Diffusivity-Mobility Relationship for Heavily Doped Semiconductors with Non-Uniform Band Structures

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Z. Naturforsch. **65a,** 882 – 886 (2010); received April 27, 2009 / revised February 22, 2010

A general relationship between the diffusivity and the mobility in degenerate semiconductors with non-uniform energy band structures has been presented. The relationship is general enough to be applicable to both non-degenerate and degenerate semiconductors. It is suitable for the study of electrical transport in heavily doped semiconductors and semiconductor devices.

Key words: Semiconductors; Heavy Doping; Diffusivity-Mobility Relationship.

1. Introduction and Background

Drift and diffusion are very important in physics, engineering, and material science [1, 2]. Diffusion in many different media has been studied since the pioneering work of Fick as described at length by Crank [3]. He proposed that diffusion of particles through a fluid obeys the phenomenological law given by

$$J_{\mathrm{D}} = -qD\left(\frac{\partial c}{\partial x}\right), \tag{1}$$

where q is the electronic charge of the particles, J_{D} is the flux of diffusion particle, and $(\partial c/\partial x)$ is the concentration gradient of the particles along the x-direction. D is the proportionality constant between the two, which is called the diffusion coefficient. Equation (1) has essentially the same form as the Fourier law of heat conduction. The diffusion coefficient, thus derived, may contain impact of interactions between particles; it may also depend on particle concentration c. Let us assume that the particles of this concentration c move with an average velocity of v; and that this movement is influenced by an external force F. Then the resulting flux is

$$J_{\mathrm{F}} = cv. \tag{2}$$

If the particle mobility is defined as the ratio of the average velocity v and the drift field F; e. g., $\mu = v/F$, then the drift flux, as given by (2), may be modified to

$$J_{\mathrm{F}} = \mu cF. \tag{3}$$

While deriving (1) – (3), a one-dimensional picture has been adopted, and the diffusion coefficient D has been introduced. It has also been assumed that the particles cross unit area per unit time as a result of the force F. Making use of (1) and (3), the total particle flux or current is given by

$$J_{\mathrm{T}} = J_{\mathrm{D}} + J_{\mathrm{F}}. \tag{4}$$

If this flux vanishes under thermal equilibrium, then

$$\mu cF = qD\left(\frac{\partial c}{\partial x}\right). \tag{5}$$

If applied to semiconductors under appropriate physical conditions, the particles under consideration would be electrons and holes, and (5) would depend on temperature, electric field, non-parabolicity [4 – 7], and degeneracy of the particles [8]. It may depend also on the doping density and the band gap narrowing of the semiconductor. However, band gap narrowing and carrier degeneracy may compete to each other [9] to dictate the electrical performances of the particles. If k_{B} is the Boltzmann constant, and T the temperature, then the particle density may be given by the Boltzmann distribution, e. g.,

$$c \approx \exp\left(-\frac{v(x)}{k_{\mathrm{B}}T}\right). \tag{6}$$

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The external force F may also be defined by $F = -(\partial v/\partial x)$. Equations (5) and (6) would then yield

$$\frac{D}{\mu} = \frac{k_B T}{q}. \quad (7)$$

This is the simplest form of the diffusivity-mobility relationship (DMR). It is nevertheless very useful for semiconductors as it allows an accurate determination of the diffusivity based on measured values of mobility, and vice versa. During the past several years, our efforts have been directed to study DMR at length [10–15]. A series of other investigations [16–48] has also been carried out to address it from many different physicochemical perspectives. Being thermodynamically independent of any scattering mechanism, it is more accurate than the individual relationship for mobility and diffusivity. Our objective in this investigation is to modify (7) and to present a general relationship for semiconductors exhibiting non-uniform band structure. Heavily doped semiconductors with such band structures have band tails, and the Gaussian density-of-states function results from random distributions of impurities [49–53]. Ion-implantation leads generally to non-uniform band structure, and band tails in this band structure [54]. Diffusivity-mobility relationships for semiconductors exhibiting non-uniform band structure are quite important for critical analysis of carrier transport and device performance in semiconductor homostructures [55, 56], semiconductor/semiconductor heterostructures [57–59], metal/semiconductor heterostructures [60–63], and insulator/semiconductor heterostructures [64–67].

2. Theoretical Model

For degenerate n-semiconductors with non-uniform Gaussian band tails, the density of states function corresponding to impurity states in the tail may be given by [47–52]

$$\rho_d = \rho_{d0} \exp\left[-\left(\frac{E - E_{d0}}{\sigma_d}\right)^2\right], \quad (8)$$

where ρ_{d0} is the amplitude; σ_d is the half-width, $\sigma_d = \sqrt{2}\sigma$, σ is the standard deviation, and E_{d0} is the energy at the center of the Gaussian band. The charged particles for these semiconductors are electrons. Let ε_s be the dielectric constant, m_e^* the effective electron mass, and N_d the doping density of the semiconductors. Then

$$\rho_{d0}\sigma_d = 2N_d/\sqrt{\pi} \quad (9)$$

with

$$\sigma_d = \frac{q^2}{\varepsilon}\sqrt{\frac{4\pi N_d}{\lambda_d}} \quad (10)$$

and

$$\lambda_d = \frac{2q}{\hbar}\left(\frac{3N_d}{\pi}\right)^{1/6}\frac{m_e^*}{\varepsilon_s}. \quad (11)$$

Assuming that the electrons are distributed both in the allowed energy levels of the conduction band and the band tail, the electron concentration may be given by

$$n_e = N_c \Im_{1/2}(\eta) + \frac{2N_d}{\sqrt{\pi}\sigma_d}\int_{-\infty}^{+\infty}\frac{\exp[-\{(E-E_{d0})/\sigma_d\}^2]\mathrm{d}E}{1+\exp[(E-E_{fe})/k_B T]}, \quad (12)$$

where η is the reduced Fermi level $\eta = E_{fe}/k_B T$, N_c is the effective density of states for electrons in the conduction band, and $\Im_{1/2}(\eta)$ is the Fermi-Dirac integral of order 1/2 given, in general, by

$$\Im_j(\eta_c) = \frac{1}{\Gamma(j+1)}\int_0^{\infty}\frac{z^j \mathrm{d}z}{1+\exp(z-\eta_C)}. \quad (13)$$

In order to solve (12) we make use of an approximation given by

$$\exp(-x^2) = \sum_{\nu=1}^{6} a_\nu e^{-\nu x}, \quad (14)$$

where x is a dimensionless parameter, $a_1 = 2.589 \times 10^{-3}$, $a_2 = -2.183$, $a_3 = 3.314 \times 10^1$, $a_4 = -7.625 \times 10^1$, $a_5 = 6.825 \times 10^1$, and $a_6 = -2.196 \times 10^1$. The comparison of the exact value of $\exp(-x^2)$ with the approximation given by (14) is shown in Figure 1, which indicates that the approximation is indeed quite excellent. If $b = k_B T/\sigma_d$, then, making use of (12) and (14), we may obtain

$$n_e = N_c \Im_{1/2}(\eta) + \frac{2N_d k_B T}{\sqrt{\pi}\sigma_d} \cdot \sum_{\nu=1}^{6} a_\nu \frac{1 - b\nu\varepsilon + b^2\nu^2\varepsilon^2/2 + b^3\nu^3\varepsilon^3/6 + \dots}{1+\exp(\varepsilon - \eta_m)}\mathrm{d}\varepsilon, \quad (15)$$

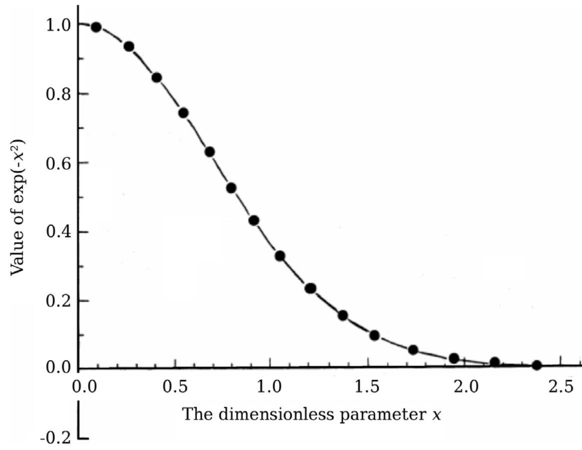

Fig. 1. Comparison of the exact value of $\exp(-x^2)$ with an approximation of it given by (14). The solid line represents the exact result, and the small solid circles represent the approximations given by (14).

where

$$\eta_{\rm m} = \frac{E_{\rm fe} - E_{\rm d0}}{k_{\rm B}T}, \quad (16a)$$

$$\varepsilon = \frac{E - E_{\rm d0}}{k_{\rm B}T}, \quad (16b)$$

$$N_{\rm m} = \left(\frac{2N_{\rm d}k_{\rm B}T}{\sqrt{\pi}\sigma_{\rm d}}\right). \quad (16c)$$

Employing (13) and (16), (15) may be rewritten as

$$n_{\rm e} = N_{\rm c}\Im_{1/2}(\eta) + N_{\rm m}\sum_{v=1}^{6} a_v[\Im_0(\eta_{\rm m}) - bv\Im_1(\eta_{\rm m}) + b^2v^2\Im_2(\eta_{\rm m}) - b^3v^3\Im_3(\eta_{\rm m})]. \quad (17)$$

Let the mobility be $\mu \equiv \mu_{\rm e}$ and the diffusivity $D \equiv D_{\rm e}$ for electrons. Similarly, $\mu \equiv \mu_{\rm h}$ and $D \equiv D_{\rm h}$ for holes. The diffusivity-mobility relationship for electrons may then be given by

$$\frac{D_{\rm e}}{\mu_{\rm e}} = \left(\frac{k_{\rm B}T}{q}\right)\frac{N_{\rm c}\Im_{1/2}(\eta) + \Re_1}{N_{\rm c}\Im_{-1/2}(\eta) + \Re_2}, \quad (18)$$

where

$$\Re_1 = N_{\rm m}\sum_{v=1}^{6} a_v[\Im_0(\eta_{\rm m}) - bv\Im_1(\eta_{\rm m}) + b^2v^2\Im_2(\eta_{\rm m}) - b^3v^3\Im_3(\eta_{\rm m})], \quad (19)$$

$$\Re_2 = N_{\rm m}\sum_{v=1}^{6} a_v[\Im_{-1}(\eta_{\rm m}) - bv\Im_0(\eta_{\rm m}) + b^2v^2\Im_1(\eta_{\rm m}) - b^3v^3\Im_2(\eta_{\rm m})]. \quad (20)$$

Equation (18) is actually the diffusivity-mobility relationship for heavily doped n-semiconductors with non-uniform band structure. The parameters $\Re_1$ and $\Re_2$ of this equation correspond to band tails. An analogous relationship may be obtained for heavily doped p-type semiconductors. Under appropriate conditions, (18) reduces to those for degenerate semiconductors without non-uniform band structure, and for non-degenerate semiconductors with parabolic band structure.

3. Results and Discussions

The diffusivity-mobility relationship for heavily doped semiconductors exhibiting Gaussian doping profile and band tail has been studied. For this study, the semiconductors have been assumed to exhibit parabolic energy band structures. It can easily be modified for degenerate semiconductors with non-parabolic energy band structures. Although formulas for carrier concentration and DMR have been developed for electrons in n-type semiconductors, analogous formulas can be developed also for holes in p-type semiconductors. These semiconductors have no compensation. Hence, at finite temperatures, the electron distribution in n-type semiconductors and the hole distribution in p-type semiconductors take place in energy states in both the allowed band (e. g., conduction band in n-semiconductor and valence band in p-semiconductor) band and the band tail. It occurs in doping regimes where the exchange interactions and the annihilation of the impurity states due to screening do not affect the semiconducting behaviour of the material. The formulas thus developed are general. For non-degenerate semiconductors, they reduce to the conventional forms. For them, the parameters $\Re_1$ and $\Re_2$ of (18) reduce to zero, and the DMR becomes

$$\frac{D_{\rm e}}{\mu_{\rm e}} = \left(\frac{k_{\rm B}T}{q}\right)\frac{\Im_{1/2}(\eta)}{\Im_{-1/2}(\eta)}. \quad (21)$$

If the reduced Fermi level $\eta < 0$, which is valid for highly non-degenerate semiconductors, (21) reduces further to

$$\frac{D_{\rm e}}{\mu_{\rm e}} = \frac{k_{\rm B}T}{q}. \quad (22)$$

In order to study the applicability of the present model, we carried out calculations for n-GaAs. The parameters used for the calculations are $\varepsilon_{\rm s} = 11.8$ and $m_{\rm e}^* = 0.067$. Figure 2 shows the variation of the Fermi level

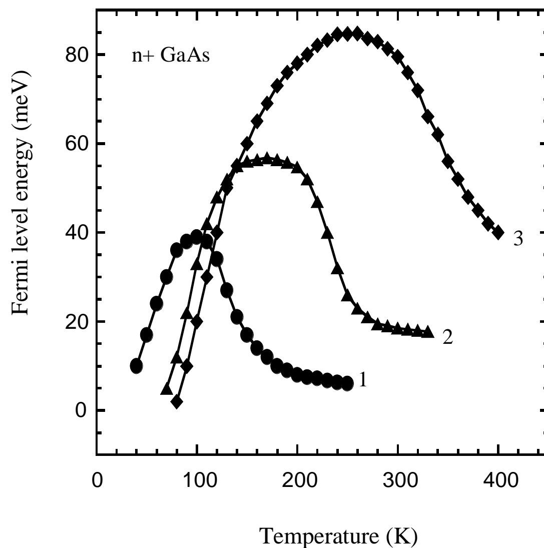

Fig. 2. Temperature dependent Fermi energies of heavily doped n-GaAs exhibiting Gaussian band tails. Curves 1, 2, and 3 correspond to doping levels of $N_d = 5 \times 10^{17}$ cm^{-3}, $N_d = 1 \times 10^{18}$ cm^{-3}, and $N_d = 3 \times 10^{18}$ cm^{-3}, respectively.

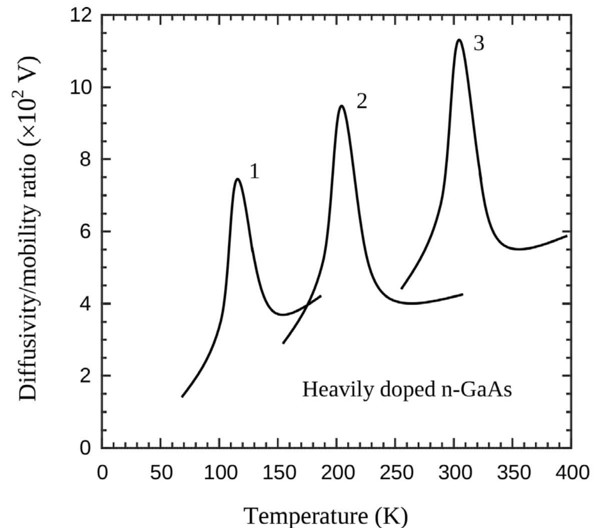

Fig. 3. Temperature-dependent diffusivity-mobility ratio of heavily-doped n-GaAs exhibiting Gaussian band tails. Curves 1, 2, and 3 correspond to doping levels of $N_d = 5 \times 10^{17}$ cm^{-3}, $N_d = 1 \times 10^{18}$ cm^{-3}, and $N_d = 3 \times 10^{18}$ cm^{-3}, respectively.

with temperature for various values of the doping level. As evident from this figure, the Fermi level increases, in general, with an increase in doping density. It increases also with temperature, reaches a peak, and then dies down with further increase in temperature. It increases as long as the Fermi level remains within the conduction band. There is a threshold temperature T_0 beyond which the Fermi level enters the band tail. At $T > T_0$, the density of states in the conduction band becomes higher than that in the band tail. Consequently, the distribution of electrons in the conduction band becomes non-degenerate. This is reflected from Figure 3, where the diffusivity-mobility ratio increases with an increase in temperature, reaches a peak, and then decreases until it reaches a value $k_B T/q$. However, for a certain temperature, the diffusivity-mobility ratio is always higher for higher doping level. Also, for each doping level, the regime of most prominent values of the diffusivity-mobility ratio is different. This regime for higher doping level occurs at higher temperature.

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