Carrier Concentrations in Degenerate Semiconductors Having Band Gap Narrowing

Atanu Das[a] and Arif Khan[b]

[a] Department of Physics and Techno Physics, Vidyasagar University, Midnapore 721 102, West Bengal, India
[b] Electrocom Corporation, P. O. Box 60317, Potomac, Maryland 20859-0317, USA

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

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The density-of-states effective mass approximation and the conduction-band effective mass approximation are employed to formulate carrier concentrations and the diffusivity-mobility relationship (DMR) for heavily doped n-semiconductors exhibiting band gap narrowing. These are very suitable for the investigation of electrical transport also in heavily doped p-semiconductors. Numerical calculations indicate that the DMR depends on a host of parameters including the temperature, carrier degeneracy, and the non-parabolicity of the band structure.

Key words: Degenerate Semiconductors; Band Gap Narrowing; Khane's Model; Diffusivity-Mobility Relationship.

1. Introduction

Carrier diffusivity and mobility are important elements of carrier transport in semiconductors. Both of them contribute to current, and depend on semiconductor band parameters such as the energy band gap E_G, the non-parabolicity of the band, and the spin-orbit coupling constants Δ. They appear to depend also on doping density, temperature, electric field, and carrier degeneracy. Band gap narrowing and carrier degeneracy compete with each other [1] to dictate the electrical performance of semiconductors. Among them, narrow band gap [2] and wide band gap [3] semiconductors exhibit special characteristics. In this investigation our objective is to study the diffusivity-mobility relationship (DMR) of carriers in semiconductors exhibiting a non-parabolic energy band structure, heavy doping and carrier degeneracy. These semiconductors are usually characterized by strong interband k.p coupling and strong interband interactions, which result in a large spin-splitting Landé factor [4]. Also, $E_\mathrm{G} \gg \Delta$ or $E_\mathrm{G} \gg \Delta$ for these semiconductors. The spin-orbit coupling tends to remove the degeneracy of states for semiconductors exhibiting the same wavefunction, but opposite spin. The determination of the effects of spin-orbit coupling on energy bands employing the k.p method simplifies the problem [4]. It indicates that even strong spin-orbit coupling will not remove the spin degeneracy for semiconductors with inversion symmetry.

There are three different approximations used to define the energy-wavevector (E-k) relationship for semiconductors with non-parabolic energy band structures. These are the conduction-band-edge effective mass approximation, the density-of-states effective mass approximation, and the conduction-band effective mass approximation. Among them, the conduction-band-edge effective mass approximation is commonly used to study the transport parameters [5 – 31], such as density-of-states, carrier concentration, diffusivity-mobility relationship, in semiconductors. In this communication we intend to invoke the density-of-states effective mass approximation and the conduction-band effective mass approximation to study carrier concentrations and diffusivity-mobility relationships for heavily doped n-semiconductors exhibiting narrow band gap and band gap narrowing due to heavy doping. Being thermodynamically independent of scattering mechanisms, the diffusivity-mobility relationship is more accurate than the individual relationships for diffusivity and mobility. The relationships may indeed be important for critical analysis of the carrier transport in semiconductor homostructures [32], semiconductor/semiconductor heterostructures [33, 34], metal/semiconductor heterostructures [35 – 38], and insulator/semiconductor heterostructures [39, 40]. The performance of devices involving such semiconductor structures is indeed influenced by carrier degeneracy and the relationship between carrier diffusivity and carrier mobility.

2. Theoretical Model

Under heavy doping the energy spectrum of electrons in n-semiconductors may assume the form [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 $\mathrm{E_c}$, m_e is the effective electron mass at the conduction-band-edge, h is Planck's constant, $\hbar = h/2\pi$, E_G is the energy band gap, and Δ is the spin-orbit coupling constant. If $E_\mathrm{G} \gg \Delta$ or $E_\mathrm{G} \ll \Delta$, (1) may be simplified to [7]

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

where $\beta = 1/E_\mathrm{G}$. The Fermi-Dirac integral of order j is given by

$$\Im_j(\eta_\mathrm{c}) = \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{z^j \mathrm{d}z}{1+\exp(z-\eta_\mathrm{c})}, \quad (3)$$

where the reduced Fermi level η_c is given by

$$k_\mathrm{B} T \eta_\mathrm{c} = E_\mathrm{n} = E_\mathrm{fn} - E_\mathrm{c}, \quad (4)$$

where k_B is the Boltzmann constant, T the absolute temperature, E_fn the Fermi energy, and E_c the conduction-band-edge.

Due to heavy doping there occurs a conduction-band shift by ΔE_c. If we assume that the valence band edge is the origin of the coordinate system, then $E_\mathrm{c} = E_\mathrm{c0} + \Delta E_\mathrm{c}$, where E_c0 is the conduction-band-edge in the absence of heavy doping. If n_e is the carrier concentration, N_d the doping density, h Planck's constant, η_c the reduced Fermi level, and N_c the effective density of states for electrons in the conduction-band, then, for heavily doped semiconductors,

$$n_\mathrm{e} \approx N_\mathrm{d} = N_\mathrm{c} \Im_{1/2}(\eta_\mathrm{c}) \quad (5)$$

with

$$N_\mathrm{c} = 2\left(\frac{2\pi m_\mathrm{e} k_\mathrm{B} T}{h^2}\right)^{3/2}.$$

Let $\lambda = (\mathrm{d}\Delta E_\mathrm{c}/\mathrm{d}N_\mathrm{d})$. Then, making use of (4) and (5), we get

$$\frac{\mathrm{d}n_\mathrm{e}}{\mathrm{d}E_\mathrm{fn}} = N_\mathrm{c}\Im_{-1/2}(\eta_\mathrm{c})\left(\frac{\mathrm{d}\eta_\mathrm{c}}{\mathrm{d}E_\mathrm{fn}}\right) \quad (6)$$

$$= \frac{N_\mathrm{c}\Im_{-1/2}(\eta_\mathrm{c})}{k_\mathrm{B}T - \lambda N_\mathrm{c}\Im_{-1/2}(\eta_\mathrm{c})}. \quad (7)$$

Note that $\Im_{-1/2}(\eta_\mathrm{c})$ of (6) and (7) resulted from the derivation of $\Im_{1/2}(\eta_\mathrm{c})$ with respect to η_c: $\Im_{-1/2}(\eta_\mathrm{c}) = \mathrm{d}\Im_{1/2}(\eta_\mathrm{c})/\mathrm{d}\eta_\mathrm{c}$. In the density of states effective mass m_d approximation, (2) may be rewritten as

$$\frac{\hbar^2 k^2}{2m_\mathrm{d}} = E, \quad (8)$$

where

$$m_\mathrm{d} = m_\mathrm{c}(1+\beta E_\mathrm{n}). \quad (9)$$

Making use of (8), the density of states for electrons in the conduction-band is

$$\delta_\mathrm{e} = \left(\frac{k}{\pi}\right)^2 \frac{\mathrm{d}k}{\mathrm{d}E} \quad (10)$$

$$= 4\pi\left(\frac{2m_\mathrm{d}}{h^2}\right)^{3/2} E^{1/2}. \quad (11)$$

Note that (11) is an approximation of the true density of states obtained by taking only the density near the bottom of the conduction-band for low enough carrier densities and temperatures into account. The effective mass m_d takes into account the equivalent minima in the conduction-band and the effective masses along the principal axes' ellipsoidal energy surface. The carrier concentration n_e is

$$\begin{aligned} n_\mathrm{e} &= N_\mathrm{c}(1+\beta E_\mathrm{n})^{3/2}\Im_{1/2}(\eta_\mathrm{c}) \\ &= N_\mathrm{cd}\Im_{1/2}(\eta_\mathrm{c}), \end{aligned} \quad (12)$$

where

$$N_\mathrm{cd} = N_\mathrm{c}(1+\beta E_\mathrm{n})^{3/2}.$$

For heavily doped n-semiconductors with band gap reduction due to the extension of the conduction-band-edge, but no band gap reduction due to the extension of the valence band edge, the energy band gap E_G is actually $E_\mathrm{G0} - \Delta E_\mathrm{c}$. If we take this into account and define

$$\zeta_1 = (1+\beta E_\mathrm{n})^{3/2}\Im_{-1/2}(\eta_\mathrm{c}), \quad (13a)$$

$$\zeta_2 = \frac{3}{2}\beta\Im_{1/2}(\eta_c)(1+\beta E_n)^{1/2}, \tag{13b}$$

$$\zeta_3 = k_B T + \beta\lambda E_n N_c \Im_{-1/2}(\eta_c), \tag{13c}$$

$$\zeta_4 = 1 - \lambda N_c \Im_{-1/2}(\eta_c)/(k_B T), \tag{13d}$$

then

$$\frac{dn_e}{dE_{fn}} = \frac{N_c(\zeta_1 + \zeta_2\zeta_3)}{\zeta_4 k_B T}. \tag{14}$$

If q is the electronic charge, then the diffusivity-mobility relationship (hereafter referred to as DMR-1) between the carrier diffusivity D_e and the carrier mobility μ_e is

$$\frac{D_e}{\mu_e} = \frac{1}{q}\left(\frac{n_e}{dn_e/dE_{fn}}\right) \tag{15}$$

$$= \left(\frac{k_B T}{q}\right)\left[\frac{\zeta_1\zeta_4}{\zeta_1 + \zeta_2\zeta_3}\right]\frac{\Im_{1/2}(\eta_c)}{\Im_{-1/2}(\eta_c)}. \tag{16}$$

It is interesting to note that the DMR-1, (16) reduces to the well-known diffusivity-mobility relationship for heavily doped degenerate semiconductors if $[\zeta_1\zeta_4/(\zeta_1 + \zeta_2\zeta_3)] \to 1$.

According to the density-of-states effective mass approximation m_s, (2) may be written as

$$\frac{\hbar^2}{m_0}\left(\frac{1}{k}\frac{dk}{dE}\right)^{-1} = \frac{m_c}{m_0}(1 + 2\beta E_n) = \frac{m_s}{m_0}, \tag{17}$$

where m_0 is the free electron mass, and

$$m_s = m_c(1 + 2\beta E_n). \tag{18}$$

Based on (17) the density of states for electrons in the conduction-band is

$$\begin{aligned}\delta_e &= \left(\frac{k}{\pi}\right)^2\frac{dk}{dE}\\ &= 4\pi\left(\frac{2m_c}{h^2}\right)^{3/2}(1 + 2\beta E_n)E^{1/2}\left(1 + \frac{\beta E}{2}\right).\end{aligned} \tag{19}$$

Equation (19) is based on a first-order Taylor's series expansion of $(1+\beta E)^{1/2}$. Higher-order terms can be included in the expansion series without much complication if it is called for higher accuracy of the end results. The electron concentration may be given by

$$\begin{aligned}n_e &= 4\pi\left(\frac{2m_c}{h^2}\right)^{3/2}\\ &\cdot(1 + 2\beta E_n)\int_0^\infty \frac{E^{1/2}(1+\beta E/2)dE}{1+\exp[(E - E_{fn})/k_B T]}\end{aligned} \tag{20}$$

$$= N_{ce}\left[\Im_{1/2}(\eta_c) + \frac{3}{4}\beta k_B T \Im_{3/2}(\eta_c)\right] = N_{ce}\xi_1 \tag{21}$$

with

$$\xi_1 = \Im_{1/2}(\eta_c) + \frac{3}{4}\beta k_B T \Im_{3/2}(\eta_c), \tag{22a}$$

$$N_{ce} = N_c(1 + 2\beta E_n). \tag{22b}$$

As apparent from (21), the carrier concentration in the density-of-states effective mass approximation takes non-parabolicity of the band and the carrier degeneracy into consideration. Fermi-Dirac integrals of only order 1/2 and 3/2 are included in the formula. Taking higher-order terms into account in the expansion of $(1+\beta E)^{1/2}$, Fermi-Dirac integrals of higher orders 5/2, 7/2, etc. would also be involved in this formulation. Following the same procedure as for (14) we get

$$\frac{dn_e}{dE_{fn}} = \frac{N_c[2\beta\xi_1\xi_2 + (1+2\beta E_n)(\xi_3 + \xi_4)]}{k_B T \zeta_4}, \tag{23}$$

where

$$\xi_2 = k_B T + \beta\lambda E_n N_c \Im_{-1/2}(\eta_c), \tag{24a}$$

$$\xi_3 = \Im_{-1/2}(\eta_c) + \frac{3}{4}\beta k_B T \Im_{1/2}(\eta_c), \tag{24b}$$

$$\xi_4 = \frac{3}{4}k_B T \lambda \beta^2 N_c \Im_{3/2}(\eta_c)\Im_{-1/2}(\eta_c). \tag{24c}$$

The Einstein relation between the carrier mobility μ_e and the diffusivity D_e (hereafter referred to as DMR-2) is

$$\frac{D_e}{\mu_e} = \frac{1}{q}\left(\frac{n_e}{dn_e/dE_{fn}}\right) \tag{25}$$

$$= \left(\frac{k_B T}{q}\right)\frac{(1+2\beta E_n)\xi_1\zeta_4}{2\beta\xi_1\xi_2 + (1+2\beta E_n)(\xi_3+\xi_4)}. \tag{26}$$

3. Results and Discussion

We have developed analytical relationships between μ_e and D_e for n-semiconductors based on the density-of-states effective mass approximation and the conduction-band effective mass approximation. 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. Because of

j	η_c Range	a_0	a_1	a_2	a_3
$1/2$	$0 \leq \eta_c \leq 20$	-1.7557	1.3890	$9.9702 \cdot 10^{-2}$	$-1.7557 \cdot 10^{-4}$
$-1/2$	$0 \leq \eta_c \leq 10$	1.0281	$8.8135 \cdot 10^{-1}$	$-4.9367 \cdot 10^{-2}$	$1.3865 \cdot 10^{-3}$
$-1/2$	$10 \leq \eta_c \leq 20$	2.2393	$5.1008 \cdot 10^{-1}$	$-1.2083 \cdot 10^{-2}$	$1.6597 \cdot 10^{-4}$

Table 1. List of parameters for the analytical expression of the Fermi-Dirac integral $\Im_j(\eta_c)$.

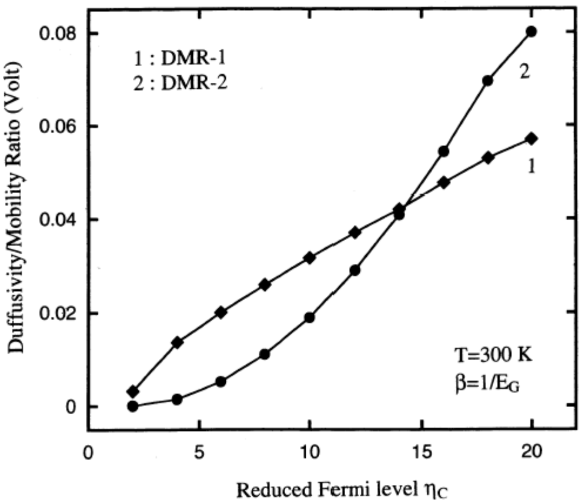

Fig. 1. Variation of DMR-1 and DMR-2 with the reduced Fermi level η_c.

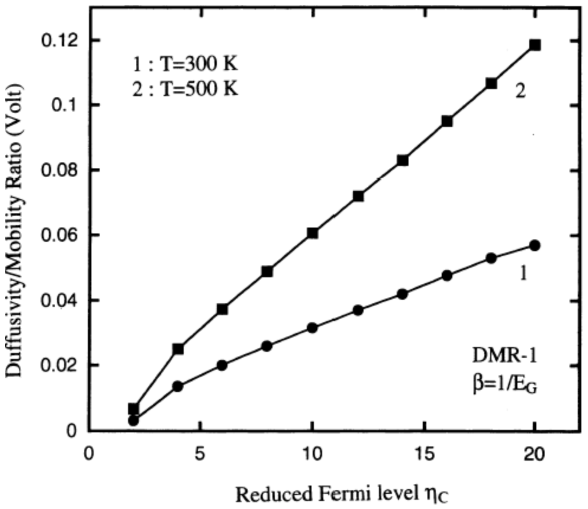

Fig. 2. Dependence of DMR-1 on the temperature T.

the assumption that the spin-orbit splitting constant Δ is either much larger or much smaller than the energy band gap E_G, they would be more applicable to narrow band gap semiconductors, such as InSb and InAs [2], and wide band gap semiconductors, such as BN and AlN [3], than to semiconductors exhibiting neither wide nor narrow energy band gaps [33]. Nevertheless, they provide a framework for the analysis of carrier concentrations and diffusivity-mobility relationships for heavily doped narrow band gap and wide band gap semiconductors exhibiting band gap narrowing and carrier degeneracy under density-of-states effective mass approximation and conduction-band effective mass approximation.

In order to carry out some numerical calculations on the carrier concentrations and the diffusivity-mobility relationships, we made use of an analytical approximation of $\Im_j(\eta_c)$ given by [41]

$$\Im_j(\eta_c) = a_0 + a_1\eta_c + a_2\eta_c^2 + a_3\eta_c^3, \tag{27}$$

where a_0, a_1, a_2 and a_3 are various parameters listed in Table 1. InAs was chosen to be the test system. Various parameters for InAs as used for the calculations are: energy band gap $E_G = 0.36$ eV, temperature $T = 300$ K, effective electron mass $m_e = 0.023$, dielectric constant $\varepsilon = 14.6$. The numerical calculations require also the knowledge of $\lambda = (\mathrm{d}\Delta E_c/\mathrm{d}N_d)$, which is different for different semiconductors. To a first approximation one may assume that the downward shift ΔE_c of the conduction-band-edge E_c is equal to the band gap narrowing ΔE_G, and that the impurities were fully ionized, producing one free electron by each dopant atom. A number of approximations are available for this band gap narrowing ΔE_G. One of them, due to Rogachev and Sablina [42] and due to Zverev et al. [43], is

$$\Delta E_G = a_G \left(\frac{N_d}{10^{24}}\right)^{1/3} \text{ eV}, \tag{28}$$

where a_G is a fitting parameter with different values for different parameters: $a_G = 3.00$ for n-Si, 1.5 for n-Ge, 1.6 for p-GaAs, 2.25 for n-InGaAs, and 1.2 for n-InAs. Equation (28) was used to calculate λ.

The variation of DMR-1 and DMR-2 as a function of the reduced Fermi level η_c is shown in Figure 1. The reduced Fermi level depicts the influence of heavy doping. It is higher for heavier doping. Figure 1 indicates that both DMR-1 and DMR-2 increase with increasing reduced Fermi level. Interestingly, DMR-2 is smaller than DMR-1 until the reduced Fermi level is about 15. But DMR-2 is larger than DMR-1 for the

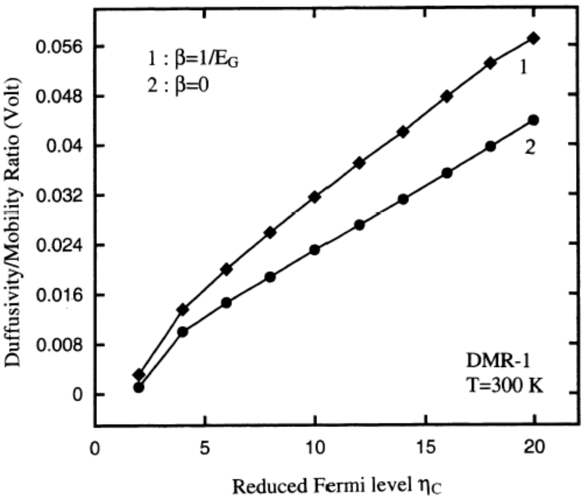

Fig. 3. Dependence of DMR-1 on the non-parabolicity parameter β.

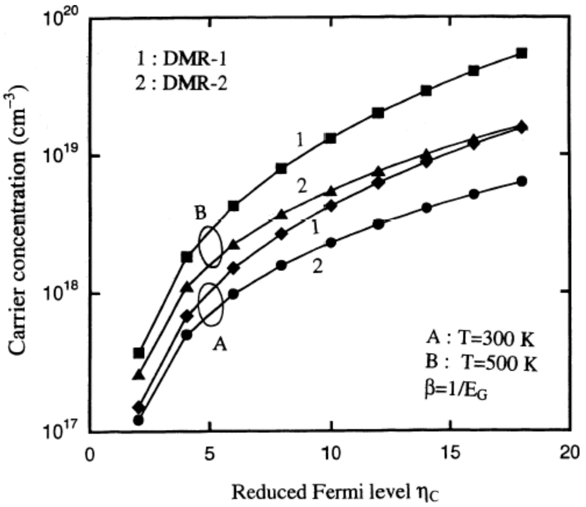

Fig. 4. Variation of the carrier concentration with the reduced Fermi level for two different-density-of-states approximations, and for $T = 300$ K and 500 K, respectively.

reduced Fermi level exceeding 15. The dependence of the DMR-1 on the temperature is shown in Figure 2. One can see that indeed DMR-1 is very sensitive to the temperature, and that, for example, for $\eta_c = 20$, the DMR-1 value at 500 K is almost twice the DMR-1 value at 300 K. Although not shown graphically, we found that DMR-2 is equally sensitive to the temperature as DMR-1. For example, for $\eta_c =$ 20, the DMR-2 value at 500 K is 0.163 eV, while that at 300 K is 0.095 eV. This dependence stems primarily from the presence of k_BT in both DMR-1 and DMR-2. The dependence of DMR-1 on the non-parabolicity parameter β is shown in Figure 3. This figure shows that indeed the diffusivity-mobility relation depends strongly on the non-parabolicity parameter β. The diffusivity D_e, as compared to the mobility μ_e, increases gradually with increasing reduced Fermi level η_c and the non-parabolicity parameter β. The variation of the carrier concentration with the reduced Fermi level η_c for the density of states approximation (APPROX-1) representing DMR-1 and the density of states approximation (APPROX-2) representing DMR-2 is shown in Figure 4. As is evident from this figure, for a certain temperature T, the carrier concentration is higher for APPROX-1 than for APPROX-2. This carrier concentration increases rapidly with η_c for $\eta_c \leq 6$. It increases slowly with η_c for $\eta_c \geq 6$.

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