Solid State Devices I - Purdue ECE-606

Homework No. 3

Student name: _____

Student ID: _____

I solved the homework assignment myself without copying a solution from someone else or from the web. Student Initials here: _____

Problem 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. (4 points)

b) Show that the numerical dispersion for the plane wave $\Psi(x) = \exp(ikx)$ described by the Schrödinger equation of 1a) is given by E = U + 2t [1 - cos(ka)] (4 points)

c) Show that when the lattice constant **a** is sufficiently small, it gives the parabolic dispersion. (2 points)

d) Derive the group velocity using the numerical dispersion and compare it with the parabolic one. (2 points)

e) Derive the effective mass using the numerical dispersion and compare it with the parabolic (2 points)

f) Sketch by hand the energy dispersion, group velocity and effective mass as function of k. Comment if they agree well with the continuum Schrödinger case. (8 points)

g) 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. (4 points)

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Problem 2.

This exercise uses the Periodic Potential Lab on nanoHUB. You can launch the tool by following the link http://nanohub.org/resources/3847.

Follow the steps outlined and supply answers to the questions presented.

i. Choose the potential type as "step" (potential type tab)

ii. Set the maximum barrier height (U) to 2eV, the minimum to zero (energy details tab)

iii. Set the width of single periodic cell to 12A (well geometry tab)

iv. Use "a" equal to 8A (well geometry tab)

v. Set the effective mass to unity.

a. Launch the tool for U = 2eV. Estimate the band-gap between the first and second energy bands. You should choose the "Allowed Bands" option from the drop down menu to answer this question. (3 points)

b. Repeat part a) with U = 4eV. Did the band gap between the first and second bands (3 points)

c. Did the bands themselves become wider (bandwidth) or narrower than in part a)? (3 points)

d. Use the drop down menu to look at the effective mass, you might notice certain values are negative; provide a physical interpretation of the change in sign of the effective mass (3 points)

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Problem 3

Use the Band structure Lab (https://nanohub.org/resources/bandstrlab directly or in ABACUS https://nanohub.org/tools/abacus), follow the steps outlined and answer the following questions

Simulate "Bulk (3D-periodic)" Choose material as Si
Click on "Physics"
Click on Electronic Structure tab to move to the next screen
Set the Tight Binding model to sp3s*d5 and make sure the Spin-Orbit coupling is ON
Note that some of the options given here would be preset as default, you need to leave them unchanged.
Click on "k-space" or "Simulate" (no changes needed in k-space)
Click on "Numerics" or "Simulate" (no changes needed in Numerics)
Click on "Simulate" (if you have not done so yet)

a) [1 point] What is the crystal structure of Si?

b) [1 point] How many atoms are there in the unit cell of Si?

c) [3 points] Zoom into the bandstructure blot in an energy range of [-2eV,4eV] by clicking on the left/vertical axis. Locate the Gamma, L, and X point. What are the corresponding electron energies at these points?

d) [3 points] Obtain the band gap information from the plot you used for the previous sub-parts

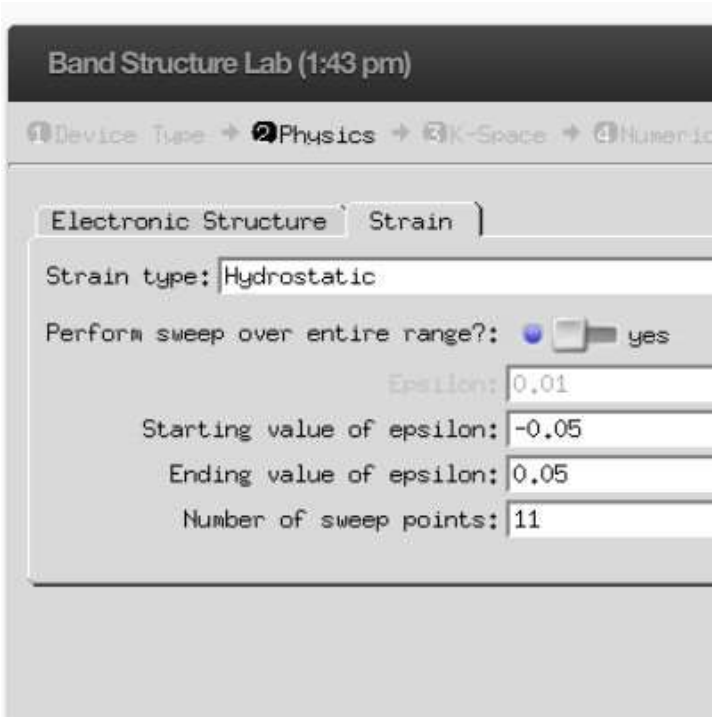
e) [3 points] On the same plot you will notice three bands below the 0eV mark, what are these bands called and how are they classified.?

f) [1 point] You will notice a split in the bands you identified in the previous part, how is it commonly known

g) [1 point] How much is the split measured on the plot?

h) [6 points]From the effective mass table information, write down the effective masses at the X and L point. What quantitative difference do you see?

i) [9 points] Let us consider the effects of the most "simple" strain: Hydrostatic. Here the lattice constant is compressed or expanded equally in all three directions. Let us configure Bandstructure lab to seep a hydrostatic strain from -5% to +5%.



Run the simulation and examine the results of the "Bands" output as a function of strain. (make sure you zoom into the [-2eV,4eV] energy range).
The plot / dataset "Bands vs. Strain" currently has a bug. You will now need to extract the various band-edges at the valence bands and the Gamma, X, and L points as a function of strain by "hand" and plot these data on a separate plot.
Plot the band edges as a function of strain.
Plot the bandgaps as a function of strain.
Can you comment on the behavior of the bandgaps? [9 points]

j) [14 points] Let us consider a more realistic strain effect: Bi-axial strain. This typically occurs when a material is grown on a substrate with a slightly different lattice constant. In the growth plane the newly grown crystal will fit into the lateral lattice constant of the substrate and in the growth direction the lattice constant will adjust to roughly contain the same volume of the unit cells. So the lateral and the vertical lattice constants will be different. Let's configure Bandstructure Lab to look in two different X directions as biaxial strain is applied
Choose biaxial strain in the [100] direction and sweep the strain from -5% to +5%.

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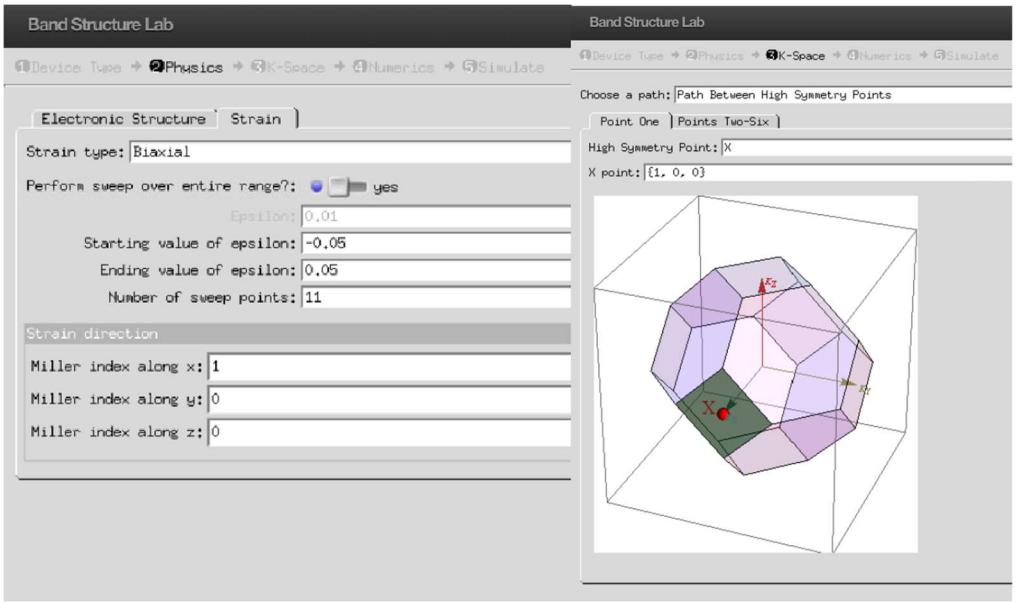
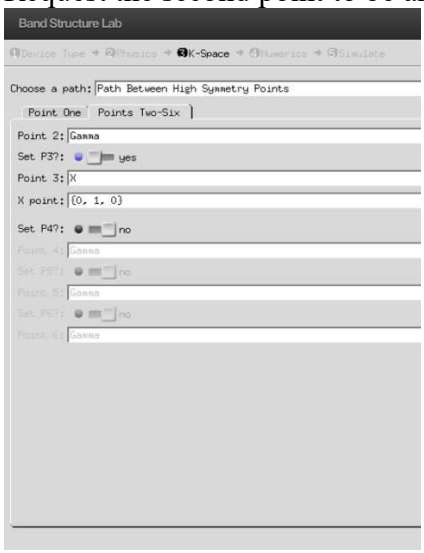


Request the second point to be another X point in an orthogonal direction:



Run the simulation and examine the results of the "Bands" output as a function of strain. (make sure you zoom into the [-2eV,4eV] energy range).

The plot / dataset "Bands vs. Strain" currently has a bug. You will now need to extract the various band-edges at the valence bands and the two X points as a function of strain by "hand" and plot these data on a separate plot.

Comment on the behavior of the two different X valleys.
How many equivalent X valleys exist?
What is the implication on the available number of states in the different crystal directions given the applied strain?
Can you comment on the behavior of the valence bands? (14 points)

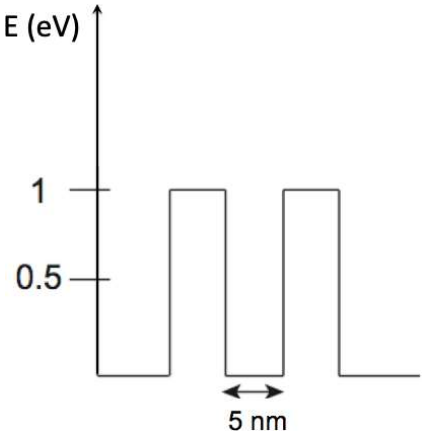
Homework No. 4

Problem 4

This question deals with quantum mechanics. (12 points)

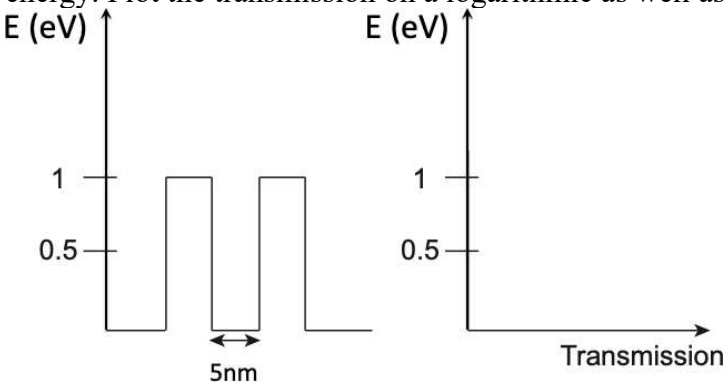
a. Compute the lowest three eigen energies in units of eV for a particle in an infinite potential well, where the well width is 5.0 nm. Assume the effective mass of the particle to be 0.1m0. You may find the following expression and approximation helpful to avoid using a calculator: $C = \frac{\hbar^2\pi^2}{2m_0} = 0.376 \text{ eV nm}^2 \approx 0.4 \text{ eV nm}^2$
(1 points)

b. Consider a double barrier structure as shown below



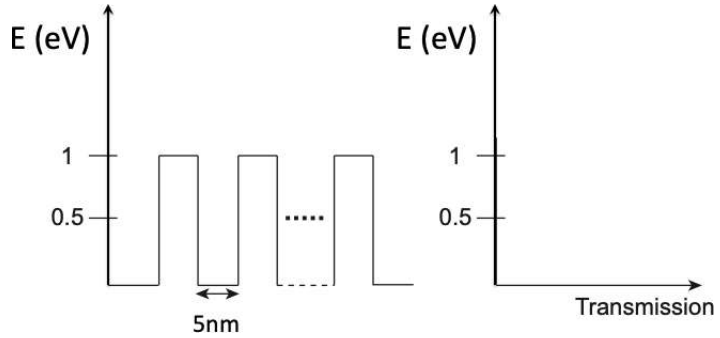
Sketch the eigen energies levels of the structure (using solid line) and that of part a) (using dashed line). Explain the relative position of the new energies compared to the ones computed in part a). Sketch your answer for part b) on the figure above. (2 points)

c. Use the tool Piece-Wise-Constant-Potential-Lab (https://nanohub.org/tools/pcpbt). Well 5nm and barriers 2nm. Plot the transmission through the double barrier structure as a function of energy. Plot the transmission on a logarithmic as well as a linear scale. (2 points)



d. Consider now a similar quantum structure like c), but now with 8 barriers instead. Use the PCPBT tool again. Plot the transmission again on a linear and a logarithmic scale. How many resonance energies are we expecting to get in this case? (3 points)

Homework No. 4



e. Consider now a similar quantum structure like d), but increase the barrier width to 4nm. Use the PCPBT tool again. Plot the transmission again on a linear and a logarithmic scale. Plot the transmission coefficient of d) and e) on the same plot (clicking on "All" on the bottom left of the graph). Document and comment on the width of the bands and the definition / sharpness of the bands (4 points)

Homework No. 4

Problem 5

In a previous homework, we introduced a material called graphene; we shall probe it further here.

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

$$\overrightarrow{a_1} = \begin{pmatrix} 1.5 \\ -\sqrt{3}/2 \\ 0 \end{pmatrix} L \qquad \overrightarrow{a_2} = \begin{pmatrix} 1.5 \\ \sqrt{3}/2 \\ 0 \end{pmatrix} L$$

Work out its reciprocal lattice vectors using the following formula

$$\overrightarrow{b_1} = 2\pi \frac{\overrightarrow{a_2} \times \overrightarrow{a_3}}{\overrightarrow{a_1} \cdot (\overrightarrow{a_2} \times \overrightarrow{a_3})} \quad \text{and} \quad \overrightarrow{b_2} = 2\pi \frac{\overrightarrow{a_3} \times \overrightarrow{a_1}}{\overrightarrow{a_1} \cdot (\overrightarrow{a_2} \times \overrightarrow{a_3})} \quad \text{where} \quad \overrightarrow{a_3} = \begin{pmatrix} 0 \\ 01 \end{pmatrix}$$

(4 points)

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. (4 points)

c) Using the following energy dispersion for graphene,

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

Plot the energy dispersion from Γ point to one of the corner where t=3eV. (4 points)

d) What is the effective mass and velocity v in the vicinity of the corner at E=0? (2 points)

e) Verify that it is a good estimate to write the energy dispersion at the corner (valley) as E= $\hbar$vk (2 points)

f) What is the valley degeneracy for graphene? (2 points)

g) Derive the density of states and zero temperature electron density as function of energy for only a single valley Graphene: E= $\hbar$vk (6 points)

h) Derive the density of states and zero temperature electron density as function of energy for only a single valley for a parabolic band semiconductor in 2 dimensions: $E = \frac{\hbar^2 k^2}{2m}$ (6 points)

Homework No. 4

Problem 6

A particle of mass m and fixed total energy E, where $0 < E < U_0$, is placed in the one-dimensional potential well pictured in Fig. P2.6.

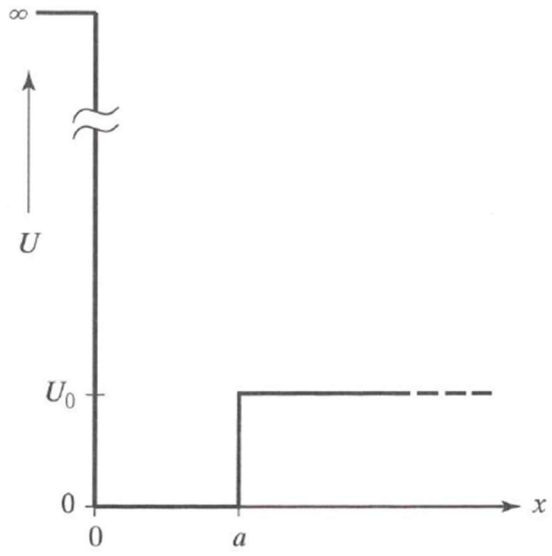


Figure P2.6

(a) Write down the simplified form of Schrodinger's equation appropriate for the various spatial regions.
(b) Indicate the general solutions to your part (a) equations.
(c) List the boundary conditions appropriate for the given problem.
(d) Establish the simultaneous equations that result by applying the part (c) boundary conditions.
(e) Obtain the equation that must be solved to determine the allowed particle energies.