Calculation of the Fermi Level, Minority Carrier Concentration, Effective Intrinsic Concentration, and Einstein Relation in n- and p-Type Germanium and Silicon

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For the basic understanding of the physics of any semiconductor device an up-to-date knowledge of the various basic parameters is highly essential. Theoretical calculations are made of the Fermi level, minority carrier concentration, effective intrinsic concentration, and Einstein relation in n- and p-type germanium and silicon at 300 K. The reported work is based on the recently developed new transport theory of heavily doped silicon by van Overstraeten et al.. It is found that the results are significantly different from the classical results.


1. Introduction

A lightly doped crystal is theoretically characterized by a perfect periodicity of the lattice. In this case it can be proved that the edges of the conduction and valence bands are well defined and that the density of quantum states obeys a square root dependence on energy. Since the concentration of the impurity atoms is strongly diluted, the wave functions associated with the electrons of the impurity atoms do not overlap. Consequently the energy levels of the impurity atoms are discrete. Under such circumstances the semiconductor crystal is called nondegenerate.

At higher impurity concentrations the impurity atoms are beginning to interact with each other so that the wave functions of their associated electrons are going to overlap. This causes a splitting of the impurity energy levels, which at higher concentrations results in the formation of an impurity band [1]. As the impurity concentration increases, the electron concentration also increases and the interaction between electrons and atomic cores may not be neglected any more. The result of this interaction is a modification of the lattice periodicity and consequently a change in the number of allowed states. Instead of a well defined conduction band edge, we now have a band tail. The equation of this modified conduction band has been calculated in [2, 3]. Therefore, at very high impurity concentrations the semiconductor crystal is called degenerate, and for optimum impurity concentrations it is called semi-degenerate.

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The purpose of the present work is to report the theoretical calculations of the Fermi level, minority carrier concentration, effective intrinsic concentration, and Einstein relation in n- and p-type germanium and silicon at 300 K. For the basic understanding of the physics of any semiconductor device an up-to-date knowledge of the various basic parameters considered here is highly essential. The reported work is based on the recently developed new transport theory of heavily doped semiconductor by van Overstraeten et al. [4]. Heavy doping effects are mainly characterized by considering the dependence of the density of quantum states or impurity states on the impurity concentration. Classical calculations never consider such a dependence. It has been found that our results based on position-dependent band structure phenomena are significantly different from the well-known classical results available until now.

2. Summary of the Basic Approach

The important basic parameters, namely the Fermi level, minority carrier concentration, effective intrinsic concentration, and Einstein relation, have been evaluated using the basic approach. This approach is nothing but to consider heavy doping effects in a quantitative manner. van Overstraeten et al. [4] have recently described this approach in detail by considering the mathematical equations describing the formation of band edge tailing and impurity band after Morgan [1] and Kane [2]. We have also considered the same method to evaluate the parameters considered in the present work in n- and p-type germanium and silicon at 300 K. Therefore, we have omitted the detailed mathematical description of the basic approach and considered the final results and their physical significance. We have considered phosphorus and boron as donor and acceptor impurities, respectively, but the present results can also be considered for arsenic, since its energy level is close to the phosphorus level. All calculations have been done using IBM 370/158 computer.

3. Calculation of the Fermi Level

The Fermi level is a unique important parameter which often occurs at several stages in semiconductor physics. It can be calculated accurately if the energy band structure of a heavily doped semiconductor is well understood. We have calculated the Fermi level by solving numerically the neutrality condition in a doped semiconductor material as

\[ n - p = N_D - N_A, \]  

where \( n \) and \( p \) are electron and hole concentration, respectively, and can be defined in terms of concentration-dependent density of states:

\[ n = \int_{-\infty}^{+\infty} g_n(E) f(E) \, dE, \]  
\[ p = \int_{-\infty}^{+\infty} g_p(E) [1 - f(E)] \, dE, \]

where \( g_n(E) \) and \( g_p(E) \) are respectively the total electron and hole density of states and \( f(E) \) is the Fermi-Dirac distribution function. \( N_D \) and \( N_A \) are the donor and acceptor concentrations, respectively. In Fig. 1a we have plotted the Fermi level dependence on impurity concentration in germanium, while Fig. 1b shows these results in silicon. From Fig. 1 we observe that even at high concentrations the Fermi level is in the band gap (unlike classical results) and is approaching the nondegenerate impurity level.
Fermi Level, Minority Carrier Concentration, and Einstein Relation

Fig. 1. Theoretical plots of the Fermi level \( E_F \) as a function of the net donor and net acceptor concentration considering position-dependent band structure at 300 K a) in germanium, b) in silicon

4. Calculation of the Minority Carrier Concentration

The minority carrier concentration can be calculated easily and accurately if we have a knowledge of the Fermi level position and then use either equation (2) or (3). As discussed earlier, first the \( E_F \) (Fermi level) has been evaluated for a given set of impurity concentrations and then the carrier concentrations have been calculated. Fig. 2a shows the plots of the hole (minority carrier) concentration versus net donor or electron (majority carrier) concentration in germanium and silicon, while Fig. 2b shows the plots of the electron (minority carrier) concentration versus net acceptor or hole (majority carrier) concentration. For comparison we have also plotted the classical results \((p_0 = n_i^0/p_0)\) in Fig. 2, where \( n_i \) is the intrinsic carrier concentration and has been considered after Morin and Maita [5]. From Fig. 2 we observe that our results based on the heavy doping approach are completely different

Fig. 2. a) Theoretical plots of the minority carrier (hole) concentration as a function of the net donor or electron concentration taking into account heavy doping effects at 300 K in germanium (---) and silicon (----). (a) \( N_A = 10^{17} \), (b) \( 10^{18} \), (c) \( 5 \times 10^{18} \), (d) \( 10^{19} \) atoms/cm\(^2\); (e) classical results. b) Theoretical plots of the minority carrier (electron) concentration as a function of the net acceptor or hole concentration taking into account heavy doping effects at 300 K in germanium (---) and silicon (----). (a) \( N_D = 10^{17} \), (b) \( 10^{18} \), (c) \( 5 \times 10^{18} \), (d) \( 10^{19} \) atoms/cm\(^2\); (e) classical results
from classical results, although at low donor and acceptor concentrations they are the same. At high impurity concentration we found a big increase in the minority carrier concentration, while classically it decreases. Classical results also do not find any effect of the compensating impurity on the minority carrier concentration. It must be remarked here that there is not much difference in the results considered in Fig. 2a and b.

5. Calculation of the Effective Intrinsic Concentration

The intrinsic concentration is also one of the important basic parameters. Classically it is only a function of temperature, but we have found its impurity concentration dependence and therefore we call it effective intrinsic concentration \( n_{ie} \). We have calculated this quantity in a usual way: \( n_{ie} = (np)^{1/2} \). Fig. 3a shows the plots of the \( n_{ie} \) versus the net donor concentration in germanium and silicon, while Fig. 3b shows these results, but as a function of the net acceptor concentration. Again we find that there is not much difference in the results plotted in Fig. 3a and b. For comparison, in Fig. 3 we have also shown the classical Morin and Maita's [5] results for the intrinsic concentration. We observe that the heavy doping effects predict a strong impurity concentration dependence of the intrinsic concentration at higher doping levels. For lower donor and acceptor concentrations our results are in quite good agreement with the classical results [5].

6. Calculation of the Einstein Relation

Einstein's [6] work on diffusion about make than seventy years ago led to a fundamental relation between the diffusivity and mobility of charged carriers, which is called Einstein relation. It has been found that Einstein's equation is of great importance in semiconductor physics for the device analysis and design and can be defined in a usual way as

\[
\frac{D}{\mu} = \frac{kT}{q},
\]

Fig. 3. a) Theoretical plots of the effective intrinsic concentration \( n_{ie} \) as a function of the net phosphorus concentration at 300 K in germanium (-----) and silicon (-- - -). (a) \( N_A = 10^{17} \), (b) \( 10^{18} \), (c) \( 5 \times 10^{18} \), (d) \( 10^{19} \) atoms/cm\(^2\); (e) Morin and Maita [5]. b) Theoretical plots of the effective intrinsic concentration \( n_{ie} \) as a function of the net boron concentration at 300 K in germanium (-----) and silicon (-- - -). (a) \( N_D = 10^{17} \), (b) \( 10^{18} \), (c) \( 5 \times 10^{18} \), (d) \( 10^{19} \) atoms/cm\(^2\); (e) Morin and Maita [5]
where $D$ and $\mu$ are the diffusion coefficient and mobility of the charged carrier, respectively, $k$ is the Boltzmann constant, $T$ the absolute temperature, and $q$ the electron charge. Equation (4) is valid only for nondegenerate semiconductors. In the last two decades enough modified relations for the Einstein relation have been emerged for the case of degenerate semiconductors [7 to 16]. Anyhow, the analysis presented in these previous references is based on the assumption of the parabolic density of states function, i.e., no heavy doping effects have been considered. In their recent work on the transport theory of heavily doped silicon van Overstraeten et al. [4] have shown qualitatively that the ratio of the electron diffusivity to mobility in a degenerate semiconductor material can be defined as

$$\frac{D_e}{\mu_e} = \frac{1}{q} \int_{-\infty}^{+\infty} \frac{Q_e(E)}{1 + \exp \left( \frac{(E - E_F)}{kT} \right)} dE.$$

(5)

Similarly a relation for the ratio of the hole diffusivity to mobility ($D_h/\mu_h$) can also be written. The generalized Einstein relation given by (5) can also be written simply in this way as

$$\frac{D_e}{\mu_e} = \frac{kT}{q} \int_{-\infty}^{+\infty} \frac{1}{1 + \exp \left( \frac{(E - E_F)}{kT} \right)} dE$$

$$\int_{-\infty}^{+\infty} \frac{Q_e(E) \exp \left( \frac{(E - E_F)}{kT} \right)}{1 + \exp \left( \frac{(E - E_F)}{kT} \right)^2} dE.$$

(6)

Fig. 4a shows the plots of the electron diffusivity to mobility ratio as a function of net donor concentration in germanium and silicon, evaluating equation (6) numerically. Similarly Fig. 4b shows the plots of the hole diffusivity to mobility ratio as a function of net acceptor concentration in germanium and silicon. From Fig. 4 we observe that the hole diffusivity to mobility ratio is more than the electron diffusivity to mobility ratio. We also find that the carrier diffusivity to mobility ratio is more for the case of germanium as compared to silicon. All the results plotted in Fig. 4

![Fig. 4](image-url)

**Fig. 4. a)** Theoretical plots of the ratio of the electron diffusivity to mobility as a function of the net donor concentration in (1) germanium and (2) silicon at 300 K based on heavy doping approach. $N_A = 10^{17}$ atoms/cm$^3$. **b)** Theoretical plots of the ratio of the hole diffusivity to mobility as a function of the net acceptor concentration in (1) germanium and (2) silicon at 300 K based on heavy doping approach. $N_D = 10^{17}$ atoms/cm$^3$. 

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approach the classical value of $kT/q$ at low impurity concentrations. The asymptotic lines drawn on the results shown in Fig. 4 give an approximate idea of the order of the impurity concentration after which the classical Einstein relation starts failing. It must also be remarked that the impurity concentration dependence of the Einstein relation predicted by Lindholm and Ayers [11], assuming parabolic density of states, is more pronounced than our results plotted in Fig. 4, which is due to the fact that we have considered heavy doping effects.

7. Conclusions

In the present work various important basic parameters of the semiconductor physics have been evaluated theoretically considering position-dependent band structure in the two important elemental semiconductor materials. It is found that our results are quite different from the available classical results. It is hoped that the present concentration dependence of the different parameters may lead to a better explanation of the experimental results; this has been reported recently [17 to 19]. Future efforts using the approach described here are in progress and will be considered in subsequent papers.

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