A GUI Program for the Calculation of Mobility and Carrier Statistics in Semiconductors

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Student Paper Abstract

Researchers at the University of Notre Dame and elsewhere working on the development of high-speed semiconductor devices find it desirable to know how the mobility in these semiconductors (Silicon, GaAs, GaN, etc) varies as a function of growth parameters such as doping density and temperature. This information is crucial in the layer-structure design of ultrafast transistors. Up until now, there have been no software tools available to semiconductor device physicists and engineers to automatically do the calculations necessary to gain such information. Researchers are therefore forced to either look up data on similar materials which have previously been determined, go through the lengthy calculations themselves, or determine it experimentally.

My task was to create a program which would:

a) Calculate the mobility, carrier density, conductivity, and Fermi energy for any given semiconductor,
b) In an easily navigable GUI (Graphical User Interface) to allow the user to choose the semiconductor, doping densities, the temperature, and similar physical parameters, and
c) In addition, it was to calculate and plot mobilities and carrier concentrations as a function of temperature, ionized acceptor & donor concentration, and the activation energy of the donors and acceptors.

In order to achieve these goals, it was necessary to read and learn the methods by with others have calculated these values, and to alter them where the assumptions under which they operate are not valid for the range of parameters to be used by the program. I then created the program which was to do the calculations. This involved simultaneously numerically integrating and solving the charge-neutrality equation with Fermi-Dirac statistics for the Fermi energy, as well as compiling a table of known parameters of various semiconductors. I also created a GUI to interface between this program and the user.

This program is currently known to be in use by researchers at Notre Dame as well as two other universities, and is freely down-loadable at the Notre Dame website: www.nd.edu/~demand. It is called “Mobility”, and it currently calculates all the above quantities (mobilities, carrier statistics, etc) for a range semiconductors. The type of semiconductor, the doping densities are user-defined, and the entire software runs in an easy-to-use GUI mode. The next generation of the program will incorporate heterostructures and will enable the calculation of mobilities and carrier statistics in quantum wells and 2-dimensional electron gases, which form the backbone of the fastest transistors in existence today.

Key Words

Student Paper, Electrical Engineering

A GUI Program for the Calculation of Mobility and Carrier Statistics in Semiconductors

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Introduction

Researchers at the University of Notre Dame and elsewhere working on the development of high-speed semiconductor devices find it desirable to know how the mobility in these semiconductors (Silicon, GaAs, GaN, etc) varies as a function of growth parameters such as doping density and temperature. This information is crucial in the layer-structure design of ultrafast transistors. Up until now, there have been no software tools available to semiconductor device physicists and engineers to automatically do the calculations necessary to gain such information. Researchers are therefore forced to either look up data on similar materials which have previously been determined, go through the lengthy calculations themselves, or determine it experimentally.

This program is meant to save time by providing an easy to use and automated method for the calculation and plotting of Mobility, Carrier Concentration, Conductivity, and the Fermi Energy in a variety of semiconductors.

Mobility, $\mu(\frac{cm^2}{V \cdot s})$, is a measure of how well charge carriers are able to move through a substance.

Together with carrier concentration (n for electrons, p for holes), mobility is important for determining the conductivity, $\rho(\frac{1}{\Omega \cdot cm})$, of a substance. Conductivity is found by the equation,

$$\rho = qn\mu_n + qp\mu_p. \tag{1}$$

In addition, electrons are able to flow more quickly in materials with higher mobility. Since the speed of an electronic device is limited by the time it takes a carrier to move from one side to the other, devices composed of materials

with higher mobility are able to achieve higher speeds. For this reason, it is useful to maximize the mobility of materials used.

Though methods for calculating the mobility have been practiced for years, there has not been a tool available for calculating it automatically. The Mobility program solves this problem by providing an intuitive interface through which a user can specify various parameters from which it calculates the mobility along with related values such as the conductivity and carrier density. The program is open source, and users may add any semiconductor they wish, provided that they have the necessary data.

Theory

The Mobility is determined by the rate at which electrons are scattered by impurities and defects within the crystal structure of the semiconductor. This rate, $1/\tau(s^{-}1)$, is the reciprocal of the relaxation time, τ (s), the average time between collisions. The relaxation time can be adjusted to account for the varying degrees of scattering on any given collision. This is called the momentum relaxation time, τ_m. The mobility is dependent upon τ_m by the equation,

$$\mu = \frac{q\tau_m}{m^*}. \tag{2}$$

There are several mechanisms by which the electrons are scattered. Ionized impurities interact with electrons and holes, attracting/repelling them via the electric force. Electrons can also be scattered by neutral impurities, dislocations in the crystal structure, and by acoustic and optical phonons. The equations for the momentum relaxation times are given in Table 1 in the form,

$$\tau_i(x) = \tau_i x^{ri}, \tag{3}$$

where $x = \frac{E}{kT}$.

In Table 1, N_I = concentration of ionized impurities; $g(n*, T, x) = ln(1 + b) - b/(1 + b)$; $b = 4.31x10^{13}[\epsilon_r(0)T^2/n*](m*/m)x$; N_n = concentration of neutral impurities; $C_l = 1/5(3C_{11}+2C_{12}+4C_{44})$; $C_t = 1/5(C_{11}-C_{12}+3C_{44})$; $\theta = h\omega_{LO}/k$.

Table 1: Momentum Relaxation Times and reduced Energy dependence for Materials with Isotropic Parabolic Bands[1]

Scattering mechanism	τ_i	r_i
Impurities		
Ionized	$\frac{0.414\epsilon_r^2(0)T^{3/2}}{Z^2N_I(cm^{-}3)g(n*,T,x)}\frac{m*}{m}^{1/2}$	3/2
Neutral	$\frac{8.16x10^6}{\epsilon_r(0)N_n(cm^{-}3)}\frac{m*}{m}^2$	0
Acoustic Phonons		
Deformation Potential	$\frac{2.4x10^{-20}C_l(dyn/cm^2)}{\xi_a^2(eV)T^{3/2}}\frac{m}{m*}^{1/2}$	$-1/2$
Piezoelectric	$\frac{9.54x10^{-}8}{h_{14}^2(V/cm)(3/C_l+4/C_t)T^{1/2}}\frac{m}{m*}^{1/2}$	1/2
Optical Phonons		
Deformation Potential	$\frac{4.83x10^{-20}C_l(dyn/cm^2)[exp(\theta/T)-1]}{\xi_A^2(eV)T^{1/2}\theta}\frac{m}{m*}^{3/2}$	$-1/2$
Polar	$\frac{9.61x10^{-15}\epsilon_r(0)\epsilon_r(\infty)[exp(\theta/T)-1]}{\epsilon_r(0)-\epsilon_r(\infty)\theta^{1/2}(\theta/T)^r}\frac{m}{m*}$	$r(\theta/T)$

n^* is given by the equation, $n^* = \frac{\partial n}{\partial \eta_c} + \frac{\partial p}{\partial \eta_v} + \frac{N_a^0 N_a^-}{N_a} + \frac{N_d^0 N_d^+}{N_d}$, where $\eta_c = \frac{E_F - E_c}{kT}$, $\eta_v = \frac{E_v - E_f}{kT}$, $\frac{\partial n}{\partial \eta_c} = n\frac{F_{-1/2}(N_c)}{F_{1/2}(N_c)}$, and $\frac{\partial p}{\partial \eta_v} = p\frac{F_{-1/2}(N_v)}{F_{1/2}(N_v)}$.

$r(\theta/T)$ is given by the equation[2],
$r = 1 - .5841\theta/T + .292(\theta/T)^2 - .037164(\theta/T)^3 + .0012016(\theta/T)^4$, when $(\theta/T) < 5$, and by $r = \frac{(3\pi^{\cdot 5})}{8}(\theta/T)^{\cdot 5}$, when $(\theta/T) > 5$.

Scattering from dislocations also occurs[3]. The momentum relaxation time, τ_{dis}, follows the equation,
$\tau_{dis} = \frac{\hbar^3\epsilon^2c^2}{N_{dis}m^*e^4}\frac{(1+4\lambda^2K_\perp^2)^{3/2}}{\lambda^4}$, where $\lambda = (\frac{\epsilon k_b T}{e^2 n^*})^{1/2}$, and $k_\perp^2 = \frac{2Em^*}{\hbar^2}$.

The total scattering rate is equal to the sum of the individual rates,

$$\frac{1}{\tau_m(x)} = \sum \frac{1}{\tau_i(x)}. \tag{4}$$

Since these scattering rates are a function of electron energy, they must be averaged over the Fermi Dirac electron distribution[1]. The procedure for averaging the relaxation time over the electron distribution is,

$$< \tau_m(x) x^t >= \frac{2}{3} \frac{\int_0^\infty \tau_m(x)(-\partial f_0/\partial x) x^{t+3/2} dx}{\int_0^\infty f_0 x^{1/2} dx}. \tag{5}$$

The equation[1] for the Fermi Dirac Distribution function f_0 is,

$$f_0 = \frac{1}{1 + exp(\frac{E-E_f}{kT})}, \tag{6}$$

where E is the electron energy, E_f is the Fermi Energy, k is Boltzmann's constant, and T is the temperature.

The Fermi Energy E_f is found by solving the charge neutrality equation, which states that the total number of positive charges equals the total number of negative charges,

$$Nd^+ - Na^- = n - p, \tag{7}$$

where $n = N_c \int_0^\infty \frac{x^{1/2} dx}{1+exp(x-\eta_n)}$, $p = N_v \int_0^\infty \frac{x^{1/2} dx}{1+exp(x-\eta_p)}$, $Na^- = \frac{N_a}{1+g_a exp[(E_a-E_f)/kT]}$, and $Nd^+ = \frac{N_d}{1+g_d exp([(E_f-E_d)/kT]}$ and where $\eta_n = \frac{E^f-E_c}{kT}$, $\eta_p = \frac{E_v-E_f}{kT}$, $Nc = 2(\frac{2\pi kTM_e}{h^2})^{3/2}$ and $N_v = 2(\frac{2\pi kTM_h}{h^2})^{3/2}$.

However, this equation cannot be solved analytically for E_f, and therefore must be solved numerically. In solving this equation for E_f, we also are able to find N_d^+, N_a^-, n, and p. From these we are able to find the total concentration of ionized impurities, $N_i = N_d^+ + N_a^-$, and the total number of neutral impuruties, $N_n = N_d + N_a - N_i$. There were assumptions used in the mobility calculations in the book, Physical Properties of Semiconductors, such as the assumption of non-degeneracy. With this assumption, the concentration of neutral impurities can be found by $N_n = N_d - N_a - n$. However, when there are more electrons than donors, due to high temperature, this assumption is no longer valid. Thus, it was necessary to use the more general form of

the charge neutrality equation in order to have accurate results over a wide range of conditions.

Note that this program does not take the effect of dislocations on the charge balance equation into account. This is a valid assumption when the dislocation concentration is low.

Additional information can be found in Physical Properties of Semiconductors[1].

Algorithm

The GUI interface (see Figure 1) allows the user to determine the semiconductor type, the temperature to be used, the doping and dislocation concentrations, as well as the ionization energies of the dopants. In addition, it allows the user to calculate over a range of values for up to 2 of these properties, yielding a 2 or 3 dimensional graph. Either the Mobility, Carrier Density, Fermi Energy, or Conductivity may be graphed.

Upon recieving the proper data from the GUI, the program first retrieves data necessary for calculations from tables 2 and 3:

Table 2: Table of Values for Selected Semiconductors

M*/M	$\epsilon_{r(0)}$	$\epsilon_{r(\infty)}$	θ	E_a	C_l	$H_{214}(3/Cl + 4/Ct)$	E_g (eV)	
0.218	9.87	5.80	1044	8.4	2.65e12	18.32e3	3.4	GaN
0.067	12.53	10.9	423	6.3	1.44e12	2.04e3	1.52	GaAs
0.13	11.10	9.11	580	13	1.66e12	1.15e3	2.26	GaP
0.082	12.38	9.55	497	6.8	1.21e12	0.137e3	1.35	InP
0.025	14.54	11.74	337	5.8	1.0e12	0.192e3	.36	InAs
0.0125	17.64	15.75	274	7.2	0.79e12	0.409e3	.18	InSb

It then sets up arrays into which it will store the values it calculates as a function of the parameters chosen by the user. Next, the program begins calculation of the Fermi energy. The Fermi energy calculation requires numerically solving the charge neutrality equation, while simultaneousy numerically integrating the individual parts. The program achieves this by calculating a wide range of Fermi Dirac integrals as a function of x, (which is E/kT) using a very small increment, so that the program could simply look up the

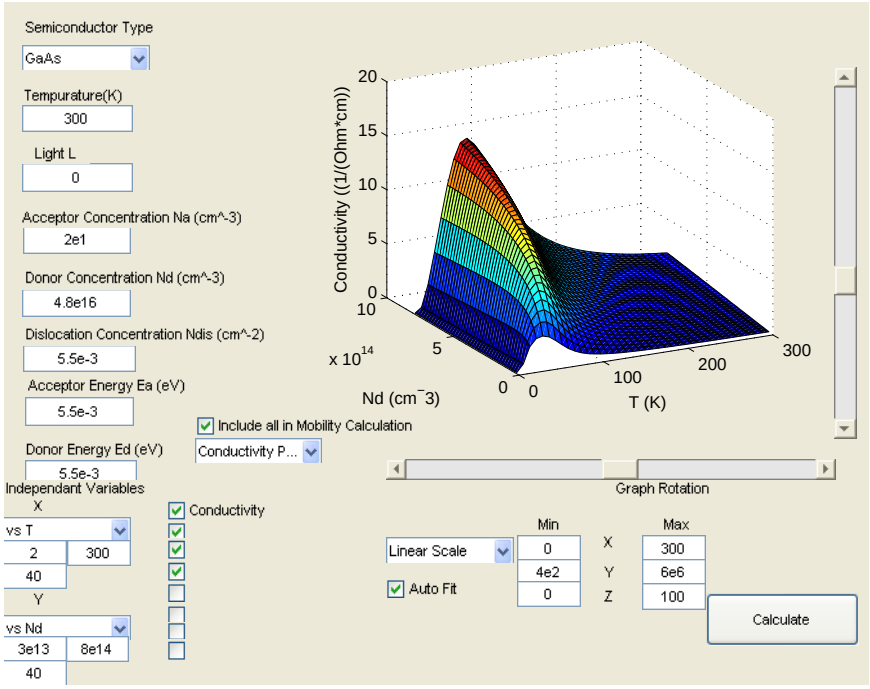

Figure 1: View of the conductivity of GaAs as a function of temperature and donor density.

Table 3: Table of Values for Selected Semiconductors

M_h/M_o	Diec	L_c	$Eg_{(0)}$	a	b	
.8	12	5.185	3.47	9.39e-4	772	GaN
.12	12.5	5.6535	1.519	5.405e-4	204	GaAs
.67	10	5.4506	2.34	6e-4	460	GaP
.4	12.1	5.8688	1.42	4.9e-4	327	InP
.33	12.5	6.0584	.415	2.76e-4	83	InAs
.18	18	6.4788	.24	6.0e-4	500	InSb

answer to a given integral. In numerically solving the equation for the Fermi energy, E_f, the program takes samples of the value of the equation with different values of the fermi energy. It finds the two samples that are the closest to the actual value, one on either side, and repeats, using the newly found smaller interval. This process repeats until a value which is sufficiently close

is found. From the Fermi energy, the carrier statistics n, p, N_d^+, N_a^-, N_n are calculated, and from them the scattering times for the various mechanisms are determined. These are then numerically averaged over the Fermi Dirac distribution and the rates are added together to find the total rate. From this total rate, the mobility is calculated. All the values which are calculated are stored in arrays and sent to the GUI to be plotted, as well as saved to a text file.

Results

Published in Physical Properties of Semiconductors[1] is a graph of the mobility of GaAs as a function of temperature using specific values for the doping etc. When these values are plugged into the program, a close replica of this graph is produced. This has served as a test of the accuracy of the program.

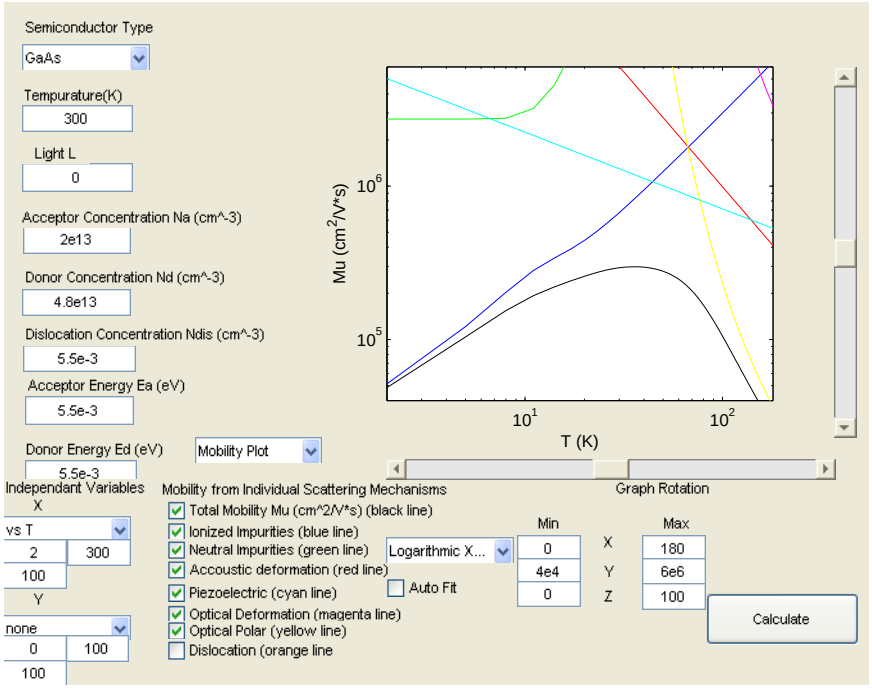

Figure 2: The mobility of GaAs as a function of temperature from 2 K to 180 K, as calculated by the program

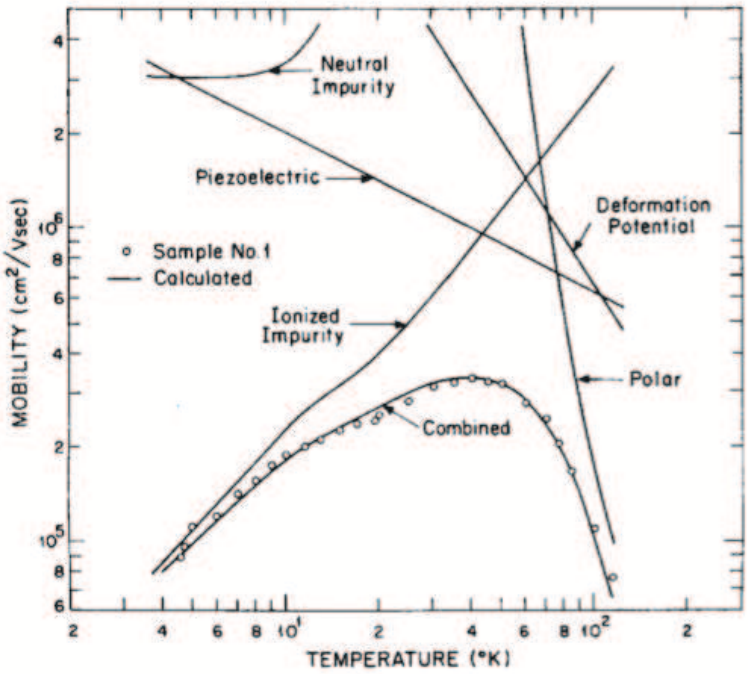

Figure 3: The published[1] plot of Mobility as a function of temperature

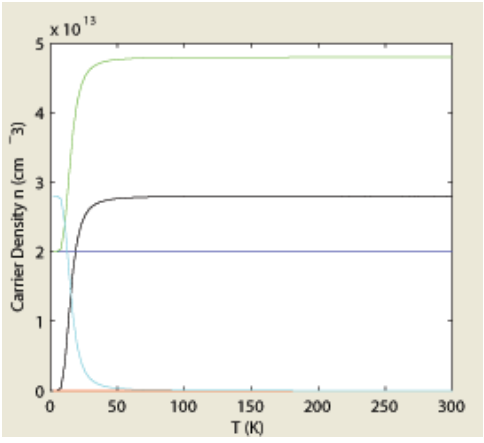

Figure 4: View of the carrier density in same calculation as above figure 2.

One unexpected result was that it appears that under extremly high doping, the mobility is dominated by neutral scattering, since there begin to be large numbers of unionized donors/acceptors. The total mobility agrees with that which was expected, but the mechanism was different, since it was expected that ionized impurity scattering would be the dominant scattering mechanism under these conditions.
This program is currently known to be in use by researchers at Notre Dame as well as two other universities, and is freely down-loadable at the Notre Dame website: www.nd.edu/ demand. It is called Mobility, and it currently calculates all the above quantities (mobilities, carrier statistics, etc) for a range semiconductors. The type of semiconductor and the doping densities are user-defined, and the entire software runs in a easy-to-use GUI mode (see screenshot in Fig 1). Currently, the program is designed to calculate the properties of bulk semiconductors. A newer version is planned which will incorporate heterostructures and will enable the calculation of mobilities and carrier statistics in quantum wells and 2-dimensional electron gases, which form the backbone of the fastest transistors in existence today.

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