EE 656: Electronics Transport in Semiconductors
Homework 5: Solution of BTE by Monte Carlo Method: High field transport in Bulk Si

In Chapter 6 of that text, the details of Monte Carlo simulation are discussed. In Chapter 7, the features of high-field transport in bulk semiconductors are described. The purpose of this assignment is to give you an opportunity to explore electron transport in bulk silicon using a Monte Carlo simulation program, SDemon, which can be accessed and operated through a WWW browser at *www.nanohub.org*

To access SDemon, go to *www.nanohub.org*, select *Tool Index* under Online Simulation. If this is your first time at the nanoHUB, you'll be asked to request an account. After filling out the form, you'll get an account automatically and then be able to log in. Use *Help* on each page for instructions on what to do. You should first run the example file, **bulk**, which you can copy from the *Exercises* subfolder in the *Examples* folder of SDemon. The simulation will take about 60 seconds. Next, examine the output (in file, **Output**, unless you renamed it). Finally, answer the following questions for an electric field of 10^5 V/cm.

1) Deduce the field-dependent electron mobility using the relationship between average velocity and applied electric field.

2) Use the expression, $D_n = 2u_{zz} \mu_n /q$, to deduce the diffusion coefficient. Compare it to the value you would expect from the conventional Einstein relation, $D_n = (k_B T_L /q) \mu_n$.

3) Estimate the drift energy. Proceed as follows. Estimate the average effective mass, $<m^*>$ using $m^*(E) = m^*(0)(1+ 2\alpha E)$. Estimate $<m^*>$ by using the average carrier energy printed in the output table *(u)* assuming that $\alpha = 0.5\ eV^{-1}$ and $m^*(0) = m_c^* = 0.26m_0$. From the average effective mass, you can estimate the drift energy. What fraction of the total carrier energy is drift energy?

4) Using the average carrier energy and the estimated drift energy, estimate the electron temperature.

5) Define the mobility as $\mu_n = q\tau_m / < m^* >$, where τ_m is the average momentum relaxation time and $<m^*>$ is the average effective mass as obtained in part 2). Estimate the momentum relaxation time.

6) The steady-state energy balance equation is $n (u - u_o) /\tau_E = J_{nz} E_z$ where τ_E is the average energy relaxation time. Use the Monte Carlo results to estimate the energy relaxation time and compare it to the momentum relaxation time.

7) It is commonly assumed that the carrier energy is equally split between the three degrees of freedom (i.e. $u_{xx} = u_{yy} = u_{zz} = u/3$). How good is this assumption?

8) Near equilibrium, the electrons populate the three sets of ellipsoids equally. What fraction of the electrons is located in the ellipsoids oriented along the z-axis, which is the

direction of the electric field too? (This quantity is labeled **n(g)/n** in the table.)

9) Examine the velocity histogram. You will need to *Post Process* the results. When you do so, type "bulk" in the Data File Tag window at the top of the page. Is the distribution function well approximated by a displaced Maxwellian? Can you explain its shape?

10) Repeat items 1) - 9) for an electric field of 10^3 V/cm. You will have to edit the file, bulk, and rerun the simulation for the new electric field. Compare the results to those for 10^5 V/cm.