

Nanowire Modeling & Design Technical Report

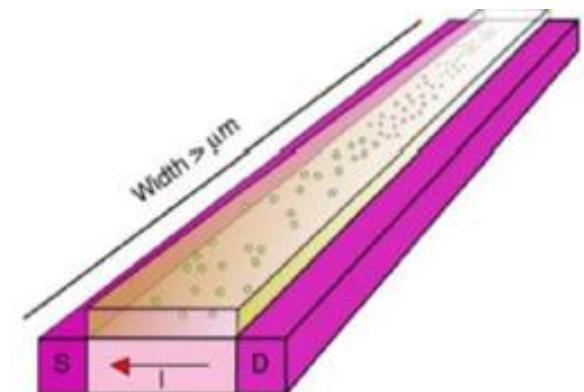
Aidan Prendergast, Claire Ryan Hagar, Imtiaz Ahmed

ajprende@purdue.edu, ryan253@purdue.edu,
ahmed202@purdue.edu



School of Electrical and
Computer Engineering

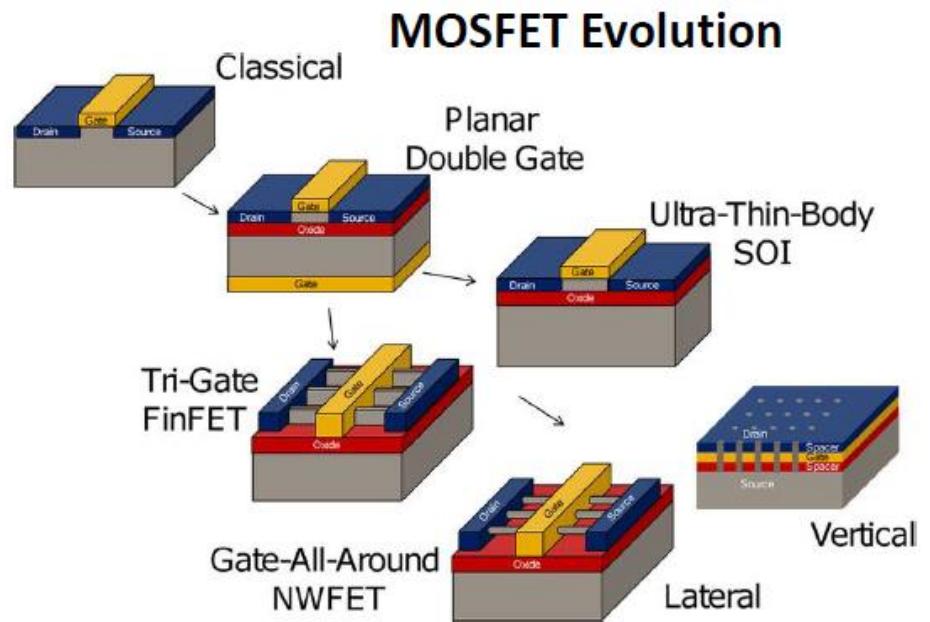
- Traditional Planar MOSFET faces several challenges as device dimensions are scaled down.
 - Increased Short channel effects
 - Increased Leakage Currents
 - Deteriorating On/Off Current ratio and Subthreshold Swing
 - Drain-Induced-Barrier-Lowering (DIBL): Drain gets control over Channel conduction
- Continuing Moore's Law—the trend of doubling transistor density approximately every two years- thus becomes more difficult
- Nanowire Transistors provide a nifty way to alleviate these challenges



Traditional
Planar MOSFET

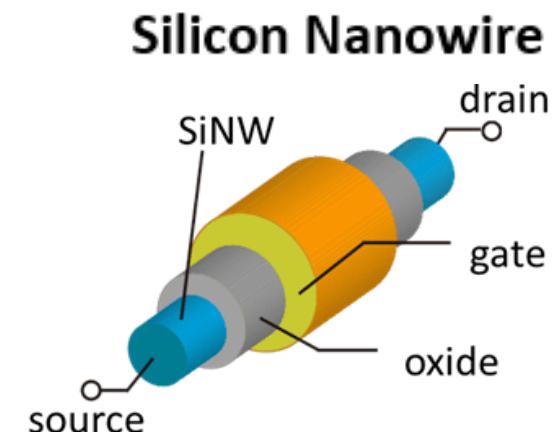
Nanowire Transistors:

- Gate surrounds Channel
- Provides greater Gate control over channel conduction leading to
 - higher switching speeds
 - lower power consumption
 - improved overall performance in terms of On/Off Current ratio and Subthreshold Swing



Goal of this Project:

- Analysis and Comparison of Gate scaling effects in Planar and Nanowire MOSFET
- Analysis of Classical (Drift-Diffusion), Semi-classical (Top-of-the-barrier), and Quantum Transport models of Nanowires
- Exploration of electron and hole nanowire characteristics



Classical MOSFET Limitations (Quad Chart 1 of 2)

Objective:

- Understand the various physical effects when scaling the gate length of a MOSFET.

Problem:

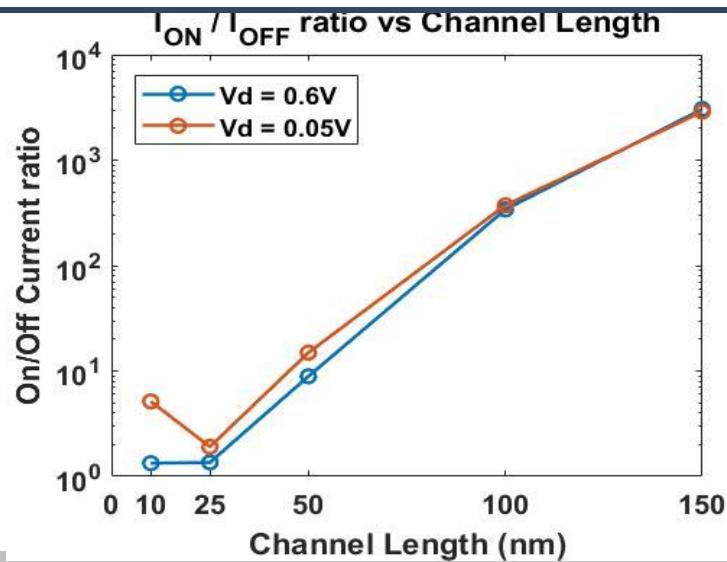
- The ON/OFF current ratio, a large ON current, and the subthreshold swing can all be affected from the gate length.

Results / Impact:

- The ON/OFF current ratio increases as the channel length increase: inverse relationship to subthreshold swing. Also, On Current and Off Current decrease as channel length increases.
- The ON/OFF current ratio is shown below. Others are shown in the Appendix ([Transistor Features](#)).
- As we scale the device down, Leakage currents become significant, resulting in high OFF currents and thus deteriorated device performance.

Approach:

- An n-type MOSFET was modeled in NanoHub's MOSFET, varying the gate length from 150nm to 5nm.
- Please see [NanoHub MOSFET Inputs](#) (located in the Appendix) for the inputs used in this simulation.



Classical MOSFET Limitations (Quad Chart 2 of 2)

Objective:

- Understand the design changes that can and have been made to increase transistor performance.

Problem:

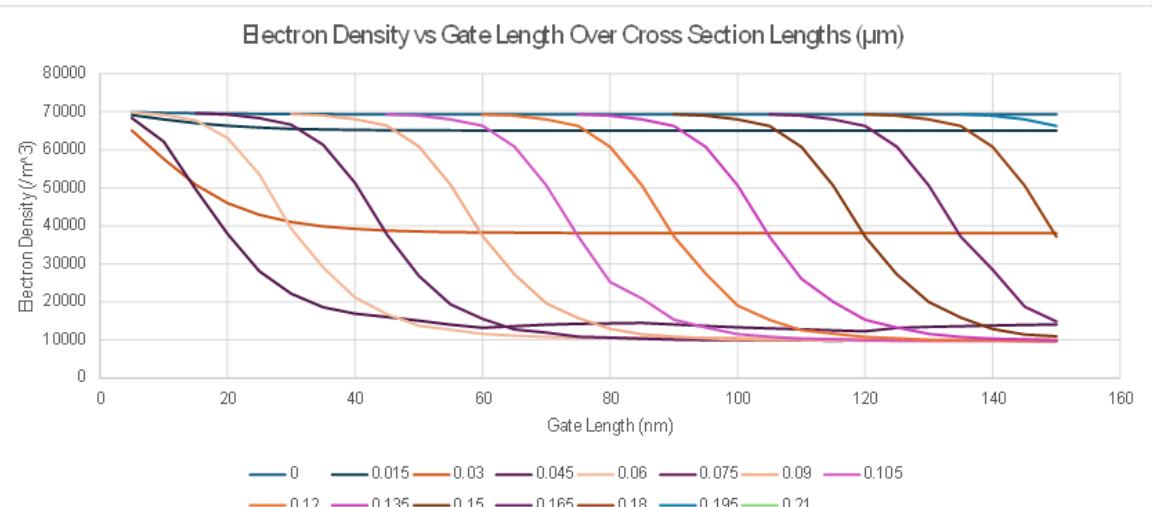
- Various characteristics can be changed to affect the transistor performance.

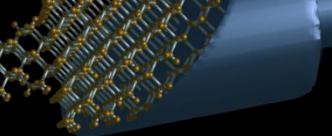
Approach:

- An n-type MOSFET was modeled in NanoHub's MOSFET, varying the gate length from 150nm to 5nm.
- Please see [NanoHub MOSFET Inputs](#) (located in the Appendix) for the inputs used in this simulation.

Results / Impact:

- Both the voltage potential and electron density is decreased with an increase of gate length.
- The relationship of electron density and gate lengths is shown below. Please see [Voltage Potentials](#) (located in the Appendix) for the relationship of voltage potential.





Nanowire with Drift Diffusion (Quad Chart 1 of 2)

Objective:

- Understand how critical transistor parameters respond to the scaling of the gate length and nanowire diameter.

Problem:

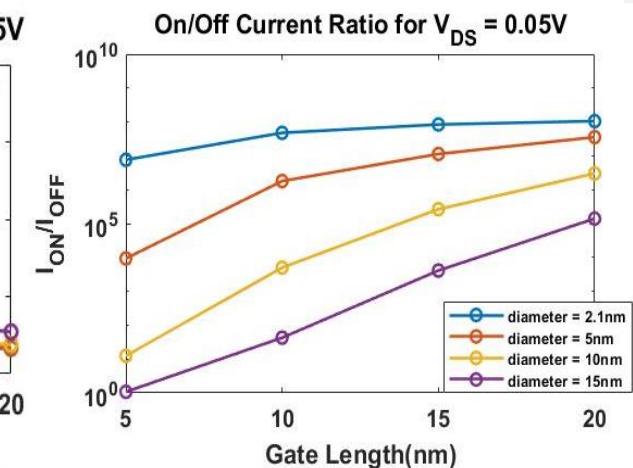
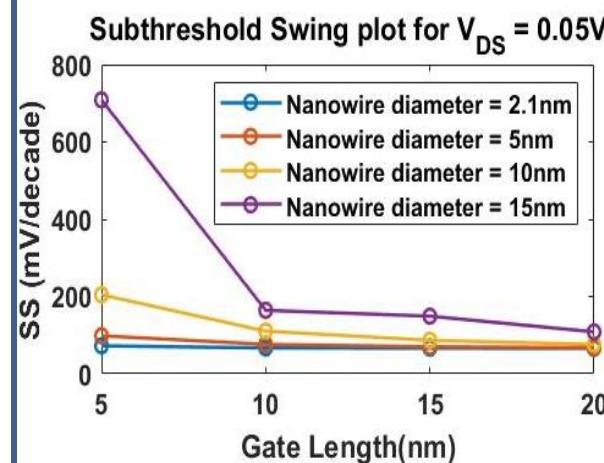
- The ON/OFF current ratio, threshold voltage, and subthreshold swing can all be impacted by changing parameters.

Approach:

- NanoHub's NANOFINFET tool was used to simulate device performance while varying the nanowire diameter and gate length.
- Please see [NANOFINFET Inputs](#) (located in the Appendix) for the inputs used in this simulation.

Results / Impact:

- The On/Off current ratio and subthreshold swing improves with decreasing diameter and increasing gate length (figure).
- The threshold voltage increases with increasing gate length and diameter (Appendix - [Nanowires with Drift Diffusion: Threshold Voltages](#)).



Nanowire with Drift Diffusion (Quad Chart 2 of 2)

Objective:

- Understand how energy band diagrams vary based on the scaling of the gate length and nanowire diameter.

Problem:

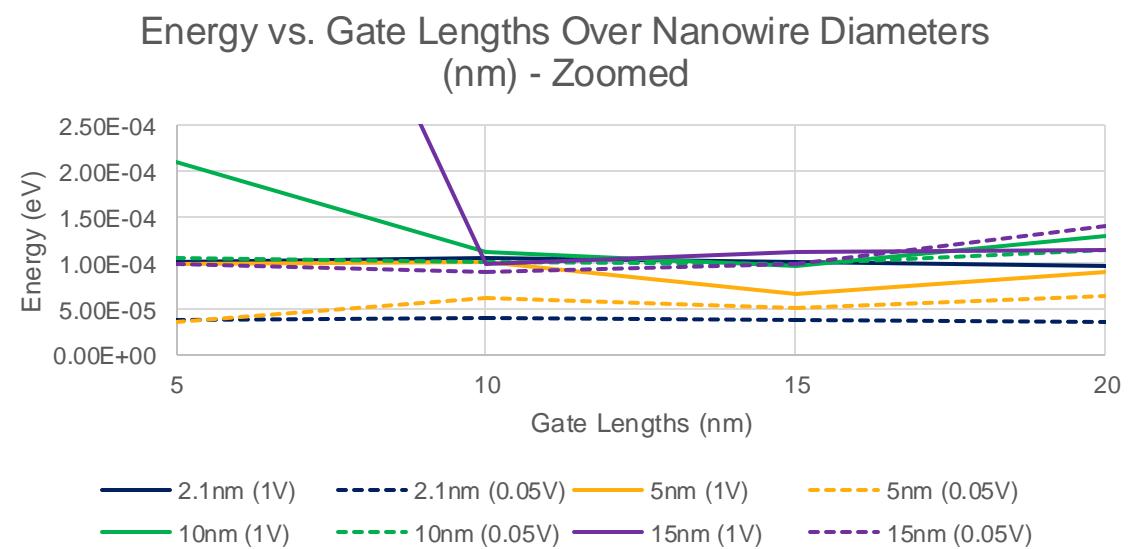
- How does the gate barrier height change as the gate length decreases?

Approach:

- NanoHub's NANOFINFET tool was used to simulate device performance while varying the nanowire diameter and gate length.
- Please see [NANOFINFET Inputs](#) (located in the Appendix) for the inputs used in this simulation.

Results / Impact:

- Please see [Energy vs. Gate Lengths](#) (located in the Appendix) for more detailed plots.
- Generally, the gate barrier height will increase as the gate length increases. Additionally, a decrease in source-drain voltage will result in a decrease of energy.



Objective:

- Understand workfunctions

Problem:

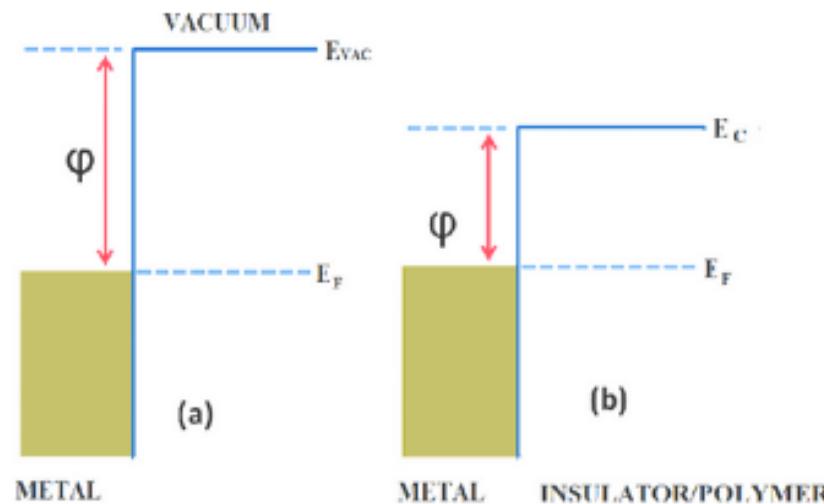
- What is the physics of "workfunction"?
- What are reasonable experimental values of workfunction?

Results / Impact:

- Workfunction is the minimum energy required to move an electron to a place away from the surface, but still close enough to be impacted by the surface's electric field. (see [1])
- For silicon, reasonable workfunction values range from 4.60 – 4.85 eV. (see [1])

Approach:

- The term workfunction was researched online to gain an understanding of its physics.



[1]

Nanowire with Drift Diffusion - Workfunction Variations and Gate Potential Analysis (Quad Chart 2 of 2)

Objective:

- Understand how a long vs short gate length nanowire effects the I-V characteristics.

Problem:

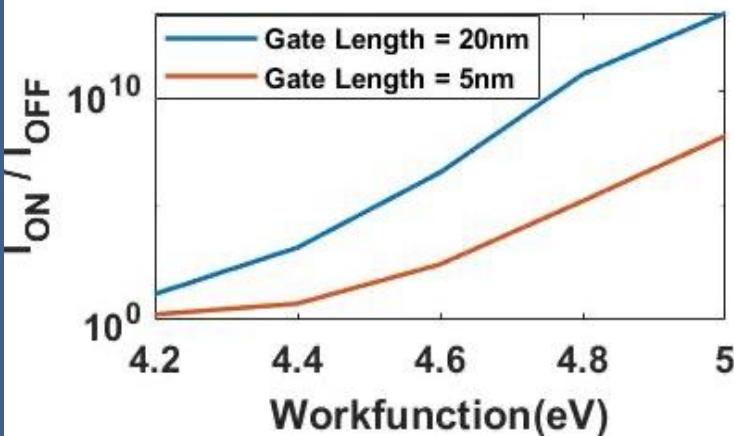
- The ON/OFF current ratio, threshold voltage, and subthreshold swing can all be impacted by changing parameters.

Results / Impact:

- As workfunction increases, the on/off current ratio increases (figure), and subthreshold swing decreases (appendix) as a result.
- Normalization of I-V data by choosing a workfunction is often done for getting rid of device-to-device variation when performing comparison
- Please see [Transistor Parameters](#) in the Appendix for additional plots.

Approach:

- NanoHub's NANOFINFET tool was used to simulate device performance while varying the gate contact workfunction.
- Please see [NANOFINFET Inputs](#) (located in the Appendix) for the inputs used in this simulation.



Smaller Gate device with low workfunction
→ barrier too low
→ higher I_{OFF}

Nanowire Modes and Gating (Quad Chart 1 of 2)

Objective:

- Understand the relationship between electron masses and nanowires.

Problem:

- As the electron masses of Silicon change from 0.91 to 0.19, what do the wavefunctions and eigen energies mean for nanowire?

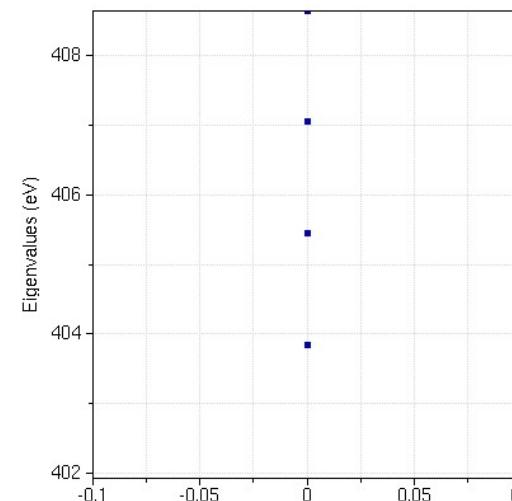
Approach:

- A flat Cylinder with height of 1nm was modeled in QuantumDotLab, varying the effective mass from 0.91 to 0.19.
- Please see [NanoHub Quantum Dot Lab Inputs](#) (located in the Appendix) for the inputs used in this simulation.

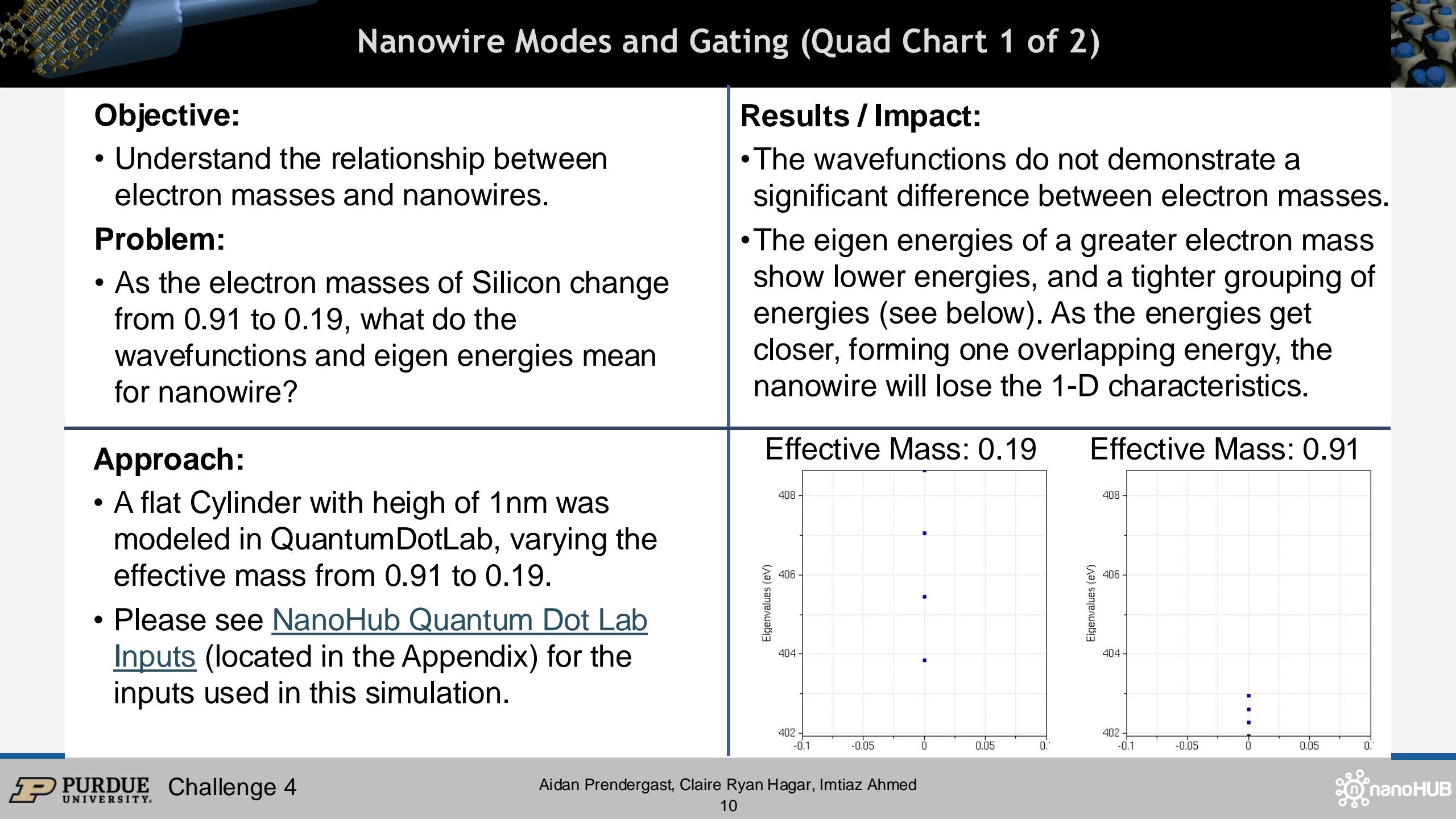
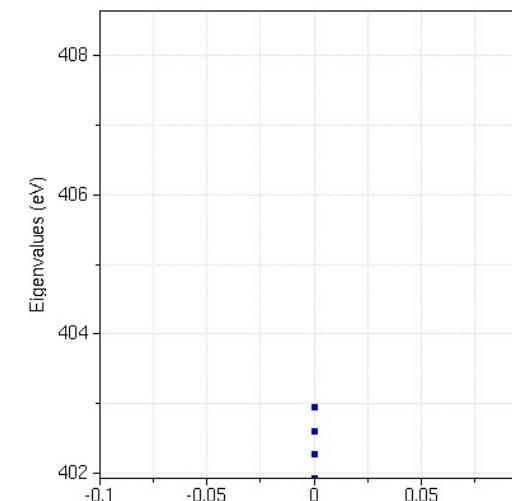
Results / Impact:

- The wavefunctions do not demonstrate a significant difference between electron masses.
- The eigen energies of a greater electron mass show lower energies, and a tighter grouping of energies (see below). As the energies get closer, forming one overlapping energy, the nanowire will lose the 1-D characteristics.

Effective Mass: 0.19



Effective Mass: 0.91



Nanowire Modes and Gating (Quad Chart 2 of 2)

Objective:

- Compare the I-Vg curves between difference crystal directions of Silicon.

Problem:

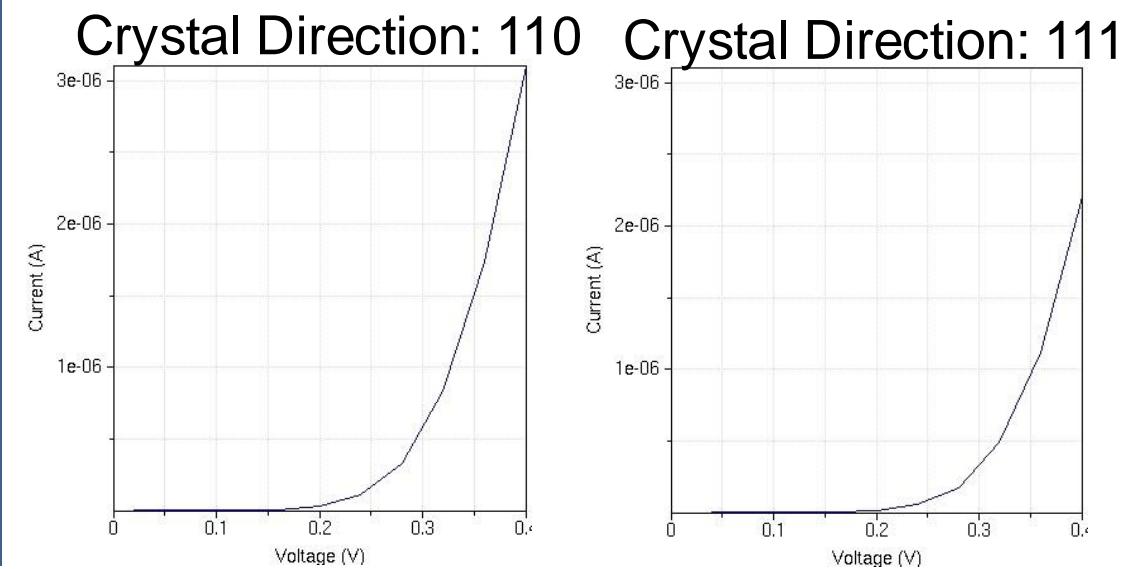
- What is the difference in I-Vg curves between 100, 110, and 111 crystal directions?

Approach:

- A silicon nanowire of diameter 2nm was modeled in Nanowire, varying the crystal direction.
- Please see [NanoHub Nanowire Inputs](#) (located in the Appendix) for the inputs used in this simulation.

Results / Impact:

- Shown below is the comparison of 110 and 111 crystal directions. The I-Vg curve of 100 does not exist.
- Shown in [1D Electron Densities](#) and [3D Electron Densities](#) (located in the Appendix) are the comparisons of the electron densities. They are very similar between crystal directions.



Nanowire Realistic Bandstructure (Quad Chart 1 of 2)

Objective:

- Understand the bandstructure of a nanowire.

Problem:

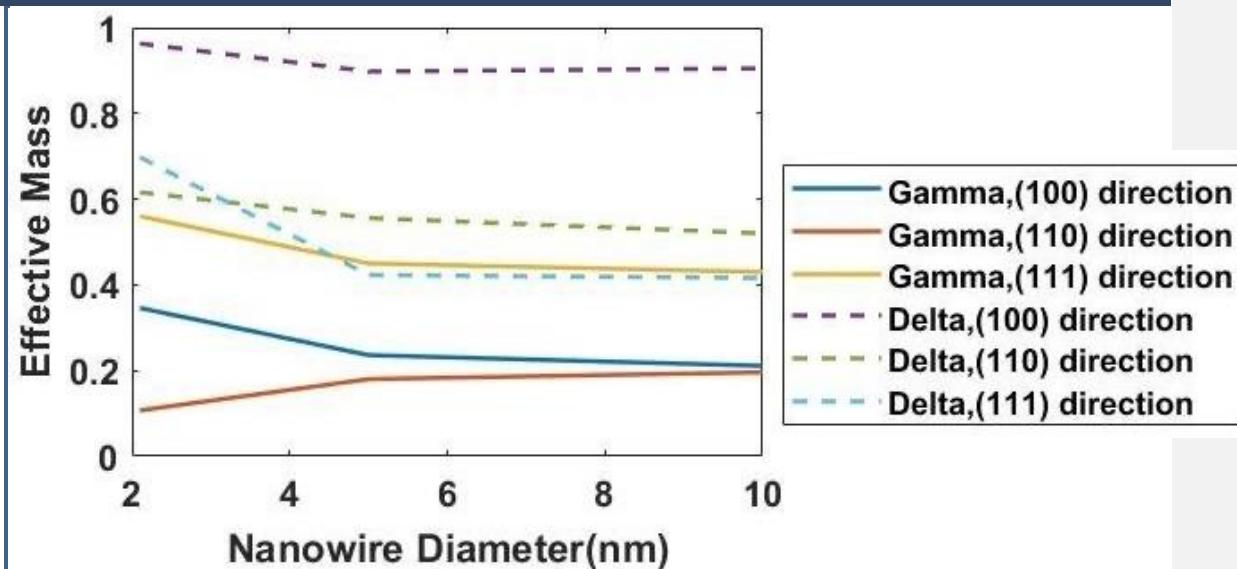
- How does the mass at the different points in a nanowire vary with diameter and transport directions?

Approach:

- A silicon nanowire was modeled in NanoHub's BandstructureLab, varying the nanowire transport direction and diameter.
- Please see [NanoHub BandstructureLab Inputs](#) (located in the Appendix) for the inputs used in this simulation.

Results / Impact:

- The mass is greater at the Delta line (when $k>0$) than at the Gamma point (when $k=0$).
- Generally, the mass will decrease as the nanowire diameter increases.
- Please see [Nanowire Realistic Bandstructure \(Masses\)](#) (in the Appendix) for more detailed plots.



Nanowire Realistic Bandstructure (Quad Chart 2 of 2)

Objective:

- Understand the bandstructure of a nanowire.

Problem:

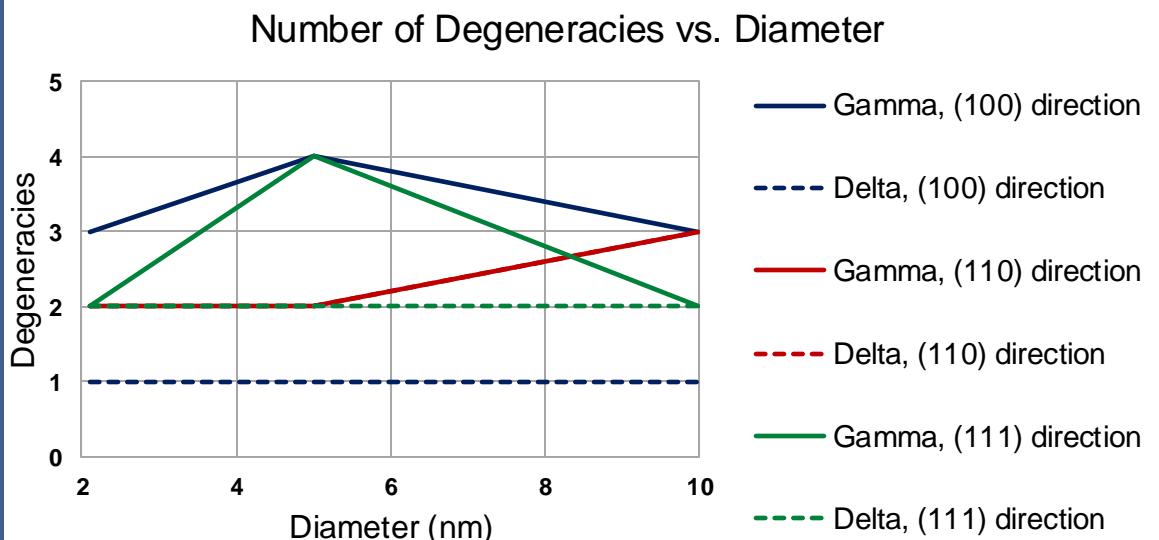
- How does the degeneracies at the different points in a nanowire vary with diameter and transport directions?

Results / Impact:

- For 100 and 111 transport directions, there are more degeneracies at the Gamma point.
- The number of degeneracies vary in no significant pattern based on nanowire diameter.
- Please see [Nanowire Realistic Bandstructure \(Degeneracies\)](#) (in the Appendix) for more detailed plots and detailed data Table

Approach:

- A silicon nanowire was modeled in NanoHub's BandstructureLab, varying the nanowire transport direction and diameter.
- Please see [NanoHub BandstructureLab Inputs](#) (located in the Appendix) for the inputs used in this simulation.



Nanowire Top-of-Barrier Transport (Quad Chart 1 of 2)

Objective:

- Understand electron transport through nanowires.

Problem:

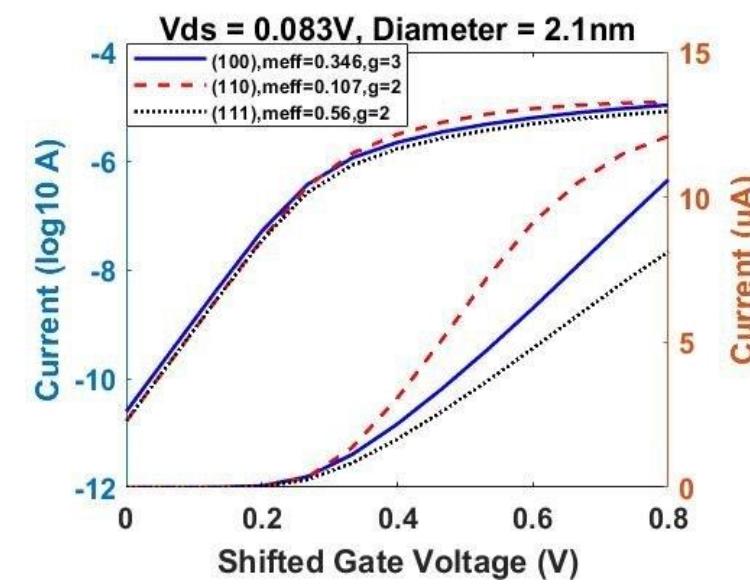
- How does the I-V curve differ between nanowire transport directions (100, 110, and 111) and differing diameters (2.1nm and 10nm)?

Approach:

- A silicon nanowire was modeled in NanoHub's FETtoy tool, varying the nanowire transport direction and diameter. The masses and degeneracies from Challenge #5 were also utilized (please see [inputs](#)).
- Please see [NanoHub FETtoy Inputs](#) (in the Appendix) for the inputs used in this simulation.

Results / Impact:

- The currents are generally largest in the 110 direction and smallest in the 111 direction.
- The currents increase with an increase in nanowire diameter.
- Please see [Nanowire Top-of-Barrier Transport \(I-V Curves\)](#) for both plots.



Nanowire Top-of-Barrier Transport (Quad Chart 2 of 2)

Objective:

- Understand electron transport through nanowires.

Problem:

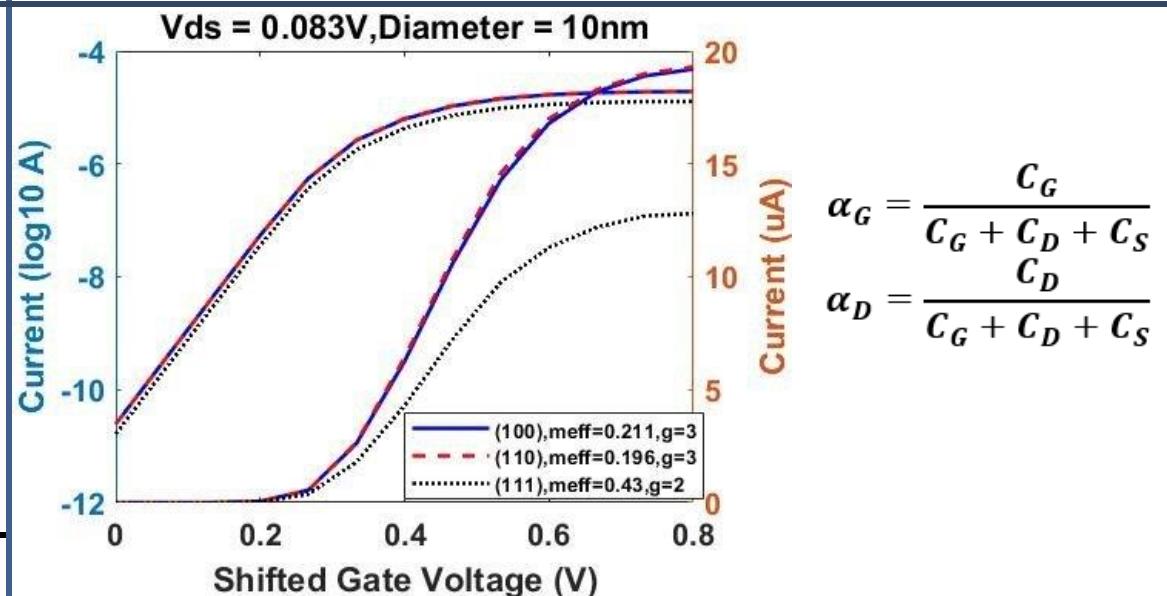
- How do the inputs alphaG and alphaD relate realistic capacitances?

Approach:

- A silicon nanowire was modeled in NanoHub's FETtoy tool, varying the nanowire transport direction and diameter. The masses and degeneracies from Challenge #5 were also utilized (please see [inputs](#)).
- Please see [NanoHub FETtoy Inputs](#) (in the Appendix) for the inputs used in this simulation.

Results / Impact:

- alphaG and alphaD quantities refer to Gate and Drain control parameter respectively.
- Ideally the Gate must have complete control over the channel and not drain. However, due to Drain Induced Barrier Lowering (DIBL), transistor sees a lowering of threshold voltage, mostly in short channel devices.
- Results in Drain control over Channel.



Fast Nanowire Quantum Transport

Objective:

- Explore Fully Quantum Mechanical Transport Calculation

Problem:

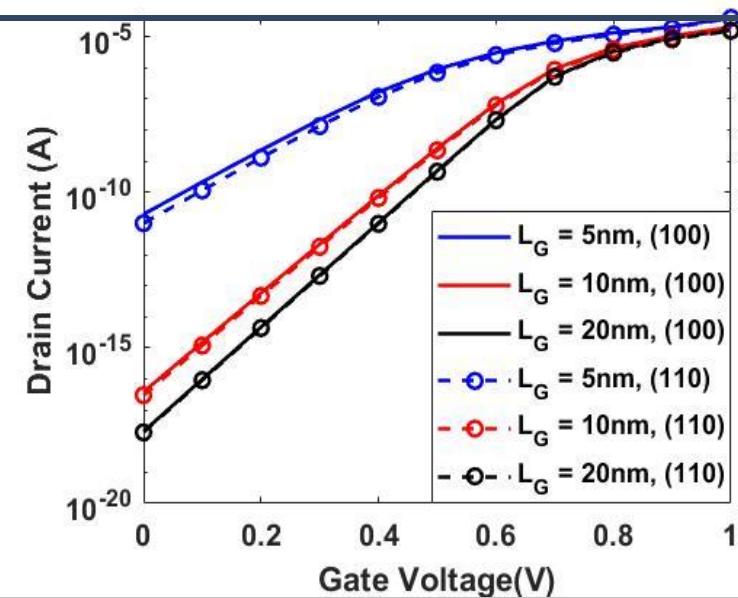
- Modeling 3nm Gate-all-around nanowires

Results / Impact:

- Gate-all-around nanowire provides better electrostatic gate control over channel
- Even for a Gate Length as short as 5nm, Off current is significantly low \Rightarrow better I_{ON}/I_{OFF}
- Charge profiles across Gate lengths and Crystal direction shown in Appendix (Charge Density Profiles)

Approach:

- 3nm Gate-all-around nanowires were modeled using Multi-gate Nanowire FET tool on nanoHub.
- Effects of varying Gate length (5nm, 10nm, 20nm) in 2 different crystal directions studied



Long Nanowire Quantum Transport (Quad Chart 1 of 2)

Objective:

- Understand atomistic quantum transport through 2.1nm cross section nanowires using a gate and channel length of 15nm.

Problem:

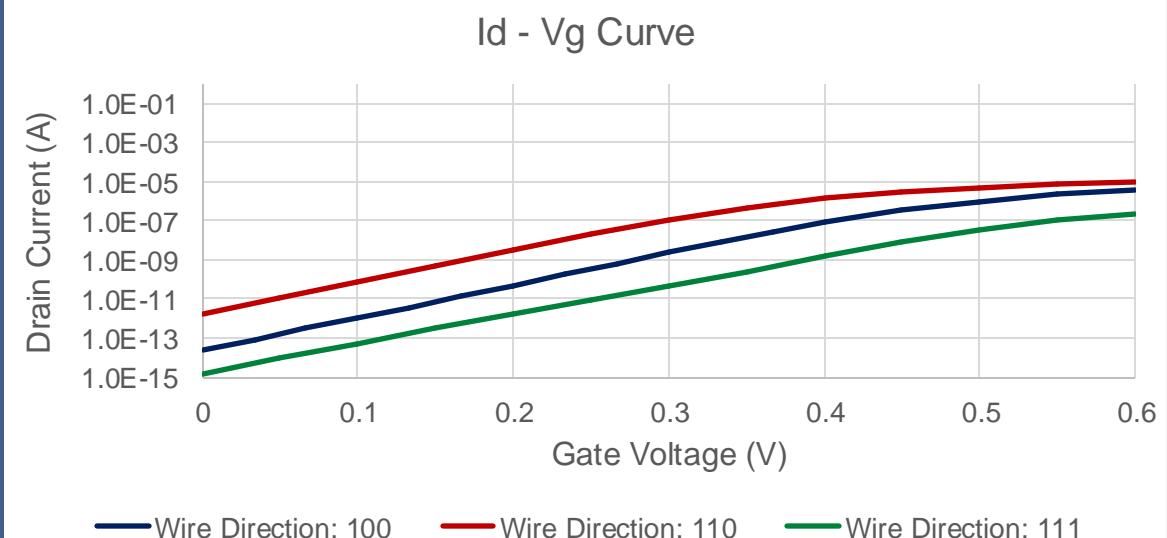
- What are the general features of the I-V curves of 100, 110, and 111 wire directions?

Approach:

- A silicon nanowire was modeled in NanoHub's Omenwire tool, varying the nanowire transport direction.
- Please see [NanoHub Inputs](#) (located in the Appendix) for the inputs used in this simulation.

Results / Impact:

- Shown below on the logarithmic plot, the drain current is the greatest in the 110 direction and lowest in the 111 direction.
- All directions start to slow their increase in current between 0.35V and 0.55V.



Long Nanowire Quantum Transport (Quad Chart 2 of 2)

Objective:

- Understand atomistic quantum transport through 2.1nm cross section nanowires using a gate and channel length of 15nm.

Problem:

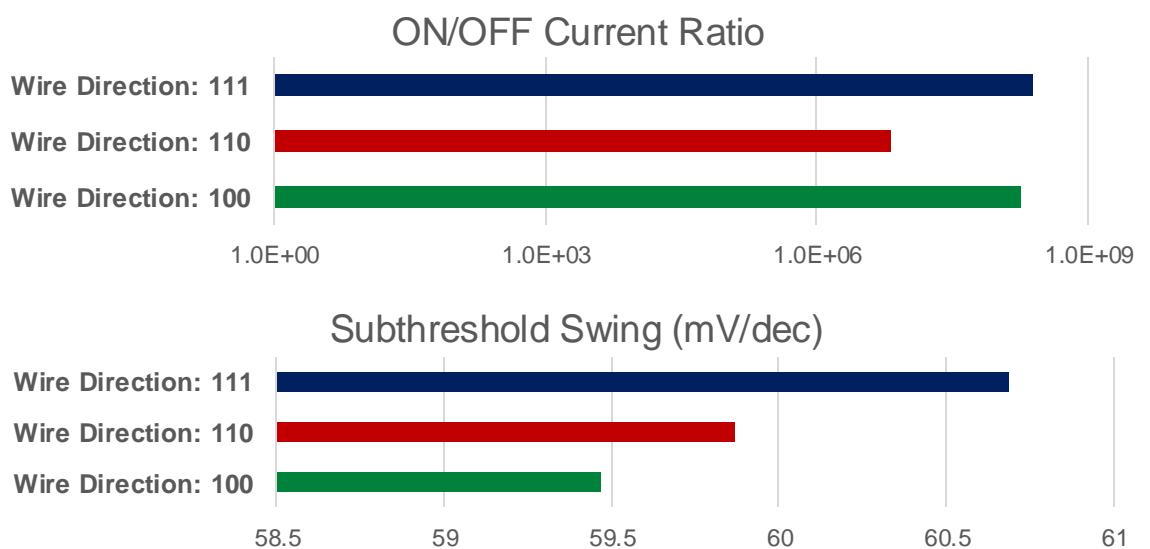
- How do the subthreshold swings and On/Off current ratios differ between 100, 110, and 111 wire directions?

Approach:

- A silicon nanowire was modeled in NanoHub's Omenwire tool, varying the nanowire transport direction.
- Please see [NanoHub Inputs](#) (located in the Appendix) for the inputs used in this simulation.

Results / Impact:

- The On/Off current ratio in the 110 direction is drastically smaller than the others.
- The subthreshold swing however has a linear change between the 100, 110, and 111 direction, steadily increasing.



Short Nanowire Quantum Transport (Quad Chart 1 of 2)

Objective:

- Understand atomistic quantum transport through 1.9nm cross section nanowires using a gate and channel length of 5nm.

Problem:

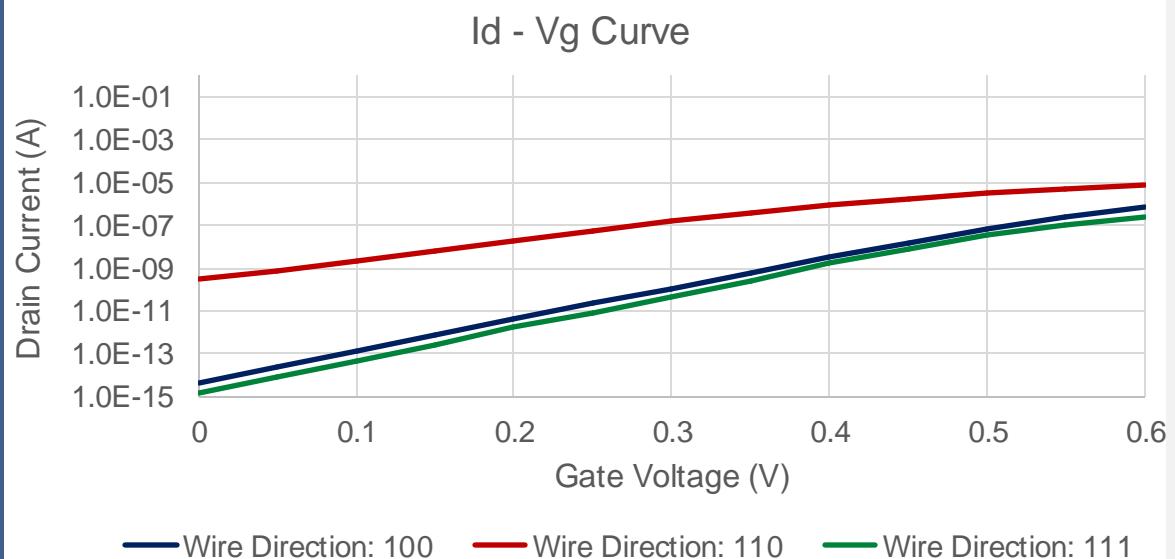
- What are the general features of the I-V curves of 100, 110, and 111 wire directions?

Approach:

- A silicon nanowire was modeled in NanoHub's Omenwire tool, varying the nanowire transport direction.
- Please see [NanoHub Inputs](#) (located in the Appendix) for the inputs used in this simulation.

Results / Impact:

- Shown below on the logarithmic plot, the drain current is the greatest in the 110 direction and lowest in the 111 direction.
- The current is very similar in the 100 and 111 directions.
- All directions don't start to slow their increase in current until after 0.55V.



Short Nanowire Quantum Transport (Quad Chart 2 of 2)

Objective:

- Understand atomistic quantum transport through 1.9nm cross section nanowires using a gate and channel length of 5nm.

Problem:

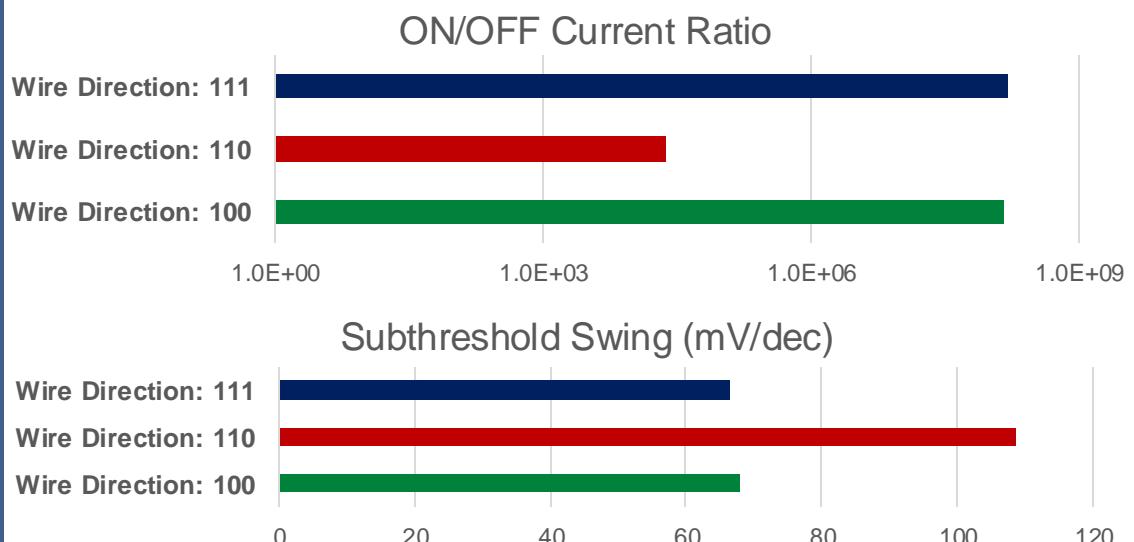
- How do the subthreshold swings and On/Off current ratios differ between 100, 110, and 111 wire directions?

Approach:

- A silicon nanowire was modeled in NanoHub's Omenwire tool, varying the nanowire transport direction.
- Please see [NanoHub Inputs](#) (located in the Appendix) for the inputs used in this simulation.

Results / Impact:

- The On/Off current ratio did not significantly change between the long and short nanowire.
- The subthreshold swing did show a large difference. With the short nanowire, the 110 direction showed a large increase.



Nanowire Dispersion Design (Quad Chart 1 of 2)

Objective:

- Understand what inputs can be used to increase the performance of a nanowire.

Problem:

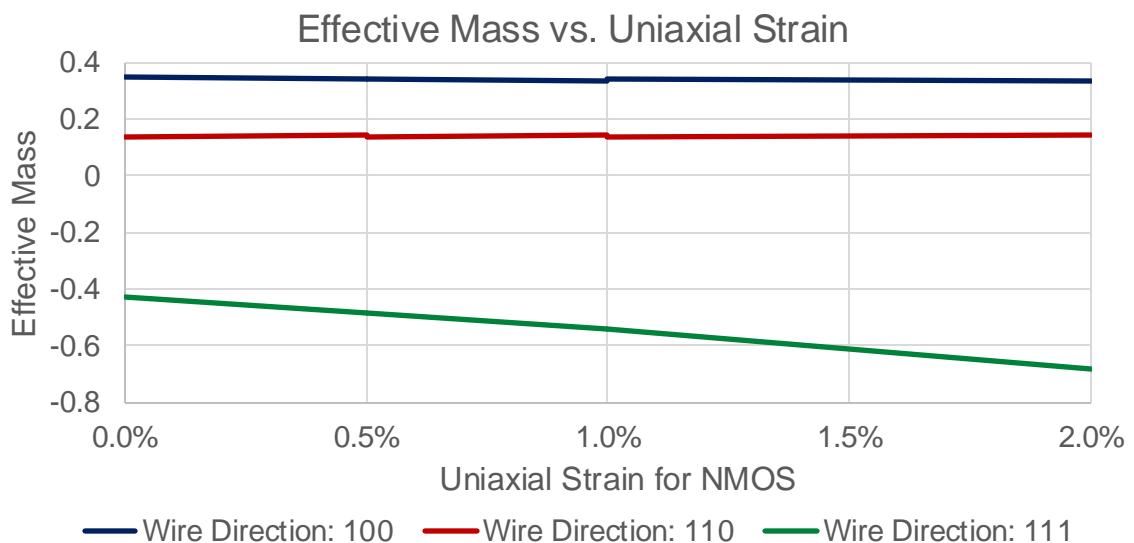
- How can the nanowire be tuned to better the transistor performance?

Results / Impact:

- The effective mass (m^*) is defined as the inverse of the second derivative of $E-k$ times the square of Plank's constant.
- m^* varies inversely with the sharpness, or curvature, of the bands. This is decreased by increasing the strain (shown below).

Approach:

- A silicon nanowire was modeled in NanoHub's BandstructureLab tool, varying the uniaxial strain from 0%, 0.5%, 1%, & 2%.
- Please see [NanoHub Inputs](#) (located in the Appendix) for the inputs used in this simulation.



Nanowire Dispersion Design (Quad Chart 2 of 2)

Objective:

- Understand what inputs can be used to increase the performance of a nanowire.

Problem:

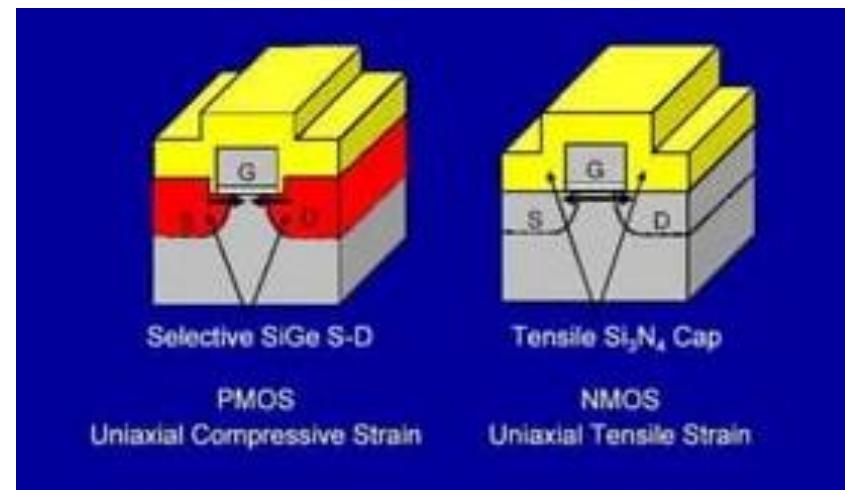
- What kinds of strain is associated with transistors? What is reasonable to do with nanowires?

Approach:

- Various publications were researched for what kind of strain is associated with transistors.
- Please see [Resources](#) 2 – 5 (located in the Appendix) for the list of publications reviewed.

Results / Impact:

- Each publication reviewed concluded that NMOS transistors should be stretched to enhance electron mobility.
- PMOS transistors should be compressed to enhance hole mobility.
- Also noted, using two separate crystal directions would be most optimal, but it is not realistic outside of a simulation.



[3]

Optimized Nanowire Quantum Transport (Quad Chart 1 of 2)

Objective:

- Understand how changes to a transistor impact performance.

Problem:

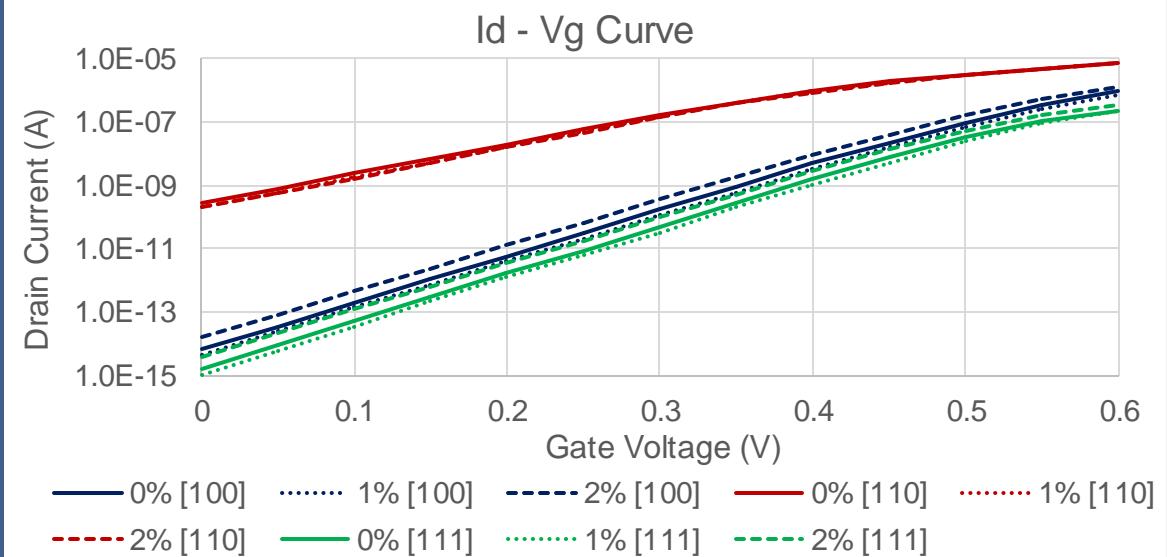
- How did the changes implemented in Challenge #10 impact the performance of the transistor?

Approach:

- A silicon nanowire was modeled in NanoHub's Omenwire tool, varying the uniaxial strain from 0%, 1%, & 2%.
- Please see [NanoHub Inputs](#) (located in the Appendix) for the inputs used in this simulation.

Results / Impact:

- Shown below and in [Id-Vg Curve](#) (located in the Appendix) in greater detail, there is not a significant difference between the I-V curves for various uniaxial strains.



Optimized Nanowire Quantum Transport (Quad Chart 2 of 2)

Objective:

- Understand how changes to a transistor impact performance.

Problem:

- What other improvements could be made to better the performance?

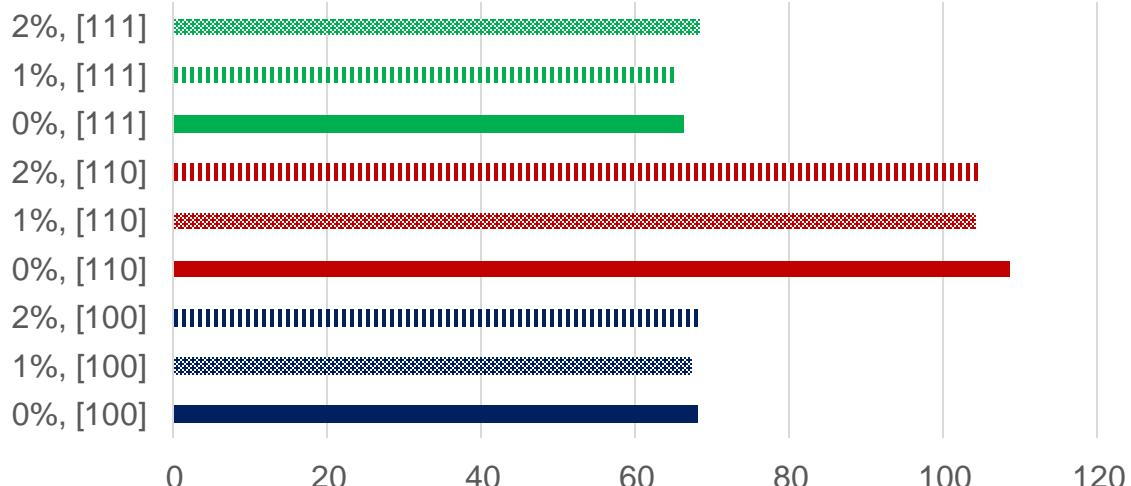
Results / Impact:

- The subthreshold swing (shown below) and the on/off current ratio (shown in the Appendix, [Critical Parameters](#)) demonstrate the best performance will occur at 1% strain (compared to 0% or 2%).

Approach:

- A silicon nanowire was modeled in NanoHub's Omenwire tool, varying the uniaxial strain from 0%, 1%, & 2%.
- Please see [NanoHub Inputs](#) (located in the Appendix) for the inputs used in this simulation.

Subthreshold Swing (mV/dec)



Hole Nanowire Bandstructure (Quad Chart 1 of 2)

Objective:

- Understand the hole bandstructure in nanowires.

Problem:

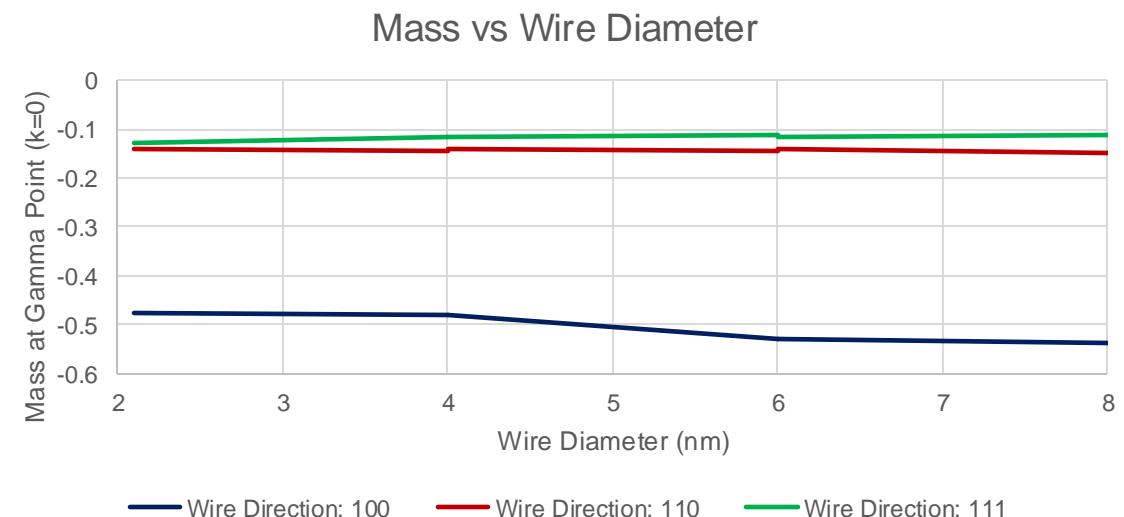
- How does the mass at Gamma Point ($k=0$) change as a function of the wire diameter?

Results / Impact:

- Shown below, for wire directions 110 and 111, the mass at the Gamma point does not have a significant change.
- For wire direction 100, the mass decreases at the Gamma point.
 - There are peaks off the Gamma point of -0.524, -0.722, and -0.518 for 2.1nm, 4nm, and 6nm diameters respectively.

Approach:

- A silicon nanowire was modeled in NanoHub's BandstructureLab tool, varying the wire diameter from 2.1nm, 4nm, 6nm, and 8nm.
- Please see [NanoHub Inputs](#) (located in the Appendix) for the inputs used in this simulation.



Hole Nanowire Bandstructure (Quad Chart 2 of 2)

Objective:

- Understand the hole bandstructure in nanowires.

Problem:

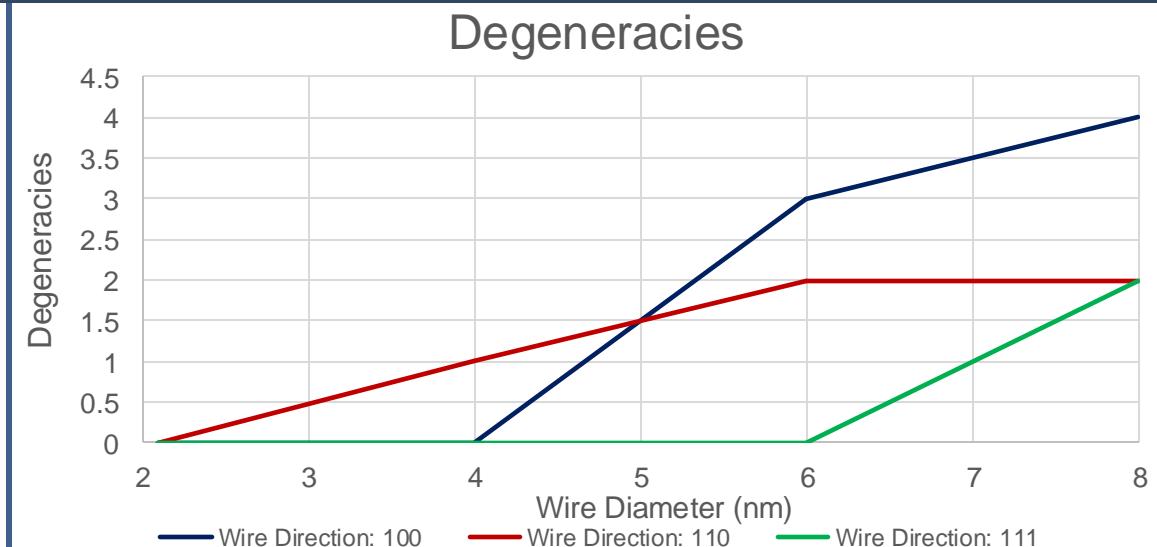
- Which wire direction is recommended at a diameter of 2.1mm?

Results / Impact:

- There are degeneracies at diameters $> 2.1\text{nm}$.
- The best wire direction for a 2.1nm diameter wire is in the 100 direction, due to the decreased mass.

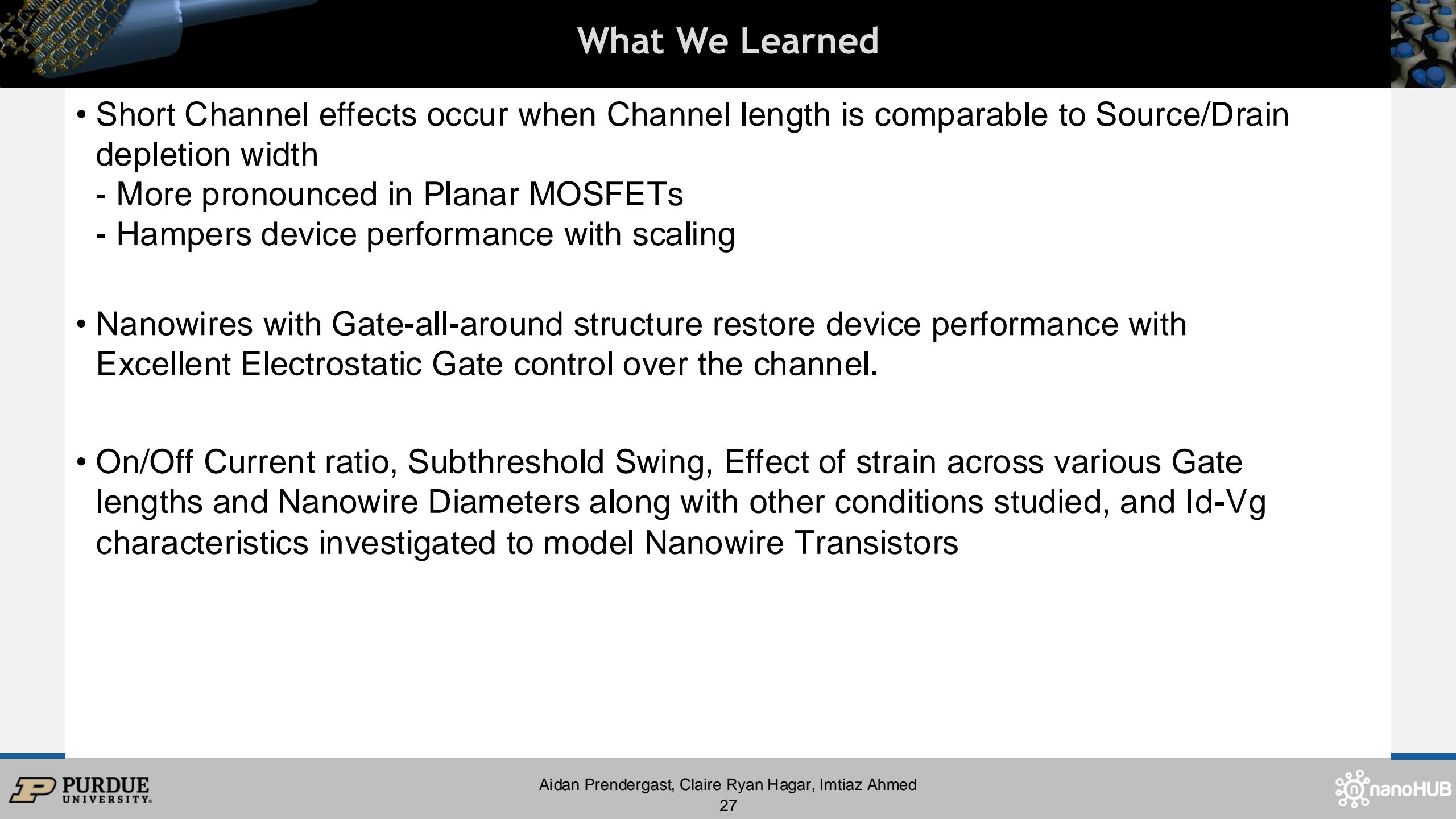
Approach:

- A silicon nanowire was modeled in NanoHub's BandstructureLab tool, varying the wire diameter from 2.1nm, 4nm, 6nm, and 8nm.
- Please see [NanoHub Inputs](#) (located in the Appendix) for the inputs used in this simulation.



What We Learned

- Short Channel effects occur when Channel length is comparable to Source/Drain depletion width
 - More pronounced in Planar MOSFETs
 - Hampers device performance with scaling
- Nanowires with Gate-all-around structure restore device performance with Excellent Electrostatic Gate control over the channel.
- On/Off Current ratio, Subthreshold Swing, Effect of strain across various Gate lengths and Nanowire Diameters along with other conditions studied, and Id-Vg characteristics investigated to model Nanowire Transistors



To Conclude

- Transistors number in the billions in individual devices that we use everyday
- You likely care about how powerful your phone is and how long its battery lasts!
- Nanowire transistors allow us to create more ideal devices for lower power and better performance
- Utilizing the design levers discussed here allows us to design the best application-specific transistors possible
- We've shown here how Nanowires outperform Planar Transistors in
 - » Leakage Currents
 - » On/Off Current Ratio
 - » Subthreshold Swing
 - » Drain-Induced-Barrier-Lowering
- Nanowire scale allows their density to continue increasing
- Nanowires look to usher in a new era of performance and efficiency!



Appendices



Team “Electron Highway”

- This team consisted of three members with distinct backgrounds split between academic research and industry experience.
- The team effort focused on collaboration rather than a division of labor.
- To build a basis for this project, every member attempted Challenge 1, 2, & 3 and collaborated on the final solution.
- All other challenges had at least two members, with members choosing challenges they were particularly interested in or had a background in. The team collaborated on the final solution.
- Utilized meetings to discuss final solutions and shared messaging app to collaborate when "stuck" on a problem



Classical MOSFET Limitations (NanoHub MOSFET Inputs)

Structural Properties | Model | Voltage Sweep |

Device Type: MOSFET n-type

Doping Profile: Uniform Doping Density

Source/Drain Length: 30nm

Source/Drain Nodes: 15

Channel Length: 150nm

Channel Nodes: 22

Oxide Thickness: 0.8nm

Oxide Nodes: 5

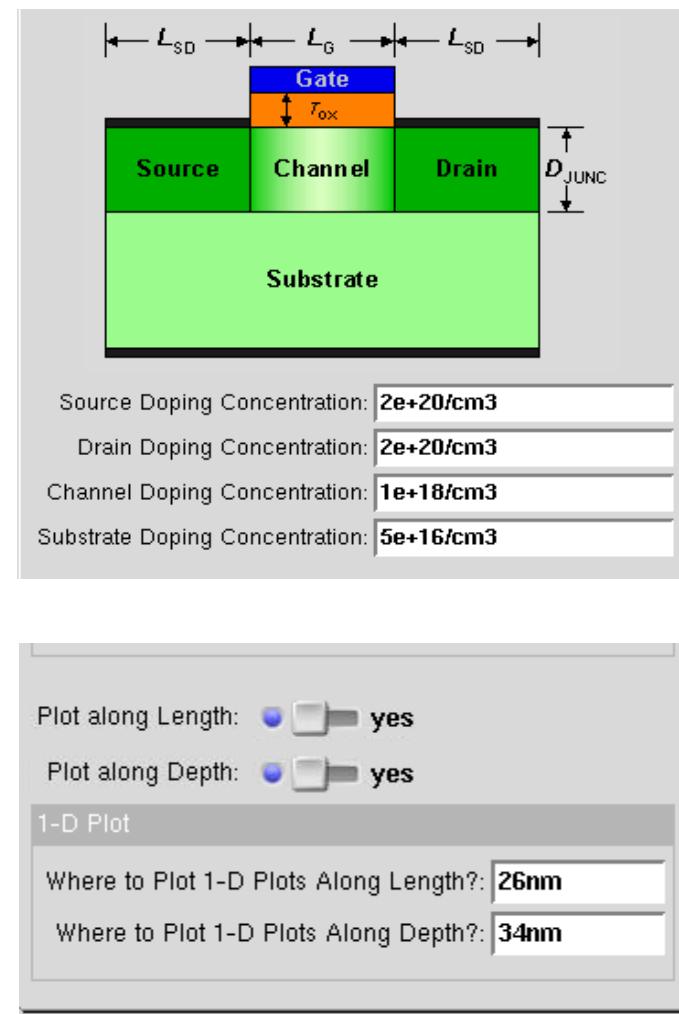
Junction Depth: 9nm

Junction Nodes: 30

Substrate Thickness: 18nm

Substrate Nodes: 10

Device Width: 1000nm



I-Vg Plot

Plot Transfer Characteristic: yes

Vg Minimum: 0V

Vg Maximum: 0.6V

Number of Points: 30

Vd Bias Minimum: 0.05V

Vd Bias Maximum: 0.6V

Number of Curves: 2

Vb Bias Point: 0V

I-Vd Plot

Plot I-Vd Characteristic: no

Vd Minimum: 0V

Vd Maximum: 1.2V

Number of Points: 15

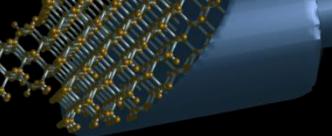
Vg Bias Minimum: 0.5V

Vg Bias Maximum: 1.2V

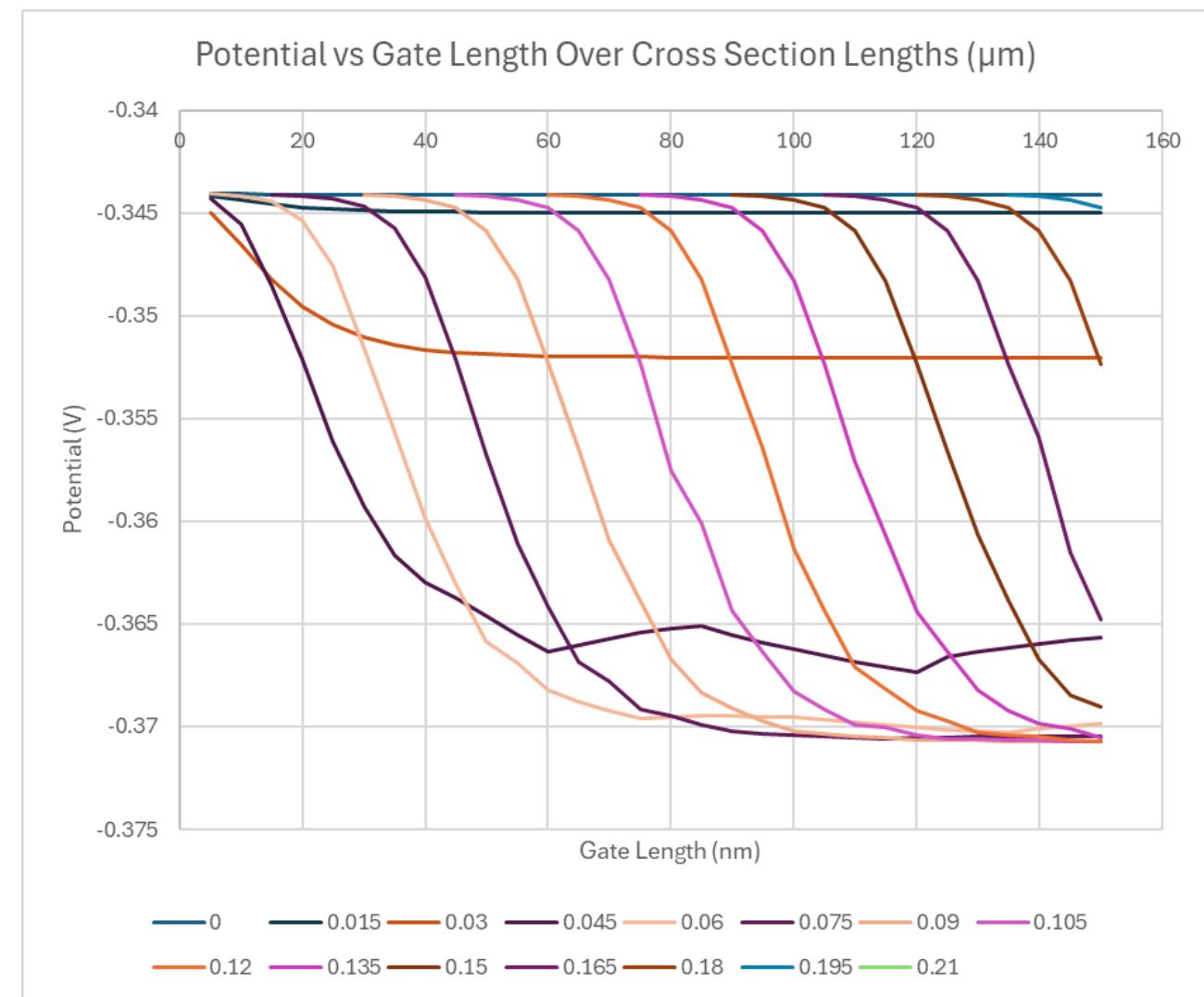
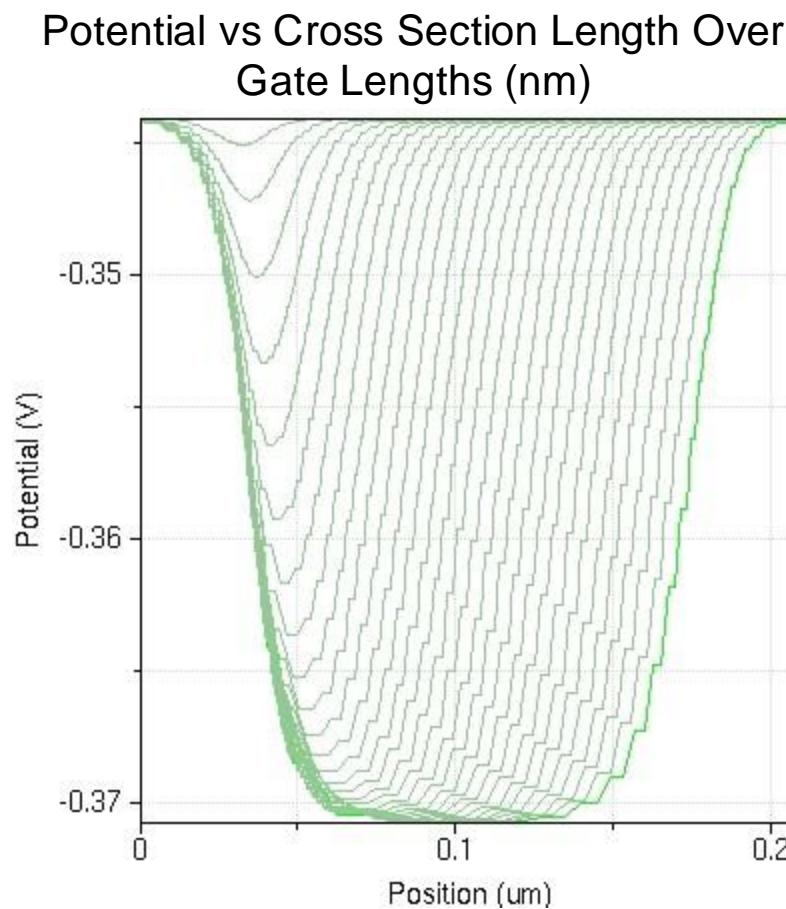
Number of Curves: 3

Vb Bias Point: 0V

Tool located at:
<https://nanohub.org/tools/mosfet>

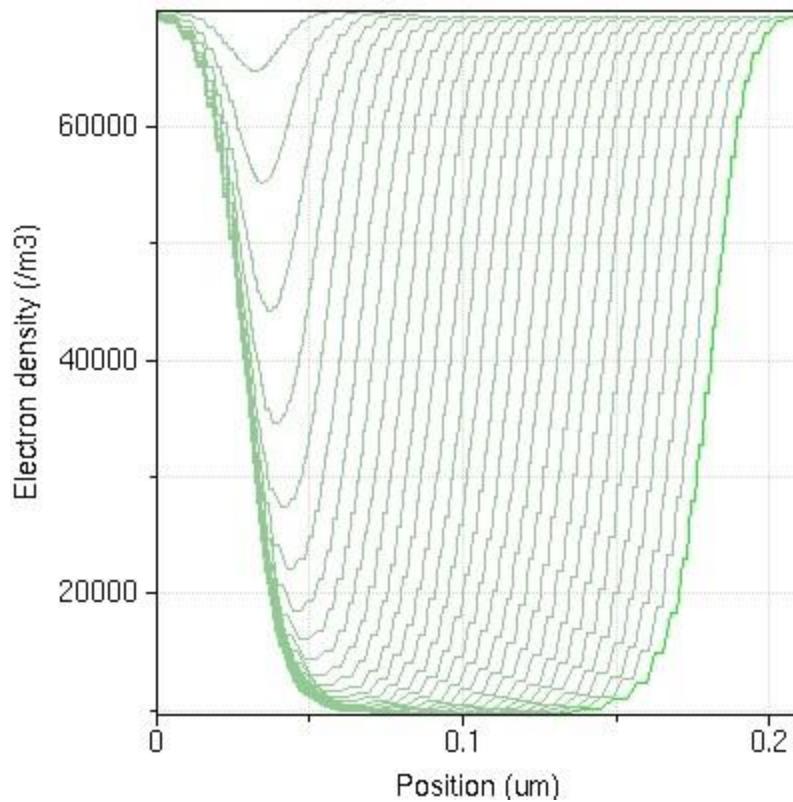


Classical MOSFET Limitations (Voltage Potentials)

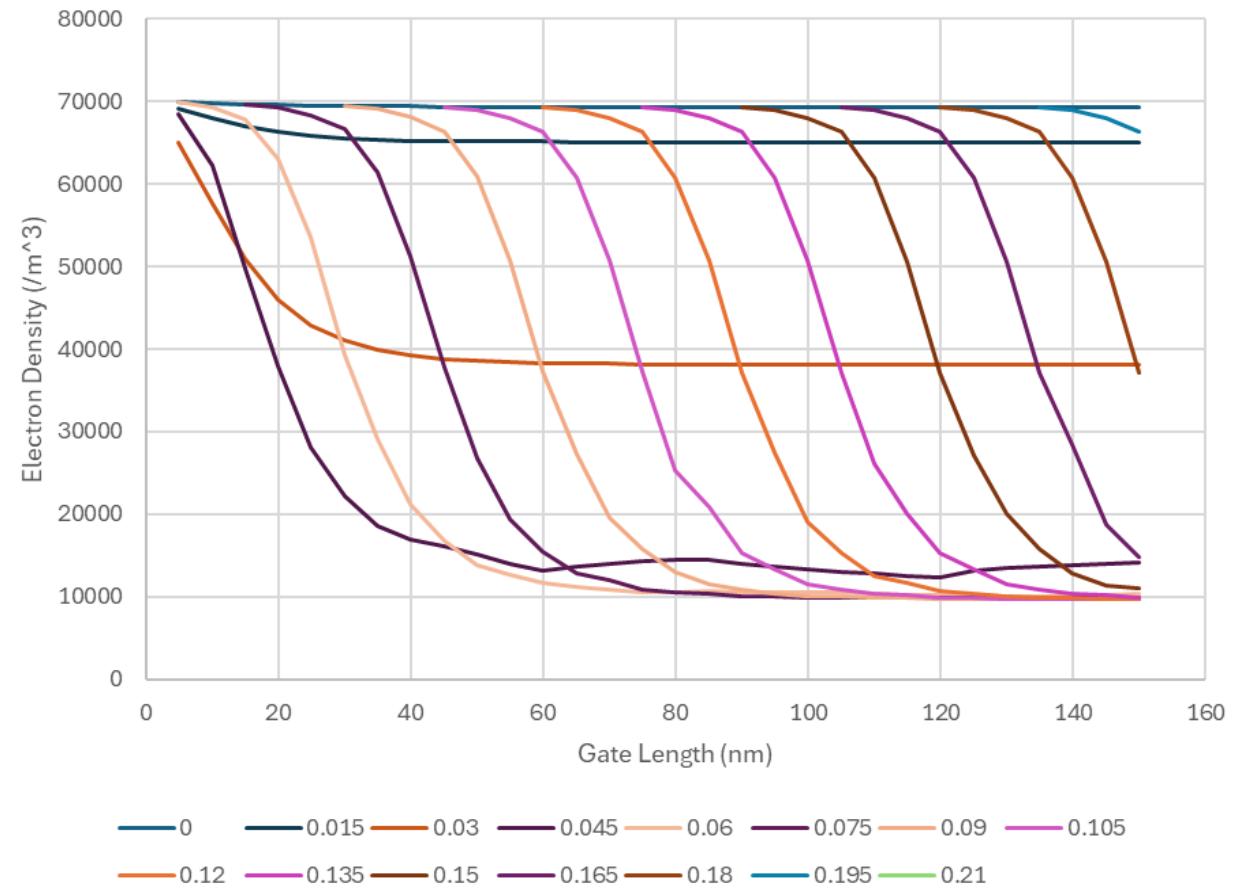


Classical MOSFET Limitations (Electron Densities)

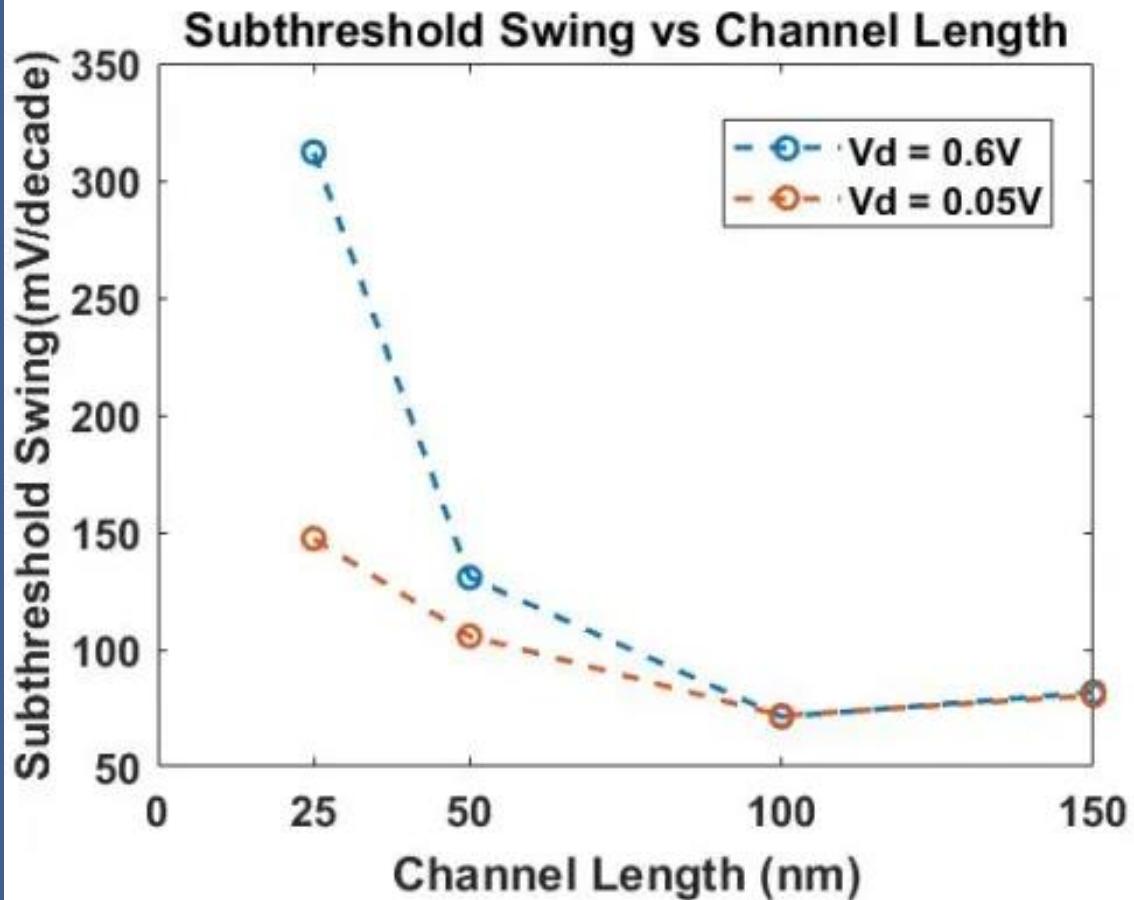
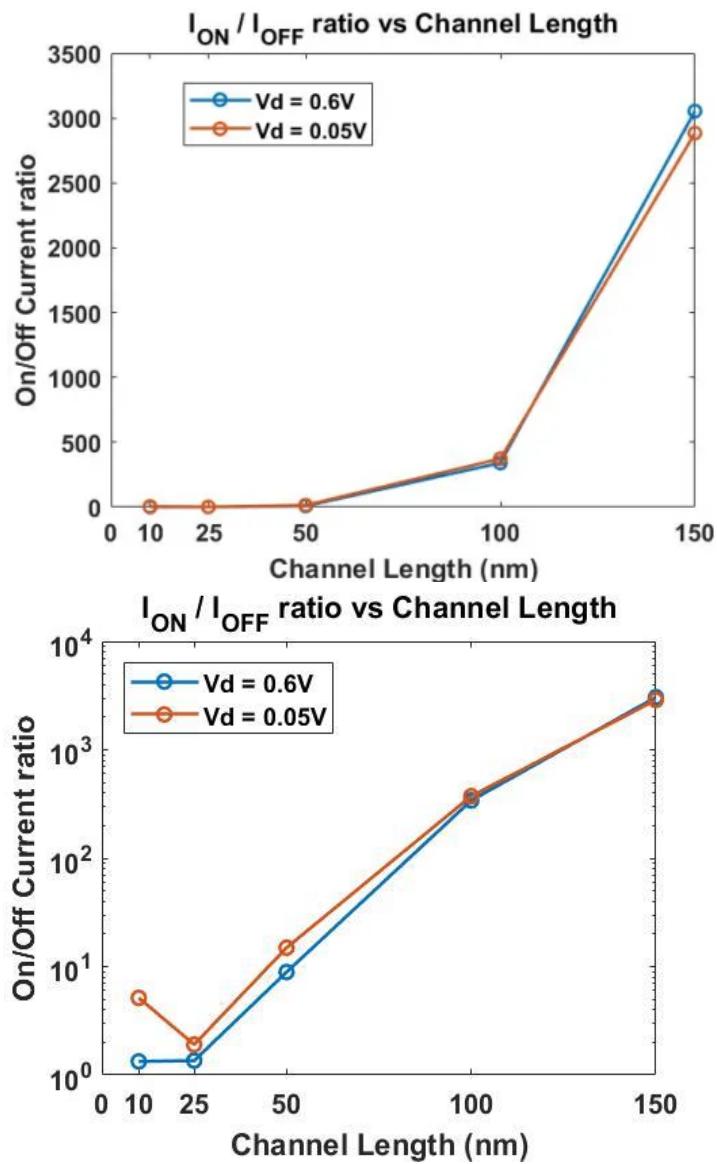
Electron Density vs Cross Section Length Over Gate Lengths (nm)



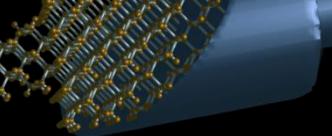
Electron Density vs Gate Length Over Cross Section Lengths (μm)



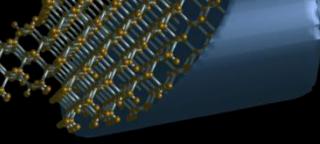
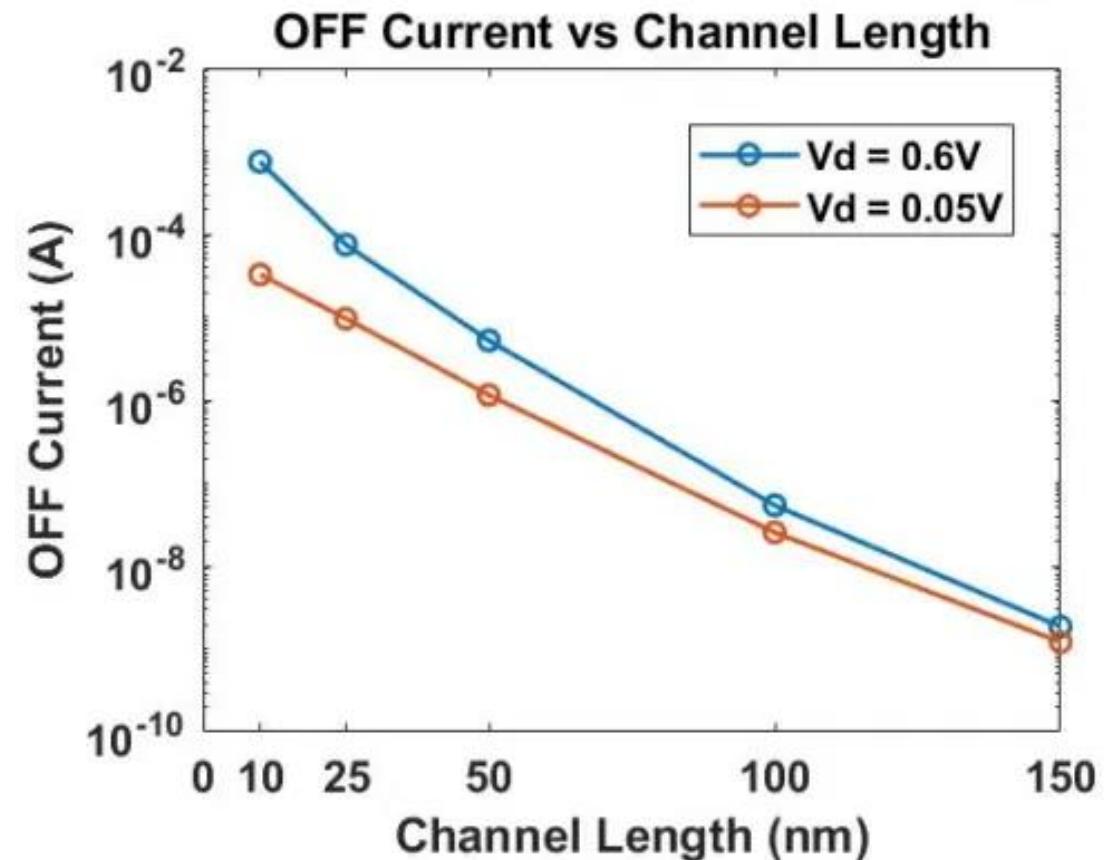
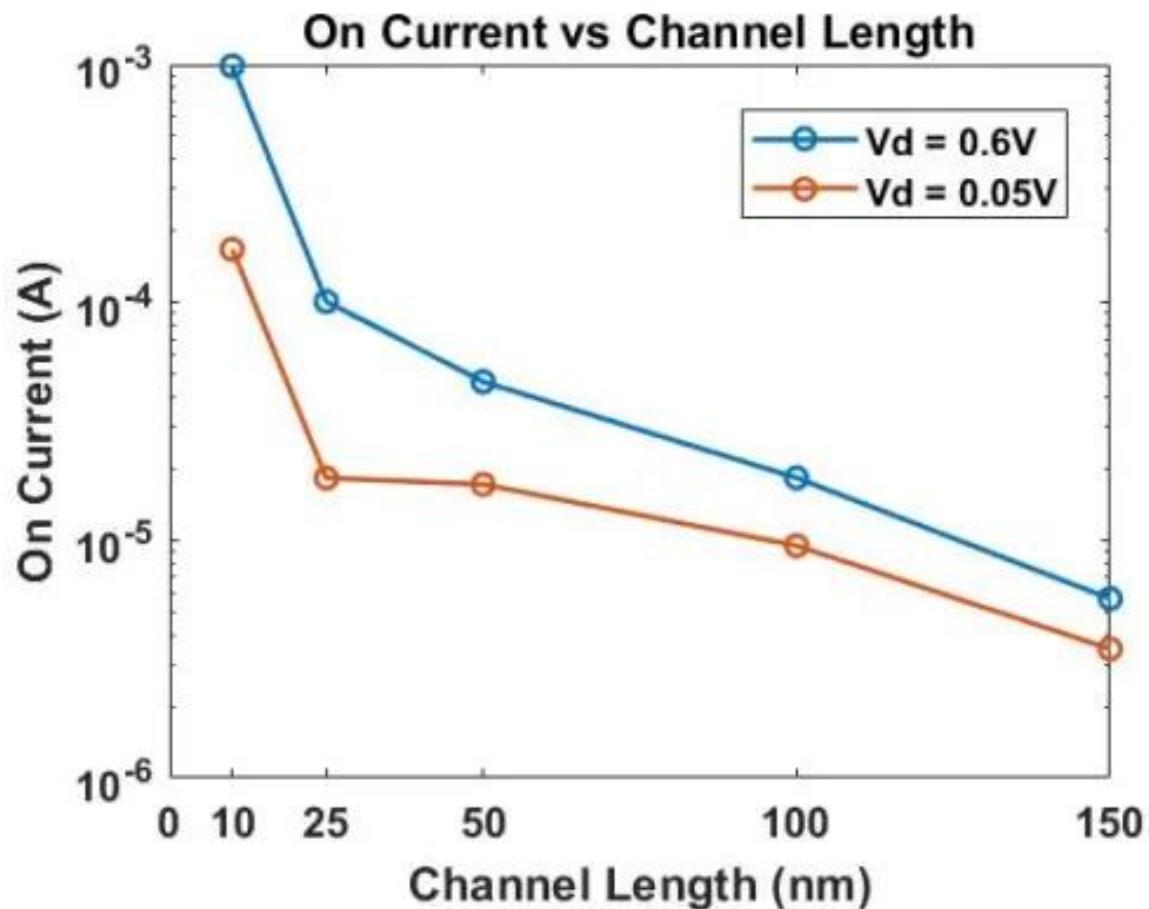
Classical MOSFET Limitations (Transistor Features)



Note, due to the increasingly high leakage currents at low channel lengths, 10nm and 5nm subthreshold swing values were excluded from the above plot.



Classical MOSFET Limitations (Transistor Features)



Nanowire with Drift Diffusion (NanoHub NANOFINFET Inputs)

All default settings were utilized, except as where shown (red boxes mark variable inputs):

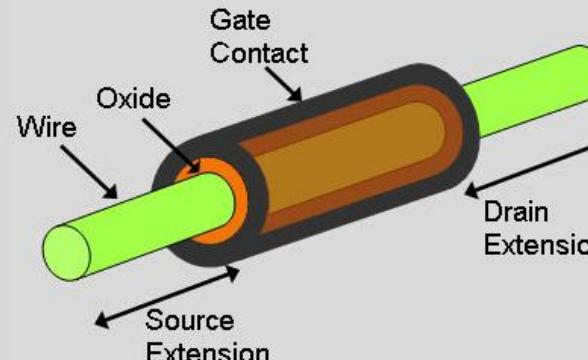
Device Type

Class: Nanowire

Spec

Gate Type: Metal

Geometry-X



Gate Contact
Oxide
Wire
Source Extension
Drain Extension

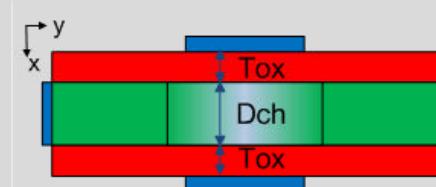
Geometry-Y

Geometry-Z

Doping

Gaussian doping

Geometry-X



Tox
Dch
Tox

Diameter - Dch: **2.1nm**

Oxide thickness - Tox: **2.5nm**

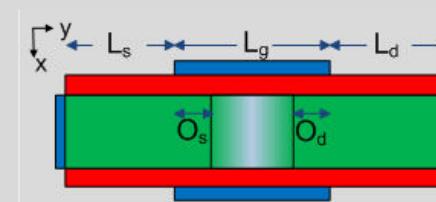
Channel width - Wch: **30nm**

Oxide thickness 1 - Tox1: **2.5nm**

Oxide thickness 2 - Tox2: **2.5nm**

Substrate - S: **100nm**

Geometry-Y



L_s **L_g** **L_d**
O_s **O_d**

Gate length - L_g: **20nm**

Source extension length - L_s: **20nm**

Drain extension length - L_d: **20nm**

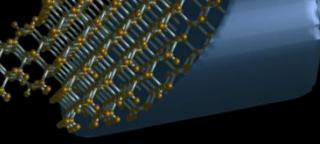
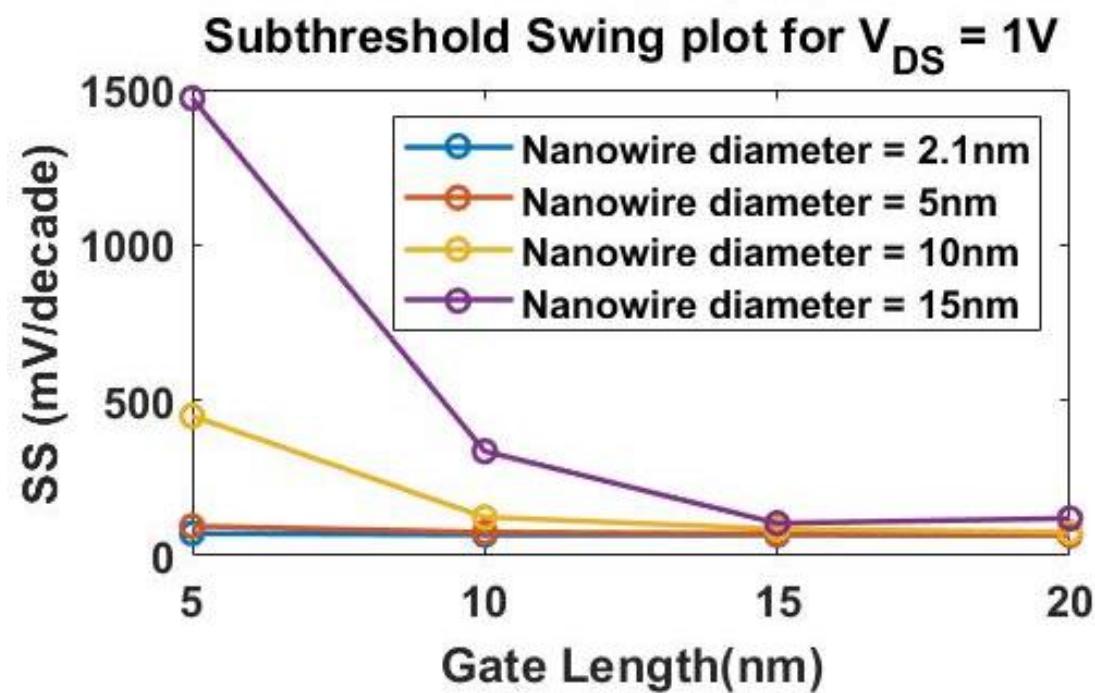
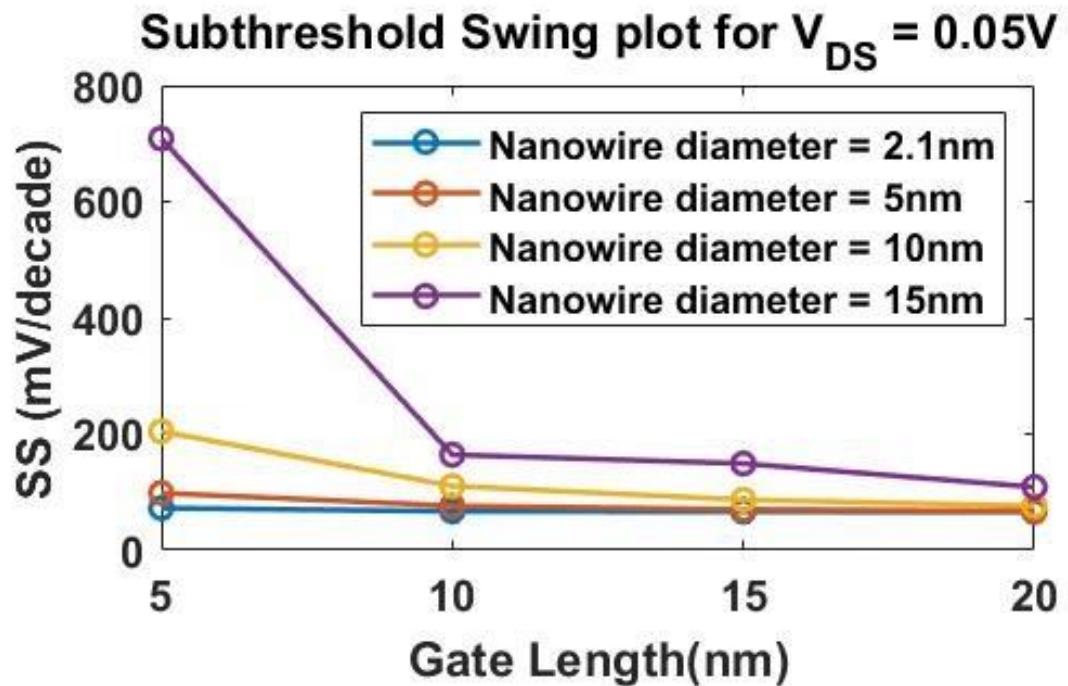
Gate overlap to source - O_s: **2nm**

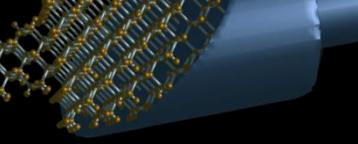
Gate overlap to drain - O_d: **2nm**

Spacer: **15nm**

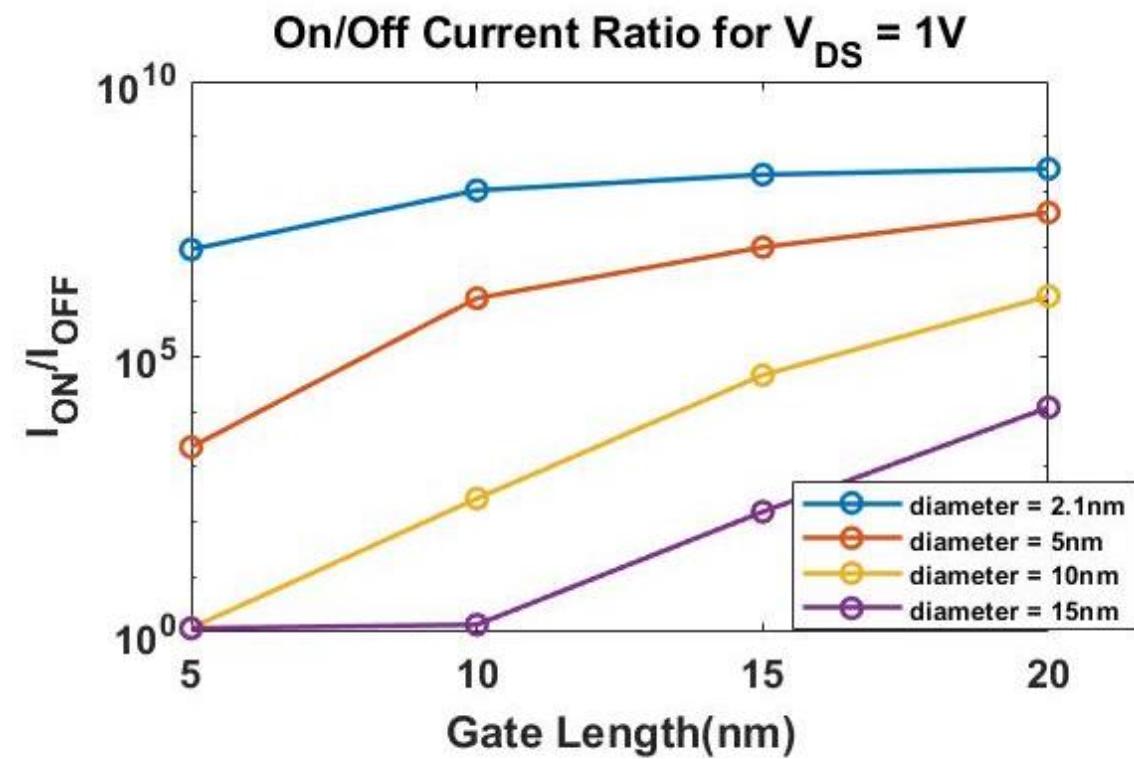
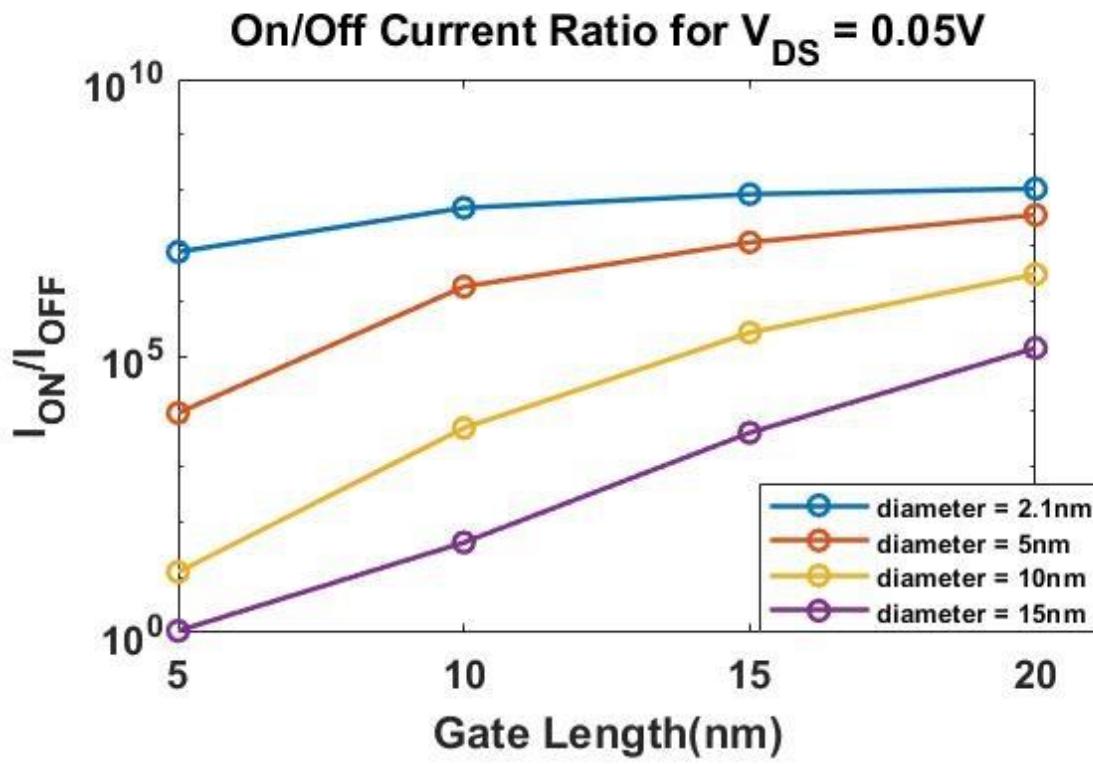
Tool located at:
<https://nanohub.org/tools/nanofinfet>

Nanowire with Drift Diffusion (Subthreshold Swing)

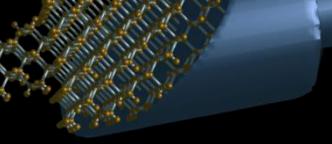
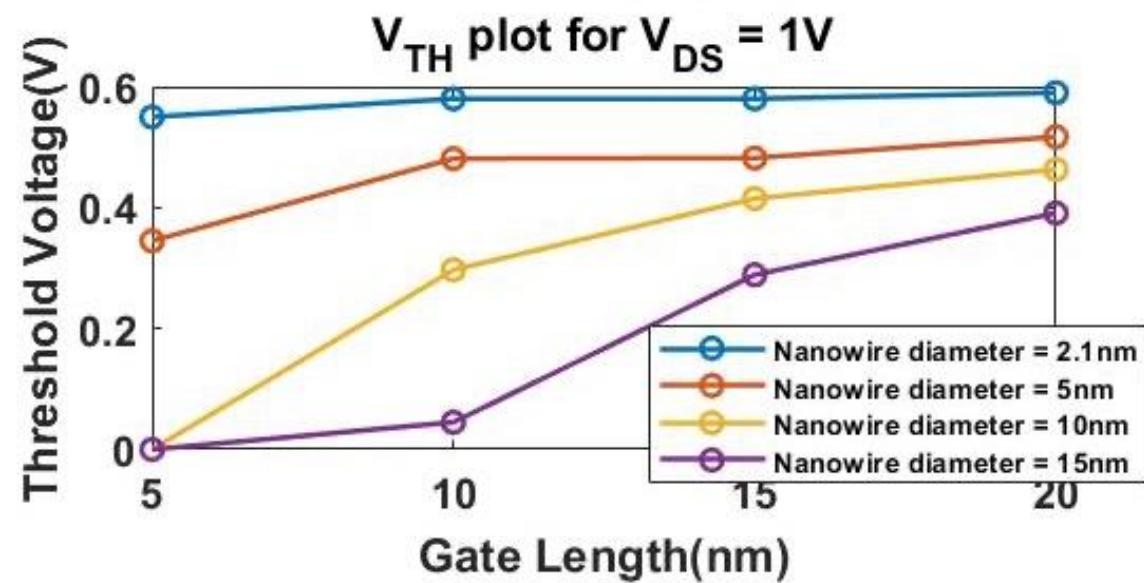
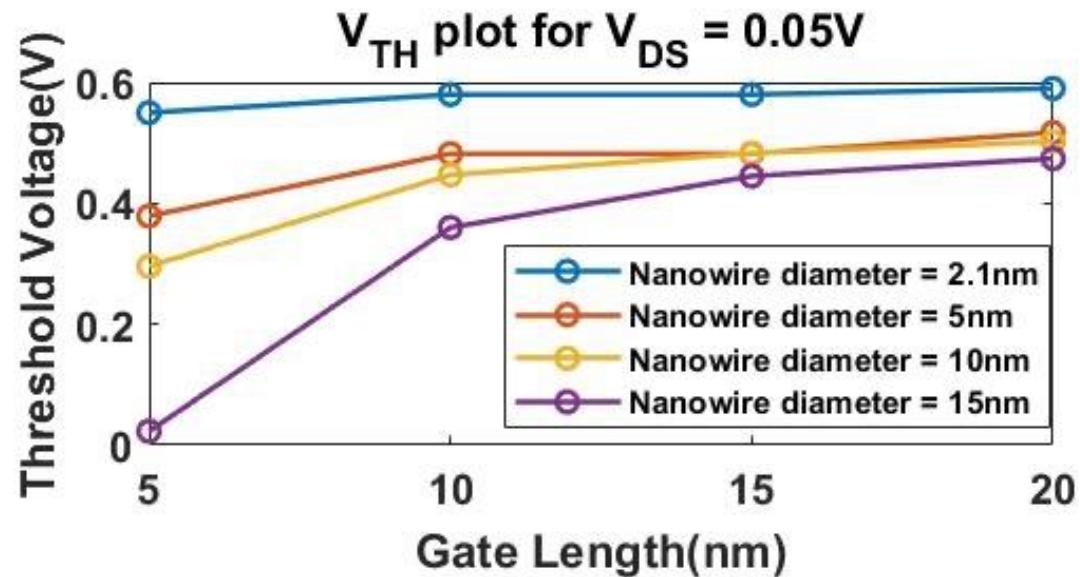




Nanowire with Drift Diffusion (On/Off Current Ratio)

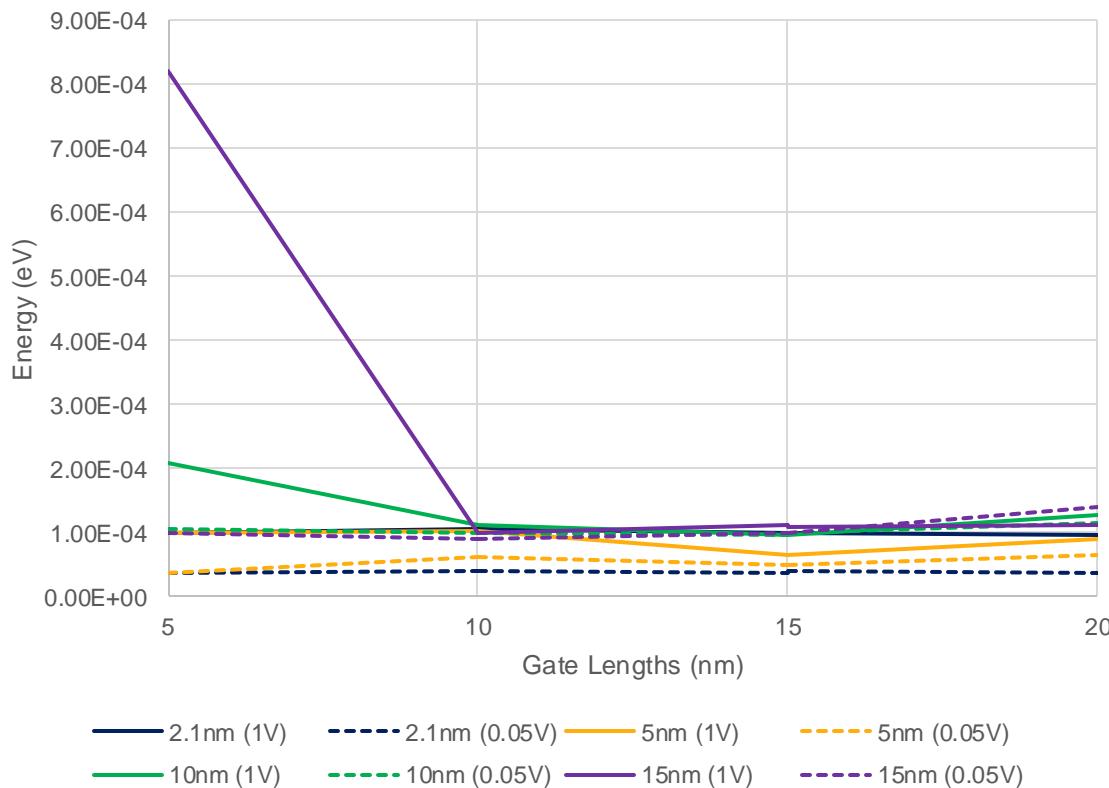


Nanowire with Drift Diffusion (Threshold Voltage)

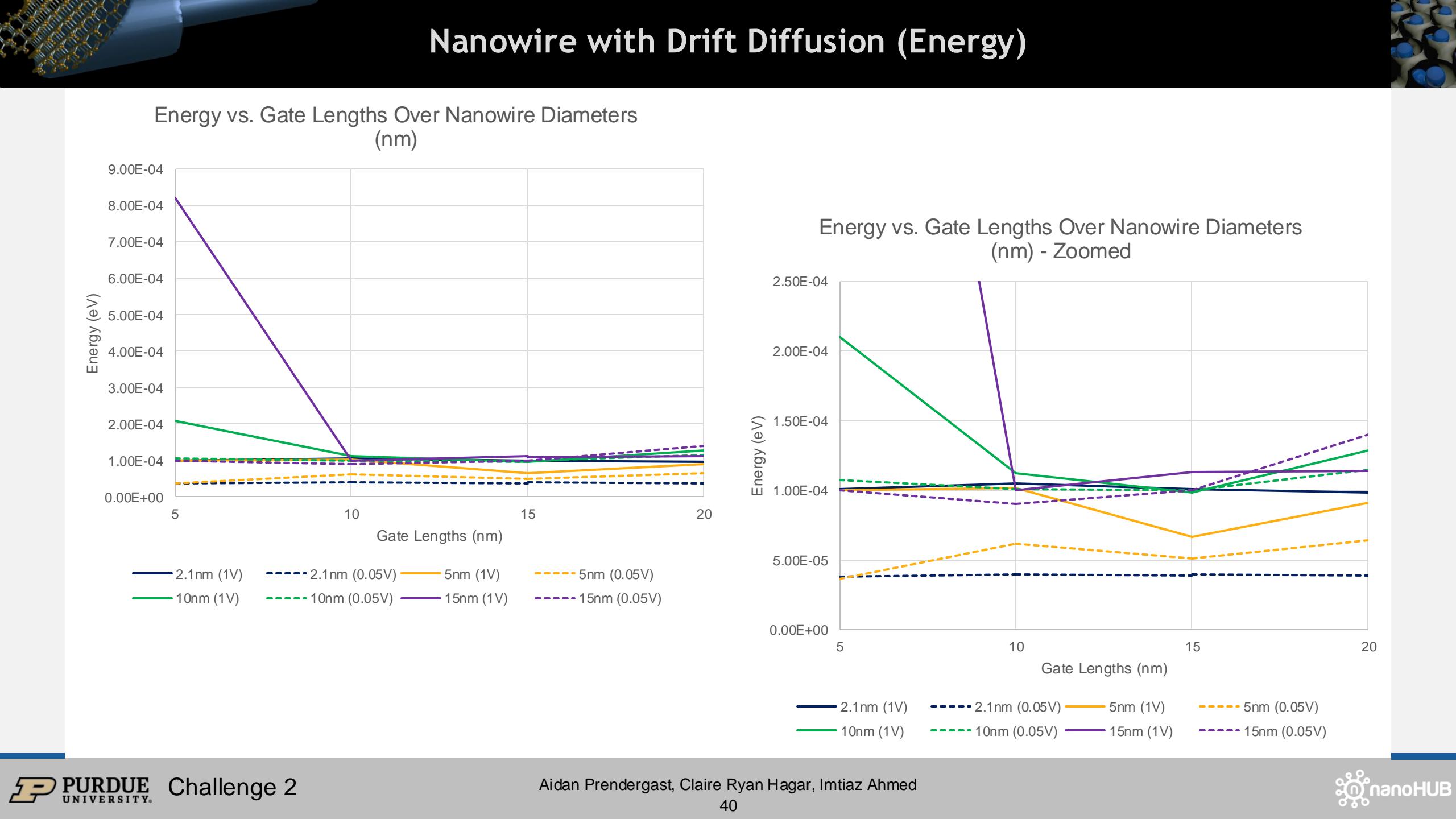
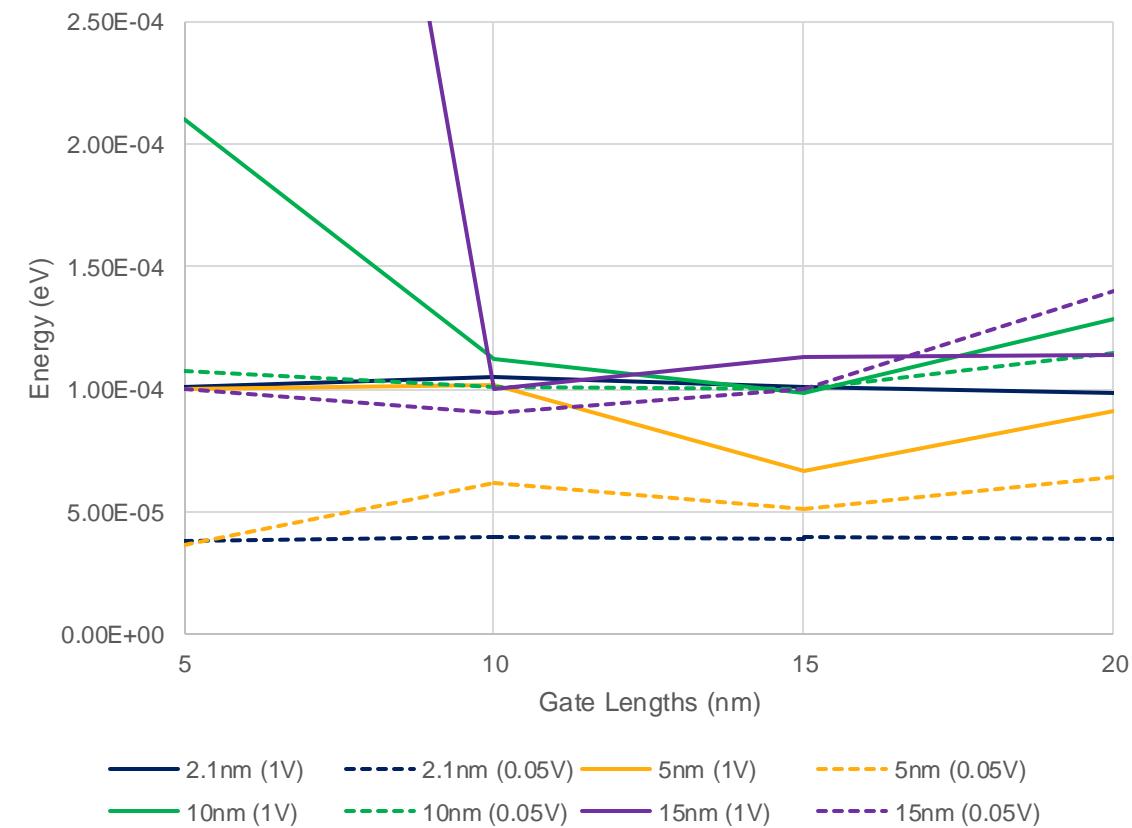


Nanowire with Drift Diffusion (Energy)

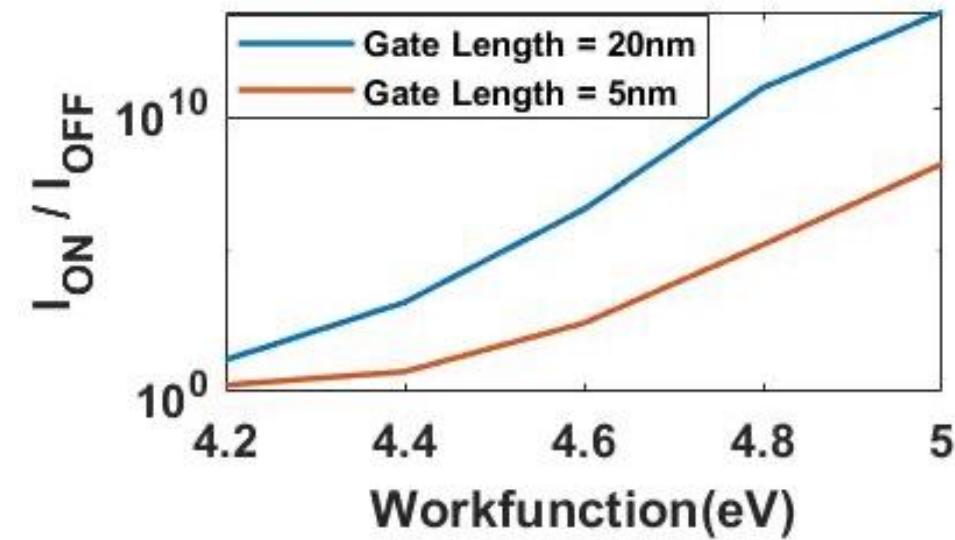
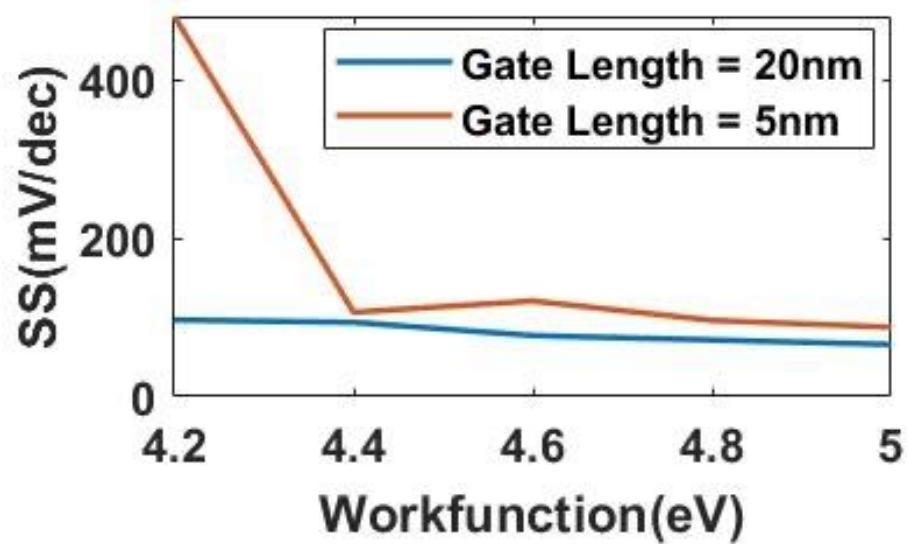
Energy vs. Gate Lengths Over Nanowire Diameters (nm)



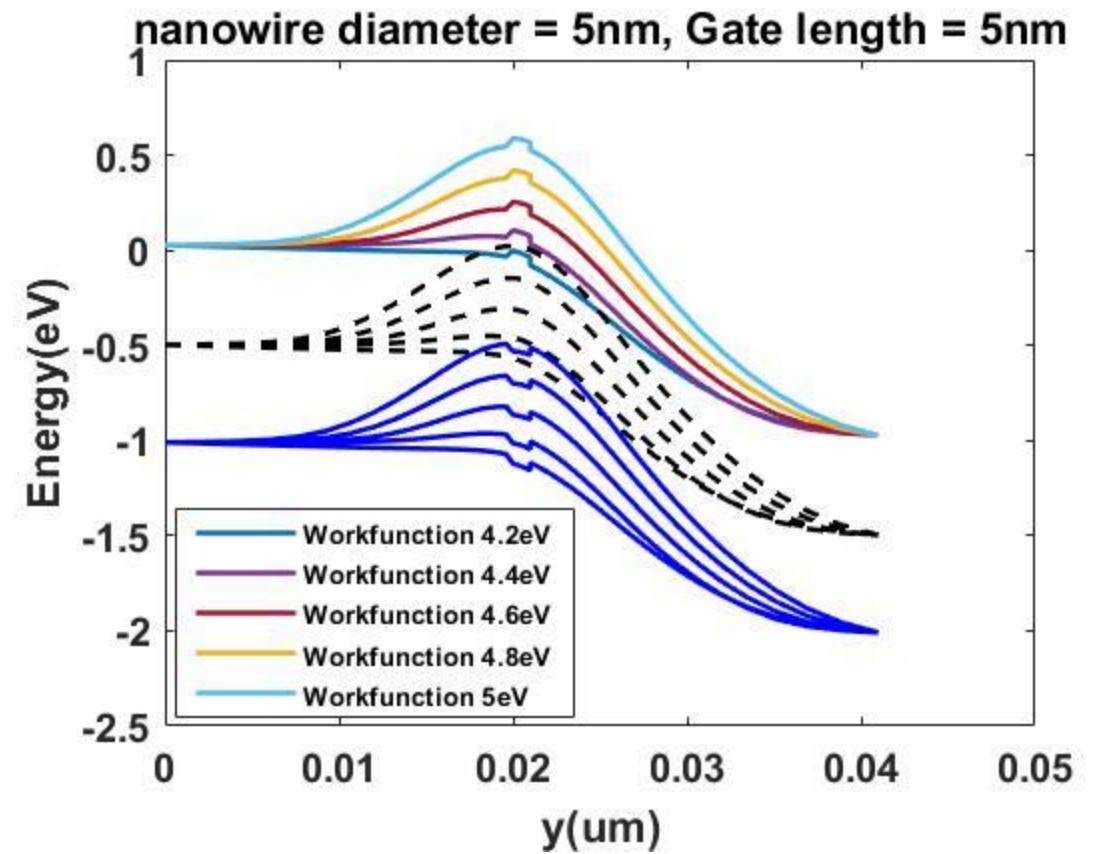
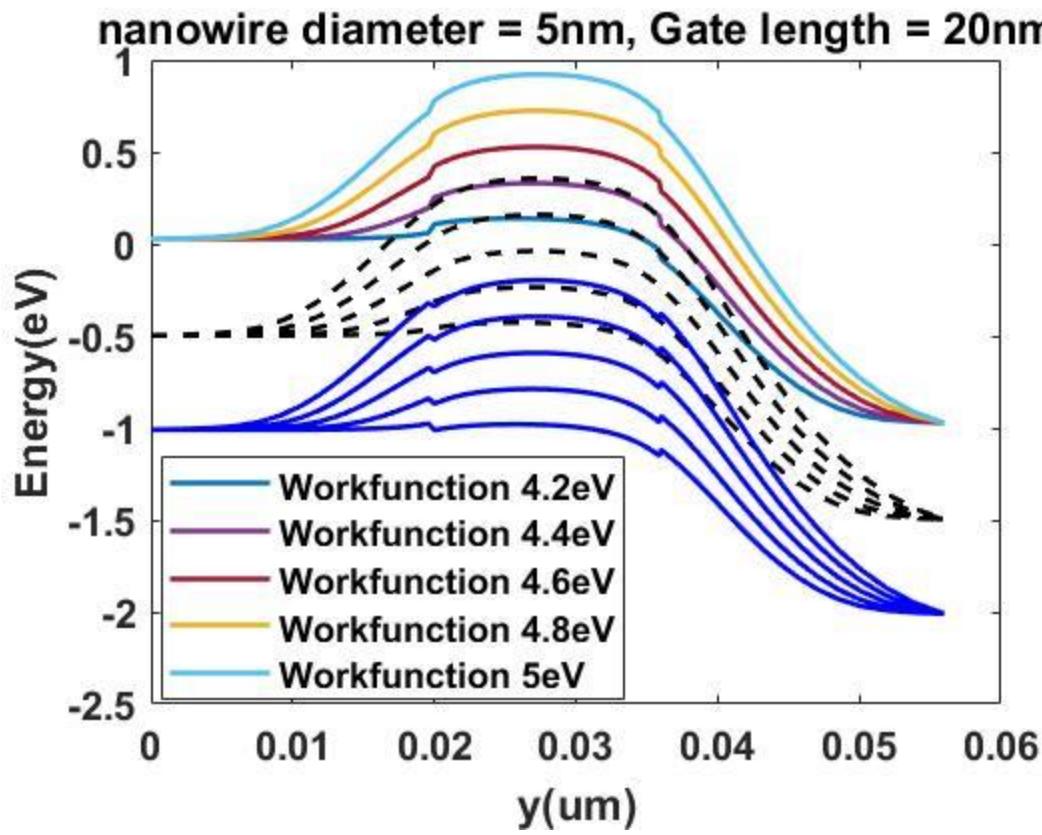
Energy vs. Gate Lengths Over Nanowire Diameters (nm) - Zoomed



Nanowire with Drift Diffusion - Workfunction Variations and Gate Potential Analysis (Transistor Parameters)



Nanowire with Drift Diffusion - Workfunction Variations and Gate Potential Analysis (Energy)



Nanowire Modes and Gating (NanoHub Quantum Dot Lab Inputs)

Quantum Dot Structure

Type of Quantum Dot Structure: Simple Quantum Dot

Simple Quantum Dot Options

Shape: Cylinder

Number of States: 8

X Dimensions: 2nm

Y Dimensions: 2nm

Z Dimensions: 1nm

Lattice Constant: 0.5nm

Effective Mass: .91

Energy gap: 1.43eV

Light Incident Angles

Angle Theta: 45deg

Angle Phi: 0deg

Sweep

Sweep Parameter: Angle phi (deg)

Minimum: 0

Maximum: 90

Number of Points: 3

Absorption

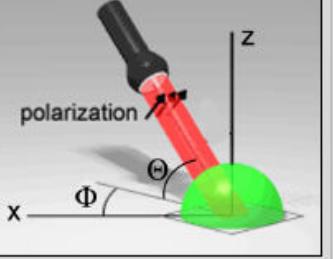
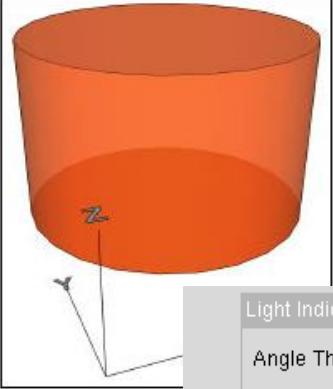
Simple Q Dot - Absolute Fermi Level: no

Simple Q Dot - Rel. or Abs. Fermi Level: 0eV

Multi-Layer - Fermi Level: 0.7eV

Temperature: 300K

State Broadening: 0.001



Output Eigenvalue HPC Specs

Output 3D Wavefunctions w/ Inner Shape: yes

Output 3D Wavefunct. w/ Outer Shapes: no

Output 3D Wavefunctions (no shapes): no

Output 3D Geometries: no

Output 3D Strain Fields (when computed): no

3D Resampling Resolution in X Direction: 20

3D Resampling Resolution in Y Direction: 20

3D Resampling Resolution in Z Direction: 20

Deformation Potential: yes

Dump Strain: yes

Messaging level (1-5): 3

Maximum number of output lines: 1000

Output Eigenvalue HPC Specs

Singleband

max_number_iterations: 2000

Convergence Limit: 1e-10

Output Eigenvalue HPC Specs

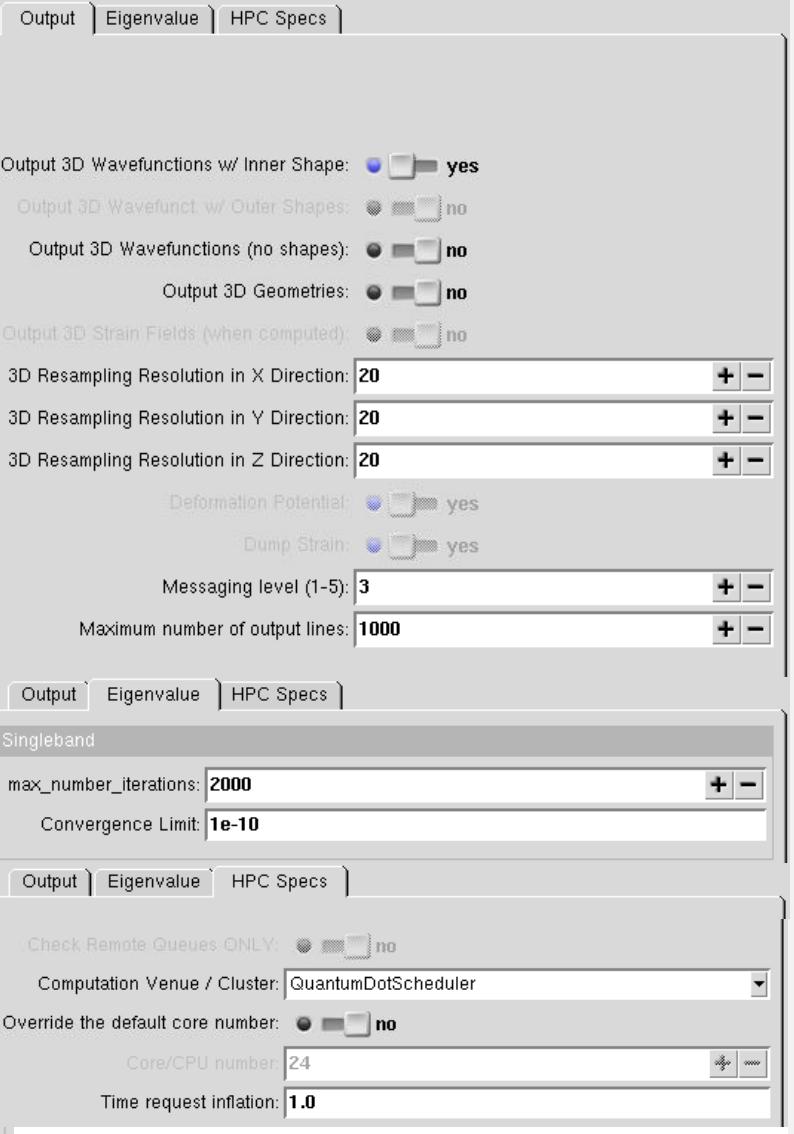
Check Remote Queues-ONLY: no

Computation Venue / Cluster: QuantumDotScheduler

Override the default core number: no

Core/CPU number: 24

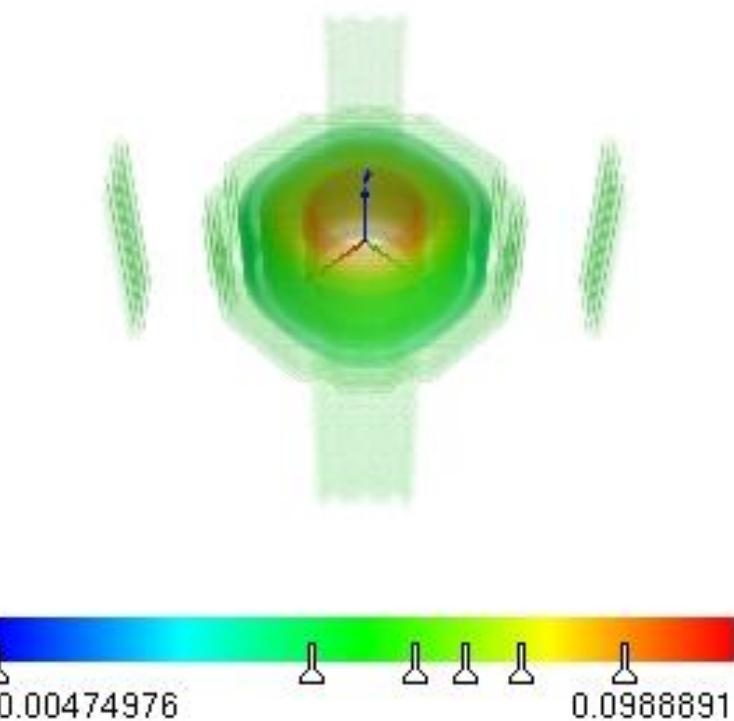
Time request inflation: 1.0



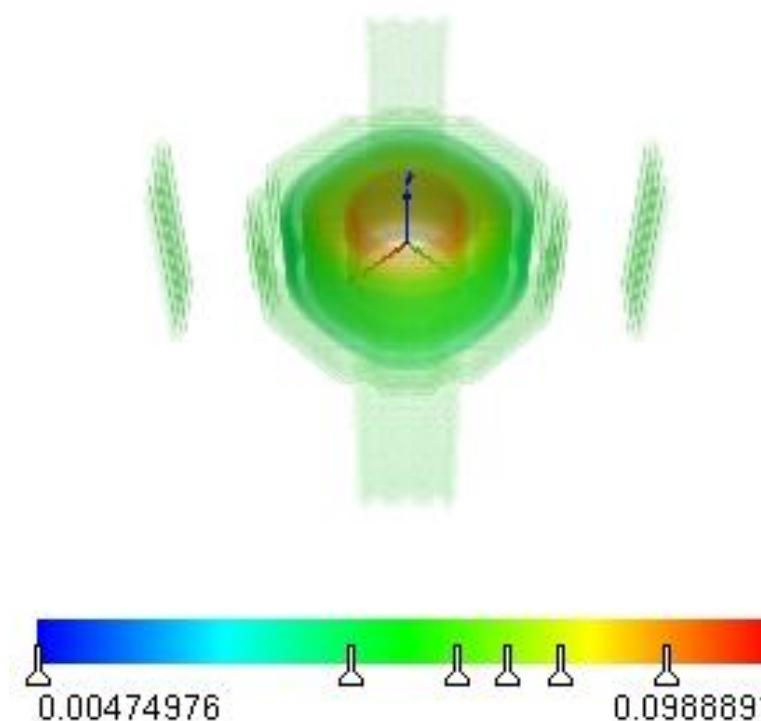
Tool located at:
<https://nanohub.org/tools/qdot>

Nanowire Modes and Gating (Wavefunctions)

Effective Mass: 0.19

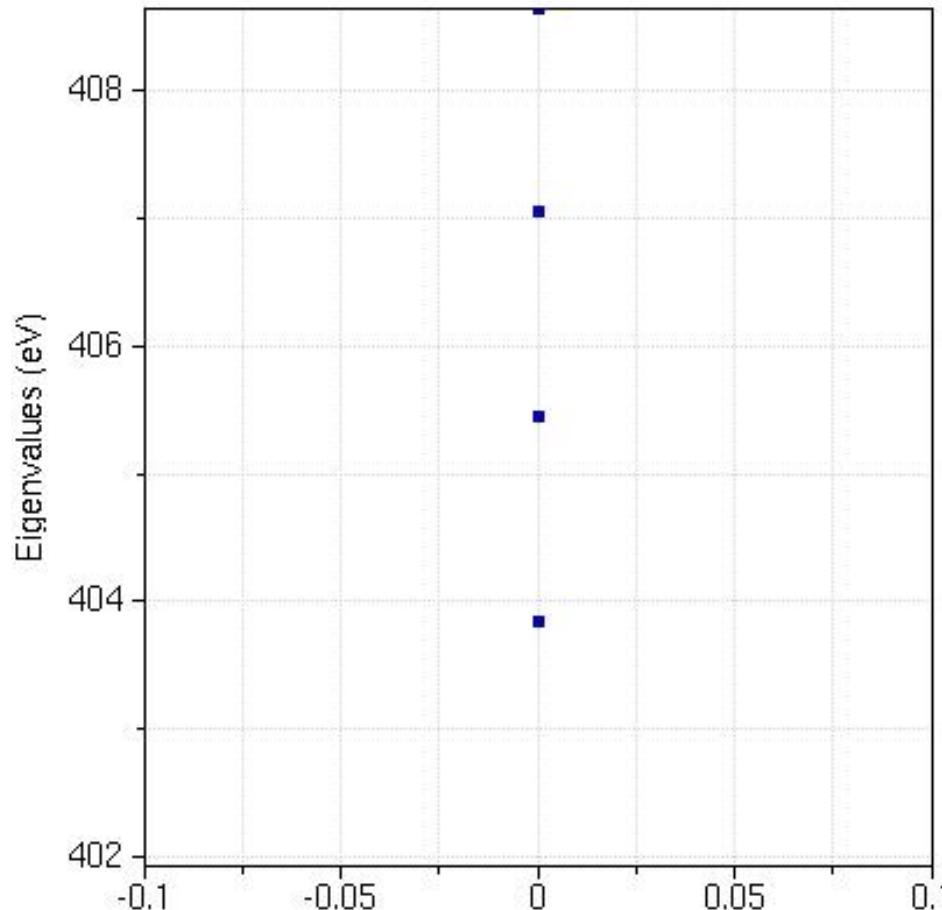


Effective Mass: 0.91

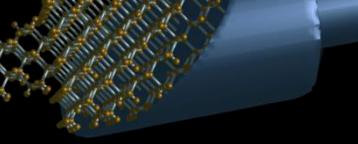
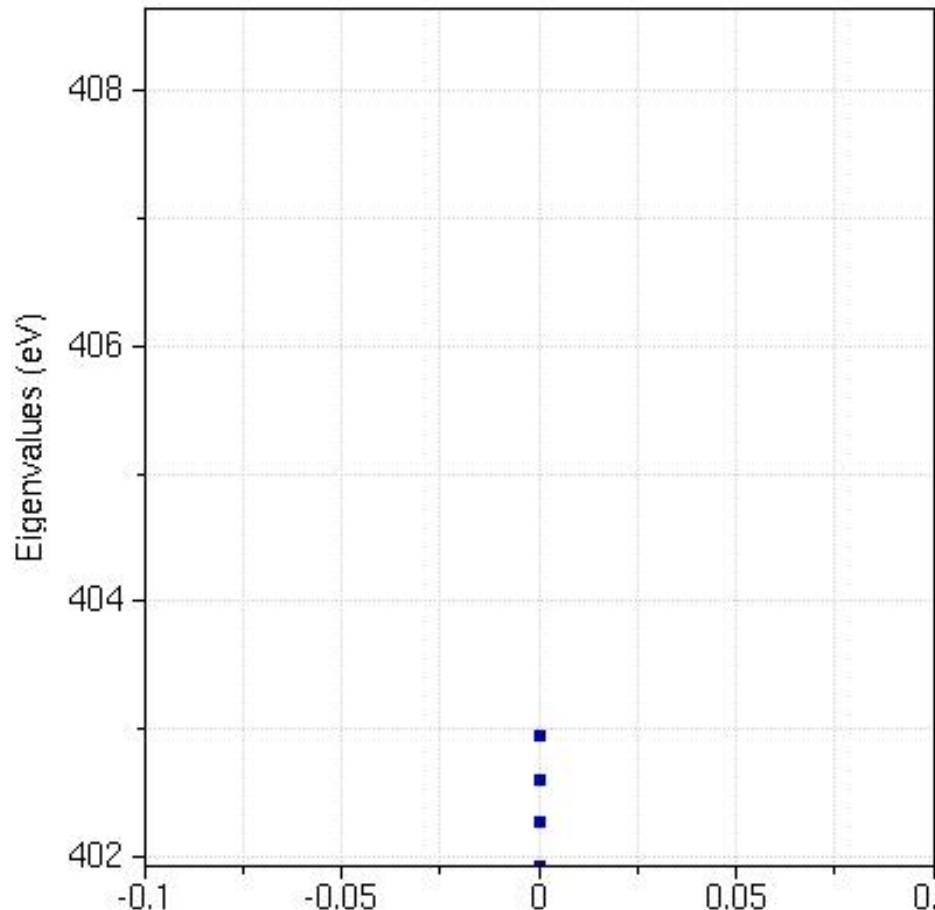


Nanowire Modes and Gating (Eigen Energies)

Effective Mass: 0.19



Effective Mass: 0.91



Nanowire Modes and Gating (NanoHub Nanowire Inputs)

Simulation parameters

Transport model: Uncoupled mode space NEGF

Include scattering: no

Number of eigenvalues: 9

Mesh fineness factor: 7

Geometry & doping | Gate | Drain |

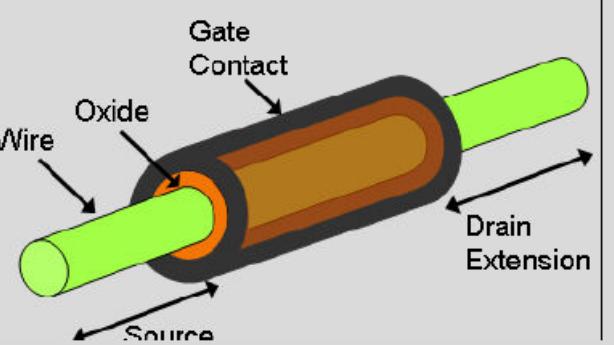
Diameter of the silicon-nanowire: 2nm

Oxide thickness: 1nm

Gate length: 8nm

Source & drain extension length: 8nm

Source & drain doping (n) in: $1e+20/cm^3$



Geometry & doping | Gate | Drain |

Gate voltage start value: 0V

Step size: 0.04V

Number of steps: 11

Geometry & doping | Gate | Drain |

Drain voltage start value: 0.4V

Step size: 0.001V

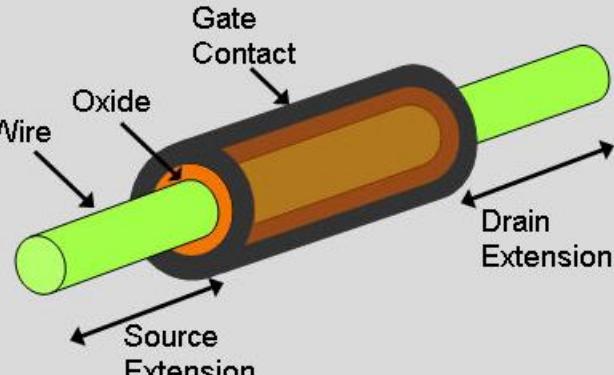
Number of steps: 1

Material Properties

Simulation materials: Silicon(Si)

Gate work function: 4.05eV

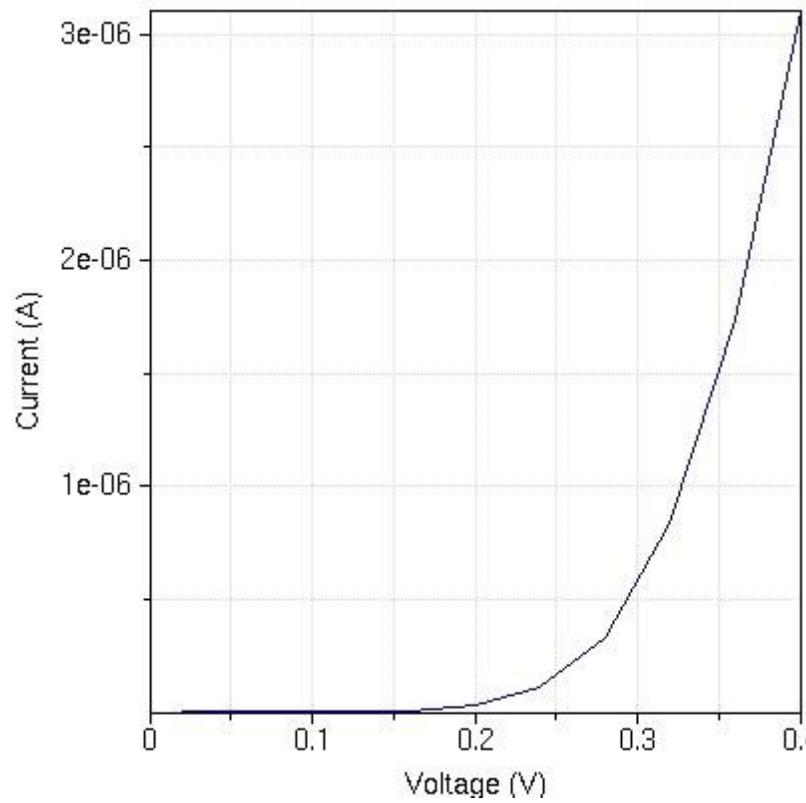
Orientation: 1 1 1



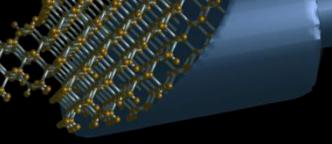
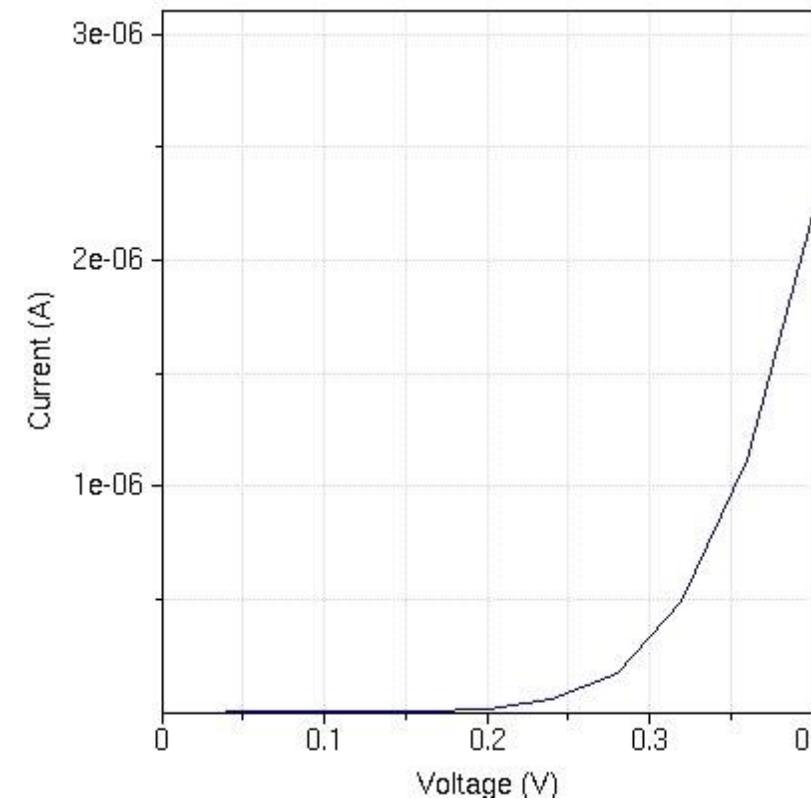
Tool located at:
<https://nanohub.org/tools/nanowire>

Nanowire Modes and Gating (I-Vg Curves)

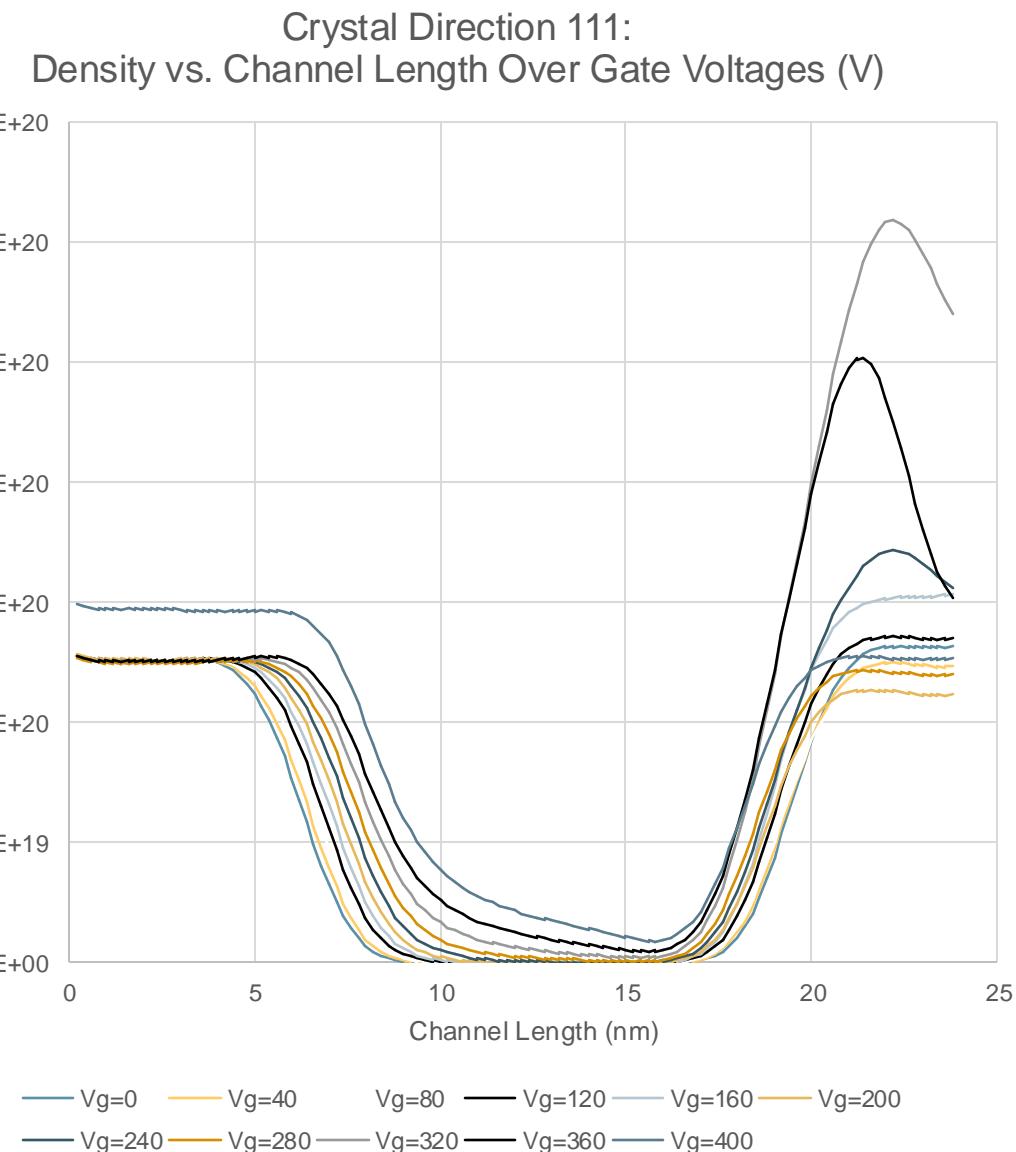
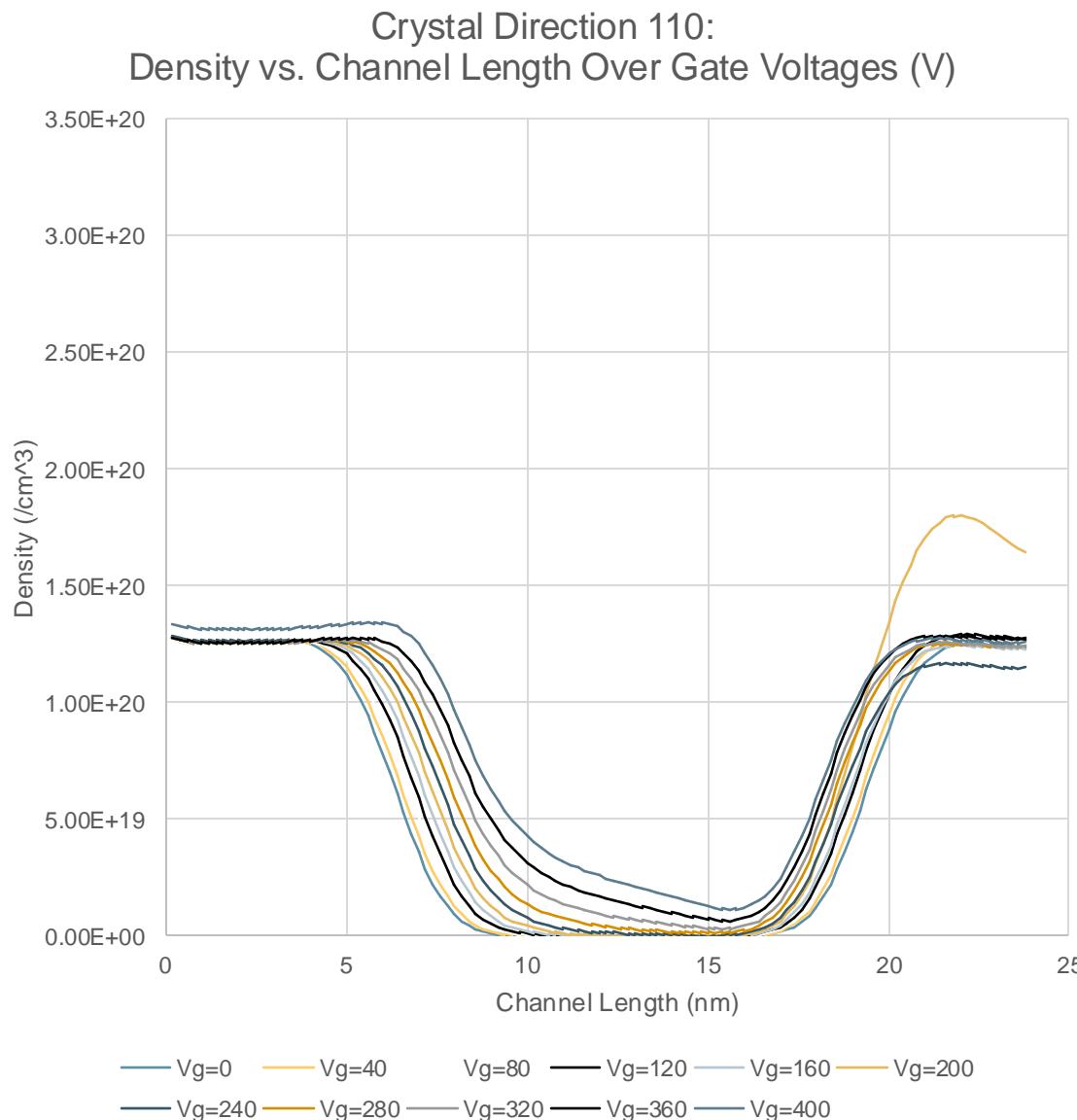
Crystal Direction: 110

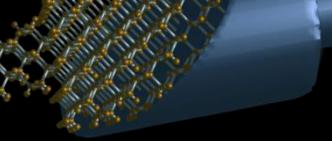


Crystal Direction: 111

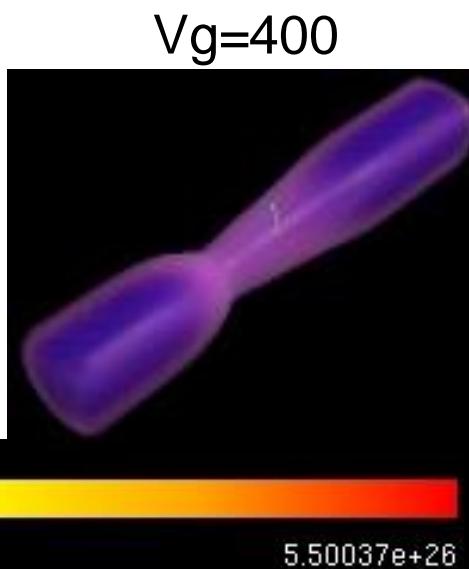
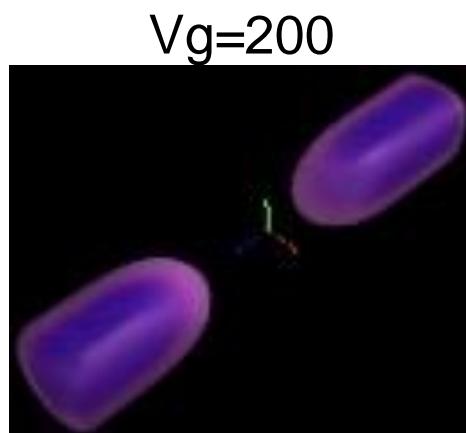
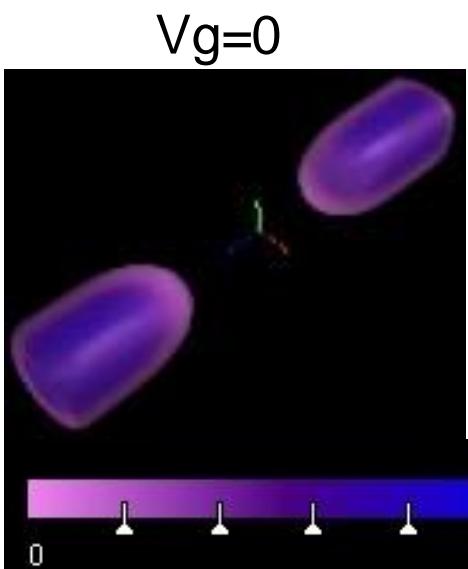


Nanowire Modes and Gating (1D Electron Densities)

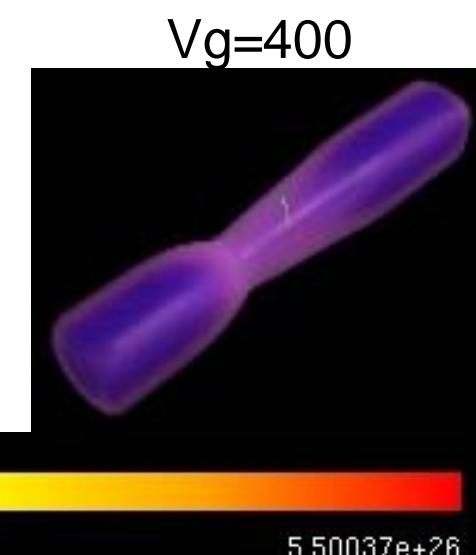
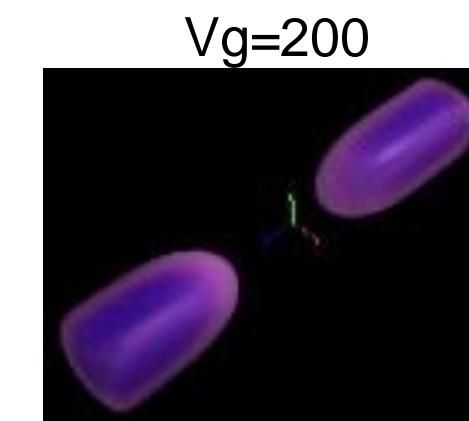
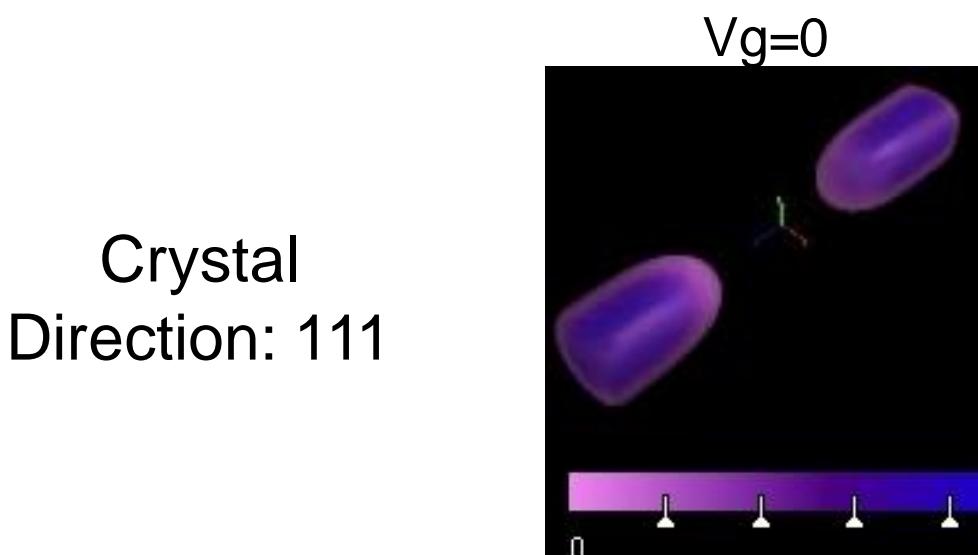




Nanowire Modes and Gating (3D Electron Densities)



Crystal
Direction: 110



Crystal
Direction: 111

Nanowire Realistic Bandstructure (Inputs)

All default settings were utilized, except as where shown (red boxes mark variable inputs):

1 Device Type → 2 Physics → 3 K-Space → 4 Numerics → 5 Simulate

Geometry: Nanowire (1D-periodic)

Calculation For: Electrons

Material: Si

Alloy Model: Virtual Crystal Approximation

Molar fraction: 0.5

Job Type: Calculate the wire band structure

Device cross section: Circle

Diameter: **2.1nm**

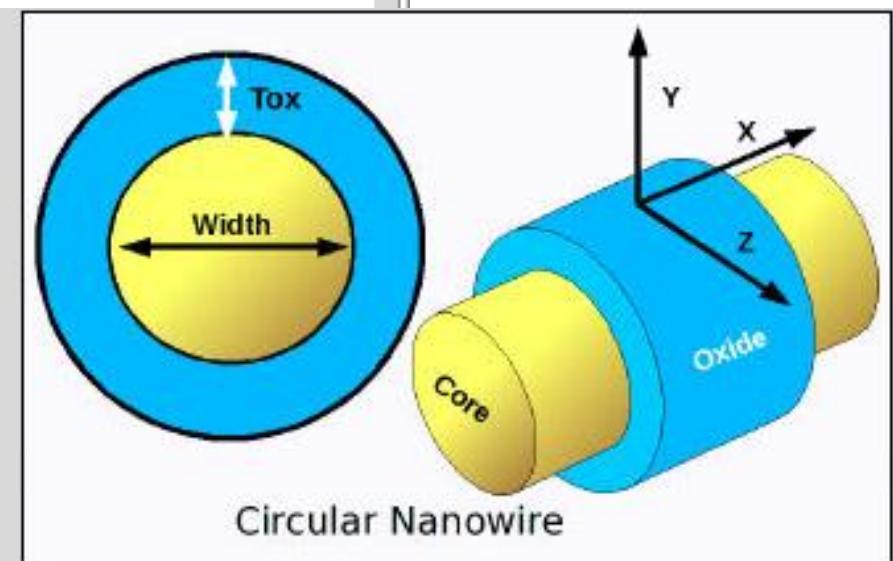
Oxide Thickness(T_{ox}): 2.2nm

Crystal Orientation

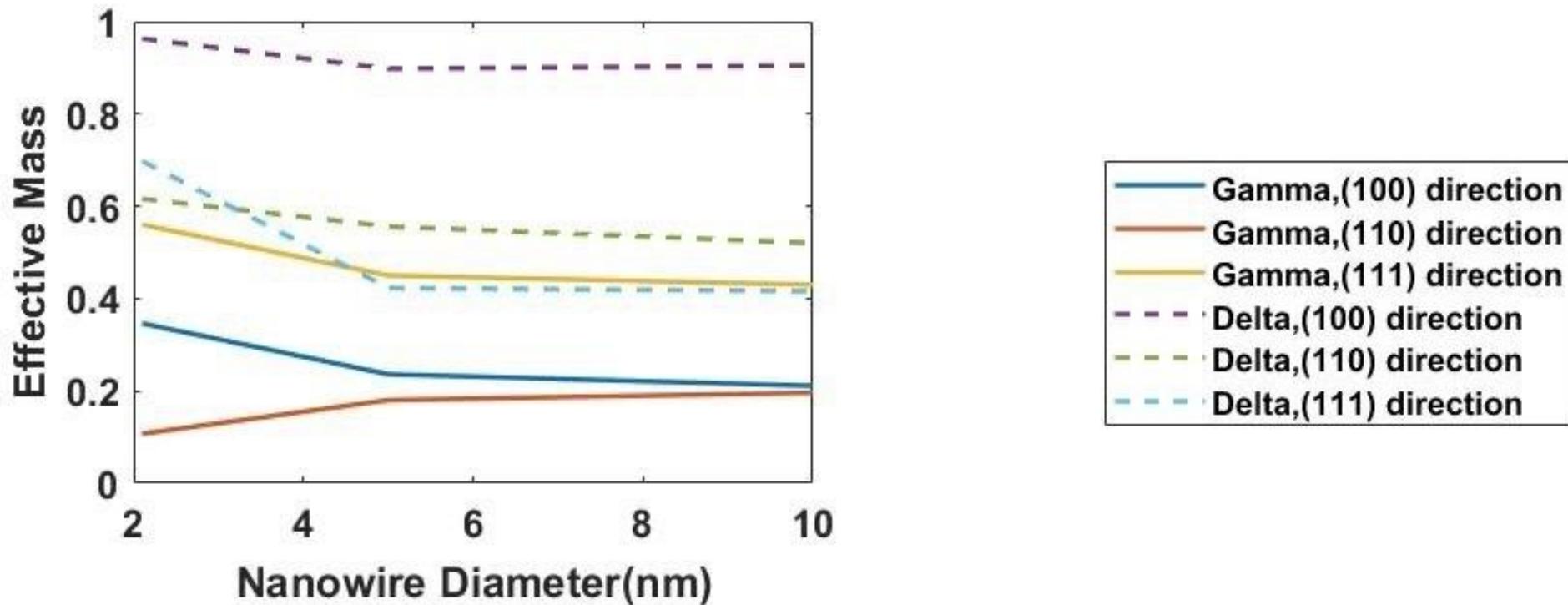
Transport direction (X): **(100)**

Confinement direction (Z): [010]

Tool located at:
<https://nanohub.org/resources/bandstrlab>



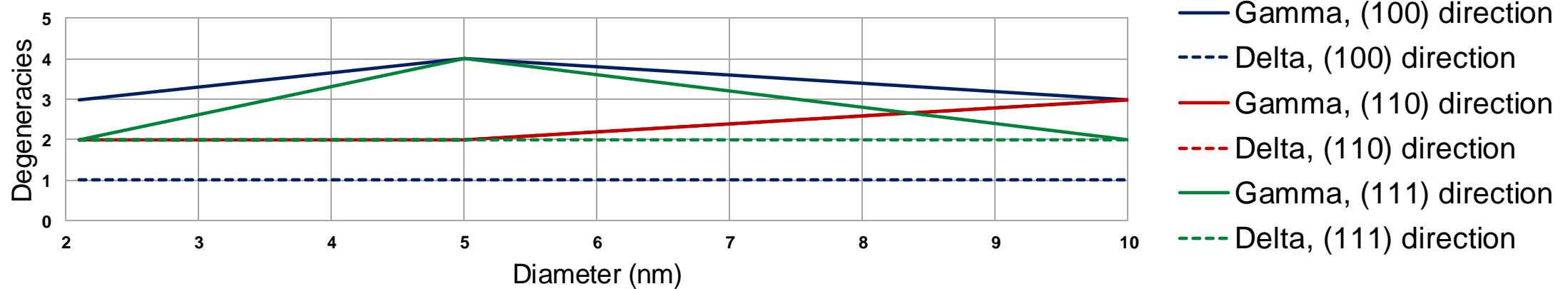
Nanowire Realistic Bandstructure (Masses)



Nanowire Realistic Bandstructure (Degeneracies)

Diameter (nm)	Region	(100) direction		(110) direction		(111) direction	
		m_{eff}	Degeneracy	m_{eff}	Degeneracy	m_{eff}	Degeneracy
2.1	Gamma	0.346	3	0.107	2	0.56	2
	Delta	0.963	1	0.616	2	0.698	2
5	Gamma	0.236	4	0.180	2	0.45	4
	Delta	0.898	1	0.556	2	0.423	2
10	Gamma	0.211	3	0.196	3	0.43	2
	Delta	0.905	1	0.52	3	0.416	2

Number of Degeneracies vs. Diameter



Nanowire Top-of-Barrier Transport (Inputs)

All default settings were utilized, except as where shown (red boxes mark variable inputs):

Device Models Environment

Model: Silicon Nanowire MOSFET

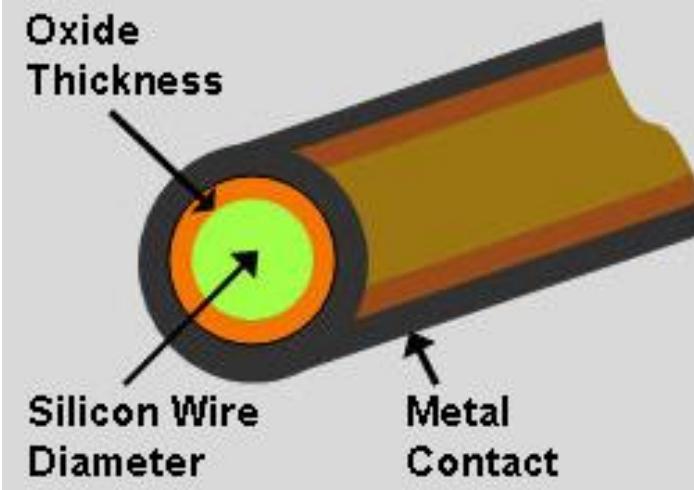
Nanowire Diameter: **2.1nm**

Gate Insulator Thickness: **1.5nm**

Gate Insulator Dielectric Constant: **3.9**

Transport Effective Mass: **.346**

Valley Degeneracy: **3** **+** **-**



Threshold Voltage: **0.32V**

Gate Control Parameter: **1**

Drain Control Parameter: **0**

Series Resistance (ohm- μ m): **0**

Ambient Temperature: **300K**

Gate Voltage Sweep

Initial Gate Voltage: **0V**

Final Gate Voltage: **1V**

Gate Voltage Bias Points: **13** **+** **-**

Drain Voltage Sweep

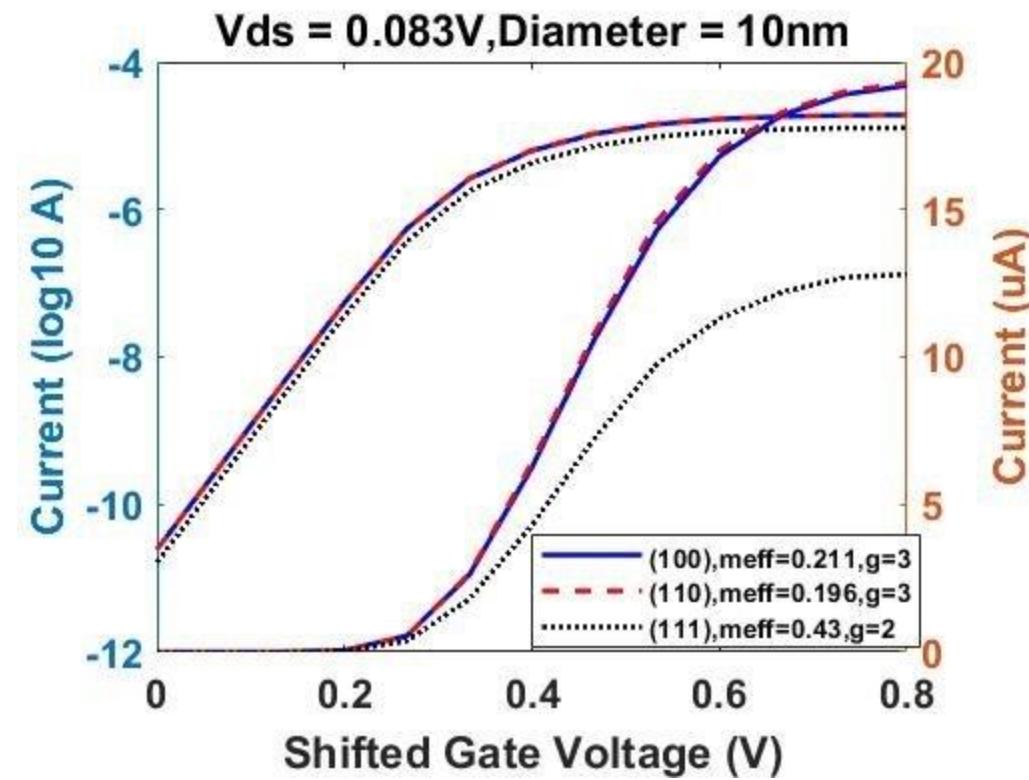
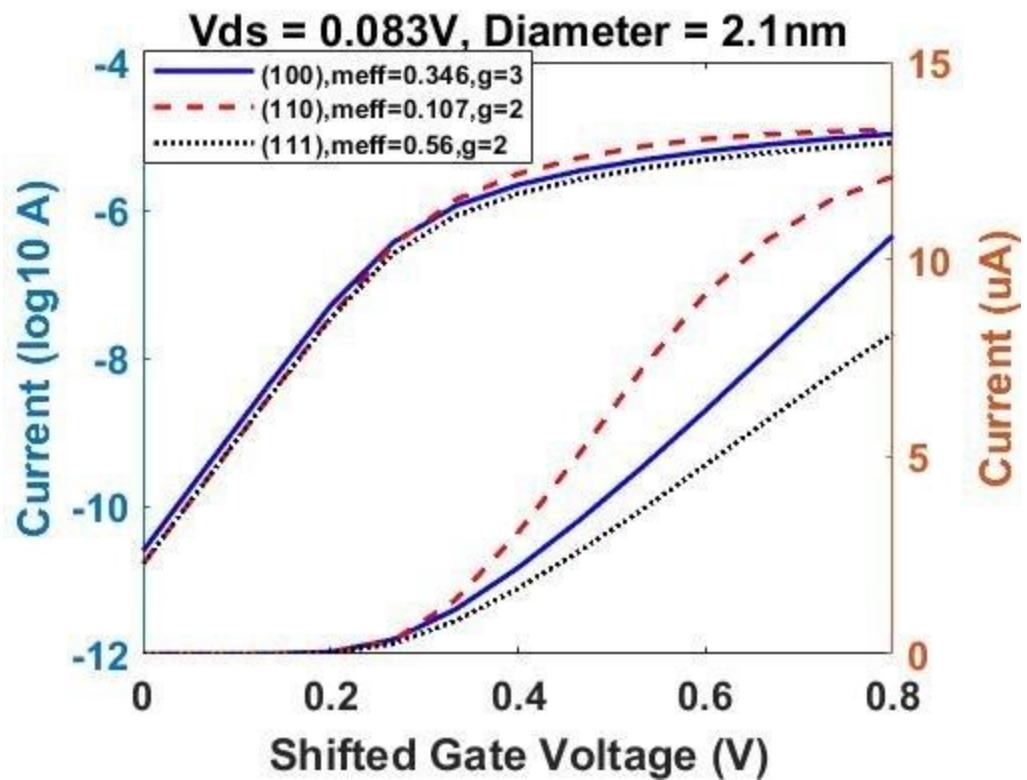
Initial Drain Voltage: **0V**

Final Drain Voltage: **1V**

Drain Voltage Bias Points: **13** **+** **-**

Tool located at:
<https://nanohub.org/resources/fettoy>

Nanowire Top-of-Barrier Transport (I-V Curves)



Fast Nanowire Quantum Transport (Input Deck)

Lsd : Source/Drain Length: **20nm**

Lc : Channel Length: **3nm**

Lg : Gate Length: **5nm** → Varied across 5nm, 10nm, 20nm

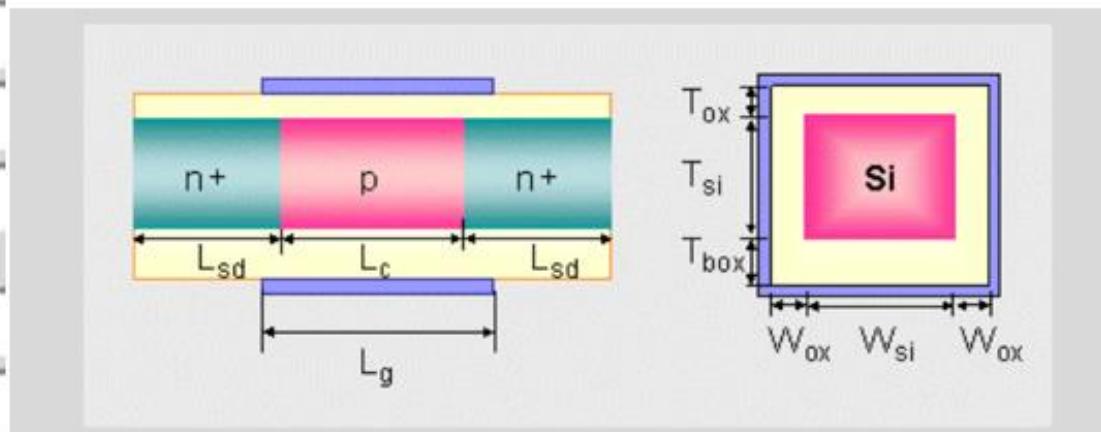
Tox : Oxide Thickness: **1nm**

Tsi : Silicon Body Thickness: **3nm**

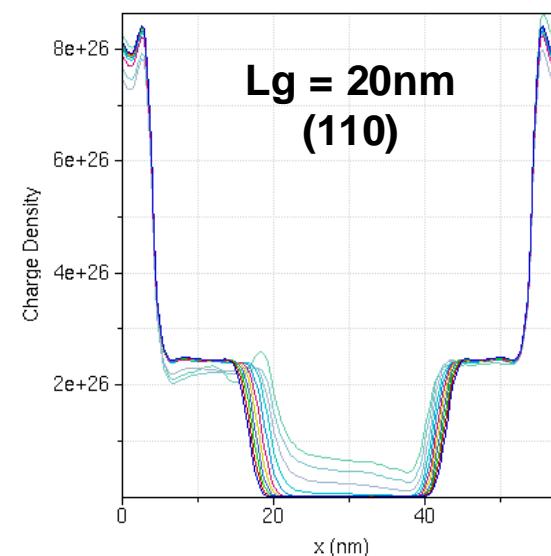
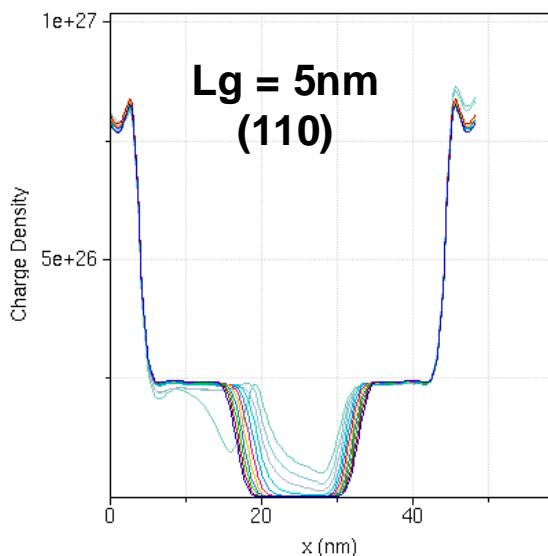
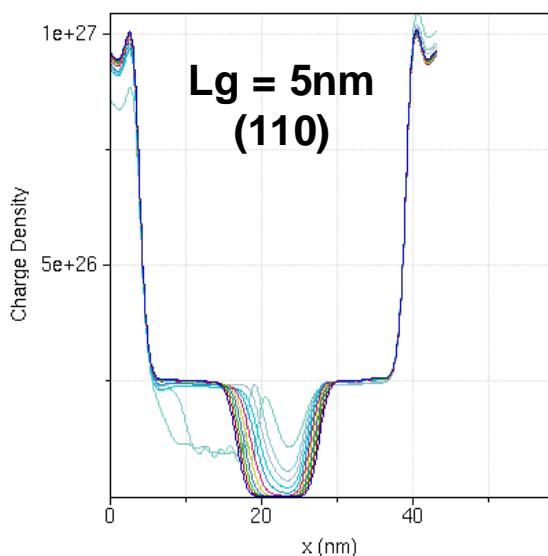
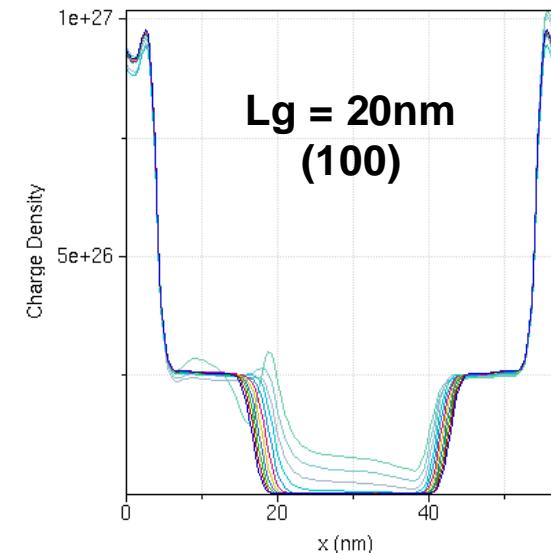
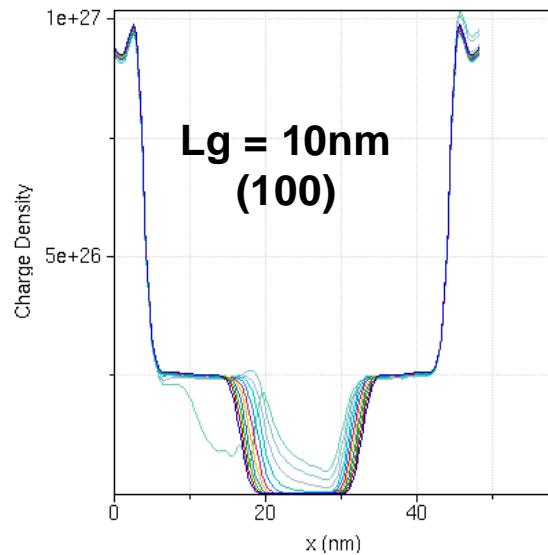
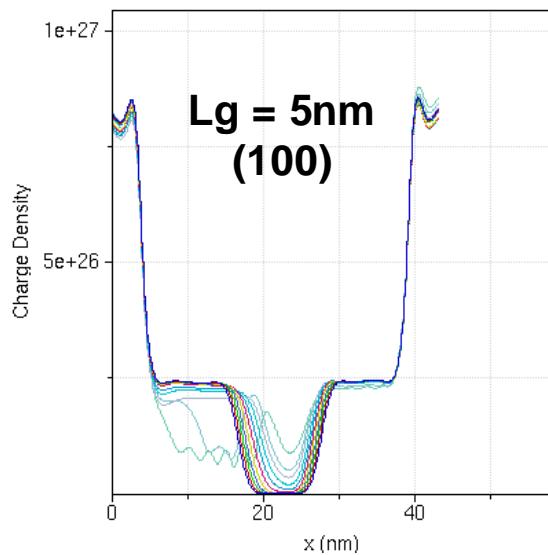
Tbox : Buried Oxide Thickness: **1nm**

Wox : Oxide Width: **1nm**

Wsi : Silicon Body Width: **3nm**



Fast Nanowire Quantum Transport (Charge Density Profiles)

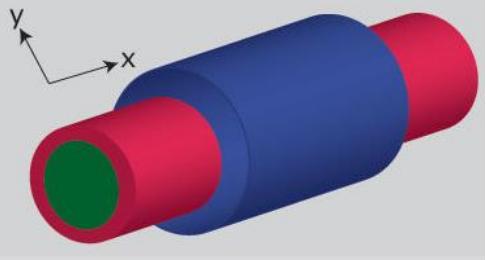


Long Nanowire Quantum Transport (Inputs)

1 Device Type → 2 Structure → 3 Material → 4 Environments → 5 Expert Options

Device Type

Class: Circular Nanowire



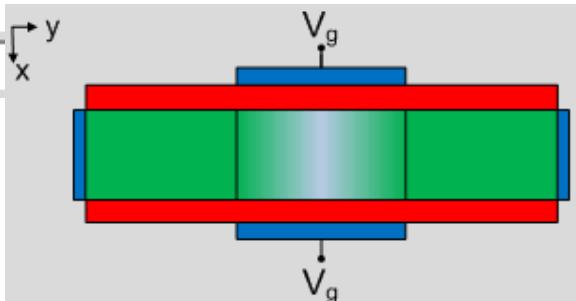
1 Device Type → 2 Structure → 3 Material → 4 Environments → 5 Expert Options

Plot options for bias Gate bias Drain bias Source bias Temperature

Minimum bias: 0V

Maximum bias: 0.6V

Number of bias points: 13



1 Device Type → 2 Structure → 3 Material → 4 Environments → 5 Expert Options

Geometry-X Geometry-Y Geometry-Z Crystal Orientation Strain Doping

Channel length - Lc: 15nm

Source length - Ls: 10nm

Drain length - Ld: 10nm

Geometry-X Geometry-Y Geometry-Z Cr...

Diameter - Dch: 2.1nm

Oxide thickness - Tox: 1nm

Channel width - Wch: 2.5nm

Left wall oxide thickness - Tox1: 1nm

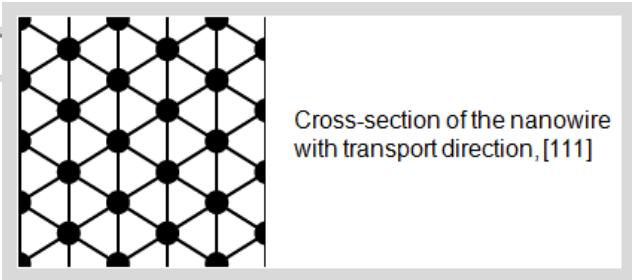
Right wall oxide thickness - Tox2: 1nm

Geometry-X Geometry-Y Geometry-Z Crystal Orientation Strain Doping

Transport direction: 1 1 1

Confinement direction in y: -1 1 0

Confinement direction in z: -1 -1 2

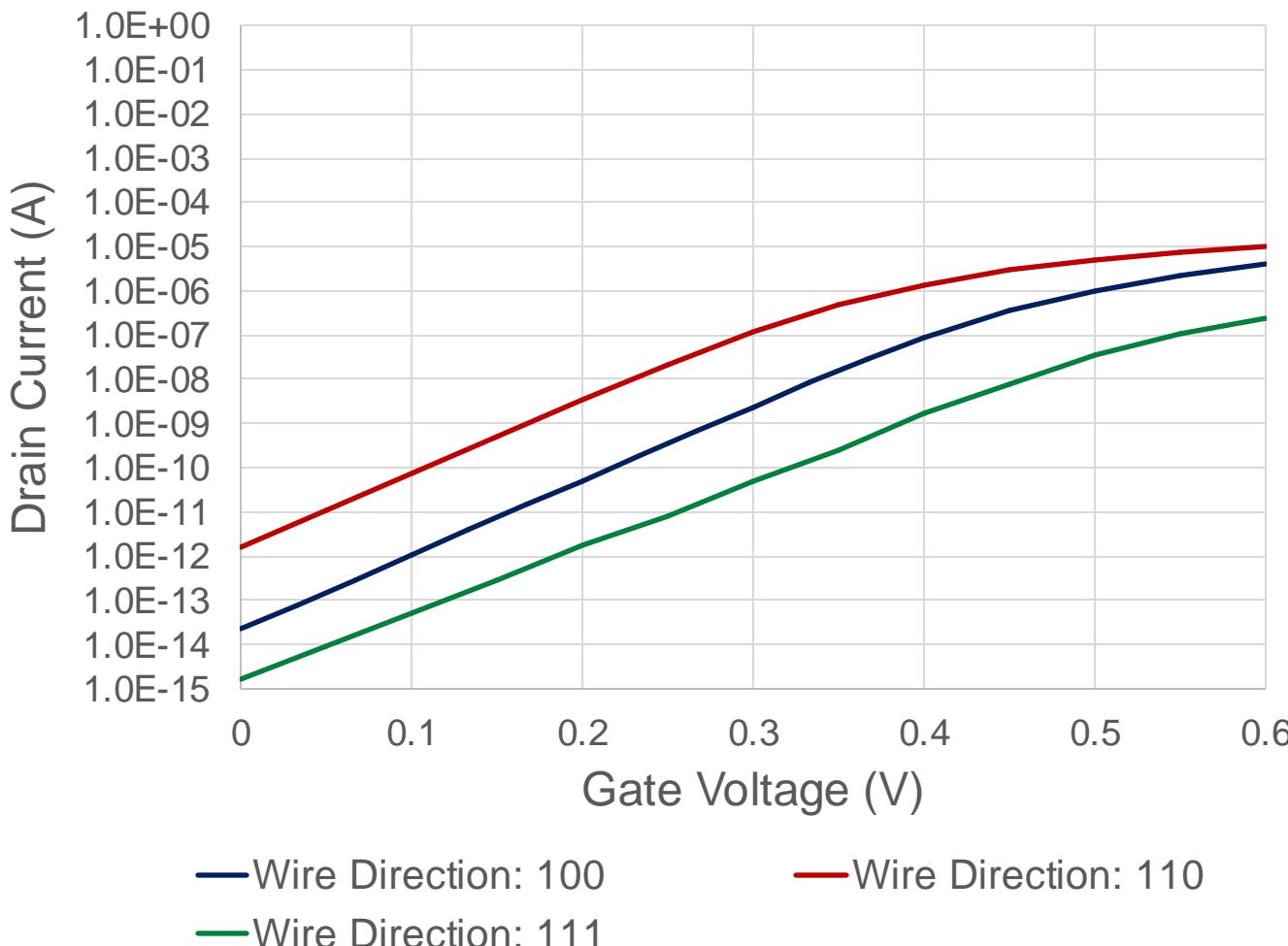


Cross-section of the nanowire with transport direction, [111]

Tool located at:
<https://nanohub.org/resources/omenwire>

Long Nanowire Quantum Transport (Id-Vg Curve)

Id - Vg Curve with 2.1nm Cross Section &
15nm Channel/Gate Lengths



Critical Parameters:

ON/OFF Current Ratio:

- Wire Direction 100 = 1.86×10^8
- Wire Direction 110 = 6.77×10^6
- Wire Direction 111 = 2.46×10^8

Subthreshold Swing:

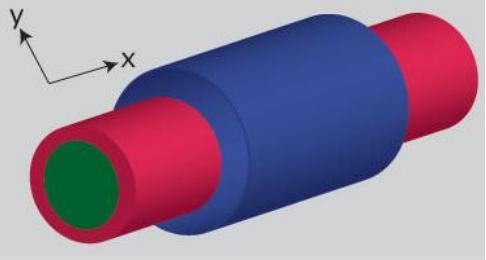
- Wire Direction 100 = 59.47 mv/dec
- Wire Direction 110 = 59.87 mv/dec
- Wire Direction 111 = 60.69 mv/dec

Short Nanowire Quantum Transport (Inputs)

1 Device Type → 2 Structure → 3 Material → 4 Environments → 5 Expert Options

Device Type

Class: Circular Nanowire



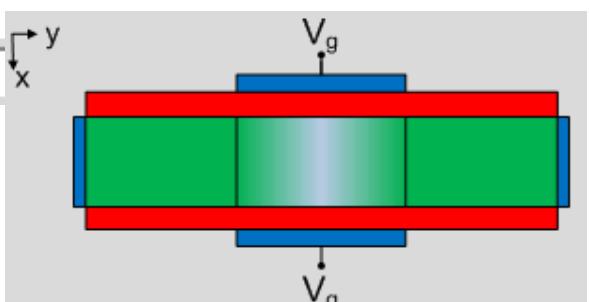
1 Device Type → 2 Structure → 3 Material → 4 Environments → 5 Expert Options

Plot options for bias Gate bias Drain bias Source bias Temperature

Minimum bias: $-1\pm 0V$

Maximum bias: $-1\pm 0.6V$

Number of bias points: 13



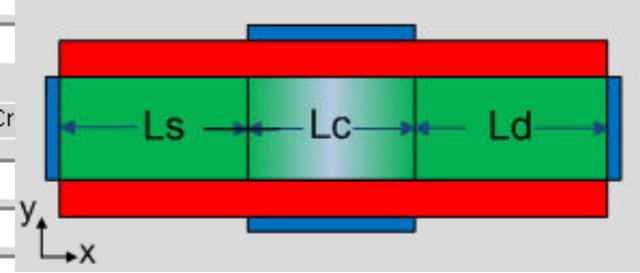
1 Device Type → 2 Structure → 3 Material → 4 Environments → 5 Expert Options

Geometry-X Geometry-Y Geometry-Z Crystal Orientation Strain Doping

Channel length - Lc: 15nm

Source length - Ls: 10nm

Drain length - Ld: 10nm



Geometry-X Geometry-Y Geometry-Z Cr Strain Doping

Diameter - Dch: 1.9nm

Oxide thickness - Tox: 1nm

Channel width - Wch: 2.5nm

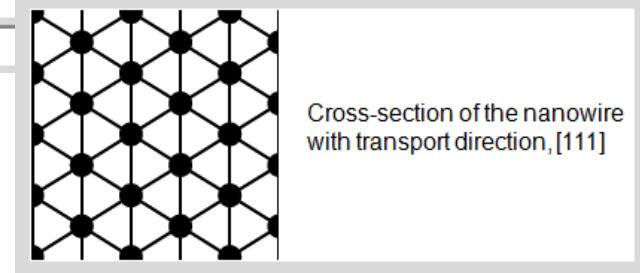
Left wall oxide thickness - Tox1: 1nm

Right wall oxide thickness - Tox2: 1nm

Transport direction: 1 1 1

Confinement direction in y: -1 1 0

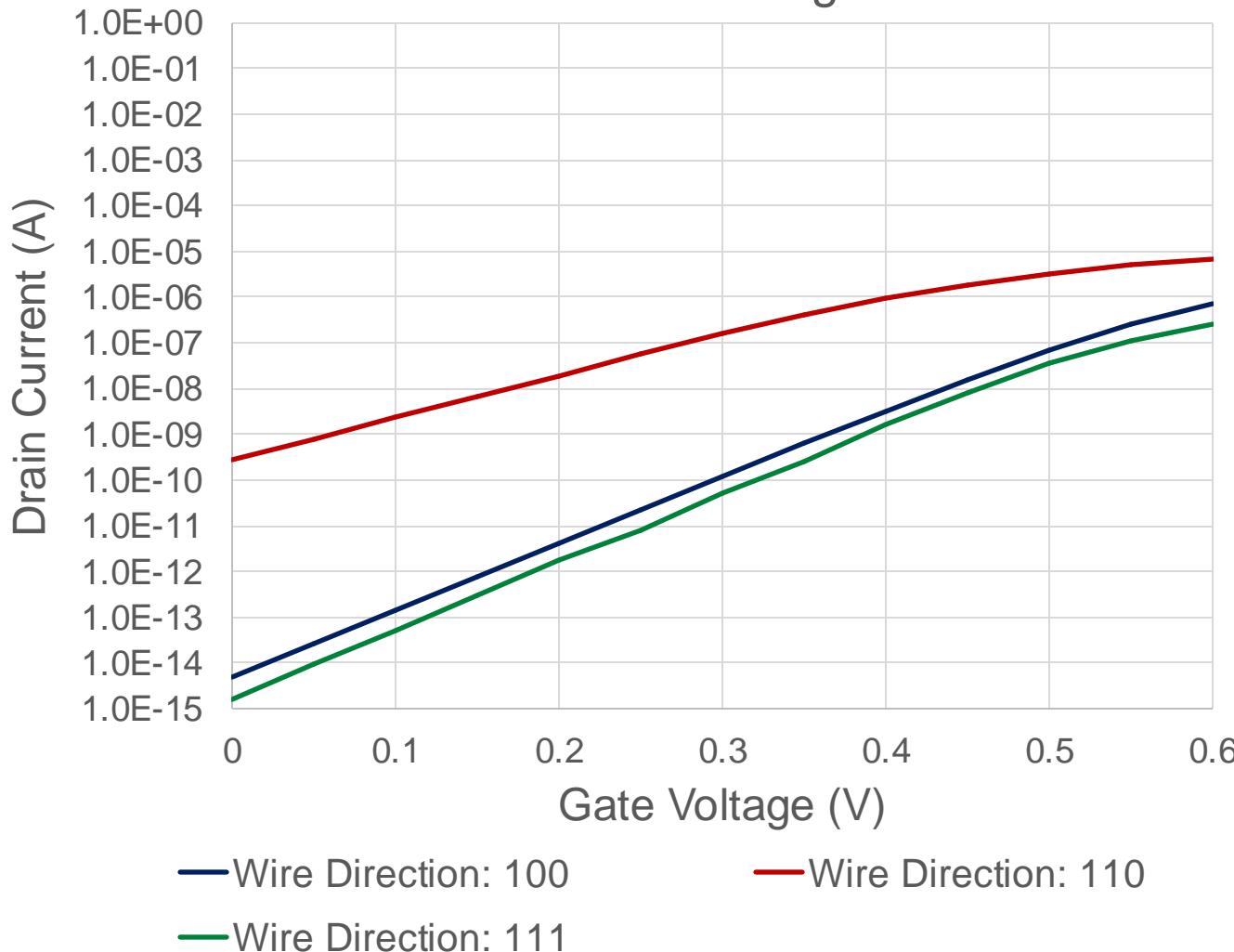
Confinement direction in z: -1 -1 2



Tool located at:
<https://nanohub.org/resources/omenwire>

Short Nanowire Quantum Transport (Id-Vg Curve)

Id - Vg Curve with 1.9nm Cross Section &
5nm Channel/Gate Lengths



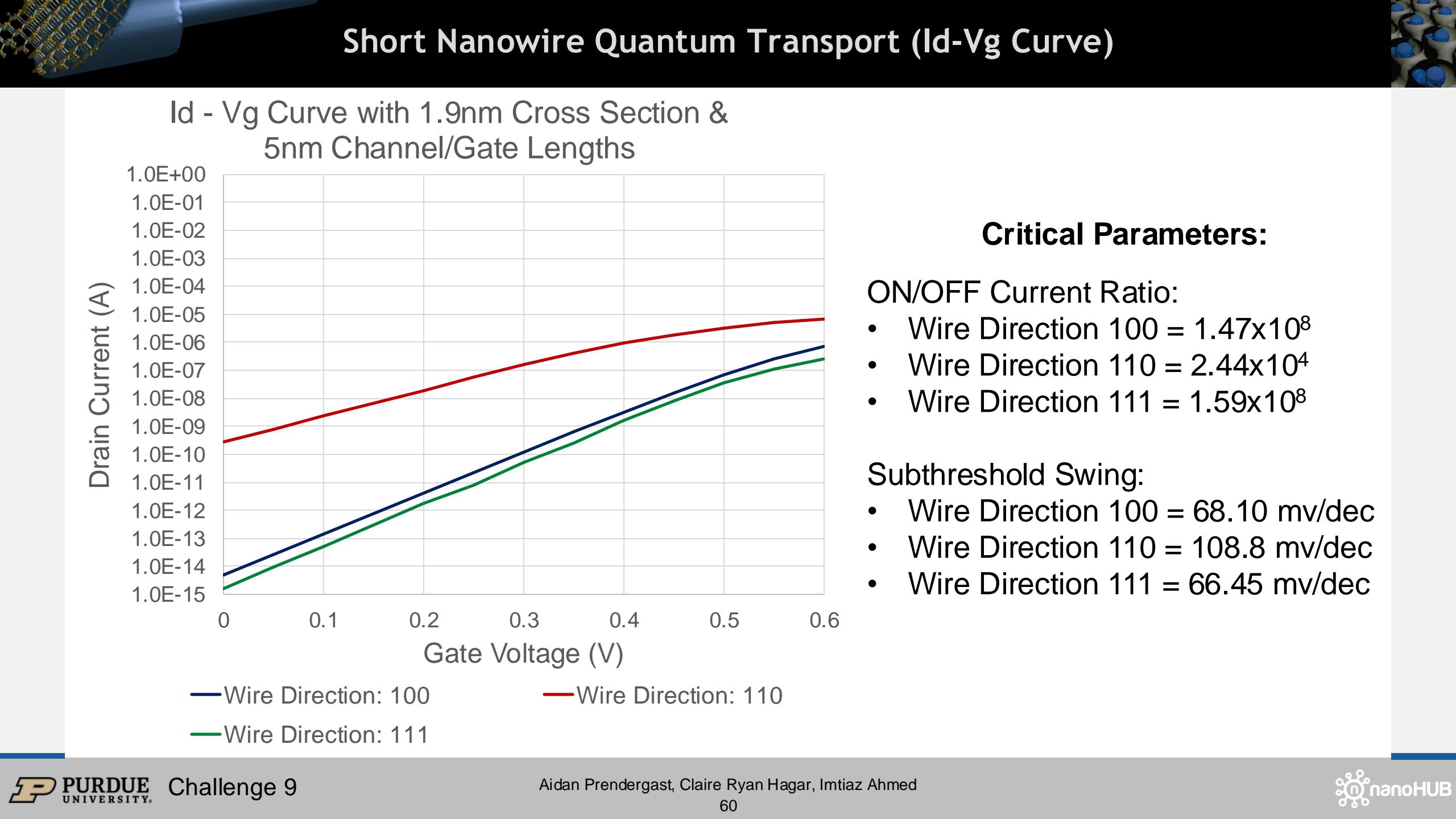
Critical Parameters:

ON/OFF Current Ratio:

- Wire Direction 100 = 1.47×10^8
- Wire Direction 110 = 2.44×10^4
- Wire Direction 111 = 1.59×10^8

Subthreshold Swing:

- Wire Direction 100 = 68.10 mv/dec
- Wire Direction 110 = 108.8 mv/dec
- Wire Direction 111 = 66.45 mv/dec



Nanowire Dispersion Design (Inputs)

All default settings were utilized, except as where shown:

1 Device Type → 2 Physics → 3 K-Space → 4 Numerics → 5 Simulate

Geometry: Nanowire (1D-periodic)

Calculation For: Electrons

Material: Si

Alloy Model: Virtual Crystal Approximation

Molar fraction: 0.5

Job Type: Calculate the wire band structure

Device cross section: Circle

Diameter: 1.9nm

Oxide Thickness(T_{ox}): 2.2nm

Crystal Orientation

Transport direction (X): (100)

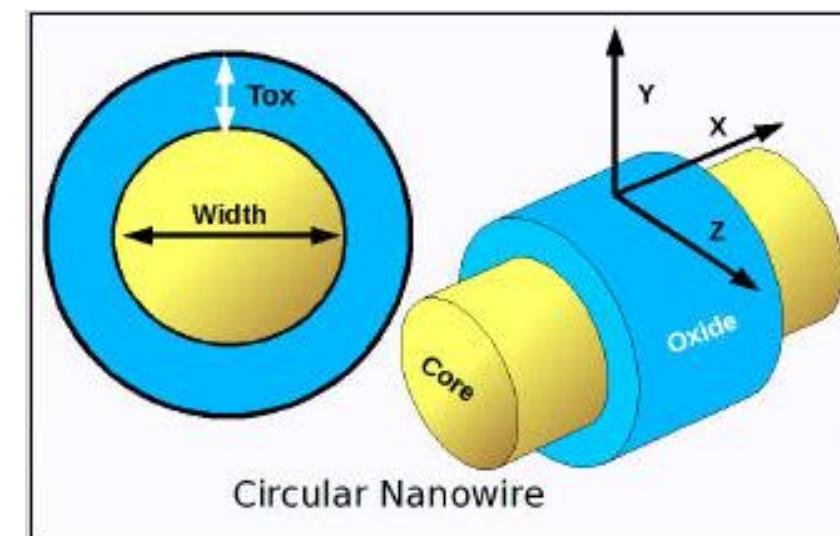
Confinement direction (Z): [010]

1 Device Type → 2 Physics → 3 K-Space → 4 Numerics → 5 Simulate

Electronic Structure Strain

Strain type: Uniaxial (along transport direction X)

Epsilon: 0.02



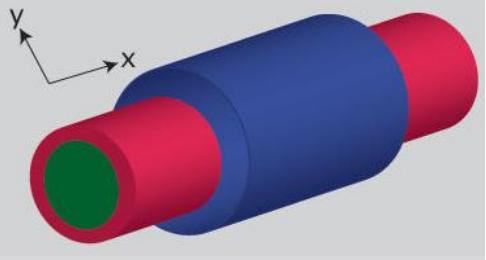
Tool located at:
<https://nanohub.org/resources/bandstrlab>

Optimized Nanowire Quantum Transport (Inputs)

1 Device Type → 2 Structure → 3 Material → 4 Environments → 5 Expert Options

Device Type

Class: Circular Nanowire



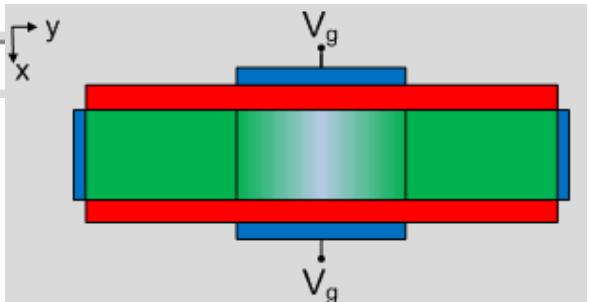
1 Device Type → 2 Structure → 3 Material → 4 Environments → 5 Expert Options

Plot options for bias Gate bias Drain bias Source bias Temperature

Minimum bias: 0V

Maximum bias: 0.6V

Number of bias points: 13



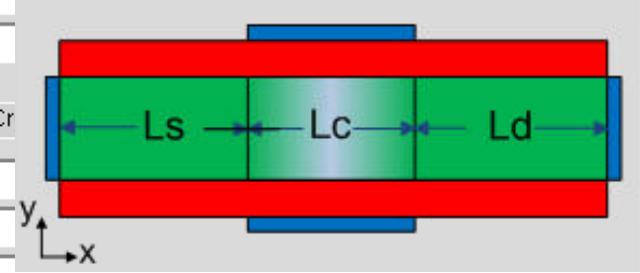
1 Device Type → 2 Structure → 3 Material → 4 Environments → 5 Expert Options

Geometry-X Geometry-Y Geometry-Z Crystal Orientation Strain Doping

Channel length - Lc: 15nm

Source length - Ls: 10nm

Drain length - Ld: 10nm



Geometry-X Geometry-Y Geometry-Z Cr Strain Doping

Diameter - Dch: 1.9nm

Oxide thickness - Tox: 1nm

Channel width - Wch: 2.5nm

Left wall oxide thickness - Tox1: 1nm

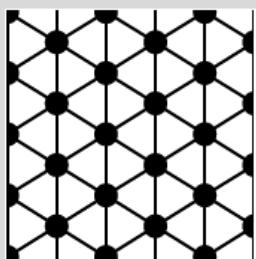
Right wall oxide thickness - Tox2: 1nm

Geometry-X Geometry-Y Geometry-Z Crystal Orientation Strain Doping

Transport direction: 1 1 1

Confinement direction in y: -1 1 0

Confinement direction in z: -1 -1 2

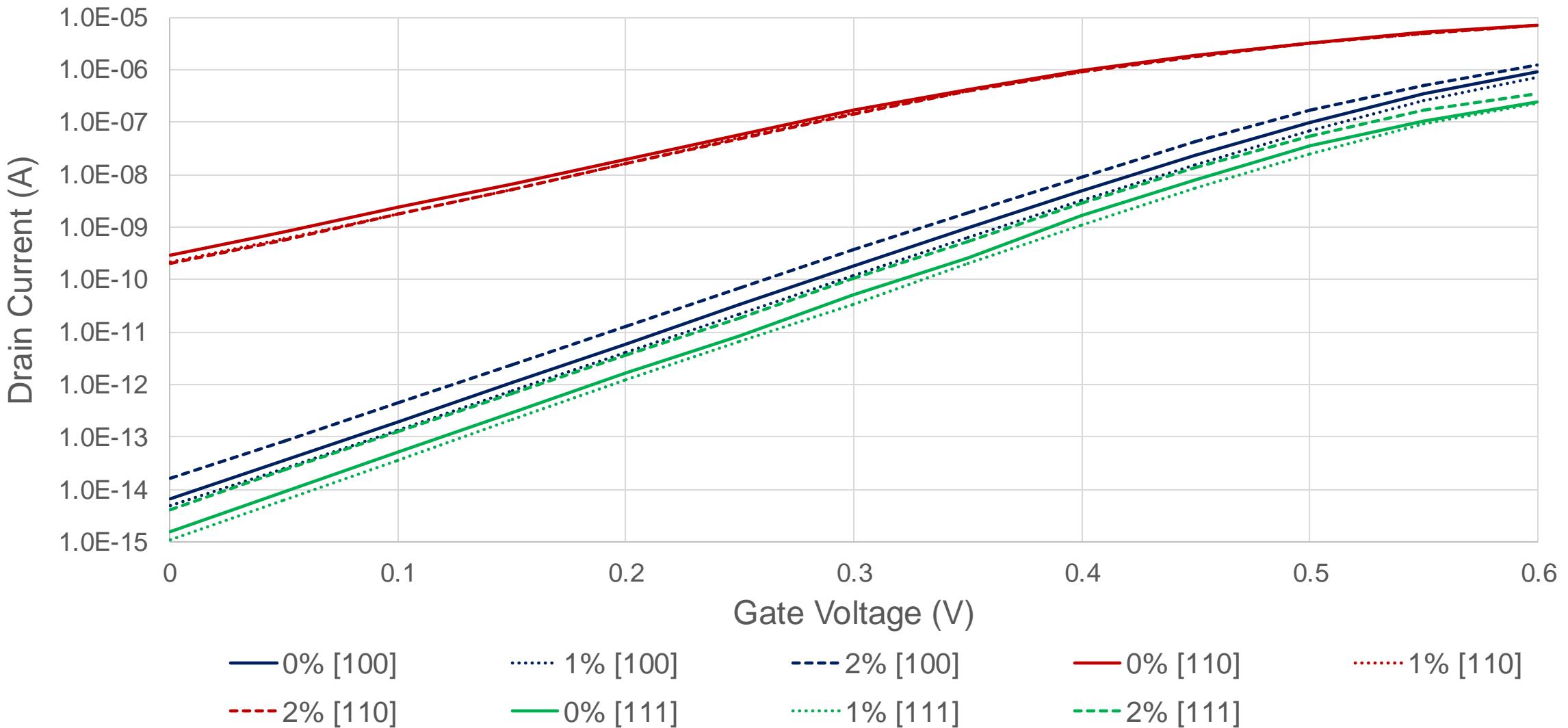


Cross-section of the nanowire with transport direction, [111]

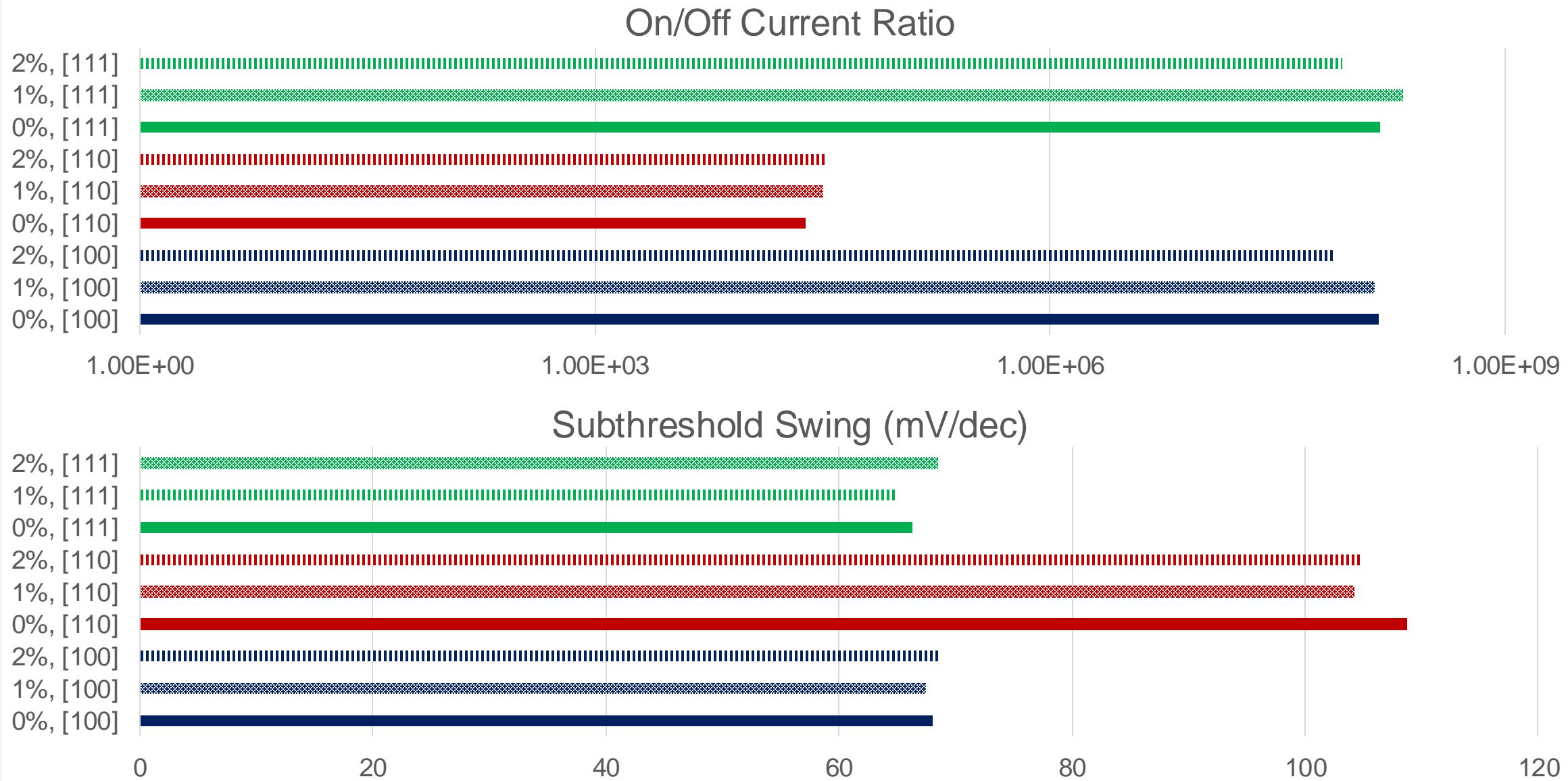
Tool located at:
<https://nanohub.org/resources/omenwire>

Optimized Nanowire Quantum Transport (Id-Vg Curve)

Id - Vg Curve with 1.9nm Cross Section & 5nm Channel/Gate Lengths



Optimized Nanowire Quantum Transport (Critical Parameters)



Hole Nanowire Bandstructure (Inputs)

All default settings were utilized, except as where shown:

1 Device Type → 2 Physics → 3 K-Space → 4 Numerics → 5 Simulate

Geometry: Nanowire (1D-periodic)

Calculation For: Electrons

Material: Si

Alloy Model: Virtual Crystal Approximation

Molar fraction: 0.5

Job Type: Calculate the wire band structure

Device cross section: Circle

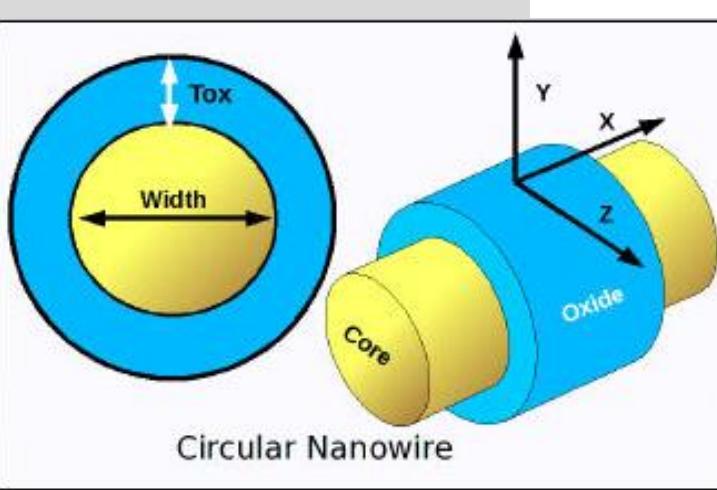
Diameter: 8nm

Oxide Thickness(Tox): 2.2nm

Crystal Orientation

Transport direction (X): (100)

Confinement direction (Z): [010]



1 Device Type → 2 Physics → 3 K-Space → 4 Numerics → 5 Simulate

Electronic Structure | Strain |

Tight Binding Model: $sp3d5s^*$

Spin-Orbit Coupling: no

Dangling Bond Energy: 30eV

Explore: Valence bands

Electronic Structure | Strain |

Strain type: Uniaxial (along transport direction X)

Epsilon: 0.02

1 Device Type → 2 Physics → 3 K-Space → 4 Numerics → 5 Simulate

Number of k-points: 10

Number of bands: 10

Manual simulation venue selection: no

Simulation Venue: nanoHUB.org (local)

Tool located at:
<https://nanohub.org/resources/bandstrlab>

Resources

- [1] W. contributors, "Work function," Wikipedia, The Free Encyclopedia., 8 February 2024. [Online]. Available: https://en.wikipedia.org/w/index.php?title=Work_function&oldid=1205050597. [Accessed 28 April 2024].
- [2] W. Lee, Y. Hwangbo, J.-H. Kim, and J.-H. Ahn, "Mobility enhancement of strained Si transistors by transfer printing on plastic substrates," *NPG Asia Materials*, vol. 8, no. 3, pp. e256–e256, Mar. 2016, doi: <https://doi.org/10.1038/am.2016.31>.
- [3] "Strained Transistors - REFERENCE PMOS-strained," www.intel.com.
https://www.intel.com/pressroom/kits/advancedtech/doodle/ref_strain/strain.htm
- [4] Y. Chen *et al.*, "Mobility Enhancement of Strained MoS₂ Transistor on Flat Substrate," *ACS nano*, vol. 17, no. 15, pp. 14954–14962, Jul. 2023, doi: <https://doi.org/10.1021/acsnano.3c03626>.
- [5] K. Mistry *et al.*, "Delaying forever: Uniaxial strained silicon transistors in a 90nm CMOS technology," *IEEE Xplore*, Jun. 01, 2004. <https://ieeexplore.ieee.org/document/1345387>

