General Diffusivity-Mobility Relationship for Heavily Doped Semiconductors

Arif Khan[a] and Atanu Das[b,c]

[a] Electrocom Corporation, P.O. Box 60317, Potomac, Maryland 20859-0317, USA
[b] Department of Physics and Techno Physics, Vidyasagar University, Midnapore 721 102, West Bengal, India
[c] Current address: Department of Electronic Engineering, Chang Gung University, Keei-Shan Tao-Yuan, Taiwan, 333, Republic of China

Reprint requests to A. K.; E-mail: a.khan123@yahoo.com or akhan@electrocom-corp.com

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A relationship between diffusivity and mobility in degenerate semiconductors is presented. The relationship is general enough to be applicable to both non-degenerate and degenerate semiconductors. It is suitable for the investigation of the electrical transport in heavily doped semiconductors.

Key words: Semiconductors; Diffusivity, Mobility.

1. Introduction

Carrier mobilities and diffusivities are integral elements of the carrier transport in semiconductors [1]. Both of them contribute to the current [2] and depend on the semiconductor band parameters [2 – 6] such as the energy band gap E_G, the non-parabolicity of the band, and the spin-orbit coupling constants Δ. Both of them determine the electronic and optoelectronic characteristics of devices [7, 8]. They seem to depend also on the doping density, the temperature, the electric field, and the carrier degeneracy [9]. Band gap narrowing and carrier degeneracy compete with each other [10] in determining the electrical performances of semiconductors. Among these semiconductors, narrow band gap [1] and wide band gap [6] semiconductors exhibit special properties. A better understanding of the mobilities and diffusivities of semiconductors is increasingly important as the electronic and optoelectronic devices are increasingly miniaturized and made of heavily doped semiconductor regions. The need to examine their relationship, called diffusivity-mobility relationship (DMR), also becomes very important. Being thermodynamically independent of scattering mechanisms, this relationship is more accurate than the individual relationships between mobility and diffusivity. During the past years a series of investigations [11 – 44] has been carried out addressed to the DMR in semiconductors. For the sake of simplicity, many of these investigations have been confined to carrier non-degeneracy, parabolic band structure, and low temperature limit. Almost all of them are based on the assumption that the spin-orbit coupling constant Δ is either much larger or much smaller than the energy band gap E_G. The scope of their applicability is consequently compromised.

Our objective in the current investigation is to present a general DMR for both lightly and heavily doped semiconductors exhibiting both parabolic and non-parabolic band structures, and involving no approximations as mentioned above. Note that only electrons and holes in bands near the quasi-Fermi level of both n- and p-type n-semiconductors participate in the conduction process of degenerate semiconductors. Also, these semiconductors do have strong interband k.p coupling and strong interband interactions, which result in large spin-splitting Landé factors [1 – 6]. The diffusivity-mobility relationship may, therefore, be important for a critical analysis of the carrier transport in all semiconductor structures, including semiconductor homostructures [45, 46], semiconductor/semiconductor heterostructures [47], metal/semiconductor heterostructures [48 – 51], metal/insulator heterostructures [52, 53], and insulator/semiconductor heterostructures [54 – 58]. For example, a change in the DMR under the influence of doping significantly influences the collector current and current gain of heterojunction bipolar transistors [47]. The DMR, affected by intermetallic diffusion in multilayer ohmic contacts [48, 49] and Schottky contacts [50], causes modifications of the carrier transport, for example, in field-effect transistors. The DMR, influenced by an appropriate choice of the insulator layer, brings about new functionalities of metal-insulator-semiconductor (MIS) transistors [54–58]. The performances of various devices involving semiconductors are indeed modified by the carrier degeneracy and, hence, by the relationship between carrier mobility and diffusivity.

2. Theoretical Model

Under heavy doping the energy spectrum of electrons in n-semiconductors may assume the form [2–6]

$$\frac{\hbar^2 k^2}{2m_{\mathrm{e}}^*}=\frac{E(E+E_{\mathrm{G}})(E+E_{\mathrm{G}}+\Delta)(E_{\mathrm{G}}+2\Delta/3)}{E_{\mathrm{G}}(E_{\mathrm{G}}+\Delta)(E+E_{\mathrm{G}}+2\Delta/3)}, \quad (1)$$

where E is the total electron energy in the conduction band of the semiconductor measured from the conduction band edge E_{C}, m_{e}^* is the effective electron mass at the conduction band edge, h is Planck's constant, and $\hbar = h/2\pi$. If $\Delta \ll E_{\mathrm{G}}$ or $\Delta \gg E_{\mathrm{G}}$, (1) may be simplified to [28]

$$E(1+\beta E)=\frac{\hbar^2 k^2}{2m_{\mathrm{E}}^*}, \quad (2)$$

where $\beta = 1/E_{\mathrm{G}}$. Otherwise, (1) may be rewritten in the form

$$\frac{\hbar^2 k^2}{2m_{\mathrm{e}}^*}=\frac{\lambda_{\mathrm{L}} E(E+E_{\mathrm{G}})(E+E_{\mathrm{G}}+\Delta)}{1+E/(E_{\mathrm{G}}+2\Delta/3)}, \quad (3)$$

where

$$\lambda_{\mathrm{L}}=\frac{3E_{\mathrm{G}}+\Delta}{3E_{\mathrm{G}}(E_{\mathrm{G}}+\Delta)(E_{\mathrm{G}}+2\Delta/3)}, \quad (4)$$

is a constant. The relative values of Δ and E_{G} are quite different for different semiconductors of different energy band gaps. For example, for InSb $\Delta = 0.803$ eV and $E_{\mathrm{G}} = 0.235$ eV; for InAs $\Delta = 0.380$ eV and $E_{\mathrm{G}} = 0.418$ eV; for Si $\Delta = 0.04$ eV and $E_{\mathrm{G}} = 1.12$ eV. This indicates that for semiconductors with medium and large energy band gaps, Δ is generally much smaller than E_{G}. For these semiconductors (4) may reasonably be approximated by

$$\lambda_{\mathrm{L}}=\frac{E_{\mathrm{G}}}{E_{\mathrm{G}}(E_{\mathrm{G}}+\Delta)(E_{\mathrm{G}}+2\Delta/3)}. \quad (5)$$

Following Mohammad [59], a simple and reasonably good approximation for an inverse parameter x may be given by

$$\frac{1}{x}=A_1\exp(-a_1x)+A_2(-a_2x)+A_3\exp(-a_3x), \quad (6)$$

where $A_1 = 15.275406$, $a_1 = 6.430790$, $A_2 = 1.728942$, $a_2 = 1.026638$, $A_3 = 0.378220$, $a_3 = 0.137109$. As shown in [59], this approximation is valid for a wide range of x. Further, it involves exponential terms which can be expanded in a Taylor series without any significant error. We believe that it can be quite useful to simplify the denominator of (3). So, making use of (6) one may obtain

$$\frac{1}{1+E/(E_{\mathrm{G}}+2\Delta/3)}=c_1-c_2E, \quad (7)$$

where

$$c_1=A_1\mathrm{e}^{-a_1}+A_2\mathrm{e}^{-a_2}+A_3\mathrm{e}^{-a_3}, \quad (8a)$$

$$c_2=\frac{a_1A_1\mathrm{e}^{-a_1}+a_2A_2\mathrm{e}^{-a_2}+a_3A_3\mathrm{e}^{-a_3}}{E_{\mathrm{G}}+2\Delta/3}. \quad (8b)$$

With some manipulations, (7) reduces (3) to the form

$$\frac{\hbar^2 k^2}{2m_{\mathrm{e}}^*}=\tau_1E+\tau_2E^2+\tau_3E^3-\tau_4E^4. \quad (9)$$

τ_1, τ_2, τ_3, and τ_4 of (9) are

$$\tau_1=\lambda_{\mathrm{L}}c_1E_{\mathrm{G}}(E_{\mathrm{G}}+\Delta), \quad (10a)$$

$$\tau_2=\lambda_{\mathrm{L}}[c_1(E_{\mathrm{G}}+\Delta)+E_{\mathrm{G}}\{c_1-c_2(E_{\mathrm{G}}+\Delta)\}], \quad (10b)$$

$$\tau_3=\lambda_{\mathrm{L}}\{c_1-c_2(E_{\mathrm{G}}+\Delta)-c_2E_{\mathrm{G}}\}, \quad (10c)$$

$$\tau_4=\lambda_{\mathrm{L}}c_2. \quad (10d)$$

Equation (9) is a power series equation quite amenable for an analytical solution of our problem. Performing differentiation with respect to the energy E, one obtains from (9)

$$k\left(\frac{\mathrm{d}k}{\mathrm{d}k}\right)=\frac{m_{\mathrm{e}}^*}{\hbar^2}\left[\tau_1+2\tau_2E+3\tau_3E^2-4\tau_4E^3\right]. \quad (11)$$

Based on (3) and (7), one may also write

$$k=\sqrt{\frac{2\lambda_{\mathrm{L}}m_{\mathrm{e}}^*}{\hbar^2}}\Big[E^{1/2}(E+E_{\mathrm{G}}+\Delta)^{1/2} \cdot (c_1-c_2E)^{1/2}(E+E_{\mathrm{G}})^{1/2}\Big]. \quad (12)$$

If we define the following parameters:

$$\tau_5 = [\lambda_{\mathrm{L}} c_1 E_{\mathrm{G}} (E_{\mathrm{G}} + \Delta)]^{1/2}, \tag{13a}$$

$$\tau_6 = \frac{1}{2E_{\mathrm{G}}} - \frac{c_2}{2c_1} + \frac{1}{2(E_{\mathrm{G}} + \Delta)}, \tag{13b}$$

$$\tau_7 = \frac{c_2}{4c_1(E_{\mathrm{G}} + \Delta)} + \left\{ \frac{c_2}{2c_1} - \frac{1}{2(E_{\mathrm{G}} + \Delta)} \right\} \left(\frac{1}{2E_{\mathrm{G}}} \right), \tag{13c}$$

$$\tau_8 = \frac{c_2}{8c_1 E_{\mathrm{G}} (E_{\mathrm{G}} + \Delta)}, \tag{13d}$$

we may simplify (12) to

$$k = \sqrt{\frac{2m_{\mathrm{e}}^*}{\hbar^2}} \tau_5 E^{1/2} \left[1 + \tau_6 E - \tau_7 E^2 - \tau_8 E^3 \right]. \tag{14}$$

The density of states function $\rho(E)$ for electrons in the conduction band is

$$\rho(E) = \left(\frac{k}{\pi} \right)^2 \frac{\mathrm{d}k}{\mathrm{d}E}. \tag{15}$$

For semiconductors with unperturbed, but simplified, non-parabolic band structure, $\rho(E)$ reduces readily to

$$\rho(E) = \rho_0 (1 + 2\beta E) E (1 + \beta E)^{1/2} \tag{16}$$

with

$$\rho_0 = \frac{(2m_{\mathrm{e}}^*/h^2)^{3/2}}{2\pi^2}. \tag{17}$$

However, if (11) and (14) are taken into consideration, an expression for the density of states function $\rho(E)$ may easily be obtained. Equation (15) is then given by

$$\rho(E) = 4\pi \left(\frac{2m_{\mathrm{e}}^*}{h^2} \right)^{3/2} \sum_{j=1}^{7} \xi_j E^{j-1/2}, \tag{18}$$

where the ξ_i $(i = 1, 2, \ldots, 7)$ are

$$\xi_1 = \tau_1 \tau_5, \tag{19a}$$

$$\xi_2 = \tau_5 [2\tau_2 + \tau_1 \tau_6], \tag{19b}$$

$$\xi_3 = \tau_5 [3\tau_3 + 2\tau_2 \tau_6 - \tau_1 \tau_7], \tag{19c}$$

$$\xi_4 = \tau_5 [-4\tau_4 + 3\tau_3 \tau_6 - 2\tau_2 \tau_7 - \tau_1 \tau_8], \tag{19d}$$

$$\xi_5 = -\tau_5 [4\tau_4 \tau_6 + 3\tau_3 \tau_7 + 2\tau_2 \tau_8], \tag{19e}$$

$$\xi_6 = -\tau_5 [4\tau_4 \tau_7 + 3\tau_3 \tau_8], \tag{19f}$$

$$\xi_7 = -4\tau_4 \tau_5 \tau_8. \tag{19g}$$

In the framework of (18), the electron carrier concentration in n-semiconductors may be expressed by

$$n_{\mathrm{e}} = 4\pi \left(\frac{2m_{\mathrm{e}}^*}{h^2} \right)^{3/2} \cdot \sum_{j=1}^{7} \xi_j \int_0^{\infty} \left[\frac{E^{j-1/2}}{1 + \exp[(E - E_{\mathrm{fe}})/k_{\mathrm{B}} T]} \right] \mathrm{d}E. \tag{20}$$

Equation (20) can be written in a compact form in terms of the Fermi-Dirac integrals $\Im_j(\eta_{\mathrm{C}})$ of order j. The general formula for these Fermi-Dirac integrals $\Im_j(\eta_{\mathrm{C}})$ of order j is

$$\Im_j(\eta_{\mathrm{C}}) = \frac{1}{\Gamma(j+1)} \int_0^{\infty} \frac{z^j \mathrm{d}z}{1 + \exp(z - \eta_{\mathrm{C}})}, \tag{21}$$

where η_{C} is the reduced Fermi level $\eta_{\mathrm{C}} = E_{\mathrm{fe}}/k_{\mathrm{B}} T$, k_{B} is the Boltzmann constant, and T is the absolute temperature. As shown by Mohammad [10], the reduced Fermi level η_{C} is a function of the carrier concentration n_{e}, which may approximately be equal to the ionized impurity concentration N_{D}. If N_{C} is the effective density of states for electrons in the conduction band [60],

$$N_{\mathrm{C}} = 2 \left[\frac{2\pi m_{\mathrm{e}}^* k_{\mathrm{B}} T}{\hbar^2} \right]^{3/2}, \tag{22}$$

then the relationship between η_{C} and $u_{\mathrm{C}} = N_{\mathrm{D}}/N_{\mathrm{C}}$ is obtained as [10]

$$\eta_{\mathrm{C}} = \log(u_{\mathrm{C}}) + \sum_{\nu=0}^{8} b_\nu u_{\mathrm{C}}^{\nu}. \tag{23}$$

The various parameters b_ν $(\nu = 1, 2, \ldots, 8)$ of (23) are given by: $b_0 = -9.048 \cdot 10^{-4}$, $b_1 = 0.354625$, $b_2 = -4.943417 \cdot 10^{-3}$, $b_3 = 1.194012 \cdot 10^{-4}$, $b_4 = -1.532784 \cdot 10^{-6}$, $b_5 = 1.274608 \cdot 10^{-8}$, $b_6 = 0.6851968 \cdot 10^{-9}$, $b_7 = -7.906237 \cdot 10^{-12}$, $b_8 = 3.0173644 \cdot 10^{-14}$.

Expressing (17) in terms of Fermi-Dirac integrals, (21) is expressed by

$$n_{\mathrm{e}} = N_{\mathrm{C}} \frac{2}{\sqrt{\pi}} \sum_{j=1}^{7} (k_{\mathrm{B}} T)^{j-1} \Gamma(j + \frac{1}{2}) \xi_j \Im_{i-\frac{1}{2}}(\eta_{\mathrm{C}}). \tag{24}$$

If q denotes the electronic charge, the relation between the carrier mobility μ_{e} and the diffusivity D_{e} is

$$\frac{D_{\mathrm{e}}}{\mu_{\mathrm{e}}} = \frac{1}{q} \left(\frac{n_{\mathrm{e}}}{\mathrm{d}n_{\mathrm{e}}/\mathrm{d}E_{\mathrm{fn}}} \right) \tag{25}$$

$$\frac{D_\mathrm{e}}{\mu_\mathrm{e}} = \left(\frac{k_\mathrm{B}T}{q}\right) \frac{\sum_{j=1}^{7}(k_\mathrm{B}T)^{j-1}\Gamma(j+\frac{1}{2})\xi_j\Im_{j-\frac{1}{2}}(\eta_\mathrm{C})}{\sum_{j=1}^{7}(k_\mathrm{B}T)^{j-1}\Gamma(j+\frac{1}{2})\xi_j\Im_{j-\frac{3}{2}}(\eta_\mathrm{C})}. \tag{26}$$

Equation (26) is a closed form solution for the DMR of electrons in semiconductors exhibiting carrier degeneracy and non-parabolic energy band structures. An analogous relationship for the DMR of holes may similarly be derived. An inspection of some earlier reports [18–22] on the DMR for semiconductors under a variety of physical, chemical, structural, magnetic, and electric conditions indicates that they are often very intractable and, hence, difficult to follow and hard to grasp. The fundamental physics is obscured by the complexity of the mathematics. The present relationships and others [14–17] obtained by our approach are remarkably simpler than similar equations by others [18–22]. For degenerate semiconductors with non-parabolic energy bands (26) reduces to the well-known Einstein equation

$$\frac{D_\mathrm{e}}{\mu_\mathrm{e}} = \frac{1}{q}\left(\frac{n_\mathrm{e}}{\mathrm{d}n_\mathrm{e}/\mathrm{d}E_\mathrm{fn}}\right) = \left(\frac{k_\mathrm{B}T}{q}\right)\frac{\Im_{-1/2}(\eta_\mathrm{C})}{\Im_{1/2}(\eta_\mathrm{C})}. \tag{27}$$

For non-degenerate semiconductors with parabolic energy bands (26) reduces to

$$\frac{D_\mathrm{e}}{\mu_\mathrm{e}} = \frac{1}{q}\left(\frac{n_\mathrm{e}}{\mathrm{d}n_\mathrm{e}/\mathrm{d}E_\mathrm{fn}}\right) = \frac{k_\mathrm{B}T}{q}. \tag{28}$$

For the sake of convenience, we call it DMR_0. The normalized DMR is defined as $\mathrm{DMR}/\mathrm{DMR}_0$.

3. Results and Discussions

To our knowledge, this is the most general analytical relationship between μ_e and D_e. An analogous relationship may be obtained for heavily doped p-semiconductors. Both of them should have significant impact on the study of carrier transport in devices. They should also be applicable to both non-degenerate and degenerate semiconductors irrespective of whether Δ is comparable to $\mathrm{E_G}$, $\Delta \gg E_\mathrm{G}$, or $\Delta \ll E_\mathrm{G}$.

To test the applicability of our model we performed numerical calculations for silicon. For these calculations we have made use of (23) and the approximations for the Fermi-Dirac integrals $\Im_j(\eta_\mathrm{C})$ given by [61]

$$\Im_j(\eta_\mathrm{C}) = \eta_\mathrm{C}^{j+1}\sum_{v=1}\frac{g_v}{\eta_\mathrm{C}^{(2v-1)}} \text{ for } \eta_\mathrm{C} > 0, \tag{29a}$$

$$\Im_j(\eta_\mathrm{C}) = \exp(\eta_\mathrm{C}) \text{ for } \eta_\mathrm{C} < 0, \tag{29b}$$

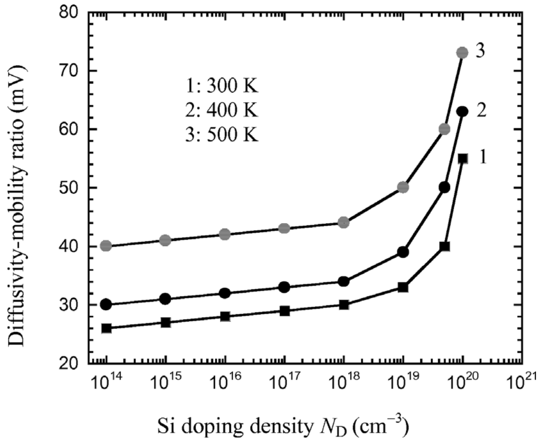

Fig. 1. Variation of the DMR values with the doping concentration for electrons in n-Si. Curves 1, 2, and 3 correspond, respectively, to T = 300 K, 400 K, and 500 K.

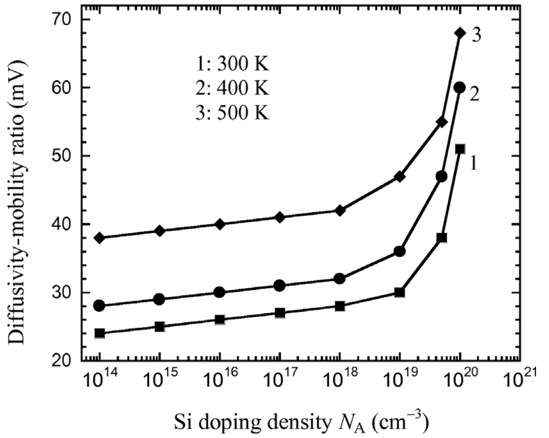

Fig. 2. Variation of the DMR values with the doping concentration for holes in n-Si. Curves 1, 2, and 3 correspond, respectively, to T = 300 K, 400 K, and 500 K.

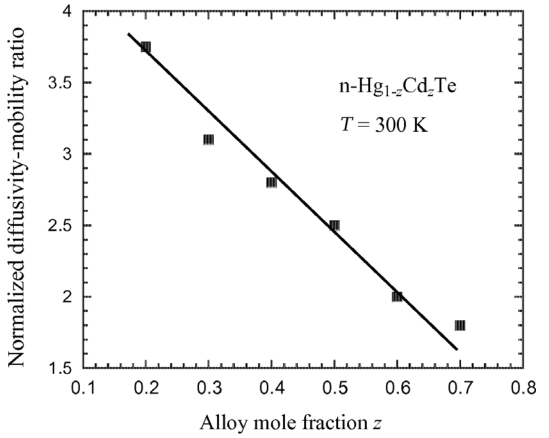

Fig. 3. Variation of the normalized DMR values with alloy composition z of $\mathrm{Hg}_{1-z}\mathrm{Cd}_z\mathrm{Te}$.

where g_v are various parameters given by Van Halen and Pulfrey [61] in their Table 2. Note that there are seven of these parameters, corresponding to each value of j in $\Im_j(\eta_C)$. Note also that, although approximate, (29a) and (29b) provide good correspondences with the exact results for a wide range of the reduced Fermi level η_C. The use of (29a) and (29b) simplifies, at the same time, our calculations for the DMR, carrier concentration, and other related parameters.

We made use of (26) to carry out calculations on the effective electron concentration and the DMR of electrons in n-Si and n-$Hg_{1-z}Cd_zTe$. These semiconductors are very widely used for technology development. The various parameters for n-Si used in our calculations are: $\Delta = 0.044$ eV [62], $E_G = 1.12$ eV [60], and $m_e^* = 0.52$ [60]. Similar parameters for n-$Hg_{1-z}Cd_zTe$ used in the present calculations are [22]:

$$\Delta = 0.63 + 0.24z - 0.27z^2 \text{ eV}, \tag{30}$$

$$\begin{aligned} E_G = \lfloor & -0.302 + 1.93z + 5.35 \cdot 10^{-4} T(1-2z) \\ & - 0.81z^2 + 0.832z^3 \rfloor \text{ eV}, \end{aligned} \tag{31}$$

$$m_e^*(z) = \frac{3\hbar^2 E_G}{4P^2(z)}, \tag{32}$$

$$P^2(z) = \frac{h^2}{2m_e^*}[18 + 3z], \tag{33}$$

where z is the mole fraction of Cd in HgCdTe. The variation of the DMR for electrons in n-Si and for holes in n-Si with doping concentration is shown in Figs. 1 and 2, respectively. One may note that the DMR value increases slowly with doping density until the semiconductor reaches degeneracy at $N_D \approx 10^{19}$ cm^{-3}. In the degeneracy regime, at $N_D > 10^{19}$ cm^{-3}, the DMR value increases very rapidly with increasing doping concentration. Also, the DMR value increases with increasing temperature. The variation of the normalized DMR with the mole fraction z of n-$Hg_{1-z}Cd_zTe$ is shown in Figure 3. For these calculations the doping concentration was chosen to be 10^{18} cm^{-3}. Interestingly, the variation is almost linear, and the higher the mole fraction, the lower is the value of the normalized DMR.

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