The Diffusivity-Mobility Relationship of Heavily Doped Semiconductors Exhibiting a Non-Parabolic Band Structure and Bandgap Narrowing

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A relationship between the mobility and diffusivity of semiconductors exhibiting bandgap narrowing has been presented. The relationship is general and applicable to both non-degenerate and degenerate semiconductors under an applied bias. It is suitable for the investigation of the electrical transport in heavily doped semiconductors.

Key words: Diffusivity-Mobility Relationship; Bandgap Narrowing; Heavily Doped Semiconductors.

1. Introduction

Heavy doping and carrier degeneracy are keys to the realization of important properties of semiconductors [1]. They are especially instrumental in dictating the characteristics of ohmic contacts [2 – 4] and Schottky contacts [5]. In fact, because of this, the performance of semiconductor devices at the device terminals and the speed of the operation of switching transistors are significantly influenced by the degree of doping and carrier degeneracy in various regions of the semiconductors. Diffusivity-mobility relationship (DMR) for electrons and holes in these semiconductors is a very useful parameter. It allows the determination of the carrier diffusity D_e from known experimental values of carrier mobility μ_e. A convenient way to understand the influence of carrier degeneracy on the performance and the operation of semiconductor devices is to take advantage of a DMR that takes bandgap narrowing under heavy doping into consideration.

During the past years a series of investigations [6 – 19] have been carried out to investigate the relationship between the carrier diffusivity and the carrier mobility in semiconductors. The two-band Kane model has been widely used for these investigations. If E is the carrier energy as measured in the vertically upward direction from the band edge of a semiconductor, and E_G is the energy bandgap of this semiconductor, then the two-band Kane model is based on the assumption that $E/E_G \ll 1$. Being a mechanism that is thermodynamically independent of any scattering, this relationship is more accurate than the individual relationships for mobility and diffusivity. The scope of their applicability is consequently drastically reduced. Our objective in this investigation is to present a modified relationship for the DMR that takes into account carrier degeneracy and bandgap narrowing, and is applicable to both wide bandgap semiconductors [20] and narrow bandgap semiconductors [21]. Such a relationship would be important for critical analysis of the carrier transport in semiconductor homostructures [22], semiconductor/semiconductor heterostructures [23], and insulator/semiconductor heterostructures [24 – 26].

2. Theoretical Model

The performance of devices involving non-parabolic band structures is significantly influenced by carrier degeneracy. Under heavy doping the energy spectrum for electrons in n-semiconductors may be [27]

$$\frac{E(E+E_G)(E+E_G+\Delta)(E_G+2\Delta/3)}{E_G(E_G+\Delta)(E+E_G+2\Delta/3)} = \frac{\hbar^2 k^2}{2m_e^*}, \quad (1)$$

where m_e^* is the effective electron mass at the conduction band edge, Δ is the spin-orbit splitting constant, h is Planck's constant, and $\hbar = h/2\pi$. If $\Delta \ll E_G$ or $\Delta \gg E_G$, which is true for many wide bandgap and narrow bandgap semiconductors, (1) may be simplified as [6 – 9]

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

with $\beta = 1/E_G$. Equation (2) is the two-band Kane model. Making use of (2), the density of states function $\rho(E)$ may be given by [6–9]

$$\rho(E) = \left(\frac{k}{\pi}\right)^2 \frac{dk}{dE}, \tag{3}$$

$$\rho(E) = \frac{1}{2\pi^2}\left(\frac{2m_e^*}{\hbar^2}\right)^{\frac{3}{2}}[E^{1/2}(1+\beta E)^{1/2}(1+2\beta E)], \tag{4}$$

and the electron density may be given by

$$n = 4\pi\left(\frac{2m_e^*}{\hbar^2}\right)^{\frac{3}{2}}$$
$$\cdot \int_0^\infty \frac{E^{1/2}(1+\beta E)^{1/2}(1+2\beta E)E^{1/2}dE}{1+\exp[(E-E_{fn})/k_BT]}, \tag{5}$$

$$n = 2\left(\frac{2\pi m_e^* k_B T}{h^2}\right)^{\frac{3}{2}}\big[\Im_{1/2}(\eta) + t_1\Im_{3/2}(\eta)$$
$$+ t_2\Im_{5/2}(\eta) + t_3\Im_{7/2}(\eta)\big], \tag{6}$$

where E_{fn} is the quasi Fermi energy,

$$t_0 = 1, \quad t_1 = \frac{15}{4}\beta k_B T, \quad t_2 = \frac{105}{32}\beta^2 k_2^2 T^2,$$
$$t_3 = \frac{315}{128}\beta^3 k_2^3 T^3, \tag{7}$$

and $\Im_j(\eta)$ is the Fermi-Dirac integral of order j:

$$\Im_j(\eta_C) = \frac{1}{\Gamma(j+1)}\int_0^\infty \frac{z^j dz}{1+\exp(z-\eta_C)}. \tag{8}$$

It may be noted that (6) thus obtained takes non-parabolicity of the band structure of heavily doped semiconductors, but not the bandgap narrowing, into account. With this bandgap narrowing the conduction band edge E_c is actually $E_{co} + \Delta E_c$, where E_{co} is the conduction band edge without bandgap narrowing, and ΔE_c is the extension of the conduction band edge due to bandgap narrowing [28]. It may simply be written as $A\Delta E_G$, where A is the asymmetric parameter and ΔE_G is the total energy bandgap narrowing [28]. Equation (6) may consequently be modified to

$$n = N_c\big[\Im_{1/2}(\eta_0 + \Delta\eta) + t_1\Im_{3/2}(\eta_0 + \Delta\eta)$$
$$+ t_2\Im_{5/2}(\eta_0 + \Delta\eta) + t_3\Im_{7/2}(\eta_0 + \Delta\eta) + \ldots\big], \tag{9}$$

where N_c, the effective density of states for electrons in the conduction, is given by

$$N_c = 2\left(\frac{2\pi m_e^* k_B T}{h^2}\right)^{3/2}. \tag{10}$$

Making use of Taylor's series expansion, one may obtain

$$\Im_j(\eta_0 + \Delta\eta) = \Im_j(\eta_0) + \Delta\eta\Im_{j-1}(\eta_0)$$
$$+ \frac{(\Delta\eta)^2}{2}\Im_{j-2}(\eta_0) + \frac{(\Delta\eta)^3}{6}\Im_{j-3}(\eta_0) + \ldots \tag{11}$$

with [29]

$$\Delta\eta = \frac{A\Delta E_G}{k_B T} = \left(\frac{3Aq^2}{16k_B T\pi\varepsilon}\right)\frac{1}{a_s}, \tag{12}$$

where q is the electronic charge, k_B is the Boltzmann constant, T the absolute temperature, ε the dielectric constant of the semiconductor, and a_s is the screening length, which is given by [29]

$$\frac{1}{a_s} = \left(\frac{\sqrt{\pi}\varepsilon k_B T}{2q^2 N_c}\right)\sqrt{\Im_{-1/2}(\eta_0)}. \tag{13}$$

Equations (12) and (13) yield

$$\Delta\eta = \lambda\sqrt{\Im_{-1/2}(eta_0)} \tag{14}$$

with

$$\lambda = \frac{3A}{32\sqrt{\pi}N_c}. \tag{15}$$

In the framework of (10)–(15) and with

$$w = \lambda[\Im_{-1/2}(\eta_0)]^{1/2}, \tag{16}$$

(9) may be rewritten as

$$n = N_c\sum_{j=1}t_{j-1}\big\{\Im_{j-1/2}(\eta_0) + w\Im_{j-3/2}(\eta_0)$$
$$+ (w^2/2)\Im_{j-5/2}(\eta_0) + (w^2/6)\Im_{j-7/2}(\eta_0)\big\}. \tag{17}$$

Note that, for $\lambda = 0$, (17) reduces to the equation for semiconductors with a non-parabolic energy band structure exhibiting no bandgap narrowing. For $\lambda = 0$ and $t_j = 0$ ($j = 1, 2, 3, 4, \ldots$), it reduces to that for semiconductors with a parabolic energy band structure. Employing (17), the Einstein relationship between the diffusivity D_e and the mobility μ_e is

$$\frac{D_e}{\mu_e} = \frac{n}{q}\left(\frac{dE_{fn}}{dn}\right), \tag{18}$$

$$\frac{D_e}{\mu_e} = \left(\frac{k_B T}{q}\right) \frac{\sum\limits_{j=1} t_{j-1}\left\{\Im_{j-1/2}(\eta_0) + w\Im_{j-3/2}(\eta_0) + (w^2/2)\Im_{j-5/2}(\eta_0) + (w^3/6)\Im_{j-7/2}(\eta_0)\right\}}{\sum\limits_{j=0} t_j\left\{\Im_{j-1/2}(\eta_0) + w\Im_{j-3/2}(\eta_0) + (w^2/2)\Im_{j-5/2}(\eta_0) + (w^3/6)\Im_{j-7/2}(\eta_0)\right\}}. \tag{19}$$

3. Results and Discussion

A relationship between the carrier diffusivity and the carrier mobility in heavily doped n-type semiconductors with non-parabolic energy band and bandgap narrowing has been developed. For this development it was assumed that the free carrier concentration n is identical to the doping concentration N_d. The relationship depends, to a large extent, on the validity of Taylor's series expansion (11). At room temperature $T = 300$ K, $k_B T \approx 25$ meV. ΔE_G is insignificantly small for non-degenerate semiconductors. However, it may exceed 100 meV for some degenerate semiconductors. This means that Taylor's series expansion (11) for degenerate semiconductors is valid only when the asymmetric parameter A is well below unity, and $\Delta\eta \ll \eta_0$. For most of the semiconductors it is indeed the case as $\Delta E_c \approx \Delta E_G$.

Following a procedure analogous to (19) a similar formula may also be obtained for p-type semiconductors. Our formula (19) is important for the study of transport properties. It is quite general and applicable to both non-degenerate and degenerate semiconductors. In the absence of bandgap narrowing it reduces to

$$\frac{D_e}{\mu_e} = \left(\frac{k_B T}{q}\right) \frac{\sum\limits_{j=1} t_{j-1}\{\Im_{j-1/2}(\eta_0)\}}{\sum\limits_{j=0} t_j\{\Im_{j-1/2}(\eta_0)\}}. \tag{20}$$

Generally bandgap narrowing does not take place in the absence of carrier degeneracy. So, the DMR D_e/μ_e may not be obtained for non-degenerate semiconductors exhibiting bandgap narrowing. In the absence of non-parabolicity and bandgap narrowing, (19) reduces to

$$\frac{D_e}{\mu_e} = \left(\frac{k_B T}{q}\right) \frac{\Im_{j-1/2}(\eta_0)}{\Im_{1/2}(\eta_0)}. \tag{21}$$

In the absence of carrier degeneracy, non-parabolicity and bandgap narrowing, (19) reduces to

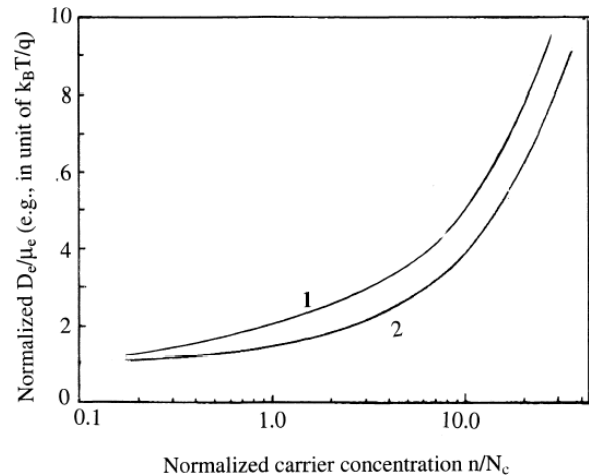$$\frac{D_e}{\mu_e} = \left(\frac{k_B T}{q}\right). \tag{22}$$

Fig. 1. Variation of the normalized diffusivity-mobility relationship (DMR) D_e/μ_e with the normalized carrier concentration (n/N_c) in germanium at 300 K with (curve 1) and without (curve 2) bandgap narrowing.

Equation (22) is the conventional diffusivity-mobility relationship. It may be noted from (22) that, for all non-degenerate semiconductors having parabolic energy band structure, the DMR D_e/μ_e is the same at any given temperature.

The dependence of the normalized DMR D_e/μ_e on the normalized carrier concentration in germanium at 300 K was calculated from (19). It is shown in Figure 1. The bandgap narrowing, the effective electron mass, and the dielectric constant for the semiconductor were obtained from [1]. The asymmetric parameter A was chosen to be 0.1. One may note that the variation in the DMR D_e/μ_e with the normalized carrier concentration remains insensitive to the carrier concentration until it reaches about 5. However, it increases rapidly with increasing carrier concentration for $n/N_c \geq 5$. There are two (D_e/μ_e) vs. (n/N_c) curves. Among them, curve 1 takes the bandgap narrowing effect into account; curve 2 does not take this effect into account. A comparison of the two indicates that bandgap narrowing does indeed influence the DMR.

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