Band Structure Lab Exercise

Gerhard Klimeck, Parijat Sengupta and Dragica Vasileska

Exercise Background

Investigations of the electron energy spectra of solids form one of the most active fields of research. Knowledge of band theory is essential for application to specific problems such as Gunn diodes, tunnel diodes, photo-detectors etc. There are several standard methods to compute the band structure of solids and confined devices (such as wells, wires, and dots) carved out of them. A brief description and some useful links to band structure calculation methods can be found here . We will use the Band structure lab to generate the band diagrams of several materials and devices. A full list of options and a brief description is available on the tool page

Exercise Objectives

When you successfully answer the questions that follow, you would have learnt the following items:

1. Understood the bulk band structures of materials such as Si, Ge, and GaAs.
2. Be able to identify key (high symmetry) points on the plots that you produce.
3. Observe differences in the nature of the band structure when confinement is introduced.
4. Influence of strain on the final band structure (strain is profitably used in the industry to optimize device performance.) .

Relevant Literature

In addition to the resources mentioned on this page and in the tool description, you may find the following text books useful:

1. J.M. Ziman, *Principles of the theory of solids*, Cambridge University Press, (1964)
   A newer reprint of this volume is also available .

2. J. Callaway, *Energy band theory*, Academic Press, New York (1964).

3. D. Long, *Energy bands in semiconductors*. J. Wiley & Sons Inc., Interscience, New-York (1968).

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Exercise: <u>Band Structure Lab</u>

1) We consider a one-dimensional wire with the following energy dispersion

$$E = U + \frac{\hbar^2 k^2}{2m} \ .$$

a) By finite difference scheme, show that the Schrodinger equation can be written in the following form,

$$E\Psi_j = (U + 2t)\Psi_j - t\Psi_{j-1} - t\Psi_{j+1} \ ,$$

where $t = \hbar^2 / 2ma^2$ and a is the lattice constant.

b) Show that the numerical dispersion for the plane wave $\Psi(x) = \exp(ikx)$ described by the Schrödinger equation is given by

$$E = U + 2t\left[1 - \cos(ka)\right] .$$

Show that when the lattice constant a is sufficiently small, it gives the parabolic dispersion.

c) Derive the group velocity and effective mass using the numerical dispersion and compare them with the parabolic one. Also, sketch by hand the energy dispersion, group velocity and effective mass as a function of k. Comment if they agree well with the continuum Schrödinger case.

d) If an electric field is applied along the x direction, state the motion of the particle (i.e. velocity and acceleration) when ka=0, π/2 and π.

2) Problem 3.6 in Advanced Semiconductor Fundamentals (ASF).

3) Problem 3.9 in ASF.

Consider a graphene material:

a) Recall that it has two unit lattice vectors given by,

$$\vec{a}_1 = \begin{pmatrix} 1.5 \\ -\sqrt{3}/2 \\ 0 \end{pmatrix} L \qquad \vec{a}_2 = \begin{pmatrix} 1.5 \\ \sqrt{3}/2 \\ 0 \end{pmatrix} L$$

Work out its reciprocal lattice vectors using the following formula

$$\vec{b}_1 = 2\pi \frac{\vec{a}_2 \times \vec{a}_3}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \qquad \text{and} \qquad \vec{b}_2 = 2\pi \frac{\vec{a}_3 \times \vec{a}_1}{\vec{a}_1 \cdot (\vec{a}_2 \times \vec{a}_3)} \quad \text{where } \vec{a}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

b) Using the Wigner-Seitz algorithm, draw the first 2D Brillouin zone and indicate the position vectors of all the corners. Indicate also the Γ point.

c) Use the following energy dispersion for graphene,

$$E = \pm t\sqrt{1+4\cos\left(\frac{3L}{2}k_x\right)\cos\left(\frac{\sqrt{3}L}{2}k_y\right)+4\cos^2\left(\frac{\sqrt{3}L}{2}k_y\right)}$$

to plot the energy dispersion from Γ point to one of the corner where t=3eV. What is the effective mass and velocity v in the vicinity of the corner at E=0? Verify that it is a good estimate to write the energy dispersion at the corner (valley) as $E = \hbar v k$. What is the valley degeneracy for graphene?

d) Derive the density of states and zero temperature electron density as function of energy for only a single valley for the following materials:

(i) Graphene: $E = \hbar v k$

(ii) Parabolic band semiconductor: $E = \frac{\hbar^2}{2m}k^2$

Comment on their differences. Do you think the electron density is temperature dependent? Invoke the Fermi Dirac function in your argument. Note: there is a spin degeneracy factor of 2.

5) Strain Distortions in Crystals

The following segments deal with numerical solutions to electronic structure. You need to use two different tools:
Periodic-Potential Lab (https://nanohub.org/tools/kronig_penney) and
Band structure Lab (https://nanohub.org/tools/bandstrlab). Both tools are also part of ABACUS (https://nanohub.org/tools/abacus) if you prefer to access them there.

5a) In the Periodic Potential Lab select the following options:

Potential Type – Columbic Potential
Energy Details: Depth of Columbic Well 15eV,
Minimum Energy -15eV,
Particle energy above the barrier: 10eV,
Well geometry: Width of single periodic cell – vary this number in steps of 0.25A from 11A to 13A,
a: 0.2A
Effective mass: 1

Read off the k=0 points of the 4th and 5th band as depicted for example in the plot "Reduced E_k compared to E_{ff} mass Ek" and plot the following:

- Band energies,
- Band-gap between these band-edges,
- Effective masses on these bands,
- Bandwidth of the 4th and 5th band at k=0 as a function of the 'Width of single cell"
- Assuming that 12A is the natural separation of these atoms, indicate the percentage of distortion on these graphs

5b) Interpret the results above. Why are the bandwidths, effective masses and band gap changing?

5c) In the Band Structure Lab select the following options:

Device Structure: Geometry: Bulk Material
Material: GaAs

Electronic Structure: defaults – sp3d5s* with spin orbit coupling
Analysis: Select Numerical Solution (Bulk) Strain Analysis, run strain sweep
Select Job to be performed: Strain Sweep
Strain Model: Hydrostatic Strain
Initial strain: -0.03
Final strain: 0.03
Number of points: 15
Adv. User Choice: default

- Look at the output of the sequence of "Lattice vs. strain". Which strain condition corresponds to compression and which to expansion?
- Now observe the "Energy Bands Vs. Strain". Compare the general behavior of the conduction and the valence bands as a function of strain in light of the results of 5b)
- Finally study the plot of the Gamma electron mass vs. strain and the HH effective mass vs. Strain
- Interpret the results in light of the results of 5b)

6) Use the Band structure Lab, follow the steps outlined and answer the following questions:

Simulate bulk material under the geometry option.
Choose material as GaAs.
Click on Electronic Structure tab to move to the next screen.
Set the Tight Binding model to sp3s*d5 and check the Spin-Orbit coupling box.
Note that some of the options given here would be preset as default, you need to leave them unchanged.
Now press the Analysis button to go forward.
Leave all preset options unchanged. Press the Advanced User option to take you to the next menu options.
Click simulate on this screen to launch the tool.

1. What is the crystal structure of GaAs?
2. How many atoms are there in the unit cell of GaAs?
3. Use the Bulk Central band plot to locate the Gamma, L, and X point. What are the corresponding energies at these points?
4. Obtain the band gap information from the plot you used for the previous sub-parts
5. On the same plot you will notice three bands below the 0eV mark, what are these bands called and how are they classified?
6. You will notice a split in the bands you identified in the previous part, how is it commonly known? How much is the split measured on the plot?
7. From the effective mass table information, write down the effective masses at the gamma and L point. What quantitative difference do you see?
8. Perform a search on the web to find how this difference in effective masses gives rise to an exotic phenomenon known as Negative Differential Resistance. Write your answer in not more than 5 sentences
9. Which device commercially uses the above phenomenon?