CHAPTER III

EMPIRICAL DIFFUSIVITY-MOBILITY RATIO

In this chapter we will discuss about Van Cong and Dabiais' empirical diffusivity-mobility ratio. They derived their empirical diffusivity-mobility ratio for any carrier concentration by approximating the general diffusivity-mobility ratio in eq.(2.10) which is strongly dependent on asymptotic behaviors of expression of Fermi energy for any carrier concentration.

3.1 A simple accurate expression of the reduced Fermi energy for any reduced carrier density[4]

From the simple relation between net carrier concentration (electron) and density of states

$$n = 2\int_{-\infty}^{\infty} \rho(E) f(E, E_f, T) dE , \qquad (3.1)$$

where n is electron concentration, $\rho(E)$ is electron density of states, E_f is Fermi energy, and E is electron energy.

For parabolic band, the density of states is

$$\rho(E) = \frac{1}{4\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\left[E-E_C\right]^{1/2}H(E-E_C), \qquad (3.2)$$

where E_C is the conduction band edge and $H(x)$ is the Heaviside step function. Suppose that $E_C = 0$, (3.2) becomes,

$$\rho(E) = \frac{1}{4\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}E^{1/2}H(E). \qquad (3.3)$$

Substituting (3.3) in (3.1) gives

$$\rho(E) = \frac{2}{4\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\int_{-\infty}^{\infty}E^{1/2}H(E)f(E,E_f,T)dE$$

$$= \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\int_{0}^{\infty}E^{1/2}\frac{1}{1+\exp\left(\frac{E-E_f}{k_BT}\right)}dE$$

$$= \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}(k_BT)^{3/2}\int_{0}^{\infty}\varepsilon^{1/2}\frac{1}{1+\exp(\varepsilon-\eta)}d\varepsilon$$

$$= 2\frac{N_c}{\pi^{1/2}}\int_{0}^{\infty}\varepsilon^{1/2}\frac{1}{1+exp(\varepsilon-\eta)}d\varepsilon\ . \qquad (3.4)$$

where[4] $N_c = \pi^{1/2}\left(\frac{1}{4\pi^2}\right)\left(\frac{2m^* k_B T}{\hbar^2}\right)^{3/2}$ is effective density of states ,

$$\varepsilon \equiv \frac{E}{k_B T},$$

$$\eta \equiv \frac{E_f}{k_B T} \quad : \text{reduced Fermi energy.}$$

We define the reduced carrier density

$$u = \frac{n}{N_c} = \frac{2}{\pi^{1/2}} \int_{-\infty}^{\infty} \frac{\varepsilon^{1/2}}{1 + exp(\varepsilon - \eta)} d\varepsilon . \qquad (3.5)$$

Equation.(3.5) is the Fermi-Dirac integrals of order ½ : $F_{1/2}(\eta)$, where

$$F_j(\eta) \equiv \frac{1}{\Gamma(j+1)} \int_0^{\infty} \frac{\varepsilon^j d\varepsilon}{1+\exp(\varepsilon - \eta)}$$

and

$$F_{1/2}(\eta) = \frac{2}{\pi^{1/2}} \int_0^{\infty} \frac{\varepsilon^{1/2}}{1 + \exp(\varepsilon - \eta)} d\varepsilon ,$$

so that

$$u = F_{1/2}(\eta) . \qquad (3.6)$$

The reversion of $u = F_{1/2}(\eta)$ is so useful to give $\eta(u)$ concerned with doped semiconductors at arbitrary impurity concentrations and temperatures.

Van Cong and Debiais stated in their paper that the accuracy of the approximation of $\eta(u)$ is strongly dependent on its asymptotic behaviors, namely in the highly degenerate ($u \to \infty$ or $\eta \to \infty$) and completely non-degenerate ($u \to 0$ or $\eta \to -\infty$) cases.

i) In the highly degenerate case.

From the Sommerfeld asymptotic expansion[7] [Appendix]

$$\int_{-\infty}^{\infty} A(E)f(E)dE = \int_{-\infty}^{E_f} A(E)dE + \sum_{n=1}^{\infty} (k_B T)^{2n} a_n \frac{d^{2n-1}}{dE^{2n-1}} A(E)\Big|_{E=E_f} , \quad (3.7)$$

we use the notation of ε and η to obtain

$$\int_{-\infty}^{\infty} A(\varepsilon)f(\varepsilon)d\varepsilon = \int_{-\infty}^{\eta} A(\varepsilon)d\varepsilon + \sum_{n=1}^{\infty} a_n \frac{d^{2n-1}}{d\varepsilon^{2n-1}} A(\varepsilon)\Big|_{\varepsilon=\eta} . \quad (3.8)$$

Replacing $A(\varepsilon)$ by $(2/\pi^{1/2})\,\varepsilon^{1/2}\,H(\varepsilon)$, where $H(\varepsilon)$ is Heaviside step function, we have

$$\frac{2}{\pi^{1/2}}\int_{0}^{\infty} \varepsilon^{1/2} f(\varepsilon)d\varepsilon = u = \frac{2}{\pi^{1/2}}\left\{\int_{0}^{\eta} \varepsilon^{1/2}d\varepsilon + \sum_{n=1}^{\infty} a_n \frac{d^{2n-1}}{d\varepsilon^{2n-1}} \varepsilon^{1/2} H(\varepsilon)\Big|_{\varepsilon=\eta}\right\}$$

$$= \frac{2}{\pi^{1/2}}\left\{\frac{2}{3}\eta^{3/2} + \frac{a_1}{2}\eta^{-1/2} + \frac{3a_2}{8}\eta^{-5/2} + \ldots\right\}$$

$$= \frac{4}{3\pi^{1/2}}\eta^{3/2}\left\{1 + \frac{3a_1}{4}\frac{1}{\eta^2} + \frac{9a_2}{16}\frac{1}{\eta^4} + \ldots\right\},$$

so that

$$\eta = \left(\frac{3}{4}\pi^{1/2}\right)^{2/3} u^{2/3}\left\{1 + \frac{3a_1}{4}\frac{1}{\eta^2} + \frac{9a_2}{16}\frac{1}{\eta^4} + \ldots\right\}^{-2/3}$$

$$= au^{2/3}\left\{1 + \frac{1}{8}\left(\frac{\pi}{\eta}\right)^2 + \frac{7}{640}\left(\frac{\pi}{\eta}\right)^4 + \ldots\right\}^{-2/3}, \qquad (3.9)$$

where $a = \left(\frac{3}{4}\pi^{1/2}\right)^{2/3}$.

Substituting η^2 found in this second member by an approximating :

$$\eta^2 = a^2u^{4/3}\left[1 + \frac{1}{8}\left(\frac{\pi}{a}\right)^2 u^{-4/3}\right]^{-1}, \qquad (3.10)$$

gives

$$\eta(u) = au^{2/3}\left[1 + bu^{-4/3} + cu^{-8/3} + \ldots\right]^{-2/3}, \qquad (3.11)$$

where $b = \frac{1}{8}\left(\frac{\pi}{a}\right)^2$, and $c = \frac{61}{1920}\left(\frac{\pi}{a}\right)^4$.

Further, a very correct asymptotic form can be obtained and represented by a function $K(u)$, as

$$K(u) = \eta(u) = au^{2/3}\left[1 + bu^{-4/3} + c^{*}u^{-8/3} + \ldots\right]^{-2/3}, \qquad (3.12)$$

where c^{*} is an empirical parameter chosen to minimize the error of this function ; c^{*} is found to be equal to[4] $(62.3739855/61)c$.

ii) Furthermore, Van Cong and Debiais remarked in the completely non-degenerate case that the asymptotic form of $\eta(u)$ can be represented by the following function

$$G(u) = \ln(u) + 2^{-3/2}u\exp(-du), \qquad (3.13)$$

where $d = 2^{3/2}\left[\frac{1}{\sqrt{27}} - \frac{3}{16}\right]$.

Therefore, as $u \to 0$, this function $G(u)$ is reduced to a very correct asymptotic form of $\eta(u)$[8] :

$$\eta(u) \approx \ln(u) + 2^{-3/2}u - \left[\frac{1}{\sqrt{27}} - \frac{3}{16}\right]u^{2}. \qquad (3.14)$$

In this communication, by basing on these correct asymptotic forms, Van Cong and Debiais purposed a simple accurate approximated expression of $\eta(u)$ for full range of u :

$$\eta_a(u) = K(u) + \frac{G(u) - K(u)}{1 + Au^B}$$

$$= \frac{G(u) + Au^B K(u)}{1 + Au^B}, \qquad (3.15)$$

where the functions $K(u)$ and $G(u)$ are defined in (3.12) and (3.13), $0 < A \leq 1$ and $B(>> 1)$ is determined by the point $\eta_a(u_0) = \eta = 0$, with $u_0 = 0.7651470246254$ [4], as

$$B = \frac{1}{\ln(u_0)} \ln\left\{\frac{1}{A}\left[\frac{F(u_0) - G(u_0)}{F(u_0)} - 1\right]\right\}. \qquad (3.16)$$

For such the values of A and B, (3.15) fulfills two correct asymptotic forms found in (3.12) and (3.13), and (3.16) shows $\Delta\eta(u_0) = \eta - \eta_a(u_0) = 0$. Therefore, all the irregularities in relative errors ($\Delta\eta/\eta_a$) are removed in the neighborhood of $\eta = 0$. So we can minimize $|\Delta\eta/\eta_a|$ as $0 < u < \infty$ by varying A from A_1, which is defined by another point : $\eta_a(1) = \eta = 0.3487473611036$ [4], as

$$A_1 = \frac{G(1) - K(1)}{\eta_a(1) - K(1)}. \qquad (3.17)$$

Here, the corresponding values of B also determined by (3.16) gives[4] $A = 0.0005372$ and $B = 4.82842262$.

For these values of A and B, the maximal relative error of (3.15) in absolute value is found to be equal to[4] 2.11×10^{-4}, which occurs at fairly large η (=3.6)

3.2 The empirical diffusivity-mobility ratio[3]

The generalized diffusivity-mobility ratio for n-type semiconductors at high temperatures T from (2.11) is

$$\frac{D}{\mu} = \frac{n}{e}\left(\frac{\partial E_f}{\partial n}\right)_{T,V}.$$

By using the notation same as in Section 3.1, it can be written in the form

$$\frac{D}{\mu} = V_T\left(u\frac{d\eta}{du}\right), \qquad (3.18)$$

where $V_T \equiv \frac{k_B T}{e}$ is the thermal potential.

From (3.18) , to obtain D/μ analytically for any u , one requires a simple and accurate formula of $\eta(u)$. $\eta(u)$ from (3.15) is used,

$$\eta(u) \cong \frac{V(u)}{W(u)}, \tag{3.19}$$

where $V(u) \equiv G(u) + Au^B K(u)$,

$$W(u) \equiv 1 + Au^B,$$

$$A = 5.372\times10^{-4}, \quad B = 4.82842262,$$

$$G(u) \equiv \ln(u) + 2^{-3/2} u\, e^{-du},$$

$$K(u) \equiv au^{2/3}\left[1 + bu^{-4/3} + c^* u^{-8/3}\right]^{-2/3},$$

$$d = 2^{3/2}\left(\frac{1}{\sqrt{27}} - \frac{3}{16}\right),$$

$$a = \left(\frac{3}{4}\sqrt{\pi}\right)^{2/3}, \quad b = \left(\frac{1}{8}\right)\left(\frac{\pi}{a}\right)^2$$

and

$$c^* = \left(\frac{62.3739855}{1920}\right)\left(\frac{\pi}{a}\right)^4.$$

Differentiating the function $\eta(u)$ with respect to u , one obtains (dη/du). Therefore (3.18) becomes :

$$\frac{D}{\mu} \cong V_T\, u\left\{\frac{V'(u)W(u) - V(u)W'(u)}{W^2(u)}\right\}, \qquad (3.20)$$

where

$$W'(u) = ABu^{B-1}$$

and

$$V'(u) = \frac{1}{u} + 2^{-3/2}e^{-du}(1-du) + \frac{2}{3}Au^{B-1}K(u)$$

$$\times\left[\left(1+\frac{3}{2}B\right) + \frac{4}{3}\left(\frac{bu^{-4/3} + 2c^{*}u^{-8/3}}{1 + bu^{-4/3} + c^{*}u^{-8/3}}\right)\right].$$

The relation(3.20) is valid for any u , Further, it is invested to examine its asymptotic forms as below .

i) As $u \to 0$ we have : $W^2 \cong 1$ and $u(V'W - VW') \cong 1$. Therefore we obtain

$$\frac{D}{\mu} \cong V_T, \qquad (3.21)$$

which is just the well-known Einstein diffusivity-mobility ratio(2.1).

ii) As $u \to \infty$ one has : $W^2 \approx A^2 u^{2B}$ and $u(V'W - VW') \approx \frac{2}{3} a\, u^{2/3} (A^2 u^{2B})$.

Therefore :

$$\frac{D}{\mu} \approx V_T \left(\frac{\pi}{6}\right)^{1/3} u^{2/3}, \qquad (3.22)$$

which is the diffusivity-mobility ratio given in the extremely degenerate case.

In order to evaluate the error of the approximated expression (3.20) , Van Cong and Debiais used the relation[6]

$$\frac{eD}{\mu k_B T} = \frac{F_{1/2}(\eta)}{F_{-1/2}(\eta)}, \qquad (3.23)$$

and accurate values of the Fermi-Dirac integral obtained by Chang and Izabelle[9] . It follows that the maximum relative error of relation(3.20) is found to be equal to 10^{-3} (in absolute value).

Advantages of the empirical diffusivity-mobility ratio

i) It is valid for any electron concentration.

ii) It is a simple expression, so that it is simple to evaluate.

iii) High accuracy in non-degenerate region (very low doping concentration) and extremely degenerate region (extremely high doping concentration).

Disadvantages of the empirical diffusivity-mobility ratio

i) It is strongly dependent on the asymptotic behavior (non-degenerate and extremely degenerate region) of the relation between Fermi energy and electron concentration, and it is dependent on the parabolic band approximation (not consider band tails), so that it may give a poor accurate result in moderately degenerate region (heavily doping concentration) in which the band tails are necessary to be considered.

ii) The standard result of D/μ that Van Cong and Dabiais used to compare with their result, is dependent on the parabolic band approximation, so that the accuracy of their result in moderately degenerate region may be unreasonable.

iii) It is dependent on the net carrier concentration (N_d - N_a) but it is not dependent on the compensation ratio (N_a/N_d). In fact while net carrier concentrations are the same values with different band tail compensation ratios, they have different density of states.

Because of disadvantages of the empirical diffusivity-mobility ratio by Van Cong and Dabiais in the moderately degenerate region, we simplify the generalized diffusivity-mobility ratio for the moderately degenerate region, using a band tail density of states (in this work we use the Kane density of states) and the Thomas-Fermi approximation of screening length in the next chapter.