of physical form
- Together: a fuller diagnostic picture connecting growth conditions to device performance
- Next: validate clusters against SEM images

Acknowledgements

- Hirandeep Kuchoor, Yugwini Deshmukh, Rashmita Baruah, Jia Li, Christopher Winkler, Lew Reynolds, Shanthi Iyer; Study of n–i–p Axial/Core–Shell Hybrid GaAsSb Dense Nanowire-Based Near-Infrared Photodetectors on Graphene. *ACS Appl. Nano Mater.* 8 November 2024; 7 (21): 24299–24314. https://doi.org/10.1021/acsanm.4c01241
- Brugnolotto, Enrico et al. “Machine Learning Inspired Nanowire Classification Method based on Nanowire Array Scanning Electron Microscope Images.” *Open research Europe* vol. 4 43. 28 Jun. 2024, doi:10.12688/openreseurope.16696.2
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