ECE 447/547 (Semiconductor Devices)
Southern Illinois University Carbondale

Project #2: Semiconductor Bandstructures and Engineering Related Parameters

Introduction:

Using this tool, you can quickly compute and visualize the band structures of bulk semiconductors, thin films, and nanowires for various materials, growth orientations, and strain conditions. Physical parameters such as the bandgap and effective mass can also be obtained from the computed $E(k)$. The band edges and effective masses of the bulk materials and the nanostructures structures can be analyzed as a function of various strain conditions.

Simulation Experiments:

Connect to the **Bandstructure Lab** on nanoHUB (https://nanohub.org/resources/bandstrlab)

A) Simulation of *Bulk* Materials

Choose the options "*bulk*" for Geometry and "electrons" and select Si, Ge, and GaAs materials (one after another).

In the K-space tab, Choose "Path Between High Symmetry Points". Essentially, you are solving the Schrodinger equation for different values of k along some defined lines/directions. For "Point One", select *L*. For "Points Two-Six", select Gamma, X, W, L, and Gamma for Silicon; and Gamma, X, K, and Gamma for Ge and GaAs.

Consider <u>three</u> sets of simulations for these three bulk materials.

In the first set, do not activate spin-orbit coupling. Also, do not apply any strain. Once you obtain the bandstructures, answer the following questions. Provide necessary figure(s) to support your answers.

1. At which points in k-space is the *electron* effective mass smallest for the three materials considered? State if the material is a direct-bandgap or an indirect-bandgap.
2. Are there points in k-space where the *electron* mass is negative? What is the physical interpretation of such observation?
3. Comment on the shape (spherical or ellipsoidal) of the constant energy surface for the conduction band minima.
4. Comment on "degeneracy" of the valence bands.
5. Which material offers the *smallest* hole effective mass?

In the second set, activate the spin-orbit coupling but do not apply any strain. Once you obtain the bulk bandstructures for the three semiconductor materials considered, answer the following question. Provide necessary figure(s) to support your answers.

6. Comment on the valence band structure behavior *with* and *without* the inclusion of spin-orbit coupling.

In the third set, consider only bulk silicon. Activate spin-orbit coupling. Apply a compressive uniaxial strain of 5% (that is set *epsilon* equal to -0.05). Answer the following question. Provide necessary figure(s) to support your answers.

7. Show that strain breaks the *degeneracy* in the valence band. What implications does this finding would have on hole transport (current) in a device?

B) Nanostructured Materials

For this part, consider silicon "nanowire" and [100] transport direction.

First, consider silicon "nanowire" and [100] transport direction. Vary diameter from 1 nm to 7 nm with a step size of 1 nm. Extract the bandgap and electron effective mass and plot these quantities against diameter. Comment on your finding.

Second, consider silicon "nanowire" and [110] transport direction and repeat the above experiment. Comment on your findings. Which particular nanowire offers the smallest effective mass? How does this mass compare to the bulk counterpart?

***Report*:**

Follow the *IEEE* style (https://www.ieee.org/conferences/publishing/templates.html) and write on the following aspects, as much as possible:

- *Abstract (a brief statement on what you plan to do in this project)*
- *Introduction (Why this project and related device is important)*
- *Design Method (i.e. the simulator used and a reference to it)*
- *Discussions on Design and Analysis*
- *Here, while describing your design and analysis, attach necessary graphs, snapshots of the simulator pages, and/or codes (if used).*
- *Conclusion*
- *Here, in short state what you have learnt from this project*
- *References (as needed)*