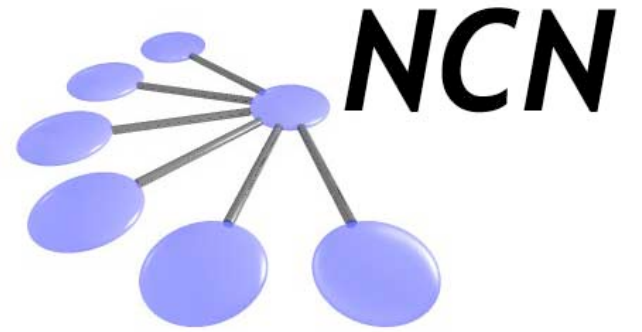
nanoHUB online simulation and more — an NCN project

Network for Computational Nanotechnology (NCN)

UC Berkeley, Univ.of Illinois, Norfolk State, Northwestern, Purdue, UTEP

First-Time User Guide to OMEN Nanowire**



PURDUE UNIVERSITY

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** https://nanohub.org/resources/5359

NCN NSF

nanoHUB online simulation and more an NCN project

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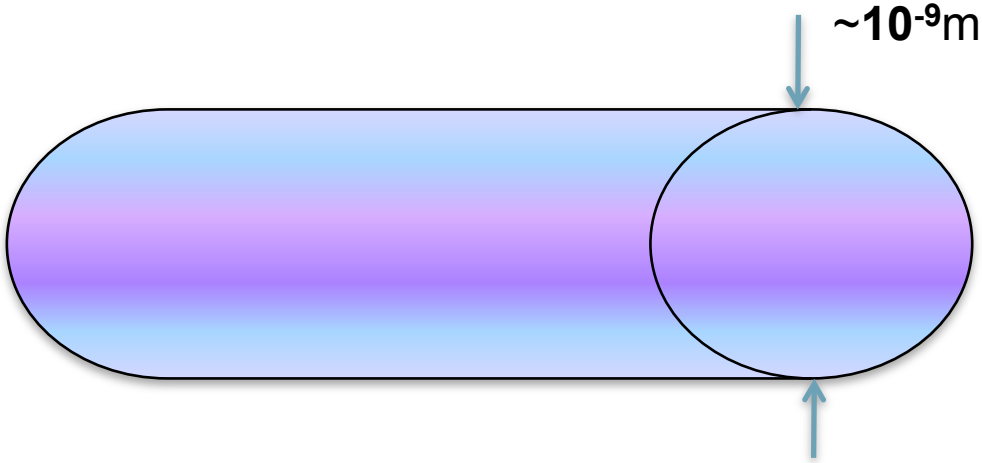
Introduction: What is a Nanowire?

nanowire: wire-like structure with diameter or lateral dimension of nanometer(10^{-9}m)



http://en.wikipedia.org/wiki/DNA

→ Various material systems can be used to fabricate nanowires.
For example: silver, gold, copper, …, etc. (metal)
Si, Ge, GaAs, GaN, …, etc. (semiconductor)

What is a Nanowire?

Application of nanowires

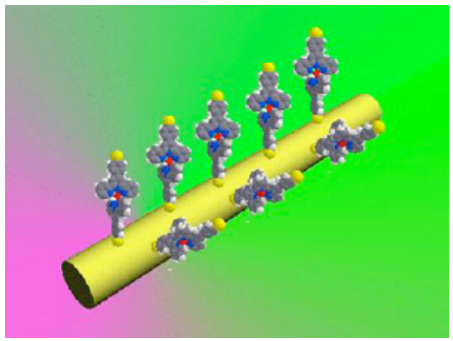


Fig. 1 **Nanowire memory cell

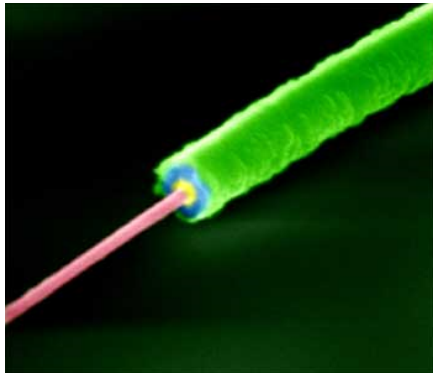


Fig. 2 ***Nanowire LED

B. Tian, Lieber Group, Harvard University

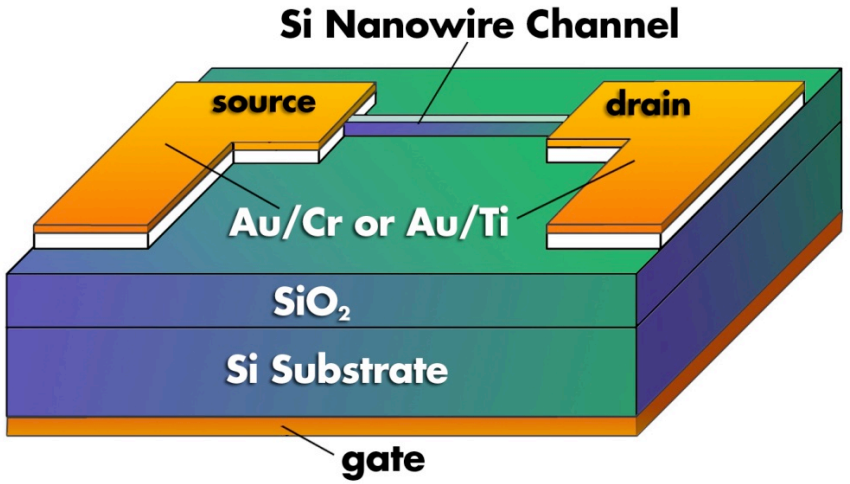


Fig. 3 Nanowire FET

National Institute of Standards and Technology

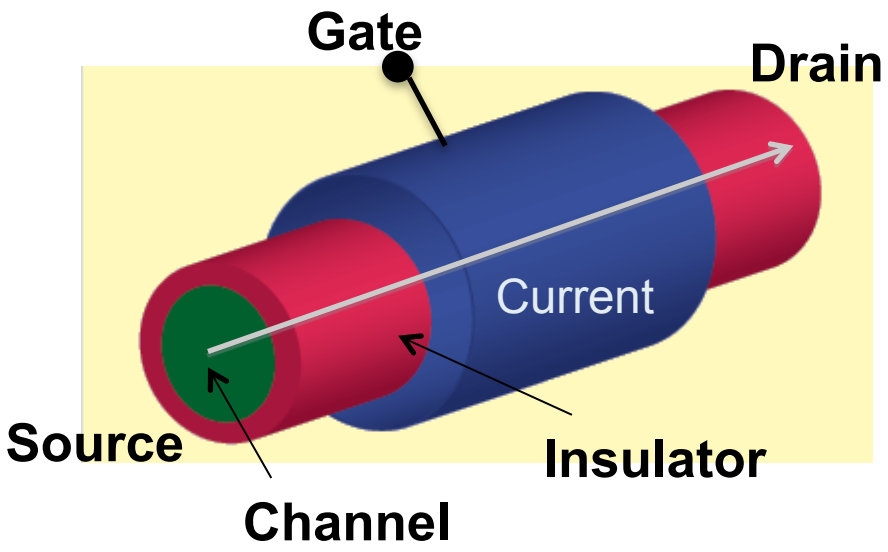
Fig 1. http://www.eurekalert.org/pub_releases/2004-04/uosc-spn042004.php

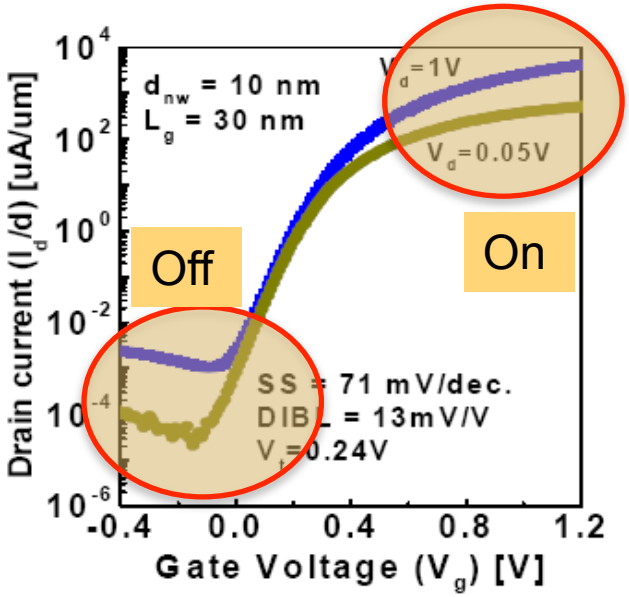
Fig 2. http://www.spectrum.ieee.org/oct07/5642

Fig 3. http://www.nist.gov/public_affairs/techbeat/tb2005_0630.htm#transistors

What is a Nanowire FET?

nanowire FET: field effect transistor(FET) using nanowire



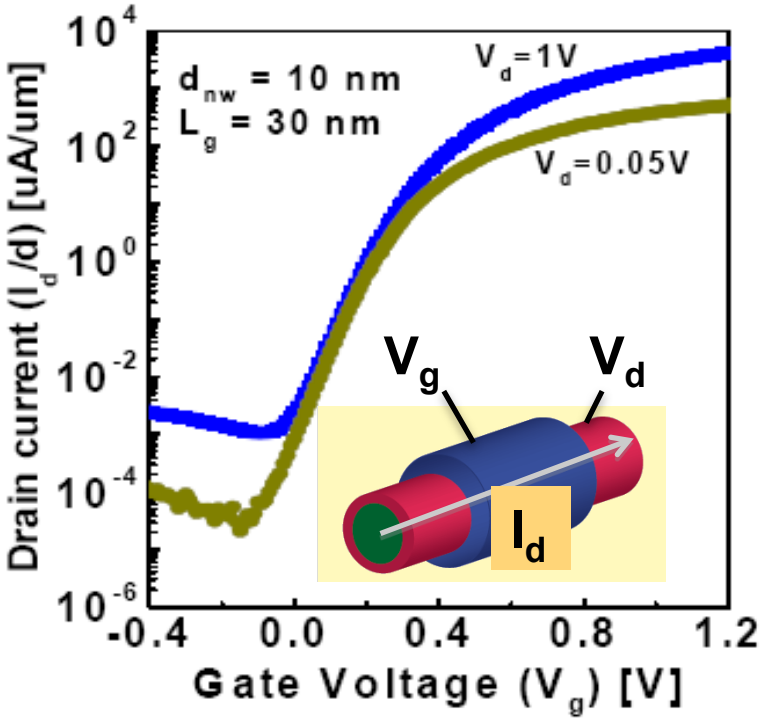


» The current from the source to the drain is turned on and off by the voltage applied to the gate.

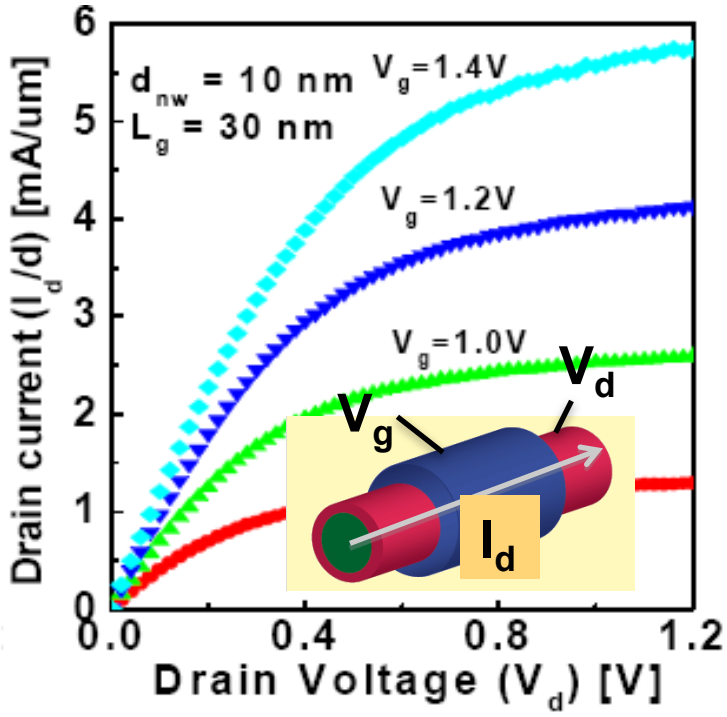
» Because the gate in nanowires is surrounding the channel, it can control the electrostatics of the channel more efficiently than the conventional MOSFET.

What Can Be Measured in a Nanowire FET?

IV Characteristics[1](Id-Vg, Id-Vd)



(a) Id-Vg



(b) Id-Vd

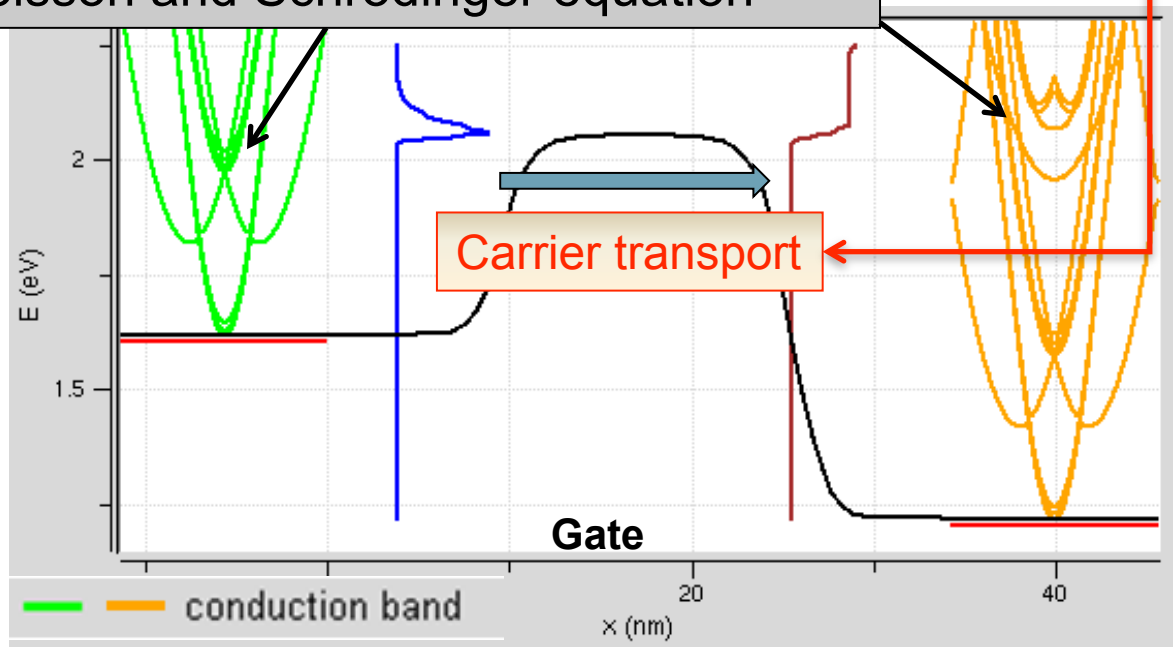
[1] Sung Dae Suk, et. al., IEDM, 2005, “High Performance 5nm radius Twin Silicon Nanowire MOSFET(TSNWFET) : Fabrication on Bulk Si Wafer, Characteristics, and Reliability

What is OMEN?

OMEN[3,4] : atomistic full-band quantum transport simulator

Atomistic description of bandstructure
– sp3d5s* tight binding model
+3D Poisson and Schrodinger equation [3,4]

Wave Function Approach[3,4]



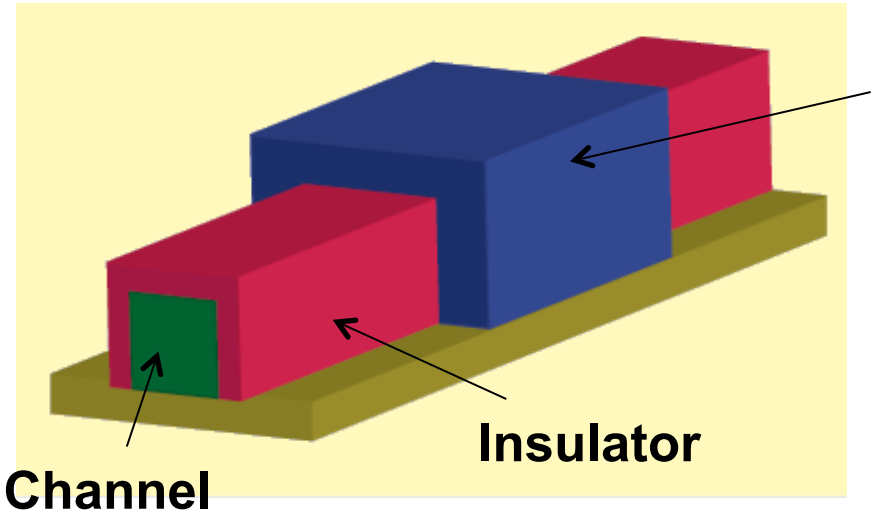
[3] Mahieu Luisier, et. al., Physical Review B, 2006
[4] http://cobweb.ecn.purdue.edu/~gekco/omen/index.html

What Can Be Simulated by OMEN Nanowire?

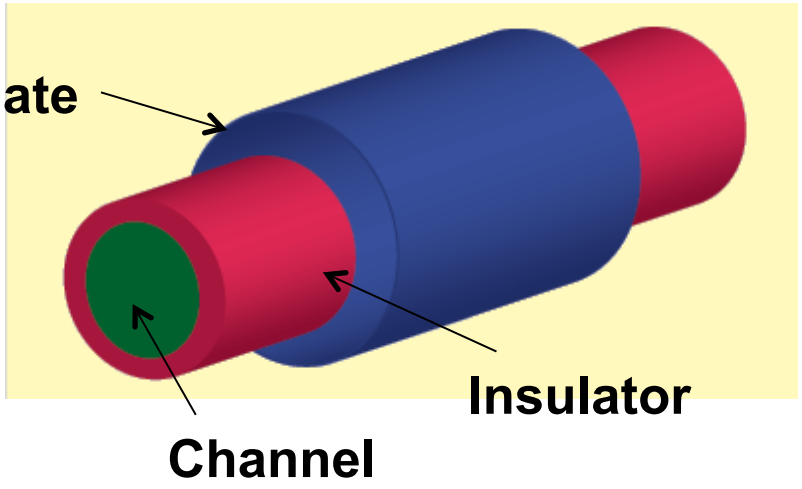
Device Type

OMEN Nanowire can simulate nanowire FETs of different types. You can choose between a rectangular nanowire and a circular nanowire.

Rectangular Nanowire



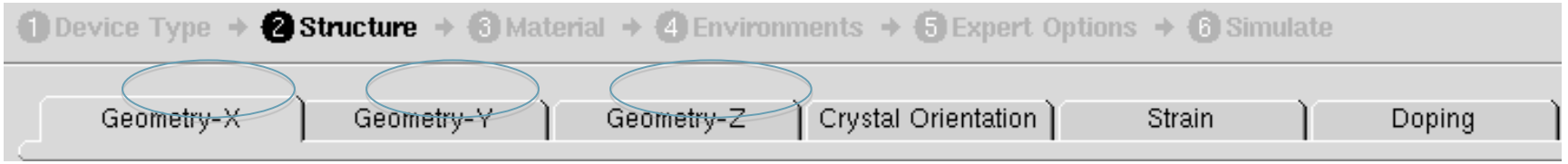
Circular Nanowire



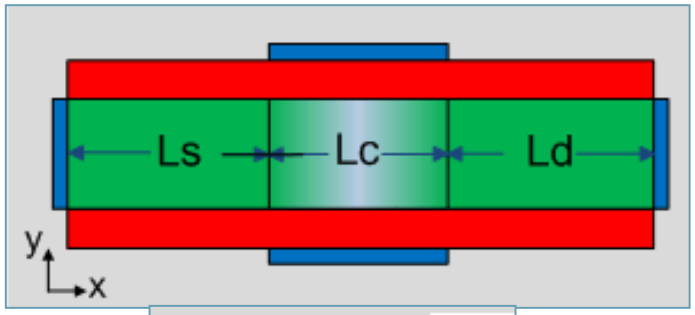
What Can Be Simulated by OMEN Nanowire?

Device Structure - Geometry

Nanowire FETs of various sizes

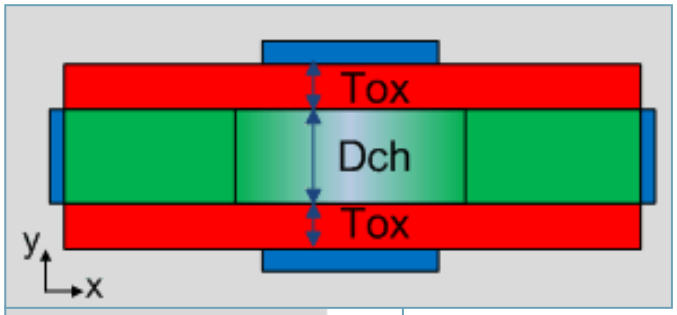


Geometry-X



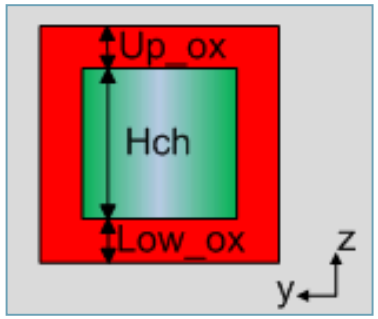
Channel length - Lc: **15nm**
Source length - Ls: **10nm**
Drain length - Ld: **10nm**

Geometry-Y



Diameter - Dch: **3nm**
Oxide thickness - Tox: **1nm**

Geometry-Z

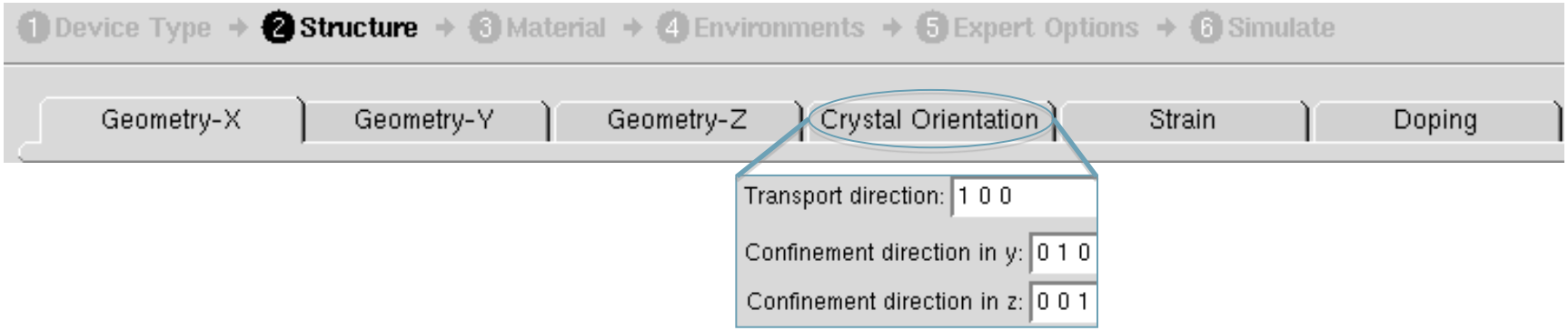


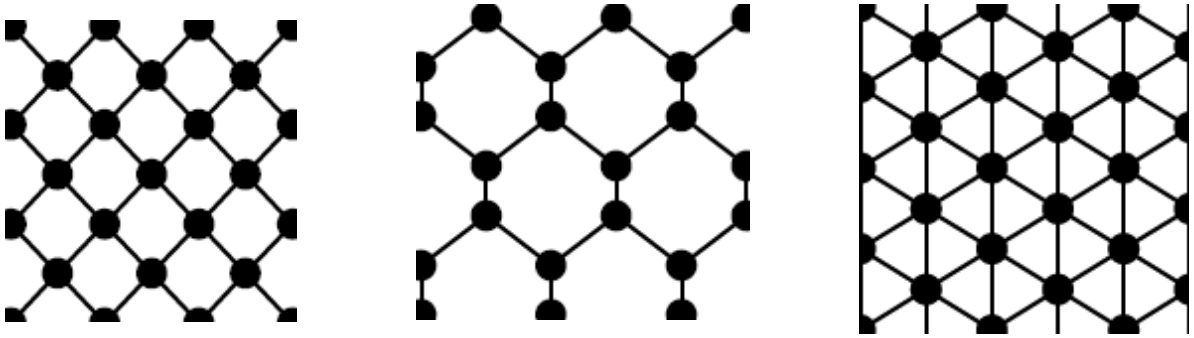
Channel height - Hch: **2nm**
Upper oxide thickness - Up_ox: **1nm**
Lower oxide thickness - Low_ox: **1nm**

What Can Be Simulated by OMEN Nanowire?

Device Structure – Crystal Orientation

Nanowire FETs of different crystal orientation





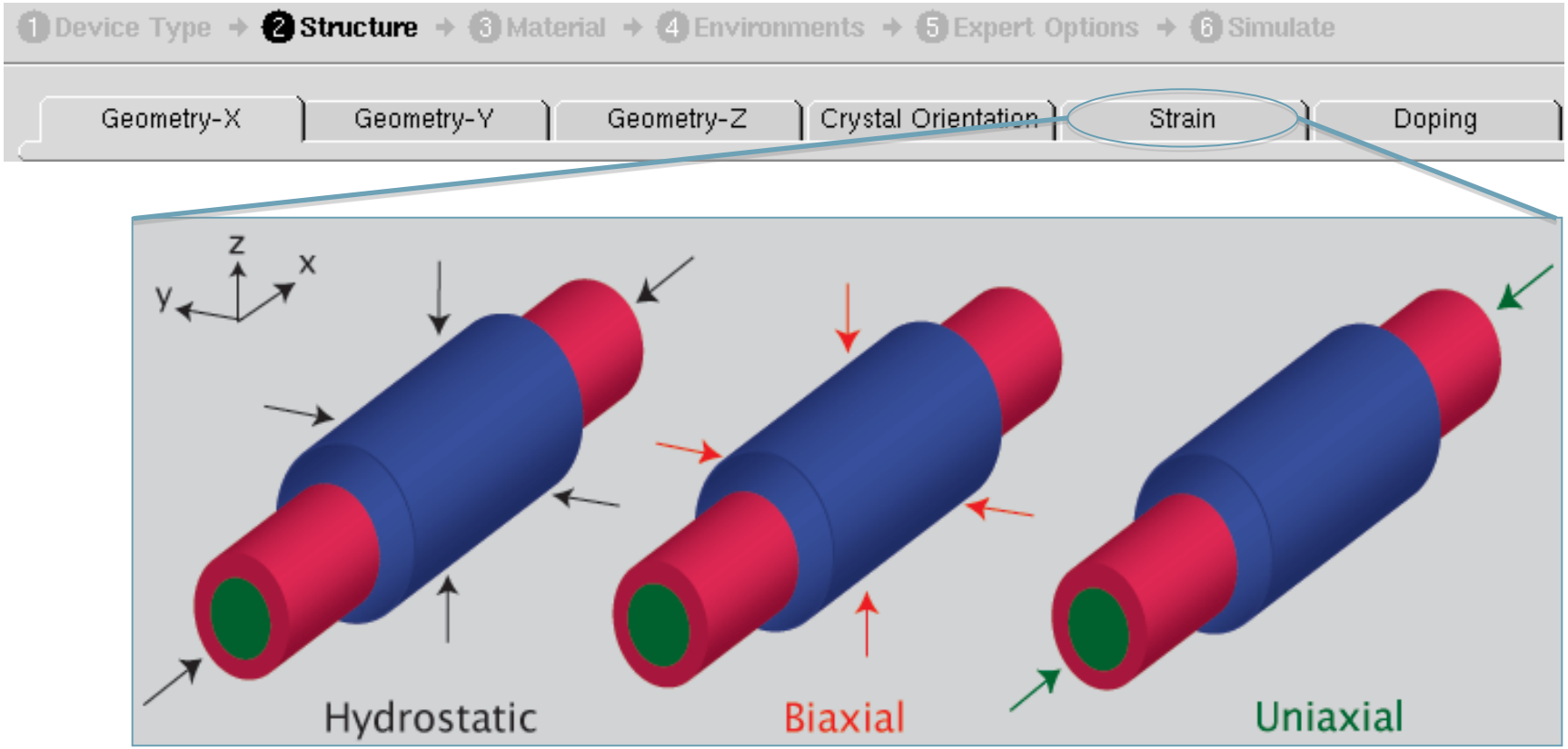
(a) [100] (b) [110] (c) [111]

cross-section of the nanowire with transport direction[3] (a) [100], (b) [110], (c) [111]

What Can Be Simulated by OMEN Nanowire?

Device Structure - Strain

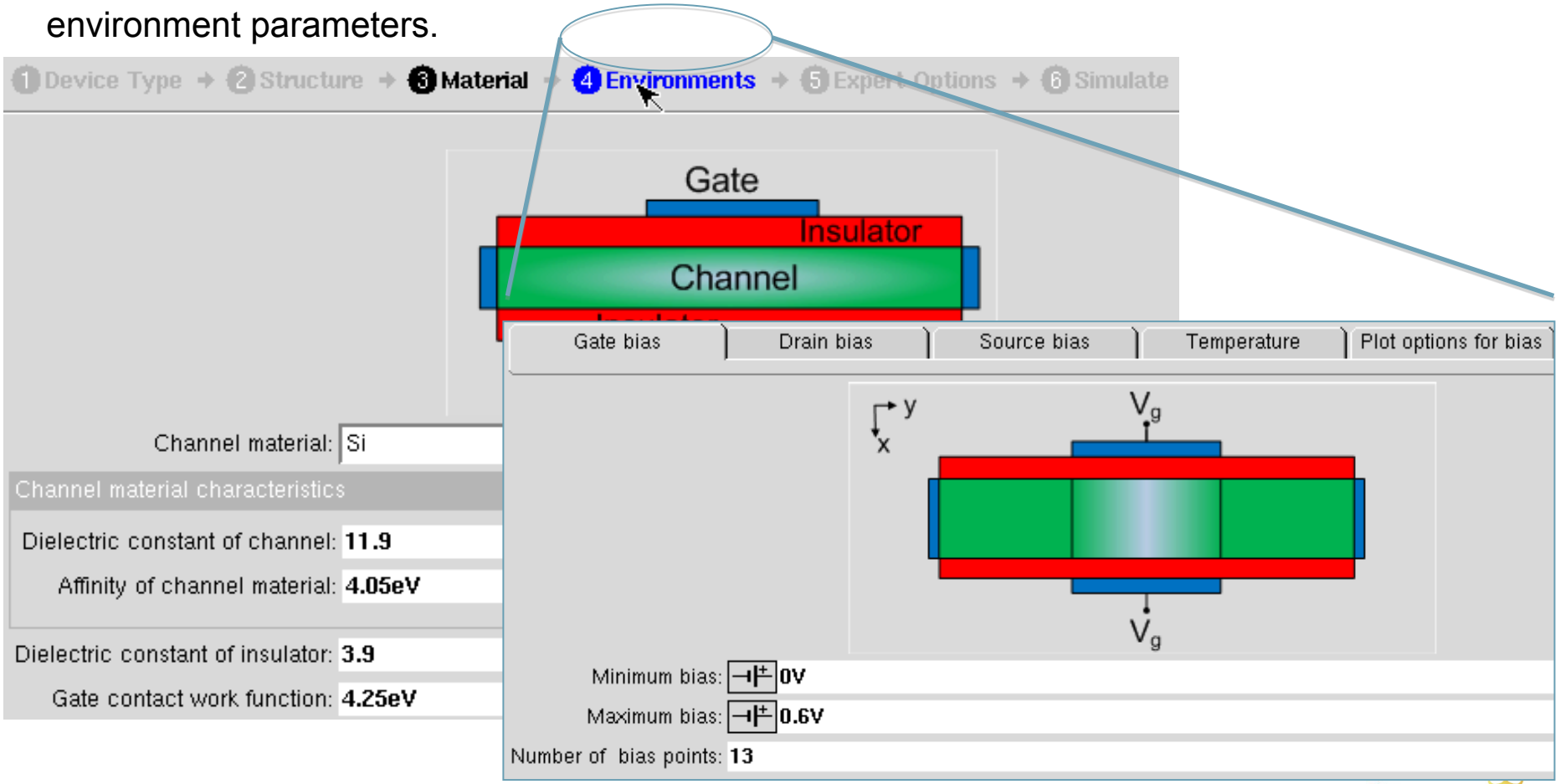
Nanowire FETs with strain



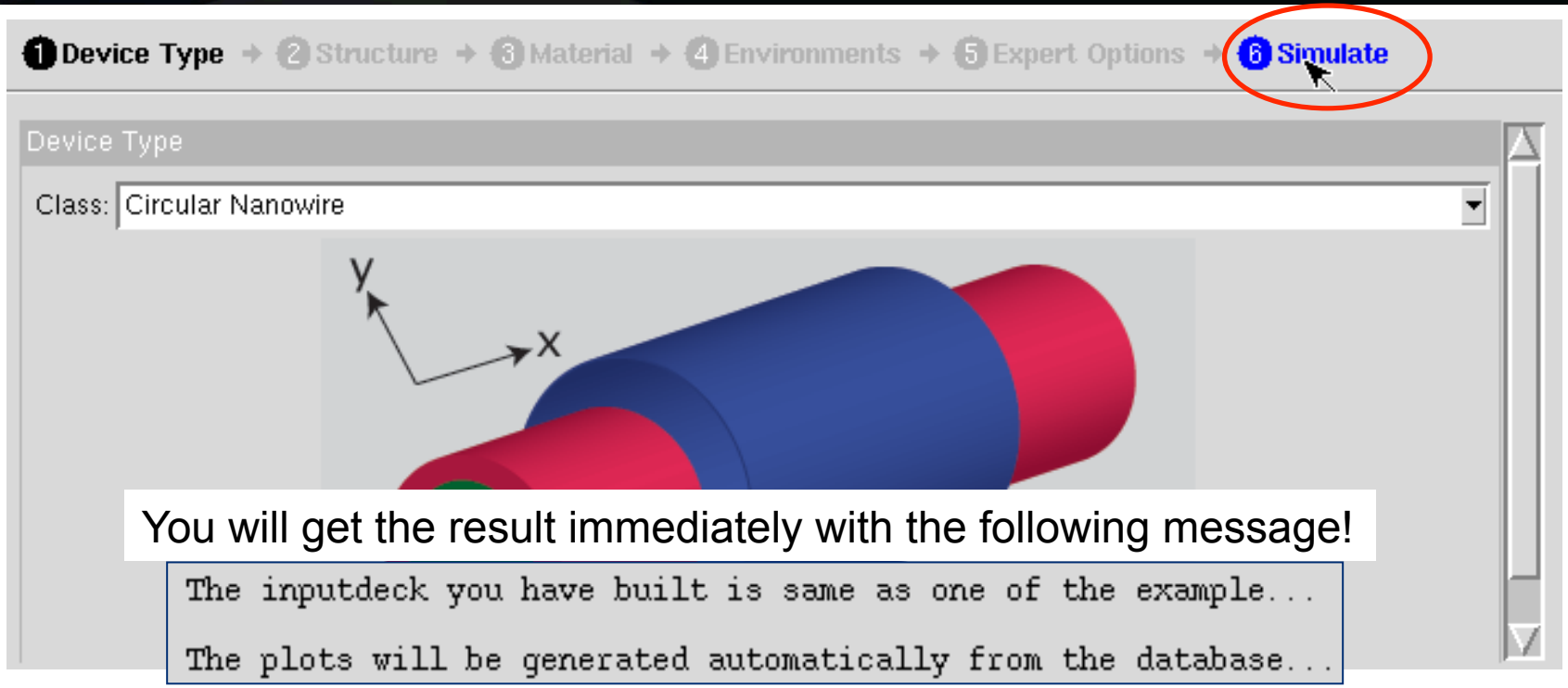
What Can Be Simulated by OMEN Nanowire?

Material/Environment

OMEN Nanowire can simulate nanowire FETs of different material and environment parameters.



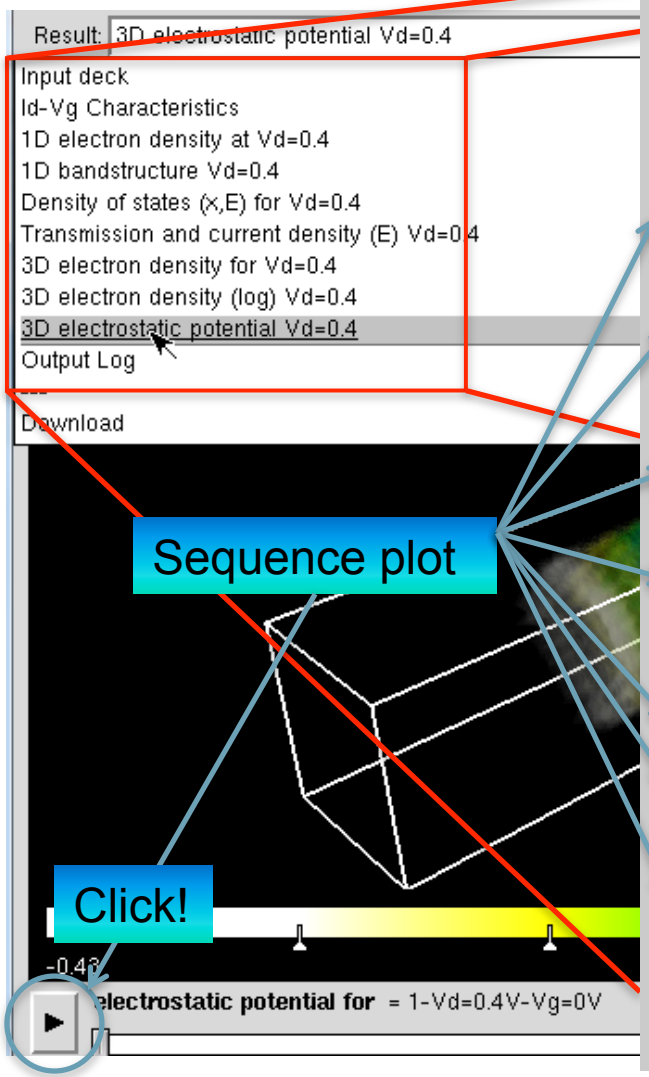
What If You Just Hit "Simulate"?



- To submit a new simulation, change other input parameters such as the structure, material, environment parameters. The estimated walltime/memory usage[5] to run the simulation will post after "Simulate" is clicked.

[5] http://cobweb.ecn.purdue.edu/~gekco/students/SungGeunKim/SungGeunKim_OMENNanowire_time_table.html

Outputs

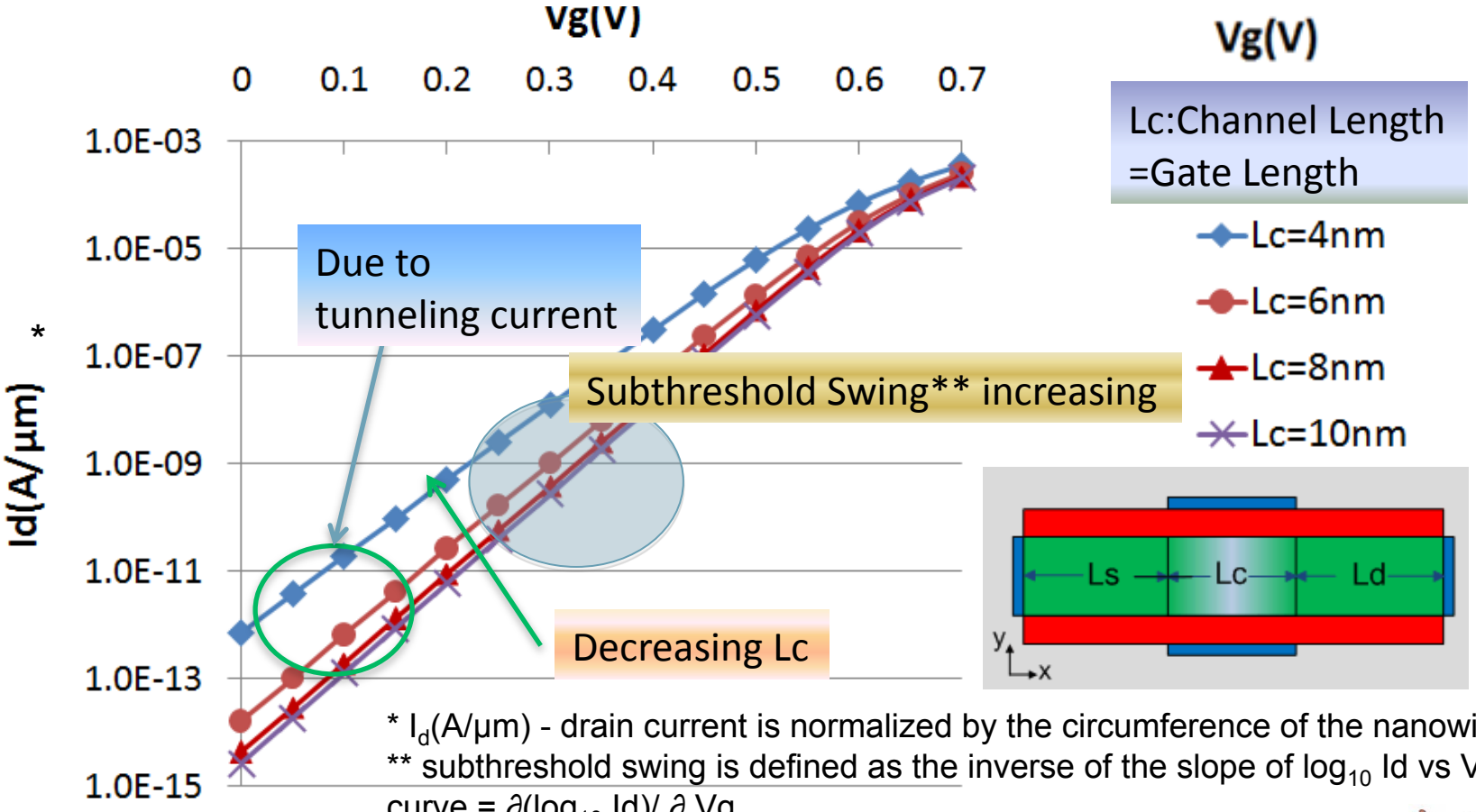


- [Inputdeck] : Input parameters translated to the format that can be used for job submission to OMEN
- [Id-Vg Characteristics] : Id-Vg curve (Id-Vd curve can be chosen to be shown in the environment input option)
- [1D electron density] : 1D electron density (/cm^3) to the transport direction
- [1D bandstructure] : 1D bandstructure/Fermi levels in the contacts/transmission coefficient/current density/conduction band edge through the nanowire
- [Density of states (x,E)] : 2D density of states as function of transport direction x and energy E
- [Transmission and current density] : Transmission coefficient and the current density(=Transmission*(f_L-f_R) fL/ fR:fermi function at the left and right contact)
- [3D electron density]
- [3D electron density(log)] : log scale of 3D electron density
- [3D electrostatic potential]
- [Output Log] : includes all the messages posted on the screen after you click “Simulate” and the output/error messages from the OMEN simulator

Example: What if the length of the channel is changed?

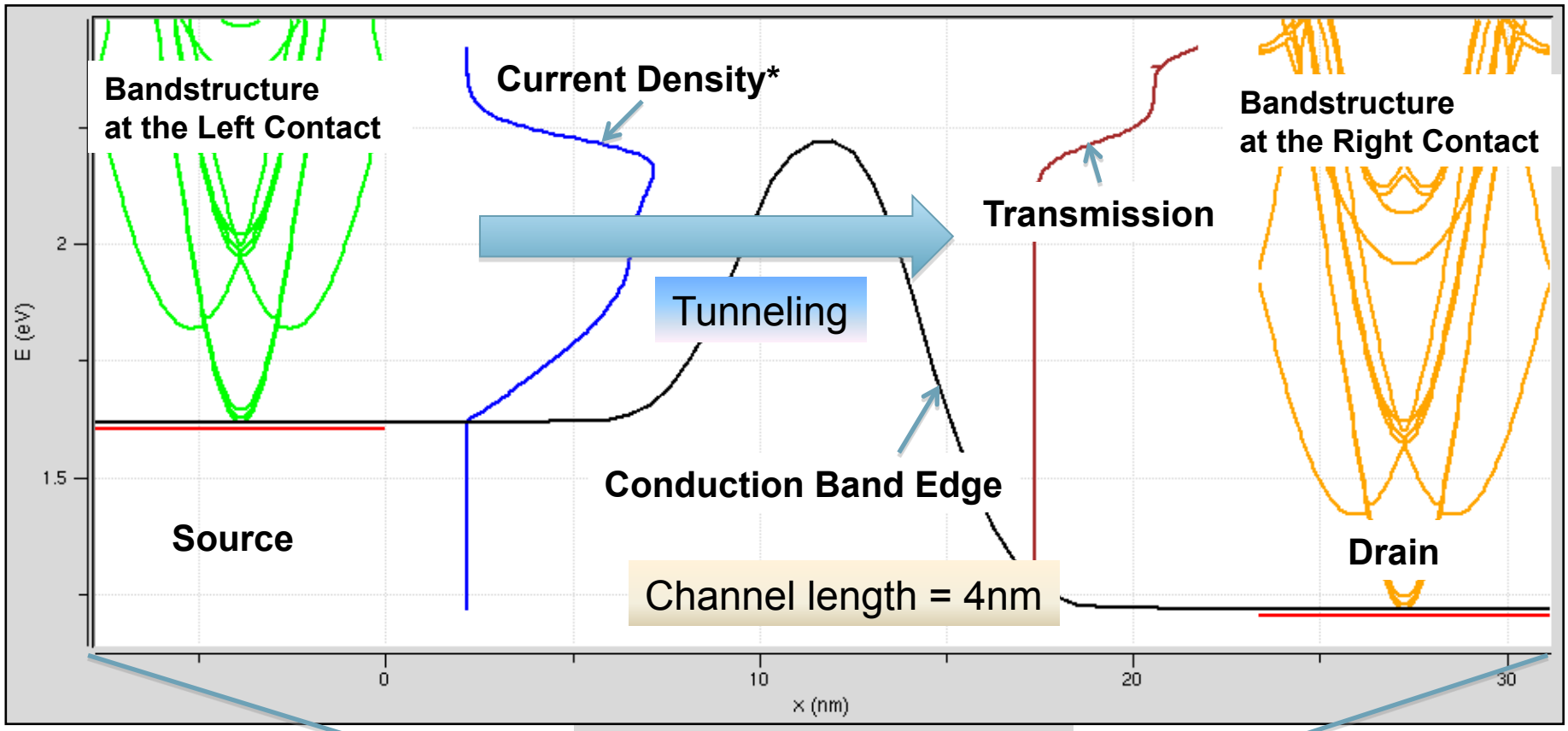
IV Characteristics

The drain current and subthreshold swing** at small Vg increases due to the tunneling current and as the channel length decreases.

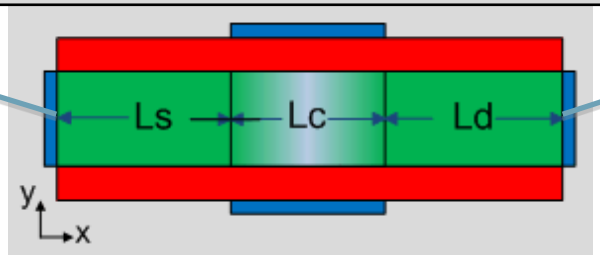


* I_d(A/μm) - drain current is normalized by the circumference of the nanowire
** subthreshold swing is defined as the inverse of the slope of $\log_{10}$ Id vs Vg curve = $\partial(\log_{10} \text{Id})/\partial \text{Vg}$

Example: What Happens at a Small Channel Length? (bandstructure)



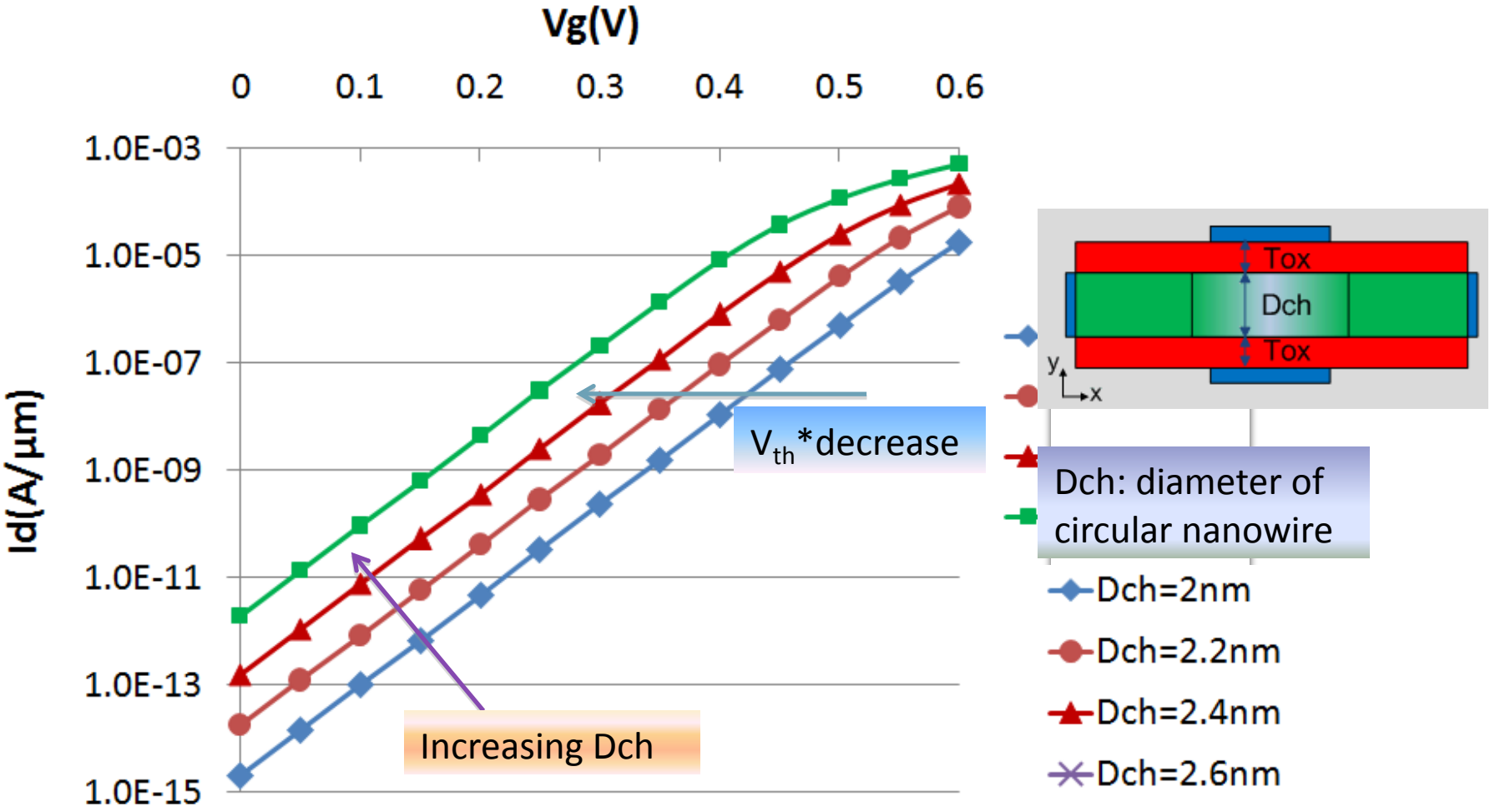
V_g=0V, V_d=0.4V



***Current Density**
=Transmission*(fL-fR)

fL:left contact fermi function
fR:right contact fermi function

Example: What if the Nanowire Diameter is Changed? (IV Characteristics)

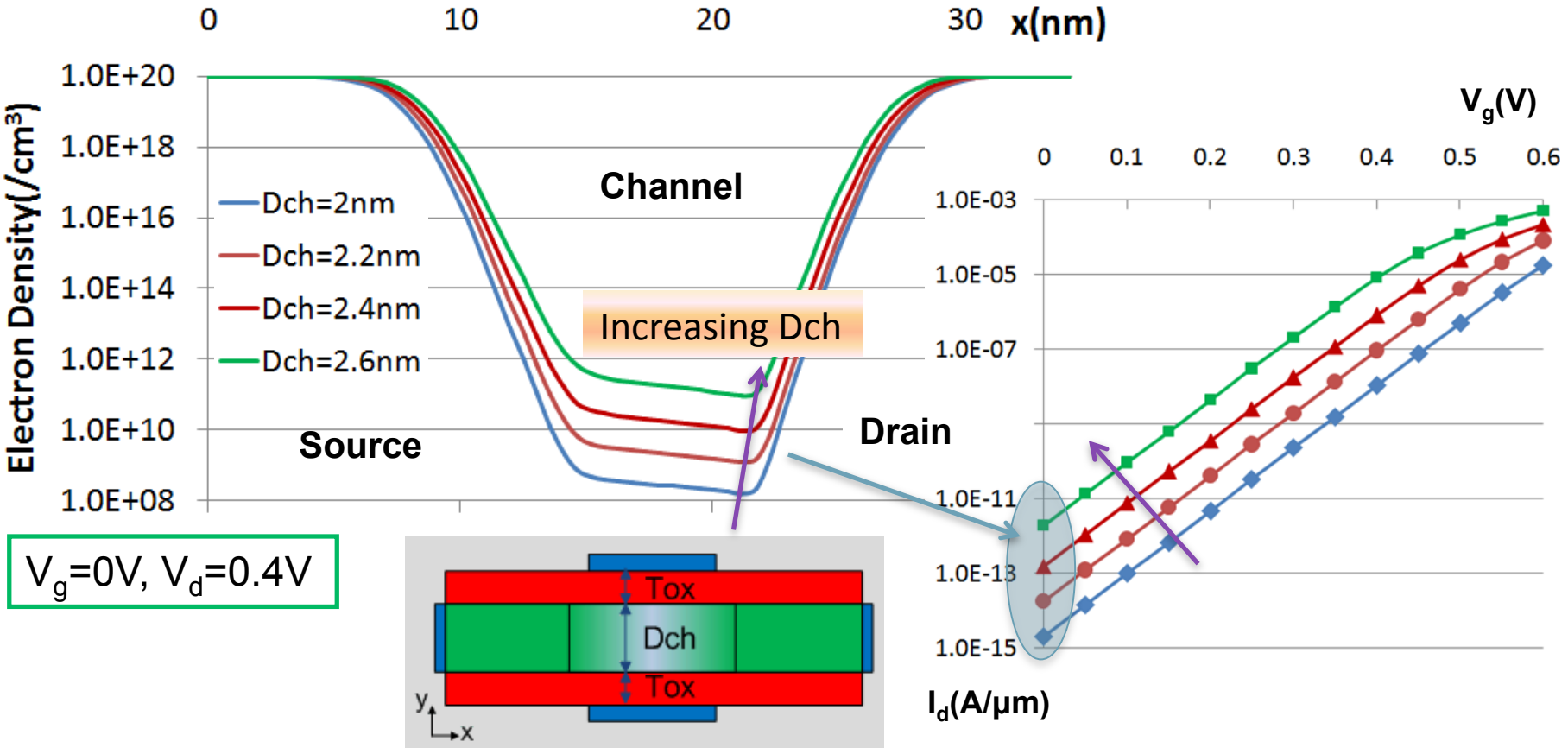


* Vth can be defined in many ways. Here we define it as a voltage where the drain current becomes larger than certain value (10^{-7}A/μm)

Example: What happens in the channel?

Electron density in the channel increases as the diameter of the nanowire increases.

→ Drain current increases at large diameter nanowire



Limitations of the OMEN Nanowire Tool

- Cross section of nanowire cannot be larger than 3X3 nm^2 or smaller than 1.5X1.5nm^2
- Length of gate should be less than 60 nm
- You can not choose which server or the number of CPUs* in that server to use
- Simulation may not be converged at high Vg (e.g. larger than 0.7V) when the potential barrier is about the same as the conduction band edge of the source side[6]

*The number of CPUs is estimated by the OMEN Nanowire according to the time table[5] database and as based on the cross section and gate length of the nanowire that user inputs.

[6] https://nanohub.org/resources/6315

On-demand Simulation

- The number of CPUs for which OMEN Nanowire can submit a job, in order to end the simulation in 4 hours* in a steele cluster, is less than 256.

- If your simulation needs more than 256 CPUs, the simulation will be aborted and the following message will appear:

```
The number of CPUs required to fullfill the simulation is more than 256

Please reduce the size of nanowire structure or reduce the number of bias points
```

- If you want to simulate structure that uses more than 256 CPUs, or if you want to simulate with a different material system than what is now provided in OMEN Nanowire, you may submit a request for a device that can manage such a job. Contact the developer team by email (kim568@purdue.edu) or by webpage

(https://nanohub.org/resources/5359/questions).

*This is the walltime limit in steele cluster

References

- Experimental Study on Nanowire FET

[1] Sung Dae Suk, et. al., IEDM, 2005, “High Performance 5nm radius Twin Silicon Nanowire MOSFET(TSNWFET) : Fabrication on Bulk Si Wafer, Characteristics, and Reliability

- Physics of Nanowire FET

[2] Wang, Jing (2006), "Device Physics and Simulation of Silicon Nanowire Transistors," http://nanohub.org/resources/1313

- OMEN

[3] Mahieu Luisier, et. al., “Atomistic simulation of nanowires in the sp3d5s* tight-binding formalism : From boundary conditions to strain calculations”, Physical Review B,2006

[4] http://cobweb.ecn.purdue.edu/~gekco/omen/index.html

- Time/memory estimation in OMEN Nanowire

[5] http://cobweb.ecn.purdue.edu/~gekco/students/SungGeunKim/SungGeunKim_OMENNanowire_time_table.html

- The Limitation of the OMEN Nanowire at high gate voltage

[6] OMEN Nanoiwre Supporting Document : Limitation of the Tool at Large Gate Voltage

- https://nanohub.org/resources/6315