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Full Length Research Paper

Comparison of low field electron transport characteristics in Ge and Si semiconductors and effects of neutron energy deposition on their crystal structure

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The transport of minority electrons up to 600 K temperature in silicon and germanium have been investigated, using an iterative approach. Theoretical expressions for electron scattering which take into account the ellipsoidal nature of the conduction band valleys have been incorporated into the model. Minority electron mobility calculations compared favorably with experimental results. The low temperature value of electron mobilty increases significantly with increasing doping concentration. The amount of neutron energy deposition in Si and Ge crystal of different sizes and at different distances from a neutron source has also been evaluated by using MCNP code. Then, the rate of atoms displacement in the crystals has been calculated using NRT Model. The damage to crystal is proportional to the energy deposition of neutron directly. Results show that the number of atoms displacement in the crystal is related to the neutron radiation damage and increased by enlarging of crystal size.

Key words: Minority electrons, ionized imurity scattering, neutron energy, atom displacement.

INTRODUCTION

Minority electron transport is an important parameter in many semiconductor devices, such as, npn bipolar transistors and HBT's to name a few. Knowledge of the transport characteristics and the mechanisms which affect it is important for proper design and simulation of semiconductor devices. Experiments have shown that minority electrons have transport properties which are much different from majority electrons in bulk semiconductors. These properties have also been shown to be dependent on the carrier concentration, electric field, temperature and material properties. For example, Tang et al. (1986) reported a considerable reduction in the zero field mobility of minority electrons in room temperature silicon when the drift field was I00 V/cm. Morohashi and coworkers observed the same reduction at temperatures from 77 to 300 K with electric fields between 25 and 700 V/cm. They attributed this reduction to the electron-hole drag effect which results in a net momentum transfer between the majority and minority carriers.

In this paper, we examine the effect of electron-hole scattering on the transient response and mobility of minority electrons injected into p-doped silicon. Simulations are performed using a lattice temperature of 300 K, a doping concentration of 10^{18} cm^{-3} and an electric field of I0 kV/cm for the transient calculations and a doping concentration of $4.5\times I0^{16}$ cm^{-3} for mobility calculations. Field are applied along the <001> crystallography direction. Semiconductor detectors have high energy resolution and are used commonly for photon and charged particles spectroscopy. Highly pure Ge semiconductors are one of the best semiconductor detectors, which can be made in large size with a very suitable high energy resolution. Although, highly pure Ge is very costly and must be kept at a low temperature, it is widely used for gamma and x-ray spectroscopy (Moglestue, 1993). When this crystal is located in a combined neutron-gamma field, neutron interactions with Ge element induce main crystal damages and distort its energy resolution (Ridley, 1997).

Depending on the energy, neutron interactions with matter may undergo a variety of nuclear processes. The main interactions of fast neutrons are elastic scattering and inelastic scattering, but neutron capture is an important interaction for thermal neutrons (Morkoc, 1999). Improved electron transport properties are one of the main targets in the ongoing study of semiconductor like Ge. The iterative technique has proved valuable for studying non-equilirium carrier transport in a range of semiconductor materials and devices (Di and Brennan, 1991). However, carrier transport modeling of Ge material has only recently begun to receive sustained attention, now that the growth of compounds and alloys is able to produce valuable material for the electronics industry. In this communication, we present iterative calculations of electron drift mobility in low electric field application. We demonstrate the effect of low electric field on the electron transport properties in these materials. The differences in transport properties are analyzed in terms of important material parameters. Most of the calculations have been carried out using a non-parabolic ellipsoidal valley model to describe transport in the conduction band.

However, the simpler and less computationally intensive spherical parabolic band scheme has also been applied, to test the validity of this approximation. The iterative calculations take into account the electron-lattice interaction through polar optical phonon scattering and deformation potential acoustic phonon scattering (treated as an elastic process). Impurity scattering due to ionized and neutral donors is also included, with the latter found to be important at low temperature due to the relatively large donor binding energy which implies considerable carrier freeze-out already at liquid nitrogen tempearure (Gonze et al., 2002). We have also calculated neutron energy deposition on Ge crystal using MCNP code. We then evaluated the damage, the atom displacements rate of Ge crystal using NRT model. It is well known that the main damages of the crystal are atom displacements and neutron activation that varied for different neutron sources (Kohn and Sham, 1965).

SIMULATION METHOD

In principle, the iterative technique give exact numerical prediction of electron mobility in bulk semiconductors. To calculate mobility, we have to solve the Boltzmann equation to get the modified probability distribution function under the action of a steady electric field. Here, we have adopted the iterative technique for solving the Boltzmann transport equation. Under application of a uniform electric field the Boltzmann equation can be written as:

$$(\frac{e}{\hbar})E.\nabla_k f = \oint [s'f'(1-f) - sf(1-f')]dk \quad (1)$$

where $f = f(k)$ and $f' = f(k')$ are the probability distribution functions and $s = s(k,k')$ and $s' = s(k',k)$ are the differential scattering rates. If the electric field is small, we can treat the change from the equilibrium distribution function as a perturbation which is first order in the electric field. The distribution in the presence of a sufficiently small field can be written quite generally as

$$f(k) = f_0(k) + g(k)\cos\theta \quad (2)$$

where $f_0(k)$ is the equilibrium distribution function, θ is the angle between k and E and $g(k)$ is an isotropic function of k, which is proportional to the magnitude of the electric field. In general, contributions to the differential scattering rates come from two types of scattering processes, elastic scattering s_{el}, due to acoustic, impurity, plasmon and piezoelectric phonons, and inelastic scattering s_{inel}, due to polar optic phonons

$$s(k,k') = s_{el}(k,k') + s_{inel}(k,k') \quad (3)$$

Generally, this scattering process cannot be treated within the framework of the relaxation time approximation because of the possibility of the significant energy exchange between the electron and the polar optic modes. In this case, s_{inel} represents transitions from the state characterized by k to k' either by emission $[s_{em}(k,k')]$ or by absorption $[s_{ab}(k,k')]$ of a phonon. The total elastic scattering rate will be the sum of all the different scattering rates which are considered as elastic processes, that is acoustic, piezoelectric, ionized impurity, and electron-plasmon scattering. In the case of polar optic phonon scattering, we have to consider scattering-in rates by phonon emission and absorption as well as scattering-out rates by phonon absorption and emission. Using Boltzmann equation and considering all differential scattering rates, the factor $g(k)$ in the perturbed part of the distribution function $f(k)$ can be given by

$$g(k) = \frac{\frac{-eE}{\hbar}\frac{\partial f_0}{\partial k} + \sum\int g'\cos\varphi[s_{inel}'(1-f) + s_{inel}f)]dk}{\sum\int(1-\cos\varphi)s_{el}dk + \sum\int[s_{inel}(1-f') + s_{inel}'f']dk} \quad (4)$$

Note, the first term in the denominator is simply the momentum relaxation rate for elastic scattering. It is interesting to note that if the initial distribution is chosen to be the equilibrium distribution, for which $g(k)$ is equal to zero, we get the relaxation time approximation result after the first iteration. We have found that convergence can normally be achieved after only a few iterations for small electric fields. Once $g(k)$ has been evaluated to the required accuracy, it is possible to calculate quantities such as the drift mobility which is given by

$$\mu_d = \frac{\hbar}{3m}\frac{\int_0^\infty k^3 \frac{g(k)}{Ed}dk}{\int_0^\infty k^2 f(k)dk} \quad (5)$$

Where d is defined as $1/d = m\nabla_k E/\hbar^2 k$. Subsequently, electron-phonon and electron-impurity mechanisms will be discussed.

ELECTRON SCATTERING MECHANISMS

Phonon scattering

The dominant scattering mechanism of electrons in polar semiconductors like Ge comes from the electron-phonon interaction except at the lowest temperatures. The electron-optical phonon interaction contributes both in the ohmic and non-ohmic mobility and provides the dominant energy-loss mechanism of electrons. First order polarization occurs in connection with the primitive unit cell, characteristic of the longitudinally polarized optical mode. In these materials, the Debye temperature is more than 800 K (Hohenberg and Kohn, 1964), hence polar optical phonon scattering must be considered as an inelastic process. Other phonon scattering processes, that is acoustic and piezoelectric scattering are considered as elastic processes. In polar optic phonon scattering the differential scattering rates for absorption and emission can be written as (Look et al., 1998)

$$S_{op}(k,k') = \frac{\sqrt{2m^*}e^2\omega_{op}}{8\pi\varepsilon_0\hbar}\left(\frac{1}{\varepsilon_\infty}-\frac{1}{\varepsilon_s}\right) \frac{1+2\alpha E'}{\gamma^{1/2}(E)}F_0(E,E')\left\{N_{op},(N_{op}+1)\right\} \quad (6)$$

where ε_s and ε_∞ are dielectric constants in low and high electric fields. N_{op} is the phonon occupation number and the N_{op} and $1+N_{op}$ refer to absorption and emission, respectively. For small electric fields, the phonon population will be very close to equilibrium, so that the average number of phonons is given by the Bose-Einstein distribution function. We have found that after a few iterations, the electron polar optical phonon scattering rate converges and becomes very close to the experimental result (Makino et al., 2001). The energy range involved in the case of scattering by acoustic phonons is from 0 to $2\hbar v_s k$, as the momentum conservation restricts the phonon wave vector q between 0 and 2k , where k is the electron wave vector. Typically the average value of k is on the order of 10^7 cm^{-1} and v_s, the velocity of sound in the medium, is on the order of 10^5 cm/s. Hence, $2\hbar v_s k \approx 1$ meV, which is small compared to the thermal energy. Hence electron-acoustic phonon scattering can be considered as an elastic process. Actually, a long wave length acoustic displacement can not affect the energy since neighboring unit cells move by almost the same amount, only the differential displacement (normally the strain) is of importance. The total differential scattering rate for acoustic phonons can be given by

$$S_{ac}(k,k') = \frac{\sqrt{2}D_{ac}^2(m_t^* m_l^*)^{1/2}K_B T}{\pi\rho v^2\hbar^4} \frac{\sqrt{E(1+\alpha E)}}{(1+2\alpha E)}[(1+\alpha E)^2+1/3(\alpha E)^2] \quad (7)$$

where D_{ac} is the acoustic deformation potential, ρ is the material density and α is the non-parabolicity coefficient. The formula clearly shows that the acoustic scattering increases with temperature.

Impurity scattering

The standard technique for dealing with ionized impurity scattering in semiconductors is the Brook-Herring (BH) technique, Meyer and Bartoli (1981)which is based on two inherent approximations. First, is the first order Born approximation and second is the single ion screening approximation. These two approximations essentially lead to a poor fit to the experimental mobility data. Several attempts have been made to modify the BH technique phenomenologically (Mansour et al., 1991). It has been shown that phase-shift analysis of electron-impurity scattering is the best way to overcome the Born approximation. Departure from the BH prediction of electron mobility is evident at higher electron concentrations. Meyer and Bartoli have provided an analytic treatment based on phase-shift analysis taking into account the multi-ion screening effect and finally been able to overcome both the approximations. All the previous techniques of impurity screening by free electrons in semiconductors were based on the Thomas-Fermi (TF) approximation, which assures that a given impurity should be fully screened.

The breakdown of the single-ion screening formalism becomes prominent in the strong screening regime, where the screening length calculated through TF theory becomes much shorter than the average distance between the impurities and hence neighboring potentials do not overlap significantly. This essentially leads to a physically unreasonable result. In the case of high compensation, the single-ion screening formalism becomes less relevant, because in order to maintain the charge neutrality condition, it would be more difficult for a given number of electrons to screen all the ionized donors separately. In the case of InP, the compensation ratio is usually quite large, and the ratio N_D^+/n is also temperature dependent. Hence, the multi-ion screening correction is very essential in InP. The effective potential of an ionized impurity scattering center is spherically symmetric in nature, so one can use phase-shift analysis to find the differential scattering rate $s(k,k')$ more accurately.

The effective potential $V(r)$ due to an ionized impurity can be expressed as $V(r) = -(Z_l e^2)/(4\pi\varepsilon_0\kappa_0 r)e^{-r/\lambda}$, where Z_l is the charge of the ionized impurity in units of e and λ is the screening length. The standard technique to find out the screening length is the TF approach which is based on single ion screening approximation. In TF one can calculate the charge contribution q_i to the screening of a single ionized donor by an electron of energy E_i and is given by $q_i = -(2e^3\lambda^2/\varepsilon_0\kappa_0 E_i V)$. In the case of multi-ion problem, the TF approach can be generalized to find out the effective charge contribution due to an electron to screen all ionized donors and can be given by $Q_i = -(2e^3 N_D^+\lambda^2/\varepsilon_0\kappa_0 E_i)$. Total screening charge exactly neutralizes the ionized donors, when Q_i is summed over all electronic states

$$\sum_i -\frac{Q_i}{e}f_0(E_i) = N_D^+ \quad (9)$$

For the sufficiently low energy electrons, Q_i can be greater than the electronic charge, which is physically unreasonable. One way to tackle, Norgett and Huck (1997) this problem is to introduce a factor S_i such that

$$S_i(E_i) = \frac{E_i}{\xi} \quad (10)$$

where $\xi = (2N_D^+ c^2\lambda^2/\varepsilon_0 k_0)$, Q_i will be modified to $Q_i' = Q_i S_i$ in Equation 9. For the low energy electrons the contribution will be –e.

Since the total contribution to the screening by the low energy electrons has been effectively decreased, Equation (9) no longer holds.

However, if the screening length λ is more than the average distance between the donors, it is not necessary to insist that each donor be fully screened, only it is required that overall charge neutrality should be preserved. Electrons in the overlap region can provide screening to both the ionized donors. Here we can define a factor p, which would be the fraction of the total charge, which is contained within a sphere of radius R surrounding the donor. Hence Equation (9) will be modified as

$$\sum_i -\frac{Q_i^{"}}{e} f_0(E_i) = pN_D^+ \quad (11)$$

where $Q_i^{"} = pQ_i$. The screening charge requirement will be fulfilled by adjusting the screening length untill Equation (11) is satisfied and is given by

$$\lambda_m^{-2} = \eta \lambda_0^{-2} \quad (12)$$

where λ_m is multi-ion screening length and λ_0 is TF screening length. The differential scattering rate for ionized impurity can be given as

$$S_{ii}(k,k') = \frac{8\pi^3\hbar^3}{m^{*2}V^2} \left|f(X)\right|^2 \delta[E(k') - E(k)] \quad (13)$$

where scattering amplitude $f(X)$ depends on the phase shift δ_l and Legendre polynomial P_l and is given by

$$f(X) = \frac{1}{2ik} \sum_{l=0}^{\infty} (2l+1)(e^{2i\delta_l} - 1) P_l(X) \quad (14)$$

It has already been mentioned that in n-type Ge the activation energy of the donors is quite large, which keeps a large number of donors neutral at low temperatures. Neutral impurity scattering has been dealt with previously using the Erginsoy expression which is based on electron scattering by a hydrogen atom and a scaling of the material parameters. It has been shown that an error as high as 45%, results in the neutral impurity scattering cross section with this simple model. Meyer and Bartoli (1981) have given a phase shift analysis treatment based on the variation results of Schwartz to calculate the neutral impurity cross section, which is applicable for a larger range of electron energy.

THEORY OF ATOM DISPLACEMENT

A primary recoil atom is produced when an energetic incident particle such as fast neutron undergoes a collision with a lattice atom. If the energy transferred to the primary knock-on atom (PKA) is large enough, E >> Ed, (where Ed=30eV; the average energy for one displacement), the PKA can continue the knock-on atom processes, producing secondary recoil atom displacements, which in turn can displace additional atoms. Such an event will result in many collision and displacement events occurring in near proximity of each other. The multiple displacement sequence of collision events is commonly referred to as a collision or displacement cascade. Transferred energy to a PKA with atomic mass number A, when occurred and that a neutron of energy E recoiled, is given by

$$T = \frac{1}{2}\left(v_1^2 + v_0^2 + 2v_1v_0\cos\theta\right) = \frac{4AE}{(A+1)^2} \quad (15)$$

where v_1 is the velocity of scattering atom after collision, and v_0 is the centre of mass velocity. The original model for displacement damage, developed initially for simple metals, is due to Kinchin and Pease, and the standard formulation of it by Norgett and Huck (1997).often referred to as the NRT model, is

$$v(T) = \begin{cases} 0 & T \le E_d \\ 1 & E_d \le T \le 2E_d \\ 0.8T/2E_d & T \ge 2E_d \end{cases} \quad (16)$$

where v(T) is the number of displaced atoms produced by a recoil atom of energy E and damage energy T, and E_d is the average threshold displacement energy for an atom in the crystal lattice. MCNP is a general-purpose Monte Carlo neutron, photon, and electron transport code. It has continuous-energy physics and is time-dependent. The geometry is any arbitrary configuration of three dimensional surfaces. It is used for radiation shielding, criticality safety, nuclear design, aerospace, medical, nonproliferation, radiation dose and other applications by several thousand users worldwide. This code is used to simulate one neutron at a time and records its history. The neutron energy deposition in the crystal has been calculated by tally F6:n for different neutron sources: mono-energy, Am-Be and ^{252}Cf sources.

RESULTS

Figure 1 shows the calculated electron mobility in bulk Ge and Si materials as a function of temperature with free electron concentration of 10^{22} m^{-3} and with the electric field applied along one of the cubic axes. It can be seen from the figure that the electron mobilities at room temperature that we find for Ge is 8000 cm^2/V-s while those for Si is about 12000 cm^2/V-s for an electric field equal to 10^4 Vm^{-1}. The results plotted in Figure 1 indicate that the electron mobility of Ge is lower than Si structure at all temperatures. This is largely due to the higher Γ valley effective mass in the Ge phase. Also, it can be seen that below 100 K, ionized impurity and piezoelectric scattering are the dominant forms of lattice scattering. The approximate $T^{-1/2}$ mobility dependence near 100 K signals the dominance of ionized impurity and piezoelectric scattering.

Figure 2 shows the calculated variation of the electron mobility as a function of free electron concentration for both crystal structures at room temperature. The mobility does not vary monotonically between free electron concentrations of 10^{20} and 10^{23} m^{-3} due to the dependence of electron scattering on free electron concentration, but shows a maximum near 10^{20} m^{-3} for all structures. We have also calculated neutron energy deposition on Ge crystal using MCNP code. The Ge and Si crystals are placed at different distances from point

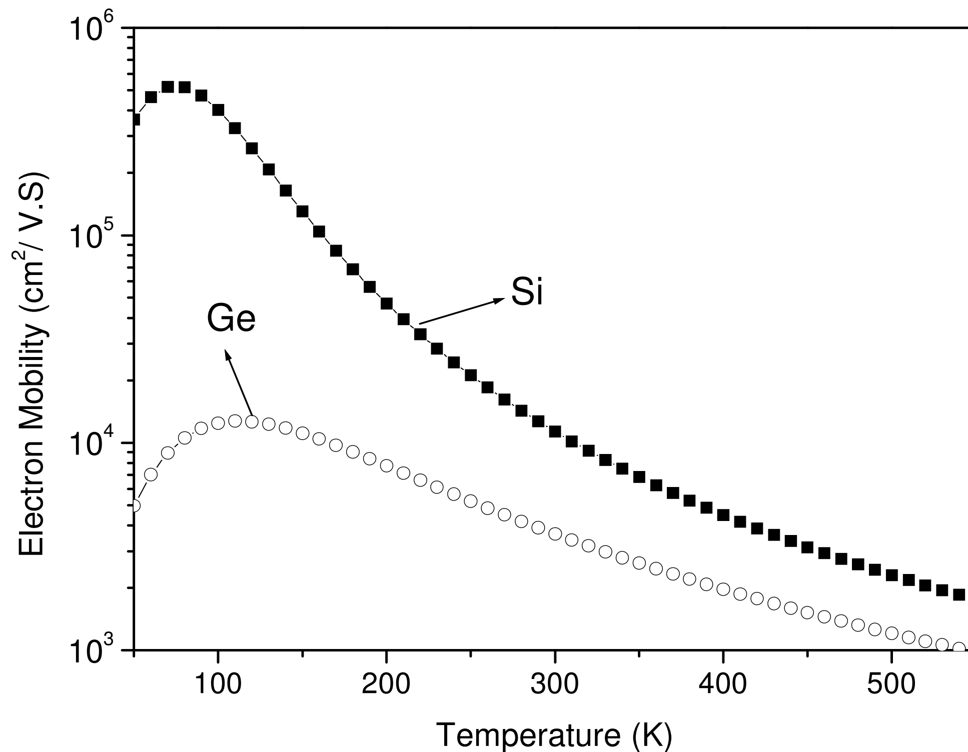


Figure 1. Electron mobility vs temperature of pure intrinsic Ge and Si. Impurity and piezoelectric scattering dominate the data below 100 K.

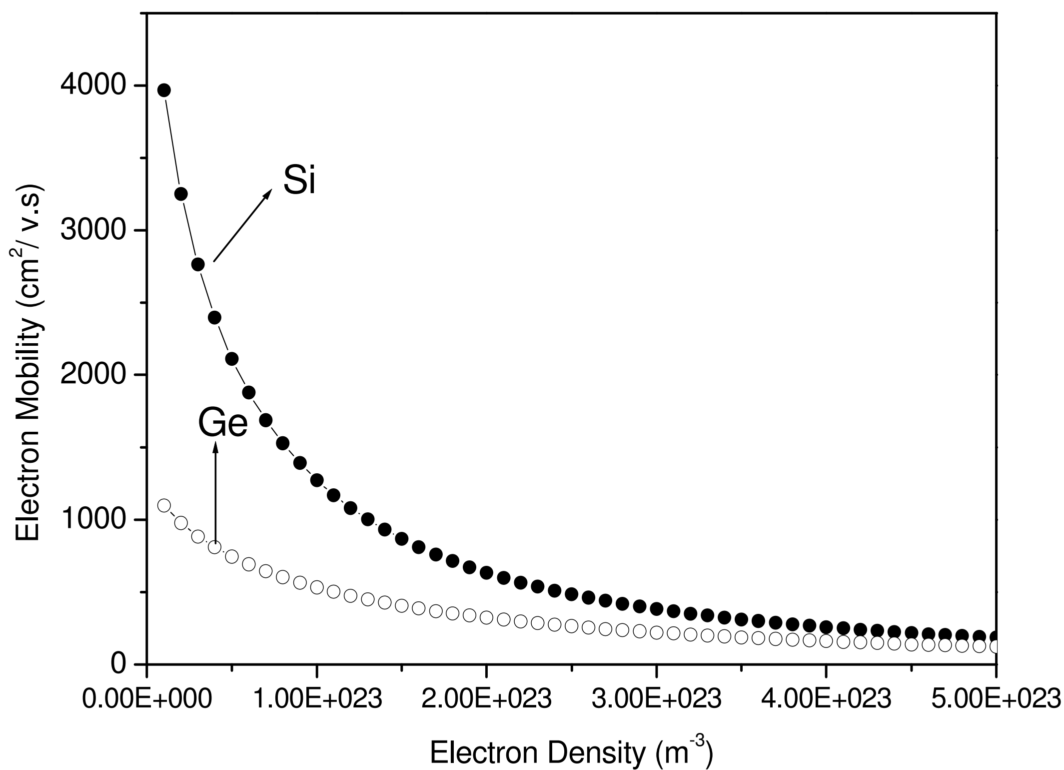
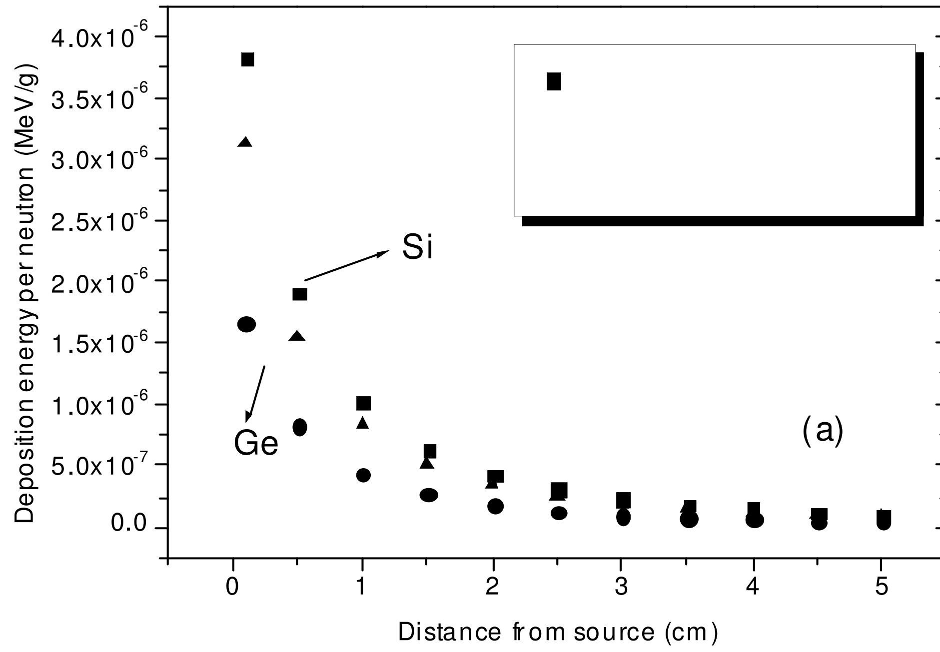


Figure 2. Calculated low-field electron mobility of Ge and Si as a function of different free electron concentration at room temperature.



Deposition energy per neutron (MeV/g)
4.0x10^-6
3.5x10^-6
3.0x10^-6
2.5x10^-6
2.0x10^-6
1.5x10^-6
1.0x10^-6
5.0x10^-7
0.0
0
1
2
3
4
5
Distance from source (cm)
Si
Ge
(a)

```
ERROR: rangecheck
OFFENDING COMMAND: .buildcmap

STACK:

-dictionary-
/WinCharSetFFFF-V2TT9BF4ACCAt
/CMap
-dictionary-
/WinCharSetFFFF-V2TT9BF4ACCAt
```