ECE 594A – Introduction to Nanoelectronics – Assignment 2

Deadline: **5/31/2013 Friday by 5 PM**.

Most problems need to be solved by MATLAB. Hand in your report (hand-written or printed) to Jiahao Kang in HFH 2152C and email all your MATLAB codes (.m) and figures (.fig) in a **compressed achieve** (.zip, .rar, .7z, etc.) to jiahao_kang@ece.ucsb.edu.

Problem 1   Quantum Well

In the lecture on 5/14/2013, we have learnt how to solve the energy states and wave functions of a 1D infinite quantum well numerically. Now we will proceed to the calculation of electron density for the system using MATLAB. In the single-electron approximation, the wavefunction or the density of the single electron represents the average distribution of the system. Therefore, density of the electrons can be estimated by the wavefunction of single electron (in the unit of #/length)

$$\rho(x) = \sum_i N_i \psi_i^\dagger(x) \cdot \psi_i(x) \quad \text{or} \quad \rho(x) = \int_E N(E)\psi_E^\dagger(x) \cdot \psi_E(x)\, dE$$

where N_i, $N(E)$ stands for the number of electrons in the ith state or the state with energy E of the system, and $\psi_i(x)$, $\psi_E(x)$ is the wavefunction of the single electron corresponding to the ith or energy E state. With regard to the Fermi-Dirac distribution, the number of the electrons in a specific state can be derived by

$$N_i = D_i \cdot f_{E_f}(E_i) \quad \text{or} \quad N(E) = D(E) \cdot f_{E_f}(E)$$

where E_i is the energy of the ith state, E_f is the Fermi level of the system. Remember that the wavefunctions have to be normalized before we calculate the density.

(1) Since we have got the eigenstate of a one-dimensional infinite potential well, please calculate the number of the electrons in each state, when we set the Fermi level exactly at the eigenenergy of the second state and consider the spin factor equals 2. Assume that the cross section has an area of 10^{-18} m^2 and neglect the cross section quantization. (Take $k_b T \approx 0.0259$ eV)

(2) Use the wavefunction numerically derived in the previous problem, and calculate the electron density of the one-dimensional infinite potential well. Plot the result along the x-axis. Check the lecture notes for the constant parameters.

Save the program as 'Problem_1.m', and save the figure as 'Problem_1.fig'.

Problem 2   Band Diagram of MOS

In this task, we will solve a real case for MOSFET using MATLAB. Recall the scheme that discretize the space and set the total length for our simulation region as [0,100) nm. The region is plotted below:
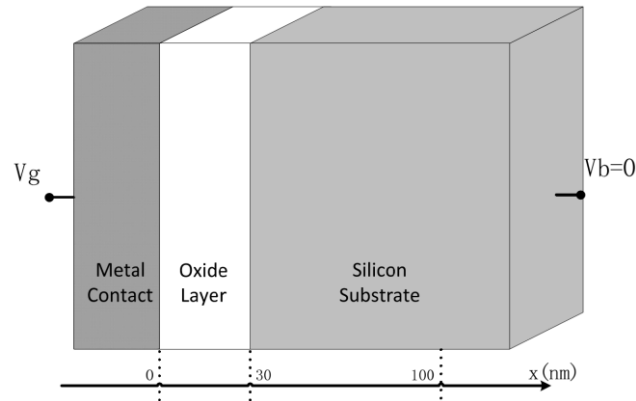
By taking the density of state in metal approaching infinity and a proper work function, we can assume that the potential at the interface between oxide layer and metal follows V_g applied to the gate. And we can take the region large enough to neglect the variation of the potential at the right edge of simulated region.

That is to say, the intrinsic Fermi level for the semiconductor satisfies:

$$E_{Fi}|_{x=0} = -V_g$$

$$\frac{\partial E_{Fi}}{\partial x}|_{x=100 \text{ nm}} = 0$$

Therefore the metal gate does not need to be included into the simulated region, but only considered as a boundary condition for Poisson's equation.

(1) Derive the discretized Poisson equation by the discretization methods taught in lecture. Note that the number of carriers inside the oxide layer is zero.

(2) Derive the discretized Jacobi matrix for the function equivalent to the equation above.

(3) Use the Jacobi matrix and the function to derive the profile of the band diagram and carriers density under V_g=0. N_a=5e17 cm-3; N_d = 0. Check the lecture notes for other constants. Plot the figure of Ec, Ev, Ef vs. x and n, p vs. x.

(4) Find V_{FB}, V_T under these assumptions and compare them with the theoretical results.

(5) Define space charge region from the interface between oxide layer and substrate to the point where the density of carrier rise to half of the doping concentration. Plot the width of the space charge region versus the gate voltage. Explain your result.

Save the program as 'Problem_2.m' that plots as required, and save the figure as 'Problem_2.fig'.

Bonus to Problem 2

Within the scheme in the previous problem, we can use a quasi-static approximation to sketch the low frequency C-V characteristics for the MOSFET. By the approximation, we assume that the charge varies with the gate voltage fast enough to keep the device in equilibrium. So to achieve the C-V characteristics, we just need to apply a gate voltage with a small difference. With the help of the charge and voltage difference, the capacitance for small signals can be easily yielded by

$$C' = \frac{\partial q'}{\partial V_g} = \frac{\Delta q'}{\Delta V_g}$$

where q' can be derived by summing up all charge in the semiconductor region. Here " ' " indicates the variable per area. Now

(1) Please derive the theoretical result of capacitance in strong inversion and accumulation region.

(2) Use your MATLAB code to show the C-V characteristics.

Save the program as 'Problem_2b.m' that plots as required, and save the figure as 'Problem_2b.fig'.

Problem 3   Lattice of Graphene

Graphite sheet is a sheet made of one single carbon atom layer. In MATLAB, Use the plot command to show the positions of all atoms within a radius of 9Å of the atoms (any one of them) in the chosen unit cell of a graphene sheet (assume the unit cell have atoms in (0,0) and (acc,0), where acc=1.44Å). Mark all the positions with blue '*' except the chosen ones in the unit cell with a red '*'. You should generate a figure similar to one of below:
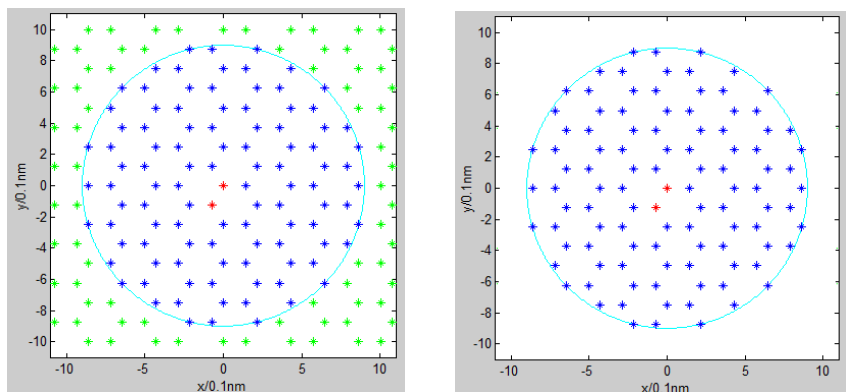
Hints: plot command takes the syntax mostly as "plot(x, y, 'line_mark_color_expression')".

Here the x and y stands for the vectors of coordinate of your points. line_mark_color_expression specifies the marks, lines, and colors.(Use help <command> in MATLAB to see the details.)

Use the unit cell and the unit lattice vector will help you to draw it.

Save the program as 'Problem_3.m' that plots as required, and save the figure as 'Problem_3.fig'.

Problem 4   Lattice of Silicon

In MATLAB, 'plot3' is used to show the data in 3D space. Use plot3 command to draw the positions of the atoms in the silicon lattice by the mark '*'. Assume that we have a cube of edge length $a=4a_{silicon}$, where $a_{silicon} \approx 5.43\text{Å}$ is the edge length of a unit cell in silicon.

Hint: "plot3(x,y,z,s)" plots in 3d-space through the points whose coordinates are the elements of x, y and z, where x, y and z are three vectors of the same length, s is a 1, 2 or 3 character string made from the characters listed under the plot command. See "help plot3" for detail.

(a) Please plot the unit cell. You should have a similar figure as below:
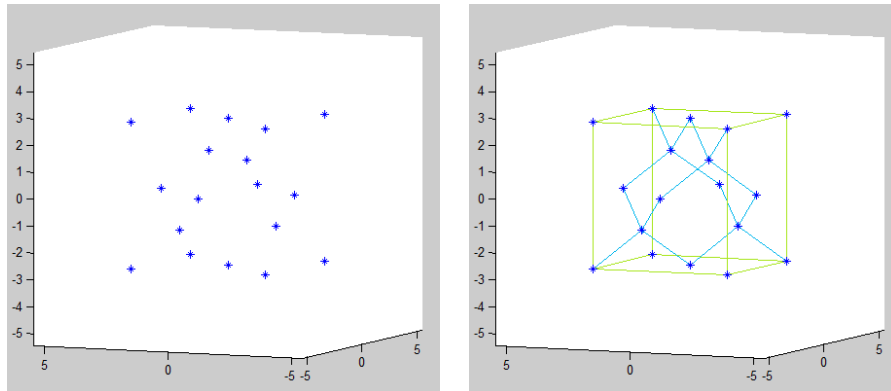
(b) Repeat the unit cell in 3 directions. Then obtain the figure for silicon lattice in (110) and (111) plane (use 'view([h l k])' command).
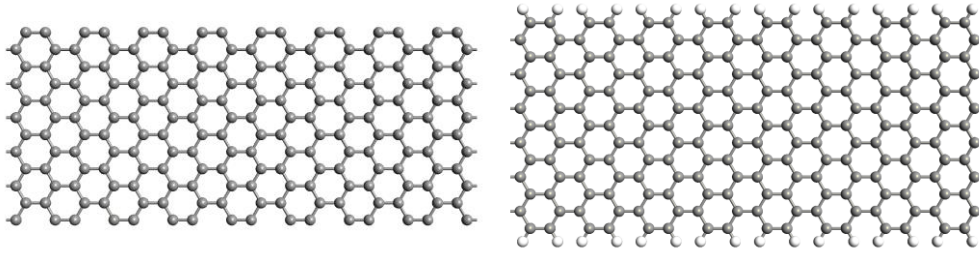
The example figures below give a view in (100) plane and random view in 3D.
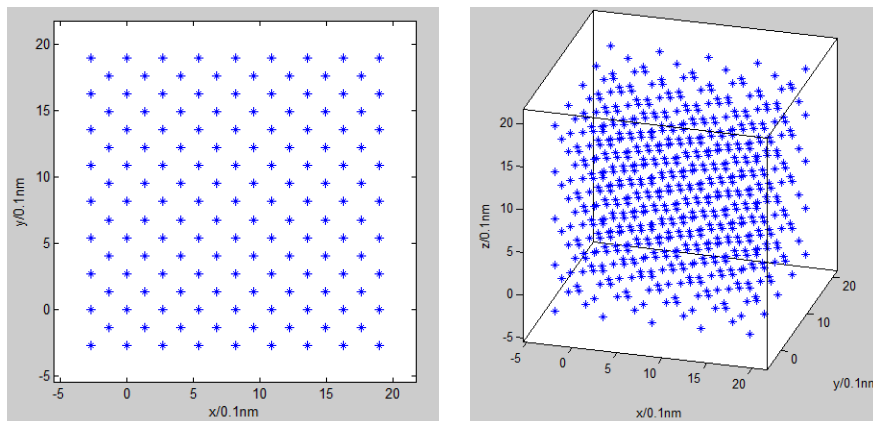
Save the program as 'Problem_4.m' that plots as required, and save the figure as 'Problem_4.fig'.

Problem 5   Band Structure of Graphene Nanoribbons

Use the method taught in class, generate the band structure of the following graphene nanoribbons (GNR) by MATLAB. Measure the band gaps.
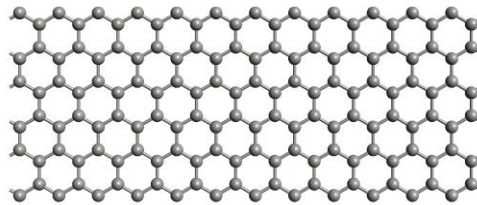

GNR 1 – armchair – 12 carbon atoms in width – edges are unsaturated
GNR 2 – armchair – 13 carbon atoms in width – edges are saturated by hydrogen atoms

Bonus to Problem 5

(a) Repeat Problem 5 for a zigzag GNR (12 carbon atoms in width – edges are unsaturated):

(b) Use the method taught in class, generate the band structure of graphene along k_x-k_y plane by MATLAB. You may use 'surf' or 'mesh' to generate a surface plot. The result should be similar to the figure below:
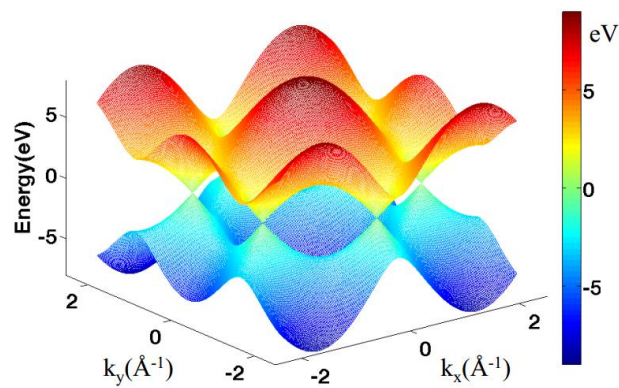
Save the program as 'Problem_5b.m' that plots as required, and save the figure as 'Problem_5b.fig'.