First-Time User Guide: Band Structure Lab

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Origin of Bands: Electrons in Vacuum

- Single electron (in vacuum) Schrödinger Equation provides the solution:
  - Plane waves as eigen vectors
  - $E(k) = Bk^2$ as eigen energy
- Eigen energy can take continuous values for every value of $k$
- $E(k)$ relationship produces continuous energy bands
Origin of Bands: Electrons in Crystal

• An electron traveling in a crystal sees an extra crystal potential, Vpp.
• Eigen vectors are \textit{no longer simple plane waves}.
• Eigen energies cannot take all the values.
• Energy bands become discontinuous, thereby producing the \textit{BAND-GAPS}.

Schrödinger equation

\[ H \psi = E(k) \psi \]
\[ H = \frac{(\hbar k)^2}{2m} + V_{pp}(r) \]

Electron Hamiltonian in a periodic crystal

Discontinuous energy bands
Abhijeet Paul

**Energy Bands, Bandgap, and Effective Mass**

- **Continuous bands**

  - **Vacuum electron**
    - $E(k) = \frac{\hbar^2 k^2}{2m_e}$
  - Electron mass in vacuum = $9.1 \times 10^{-31} \text{kg}$
  - $k$ range: $-\pi/a \leq k \leq \pi/a$.

  - **Continuous bands**

  - **Energy bands**

    - Lattice constant = $-\pi/a \leq k \leq \pi/a$. This is called the first **BRILLOUIN ZONE**.
    - E(k) relation in this zone is called **reduced E(k) relation**.

  - **Effective mass**
    - Now free electron mass is replaced by effective mass ($m^*$).
    - Effective mass provides the energy band curvature.

  - **Band Gap**

  - **Similar E(k) relationship**

  - **Effective mass**

  - **Reduced E(k) relation**

  - $E(k) = \frac{\hbar^2 k^2}{2m^*_e}$

  - $\frac{1}{m^*_e(k_o)} = \frac{1}{\hbar^2} \left( \frac{\delta^2 E_k}{\delta k^2} \right)_{k=k_o}$
Nanowires have 3 cross-sectional shapes: circular, triangular, rectangular.
- The semiconductor is represented atomistically for the E(k) calculation.
- The oxide is treated as continuum material for self-consistent simulations.
- X -> transport direction
- Y,Z -> confinement directions
How Band Structure is Calculated

[1] Select crystal dimensionality

[2] Assemble device Hamiltonian \([H]\)

[3] Diagonalized \(H\) provides eigen-energies

[4] Dispersion \((E(k))\) relation

In the Band Structure Lab, the device Hamiltonian is assembled using the semi-empirical tight-binding method.
Device Hamiltonian is assembled using **semi-empirical tight-binding (TB)**
- Each atom is represented using an onsite block [Hon_a or Hon_c].
- Coupling with nearest neighbor is taken in coupling blocks [Vac, Vca]
- Size of these blocks depends on the basis set and spin-orbit coupling
- Basis sets are made of orthogonal atomic orbitals like s,p,d,etc.
- **The Band Structure Lab uses sp3d5s* basis set with 10 basis functions**
Self-consistent E(k) Calculation Procedure

Electronic structure
20 band sp$^3$d$^5$s$^*$ model with spin orbit coupling

- Appropriate for treating atomic level disorder
- Strain treatment at atomic level
- Structural, material & potential variations treated easily

Zinc blend

Top of the barrier, ballistic transport

Self consistent iteration scheme

Solve Poisson eqn. for Potential [U]
• What is the Band Structure Lab and what does it do?:

  » A C++ based code to perform electronic structure calculation
  » A tool powered by OMEN-BSLAB, C/C++ MPI based parallel code
  » Solves single electron Schrödinger equation in different types of semiconductor crystals using the semi-empirical tight-binding method:
     ✓ For pure crystals with and without strain
     ✓ For gates semiconductor systems with applied external biases for nanowires and ultra thin bodies (UTB)
  » Provides various information on an electron in a periodic potential
     ✓ Energy bands
     ✓ Effective masses and band-gaps

This tool was developed at Purdue University and is part of the teaching tools on nanoHUB.org (AQME).
Features of the Band Structure Lab

• Calculation of energy dispersion ($E(k)$) for semiconductor materials:
  » In bulk (3D), Ultra Thin Bodies [UTB] (2D), and Nanowires (1D)
  » With and without strain in the system, it can handle:
    ✓ Hydrostatic strain (equal strain in all directions)
    ✓ Biaxial strain (equal strain on a plane)
    ✓ Uniaxial strain (strain along any arbitrary axis)
    ✓ Arbitrary strain (all directions have different strains)

• Provides following information
  » Effective masses in bulk, nanowires, and UTBs
  » 3D dispersion for bulks in 1st Brillouin zone
  » Bandgaps and bandedges

• Self-consistent simulations:
  » Provides charge and potential profile in nanowire FETs and in UTB DGMOS for the applied gate bias
  » Change in E($k$) relation due to applied bias

Screen shot from http://nanohub.org
This tool has 3 levels of parallelism, namely:

- Parallel over all the gate biases
- Parallel over the kz point calculations for each Vg point
- Parallel over the kx point calculation for each Kz point

This tool has internal job submission method, depending on the kind of job the user wants to run.

It is important for the user to understand that while they can override these internal settings, this should be done with care. For additional information on the job submission policy, see Appendix [A].
**Inputs [1]: Device Structure**

Types of geometries and related parameters are selected on this page

### [1] Geometry

<table>
<thead>
<tr>
<th>Geometry</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bulk material</td>
</tr>
<tr>
<td>Nanowire - circular cross section</td>
</tr>
<tr>
<td>Nanowire - rectangular cross section</td>
</tr>
<tr>
<td>Nanowire - triangular cross section</td>
</tr>
<tr>
<td>Ultra-thin body MCTFE</td>
</tr>
</tbody>
</table>

### [2] Device Information

#### [2.1] Job type:
- Bulk: Band structure calculation
- Nanowire & UTB:
  - [1] Band structure calculation
  - [2] Band structure calculation under an applied bias

#### [2.2] Device Dimension:
Depending on job type, select:
- [a] Dimension of NW or UTB semiconductor core in nm
- [b] Thickness of oxide in nm (This is available for self-consistent E(k) calculation.)

#### [2.3] Device Directions:
- [a] Transport direction (X) [100], [110], [111]
- [b] Confinement direction (Z)
- [c] 3rd orthogonal direction (Y) determined automatically


<table>
<thead>
<tr>
<th>Material Types:</th>
</tr>
</thead>
<tbody>
<tr>
<td>[a] Silicon</td>
</tr>
<tr>
<td>[b] Gallium Arsenide</td>
</tr>
<tr>
<td>[c] Indium Arsenide</td>
</tr>
<tr>
<td>[d] Germanium</td>
</tr>
</tbody>
</table>

5 types of geometry [periodicity]:
- [1] Bulk [3D]
- [2] Circular nanowire [1D]
- [3] Rectangular nanowire [1D]
- [4] Triangular nanowire [1D]
- [5] Ultra thin body [2D]
Properties used to obtain the electronic dispersion are set on this page.

[1] **Tight Binding Model**
This is the basis, set model used for calculating the band structure. Presently, the *sp3d5d* model is supported by the tool.

[2] **Spin Orbit (SO) Coupling**
- This produces the effect of electron spin on band structure.
- **Should be always “ON” for valence bands.**
- **Produces negligible effect on conduction bands.**
- **With SO on calculations are slower due to larger matrix sizes.**

[3] **Dangling Bond Energy**
- This is the energy barrier set at the external boundary of the structure.
- This value is utilized to remove the spurious states in the bandgap. Default value of 30 eV is good.
- Smaller value means lower barrier and larger value means higher barrier.
- **Usually there is no need to change this value.**
This page provides options for the kind of simulations that can be run, depending on the selected geometry.

Two types of simulations: bulk dispersion and strain sweep

Bulk dispersion [E(k)] calculation:
- Explore bands
  [1] Along std. symmetry directions*
  [2] Along some symmetry directions*
- Show 3D E(k)
  Produces energy isosurface plots. User can set the kx, ky, kz region, as well as the energy limit. for the bands

Strain sweep analysis:
Effect of strain on E(k)
- Select the % strain value (eps_xx, eps_yy, eps_zz) along the 3 axes
- Provide the initial and final % strain value
- Provide number of points for strain sweep

Strain Models
- [1] Bi-axial
- [2] Uniaxial
- [3] Hydrostatic

Only 3 models available for strain sweep analysis

* See Appendix [B]
Inputs [3.b] Analysis - UTB

E(k) calculation options

Select Type of Band
CB or VB

Direction along which E(k) to be calculated*

Select the number of sub-bands.

Select the number of k points.

Select the strain type and values. (Strain detail is the same as bulk)

Self-consistent calculation options

Select Type of DGMOS
N-type or P-type
Depending on source-drain doping:

Select the number of sub-bands.

Select the number of k points. (Higher k points are good for a P-type simulation, but they increase the simulation time.

Select the strain model.

Bias selection:
• Set gate bias.
• Set drain bias.
• Set gate work function.
• Set semiconductor electron affinity.
• Set device temperature.
• Set DIBL.

Select backgate configuration.

Set source/drain doping.

* See Appendix B
**Inputs [3.c] Analysis - Wire**

**E(k) calculation options**
- Select Type of Band: **CB or VB**
- Select the number of sub-bands.
- Select the number of k points.
- Select the strain type and values. Strain detail is same as bulk.

**Self-consistent calculation options**
- Select Type of Gate all-around MOS **N-type or P-type** Depending on source-drain doping:
- Select the number of sub-bands.
- Select number of k points. (Higher K points are good for a P-type simulation, but they increase the simulation time.
- Select strain model.

**Bias selection:**
- Set gate bias.
- Set drain bias.
- Set gate work function.
- Set semiconductor electron affinity.
- Set device temperature.
- Set DIBL.

**Set source/drain doping.**
Inputs [4]: Advanced User Choice

Allows the users to submit jobs on their cluster of choice
See Appendix A for more details.

Two clusters are available:

NANOHUB (less CPUs)
- Well suited for light* and medium* job types
- Has less delay in job submission
- Self-consistent jobs should not be submitted as it may result in longer turn around time.

STEELE (larger CPUs)
- Well suited for medium* and heavy* job types.
- Has longer queue delays during job submission.
- Self-consistent jobs should be submitted here.

CAUTION: Do not change this option if you are not sure. The tool will automatically decide the simulation venue depending on the job type.

* See Appendix A
What Happens When You Just Hit SIMULATE?

Default Inputs

- Geometry -> Bulk
- Material -> Silicon
- TB Model -> sp3d5s*
- Spin orbit -> on
- Dangling bond energy: 30eV
- Bulk Ek simulation
- Full Domain simulation
- Strain -> none
- Show 3D bands -> no
- Advanced user choice -> default.

Default Outputs

- [Bulk band structure]: Shows the all the energy bands.
- [Bulk central bands]: Shows only the conduction and 3 valence bands.
- [Bandgap/Bandedge information]: Provides information about band extrema and bandgap.
- [Effective mass information]: Provides conduction and valence band masses at high symmetry points.
- [Unitcell structure]: Shows 3D zinc-blend unitcell structure.
- [Atomic structure]: Shows a larger crystal of silicon.
- [Input decks]: Provides input decks used by OMEN-BSLAB.
- [Backend code log]: log of OMEN-BSLAB.
- [Timestamps]: Shows overall simulation time breakup.
- [Tool Run Log]: Shows the log of tool run.
What Happens When You Just Hit SIMULATE? (continued)

[1] Bulk Bands

[2] Central Bands

Conduction Band

Heavy hole

Valence Bands around Γ point

Light hole

Split-off hole

[3] Band Info(Si)

Conduction band minima = 1.13446eV.
Valence band maxima = 0.00244033eV.
Bandgap = 1.13202eV.

[4] Silicon Unitcell

Screen shots from http://nanohub.org
What Happens When You Just Hit SIMULATE? (continued)

---

**Silicon effective masses**

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**Effective Mass Information**

---

<table>
<thead>
<tr>
<th>band</th>
<th>valley</th>
<th>point</th>
<th>[2PI/a0]</th>
<th>direction</th>
<th>value [m0]</th>
<th>Note</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ec L</td>
<td>(0.50114, 0.50114, 0.50114)</td>
<td>111</td>
<td>3.191V</td>
<td>Longitudinal</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ec L</td>
<td>(0.50114, 0.50114, 0.50114)</td>
<td>1-10</td>
<td>0.1705</td>
<td>transverse</td>
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<td></td>
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<tr>
<td>Ec L</td>
<td>(0.50114, 0.50114, 0.50114)</td>
<td>11-2</td>
<td>0.1699</td>
<td>transverse</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ec X</td>
<td>(0.812, 0.0, 0)</td>
<td>100</td>
<td>0.8999</td>
<td>longitudinal</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ec X</td>
<td>(0.812, 0.0, 0)</td>
<td>010</td>
<td>0.1956</td>
<td>transverse</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ec X</td>
<td>(0.812, 0.0, 0)</td>
<td>110</td>
<td>0.3213</td>
<td>---</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ec X</td>
<td>(0.812, 0.0, 0)</td>
<td>111</td>
<td>0.2661</td>
<td>---</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ec Gamma</td>
<td>???</td>
<td>100</td>
<td>???</td>
<td>failed -- no minima</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ec Gamma</td>
<td>???</td>
<td>110</td>
<td>???</td>
<td>failed -- no minima</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Ec Gamma</td>
<td>???</td>
<td>111</td>
<td>???</td>
<td>failed -- no minima</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Evln Gamma</td>
<td>(0, 0, 0)</td>
<td>100</td>
<td>0.2756</td>
<td>---</td>
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<td></td>
</tr>
<tr>
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<td>0.5802</td>
<td>---</td>
<td></td>
<td></td>
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<tr>
<td>Evlh Gamma</td>
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<td>111</td>
<td>0.7329</td>
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</tr>
<tr>
<td>Evlh Gamma</td>
<td>(0, 0, 0)</td>
<td>100</td>
<td>0.2141</td>
<td>---</td>
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<td></td>
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<tr>
<td>Evlh Gamma</td>
<td>(0, 0, 0)</td>
<td>110</td>
<td>0.1521</td>
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<tr>
<td>Evlh Gamma</td>
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<td>111</td>
<td>0.1442</td>
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<tr>
<td>Evso Gamma</td>
<td>(0, 0, 0)</td>
<td>100</td>
<td>0.2457</td>
<td>---</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Evso Gamma</td>
<td>(0, 0, 0)</td>
<td>110</td>
<td>0.2457</td>
<td>---</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Evso Gamma</td>
<td>(0, 0, 0)</td>
<td>111</td>
<td>0.2457</td>
<td>---</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

---

**Timestamp and tool log**

---

**Simulation Description**

**JUP type:** Bulk EX simulation

---

**Job Type and Resource utilization Log**

**Job type:** EXsim

**Associated job no.:** 1

**Selected Simulation venue:** cluster:D

**Alloted Venue no.:** 4

**GFUs per node:** 2

**GFUs per job:** 6

---

**Screen shots from [http://nanohub.org](http://nanohub.org)**

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Default Circular Nanowire Simulation

**Inputs**

- Geometry -> circular nanowire
- Material -> silicon
- Wire diameter -> 2.1nm
- Transport direction (X) -> [100]
- Confinement direction (Z) -> [010]
- TB model -> sp3d5s*
- Spin orbit -> on
- Dangling bond energy -> 30 eV
- CB and VB simulation
- Number of bands -> 10
- Number of k points -> 61
- Strain -> none
- Advanced user choice -> no

**Outputs**

[1] Wire Band Structure
[2] Bandedge Information

Screen shots from http://nanohub.org

Conduction band minima = 1.58027 eV
Valence band maxima = -0.378968 eV
Bandgap = 1.95924 eV.
### Outputs

| Band no. (valley) | Mass dir. \( \langle k_x, k_y, k_z \rangle \) | \( |k_x, k_y, k_z| \langle \pi \rangle \) | Eff. Mass (m0) |
|------------------|------------------------------------------|-----------------------------------|----------------|
| \( n = 1 \) \( (1) \) | \( \langle 1, 0, 0 \rangle \) | \( (0, 0, 0) \) | 0.476597 | -0.378968 |
| \( n = 1 \) \( (2) \) | \( \langle 1, 0, 0 \rangle \) | \( (0.25, 0, 0) \) | 0.457326 | -0.432781 |
| \( n = 2 \) \( (1) \) | \( \langle 1, 0, 0 \rangle \) | \( (0, 0, 0) \) | 0.476597 | -0.378968 |
| \( n = 2 \) \( (2) \) | \( \langle 1, 0, 0 \rangle \) | \( (0.25, 0, 0) \) | 0.457325 | -0.432781 |
| \( n = 3 \) \( (1) \) | \( \langle 1, 0, 0 \rangle \) | \( (0, 0, 0) \) | 0.358354 | -0.451571 |
| \( n = 3 \) \( (2) \) | \( \langle 1, 0, 0 \rangle \) | \( (0.183333, 0, 0) \) | 0.334611 | -0.440564 |

### Simulation Description

**JOB_TYPE**: WIRE EK simulation

**Simulation Description**

- Inputdeck parsed: time: 0.00041 [sec] tot.time: 0.00041 [sec]
- Resources calculated: time: 0.03446 [sec] tot.time: 0.03437 [sec]
- Queue Wait/Resource Busy Time: time: 5.25308 [sec] tot.time: 5.28795
- Simulation (Run) Time: time: 24.75193 [sec] tot.time: 30.03987 [sec]
- Plotting completed: time: 0.02953 [sec] tot.time: 30.06940 [sec]
- Junkfiles cleaned: time: 0.24595 [sec] tot.time: 30.31525 [sec]

### Job Type and Resource utilization Log

- **Job Type**: WES
- **Associated job no**: 4
- **Selected Simulation venue**: clusterP
- **Allocated Venue no**: 5
- **CPU per node**: 2
- **CPUs per job**: 24

**Screen shots from http://nanohub.org**

---

**Abhijeet Paul**
Default UTB Simulation

**Inputs**

- Geometry -> Ultra Thin Body (UTB)
- Material -> silicon
- Body thickness -> 1.0 nm
- Transport direction (X) -> [100]
- Confinement direction (Z) -> [010]
- TB Model -> sp3d5s*
- Spin orbit -> on
- Dangling bond energy -> 30 eV
- CB simulation
- Full domain simulation
- Number of bands -> 10
- Number of k points -> 61
- Strain -> none
- Advanced user choice -> no

**Outputs**

[1] CB E(k) Plots

- Γ->[100](X)

[2] Band Edge

- Γ->[110](L)


Conduction band minima = 1.41314 eV.

Screen shots from http://nanohub.org
Default UTB Simulation (continued)

Outputs

[4] 2D Conduction Band

[5] Simulation Log

Simulation venue for this simulation is:clusterP

Simulation Description

JOB TYPE : UTB EK simulation

Inputdeck parsed => time: 0.00045 [sec] tot.time: 0.00045 [sec]

Resources calculated => time: 0.07595 [sec] tot.time: 0.07741 [sec]

Queue Wait/Resource Busy Time => time: 41.39259 [sec] tot.time: 41.47010


Plotting completed => time: 0.31038 [sec] tot.time: 75.40404 [sec]

Junkfiles cleaned => time: 0.18500 [sec] tot.time: 75.58905 [sec]

Job Type and Resource utilization Log
Job type : UTBEK
Associated job no : 5
Selected Simulation venue : clusterP
Alloted Venue no : 5
CPU per node : 2
CPUs per job : 8

Screen shots from http://nanohub.org
**Nanowire Self-consistent Simulation**

**Inputs**

- Geometry -> circular nanowire
- Material -> silicon
- Job type -> self-consistent E(k)
- Wire diameter -> 2.1 nm
- Transport direction (X) -> [100]
- Confinement direction (Z) -> [010]
- TB Model -> sp3d5s*
- Spin orbit -> off
- Dangling bond energy -> 30 eV
- N-type FET.
- Number of bands -> 10
- Number of k points -> 61
- Strain -> none
- $V_g = 0.2V, V_d = 0.05V$
- Gate work function = 4.25 eV
- Electron affinity = 4.05 eV
- S/D doping = 1e20 cm^-3.
- Advanced user choice -> no

**Outputs**

- Comparison of initial and final Ek at $V_{gs} = 0.2V$
- Due to the bias, the final Ek shifts lower to provide a charge.

---

**Effect of gate bias on electronic structure**

- Comparison of initial and final Ek at $V_{gs} = 0.2V$
- Due to the bias, the final Ek shifts lower to provide a charge.

---

**Screen shot from http://nanohub.org**
Nanowire Self-consistent Simulation (continued)

**Outputs**

1. **2D Charge profile [#/nm]**
2. **Ballistic current & injection velocity**
3. **Ballistic current = 1.1539e-07 muAmp**
   **Injection velocity = 84293.8 n/s**
4. **Source/Drain Fermi level**
   - Source Fermi level = 1.20296 eV
   - Drain Fermi level = 1.15296 eV

**Computational Resources**

- Simulation Description
  - JOB_TYPE : Self-consistent Wire EK simulation

- Timestamps
  - Inputdeck parsed: time: 0.00052 [sec] tot.time: 0.00062 [sec]
  - Resources calculated: time: 0.00680 [sec] tot.time: 0.00742 [sec]
  - Plotting completed: time: 0.04718 [sec] tot.time: 365.13433 [sec]
  - Junkfiles cleaned: time: 0.11807 [sec] tot.time: 365.25240 [sec]

**Job Type and Resource utilization Log**

- Job type: WSCBS
- Associated job no: 10
- Selected Simulation venue: Steele
- Alloted Venue no: 2
- CPU per node: 8
- CPUs per job: 15

**Screen shots from http://nanohub.org**

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Bulk Strain Sweep Simulation

Study the effect of biaxial strain on silicon bulk electronic structure

**Inputs**
- Geometry -> Bulk
- Material -> Silicon
- TB Model -> sp3d5s*
- Spin orbit -> on
- Dangling bond energy -> 30 eV
- Strain sweep simulation
- Strain -> Biaxial
- Start strain value = -0.01 %
- End strain value = 0.03 %
- No. of strain points = 20.
- Advanced user choice -> no

**Outputs**

Screen shots from http://nanohub.org

1. BandGap Variation
2. Band Edge Variation

CB, LH, HH, SO
Bulk Strain Sweep Silicon: Outputs

[1] X valley electron eff. mass variation along different directions

Electron masses do not vary much.

[1] Heavy Hole mass variation @ gamma valley

Heavy hole masses do vary quite a bit.

Other available plots
- L valley electron eff. mass variation
- Light and split off hole mass variation
- Variation in unitcell structure
- Output logs

Screen shots from http://nanohub.org
Case Study: Nanowire Electronic Structure

Study the effect of diameter variation on circular Silicon nanowire CB electronic dispersion

**Inputs**
- Geometry -> circular nanowire
- Material -> silicon
- **Wire diameter** -> [2.1,3.1,4.1,5.1,6.1] nm
- Transport direction (X) -> [100]
- Confinement direction (Z) -> [010]
- TB model -> sp3d5s*
- Spin orbit -> on
- Dangling bond energy -> 30 eV
- CB simulation
- Number of bands -> 10
- Number of k points -> 61
- Strain -> none
- Advanced user choice -> no

**Outputs**
- CB bandedge goes higher in energy with a decreasing diameter
- As wire diameter increases, Ec value approaches bulk Ec value
- All six silicon valleys lose degeneracy due to confinement
Case Study: Valley Splitting

Valley splitting: splitting of originally degenerate bands due to geometrical and potential confinement.

- Valley splitting has been taken at gamma point.
- In bulk the 6 CB lobes are degenerate in silicon, but split due to confinement.
- Valley splitting shows an oscillatory behavior which is expected since the number of atomic layers in the cross-section change from even to odd.

Transport mass gets heavier as the diameter reduces.


All simulations ran on either ClusterD* or ClusterF.*

Each simulation ran on 24 CPUs is automatically decided.

The simulation time increases as the diameter of the wire increases.

Screen shots from http://nanohub.org

*See Appendix A
Suggested Exercises

• Perform bulk simulation for Germanium and GaAs
  » What differences are there in their bands and effective masses?
  » How are the two unit cells different?
  » Which is zinc-blende and which is diamond lattice?

• Perform a thickness study on the silicon UTB structure and prepare similar graphs as shown in the silicon nanowire study.

• Perform a self-consistent simulation on a n-type circular silicon nanowire with a diameter of 4.1nm and an oxide thickness of 2nm.
  » Vary the gate bias from 0 to 0.6V, set the drain bias at 0.5V, and keep the source/drain doping at $1e20cm^{-3}$.
  » Plot 1D charge vs Vgs
  » Observe how the charge and potential profile changes with the applied gate bias.
Final Words about the Tool

Tool Limitations

• Presently can handle only zinc-blende crystal systems
• Cannot treat oxide atomistically for self-consistent simulations
• Cannot treat alloy type channels
• Due to computational and simulation time constraints, very large wires or UTB structures cannot be simulated. (If you would like to simulate bigger structures, please contact the developers.)

Opportunities and Input

• Use this tool to learn about electronic band structures in semiconductors as well as in electronic transport.
• Contact the developers to collaborate on work using this tool.
• Feel free to post any problems encountered using the tool or any new features you want on nanoHUB.org. You may use the following links:
  » the bugs (tool webpage)
  » new features you want (wish list)
• Check for the latest bug fixes on tool’s webpage.
References [1]

• Information on effective mass structure:

• Notes on band structure calculation:
  » Tutorial on Semi-empirical band structure Methods [https://nanohub.org/resources/4882](https://nanohub.org/resources/4882)
  » band structure in Nanoelectronics. [https://nanohub.org/resources/381](https://nanohub.org/resources/381)

• Notes on semi-empirical tight-binding method:
  » Wiki page on tight-binding formulation

• Notes on ballistic transport:
  » Simple Theory of the Ballistic MOSFET
  » Ballistic Nanotransistors
  » Notes on the ballistic MOSFETs

• Effective mass information:
• Simple 1D periodic potential model:
  » Quantum Mechanics: Periodic Potentials and Kronig-Penney Model

• Exercises on band structure calculations:
  » Computational Electronics HW - band structure Calculation
  » Periodic Potentials and Band structure: an Exercise

• Link to the simulation tool’s page:
  » https://nanohub.org/resources/1308

*Please check the tool web page regularly for the latest features, releases, and bug-fixes.*
## Appendix [A]: Job Submission Policy

<table>
<thead>
<tr>
<th>Job Type</th>
<th>Estimated Simulation Time ([T])</th>
<th>CPU Requirement ([NP])</th>
<th>Job Venue</th>
<th>Job Examples</th>
</tr>
</thead>
<tbody>
<tr>
<td>Light</td>
<td>(T &lt; 1) min</td>
<td>(NP &lt; 48)</td>
<td>ClusterD, ClusterF</td>
<td>Bulk band structure, Bulk strain sweep, most of the bulk calculations</td>
</tr>
<tr>
<td>Medium</td>
<td>(1) min &lt; (T &lt; 30) min</td>
<td>(NP &lt; 48)</td>
<td>ClusterD, ClusterF</td>
<td>E((k)) calculation wire radius ~ 5nm UTB width &lt; 4nm</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(NP &gt; 48)</td>
<td>Steele</td>
<td>E((k)) calculation wire rad &gt; 5nm UTB width &gt; 4nm</td>
</tr>
<tr>
<td>Heavy</td>
<td>(30) min &lt; (T &lt; 4) hours</td>
<td>(48 &lt; NP &lt; 128)</td>
<td>Steele</td>
<td>All self-consistent simulations and E((k)) calculations for larger wires and UTBs</td>
</tr>
</tbody>
</table>
Appendix [A]: Job Submission Policy (continued)

• Job Type description:
  » Light job: Jobs that are computationally less intensive as well as less time consuming
  » Medium jobs: Jobs that need more computational power but finish faster than heavy jobs
  » Heavy jobs: Jobs that need both higher computational power as well as more time to finish

• Estimated Simulation time: Average time needed to finish the job on 1 CPU

• CPU requirement: This is decided based on the number of k points, device size, and bias points.

• Job Venue:
  » ClusterD, ClusterF: Both are nanoHUB clusters with 48 nodes each
  » Steele: This has around 7000 CPUs belonging to Purdue University. Jobs can run for a maximum of 4 hours. Link for Steele Cluster
## Nomenclature for high symmetry points in different crystals

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Γ</td>
<td>Center of the Brillouin zone (all crystals)</td>
</tr>
<tr>
<td>M</td>
<td>Center of an edge</td>
</tr>
<tr>
<td>R</td>
<td>Corner point</td>
</tr>
<tr>
<td>X</td>
<td>Center of a face</td>
</tr>
<tr>
<td>K</td>
<td>Middle of an edge joining two hexagonal faces</td>
</tr>
<tr>
<td>L</td>
<td>Center of a hexagonal face</td>
</tr>
<tr>
<td>U</td>
<td>Middle of an edge joining a hexagonal and a square face</td>
</tr>
<tr>
<td>W</td>
<td>Corner point</td>
</tr>
<tr>
<td>X</td>
<td>Center of a square face</td>
</tr>
</tbody>
</table>

**Simple cube**

- M: Center of an edge
- R: Corner point
- X: Center of a face

**Face-centered cubic (Zinc Blende)**

- K: Middle of an edge joining two hexagonal faces
- L: Center of a hexagonal face
- U: Middle of an edge joining a hexagonal and a square face
- W: Corner point
- X: Center of a square face

# Appendix [B]: Brillouin Zone (continued)

## Nomenclature for high symmetry points in different crystals

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Body-centered cubic</strong></td>
<td></td>
</tr>
<tr>
<td>H</td>
<td>Corner point joining four edges</td>
</tr>
<tr>
<td>N</td>
<td>Center of a face</td>
</tr>
<tr>
<td>P</td>
<td>Corner point joining three edges</td>
</tr>
<tr>
<td><strong>Hexagonal</strong></td>
<td></td>
</tr>
<tr>
<td>A</td>
<td>Center of a hexagonal face</td>
</tr>
<tr>
<td>H</td>
<td>Corner point</td>
</tr>
<tr>
<td>K</td>
<td>Middle of an edge joining two rectangular faces</td>
</tr>
<tr>
<td>L</td>
<td>Middle of an edge joining a hexagonal and a rectangular face</td>
</tr>
<tr>
<td>M</td>
<td>Center of a rectangular face</td>
</tr>
</tbody>
</table>

Appendix [C]: Job Types

Job types found in the tool and their descriptions

<table>
<thead>
<tr>
<th>Job Name</th>
<th>Job Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bulk E(k)</td>
<td>Calculation of bulk E(k)</td>
</tr>
<tr>
<td>Bulk E(k) 3D</td>
<td>Calculation of 3D bulk E(k)</td>
</tr>
<tr>
<td>Bulk Straincal</td>
<td>Strain sweep in bulk</td>
</tr>
<tr>
<td>WBS</td>
<td>Wire band structure calculation</td>
</tr>
<tr>
<td>WSCCBS</td>
<td>Wire self-consistent band structure calculation at 1 bias point</td>
</tr>
<tr>
<td>SCCV</td>
<td>Wire self consistent CV simulation (<em>to be implemented</em>)</td>
</tr>
<tr>
<td>UTBEK</td>
<td>UTB band structure calculation</td>
</tr>
<tr>
<td>USCBS</td>
<td>UTB self-consistent band structure calculation at 1 bias point</td>
</tr>
<tr>
<td>USCCCV</td>
<td>UTB self-consistent CV simulation (<em>to be implemented</em>)</td>
</tr>
</tbody>
</table>