CHAPTER IV

THE DIFFUSIVITY-MOBILITY RATIO

FOR HEAVILY DOPED SEMICONDUCTORS

In Chapter II the generalized diffusivity-mobility ratio was reviewed. In this chapter we will use the result of Chapter II to derive the diffusivity-mobility for heavily doped semiconductors. Before going to our main purpose, we will consider the electrons behavior in section 4.1 and the change in density of states in section 4.2 when impurities are added to a system. Finally, we use the result of section 4.2 and Kane's density of states to derive and evaluate the diffusivity-mobility ratio for heavily doped semiconductors in section 4.3 .

4.1 Screening[7]

4.1.1 Introduction

The phenomenon of screening is one of the simplest and most important manifestation of electron-electron interactions. First, we consider screening in a free electron gas.

Suppose a positively charged particle is placed at a given position in the electron gas and rapidly held there. It will then attract, creating a surplus of negative charges in its neighborhood, which reduces (or screen) its field. In treading this screening it is convenient to introduce two electrostatic potentials. The first, ϕ^{ext}, arises solely from the positively charged particle itself, and therefore satisfies Poisson's equation in the form :

$$-\nabla^2 \phi^{ext}(\vec{r}) \;=\; 4\pi\rho^{ext}(\vec{r}),\tag{4.1}$$

where $\rho^{ext}(\vec{r})$ is the particle's charge density. The second, ϕ, is the full physical potential, produced by both the positively charged particle and the cloud of screening electrons it induces. It therefore satisfies

$$-\nabla^2 \phi(\vec{r}) \;=\; 4\pi\rho(\vec{r}),\tag{4.2}$$

where ρ is the full charge density,

$$\rho(\vec{r}) \;=\; \rho^{ext}(\vec{r}) + \rho^{ind}(\vec{r}),\tag{4.3}$$

and $\rho^{ind}(\vec{r})$ is the charge density induced in the electron gas by the presence of the external particles.

By analogy with the theory of dielectric media, one assume that ϕ^{ext} and ϕ are linearly related by an equation of the form :

$$\phi^{ext}(\vec{r}) \;=\; \int d\vec{r}'\varepsilon(\vec{r},\vec{r}')\phi(\vec{r}') . \qquad (4.4)$$

In a spatially uniform electron gas ε can depend only on the separation between the point $\vec{r}$ and $\vec{r}'$, but not on their absolute position:

$$\varepsilon(\vec{r},\vec{r}') \;=\; \varepsilon(\vec{r}-\vec{r}') . \qquad (4.5)$$

Thus (4.4) assumes the form

$$\phi^{ext}(\vec{r}) \;=\; \int d\vec{r}'\varepsilon(\vec{r}-\vec{r}')\,\phi(\vec{r}') , \qquad (4.6)$$

which implies that the corresponding Fourier transforms satisfy

$$\phi^{ext}(\vec{q}) \;=\; \varepsilon(\vec{q})\phi(\vec{q}) , \qquad (4.7)$$

where the Fourier transforms are defined by

$$\varepsilon(\vec{q}) \;=\; \int d\vec{r}\exp\left[-i\vec{q}.\vec{r}\right]\varepsilon(\vec{r}) , \qquad (4.8)$$

$$\varepsilon(\vec{r}) \;=\; \frac{1}{(2\pi)^3}\int d\vec{q}\,\exp\!\left[i\vec{q}.\vec{r}\right]\varepsilon(\vec{q})\,. \qquad (4.9)$$

The quantity $\varepsilon(\vec{q})$ is called the (wave vector dependent) dielectric constant of the electron gas.

The quantity that turns out to be the most natural to calculate directly is not the dielectric constant $\varepsilon(\vec{q})$ but the charge density $\rho^{ind}(\vec{r})$ induced in the electron gas by the total potential $\phi(\vec{r})$. We shall examine below how this can be calculated.

The Fourier transform of (4.2) and (4.1) are

$$q^2\phi(\vec{q}) \;=\; 4\pi\rho(\vec{q})\,, \qquad (4.10)$$

$$q^2\phi^{ext}(\vec{q}) \;=\; 4\pi\rho^{ext}(\vec{q})\,. \qquad (4.11)$$

Together with (4.3) these give

$$\frac{q^2}{4\pi}\left\{\phi(\vec{q}) - \phi^{ext}(\vec{q})\right\} \;=\; \rho^{ind}(\vec{q})\,, \qquad (4.12)$$

or

$$\phi^{ext}(\vec{q}) \;=\; \left\{1 - \frac{4\pi}{q^2}\frac{\rho^{ind}(\vec{q})}{\phi(\vec{q})}\right\}\phi(\vec{q})\,. \qquad (4.13)$$

Comparing this with (4.7) leads to the relation

$$\varepsilon(\vec{q}) = 1 - \frac{4\pi}{q^2} \frac{\rho^{ind}(\vec{q})}{\phi(\vec{q})}. \qquad (4.14)$$

In this work, we discuss with electrons in a semiconductor (not in vacuum) so that it is convenient to insert an effective dielectric constant, ε_0, to take into account of the effect of interband transitions, the polarization of the ion, etc., in an *ad hoc* manner to find

$$\varepsilon(\vec{q}) = 1 - \frac{4\pi}{\varepsilon_0 q^2} \frac{\rho^{ind}(\vec{q})}{\phi(\vec{q})}. \qquad (4.15)$$

Relations 4.14 and 4.15 are general results of screening and we will approximate the induced charge density and the total potential in relation 4.14 to give the Thomas-Fermi theory of screening or the Thomas-Fermi approximation in next section.

4.1.2 Thomas-Fermi theory of screening

In principle, to find the charge density in the presence of the total potential, ϕ, one must solve the one-electron Schrodinger equation,

$$-\frac{\hbar^2}{2m}\nabla^2\Psi_i(\vec{r}) - e\phi(\vec{r})\Psi_i(\vec{r}) = E_i\Psi_i(\vec{r}). \qquad (4.16)$$

The Thomas-Fermi approach is based on a simplification in this procedure that can be made when the total potential $\phi(\vec{r})$ is a very slowly varying function of $\vec{r}$. We assume it is meaningful to specify the energy versus wave vector relation of an electron at the position $\vec{r}$, and we take this relation to be

$$E(\vec{k}) = \frac{\hbar^2}{2m}k^2 - e\phi(\vec{r}). \qquad (4.17)$$

Thus we assume that the solution of (4.16) describes a set of electrons with energies of the simple classical form (4.17). To calculate the charge density produced by these electrons one places their energies into the expression,

$$n = \int \frac{d\vec{k}}{4\pi^3} \frac{1}{\exp\left\{\dfrac{\left(E(\vec{k})-E_f\right)}{k_BT}\right\}+1}, \qquad (4.18)$$

for the electron number density, to find (with $\beta = 1/k_B T$)

$$n(\vec{r}) = \int \frac{d\vec{k}}{4\pi^3} \frac{1}{\exp\left\{\beta\left(\frac{\hbar^2 k^2}{2m} - e\phi(\vec{r}) - E_f\right)\right\} + 1},$$
(4.19)

The induced charge density is just $-en(\vec{r}) + en_0$, where the second term is the charge density of the uniform positive background. The number density of the background is just the density of the electronic system when ϕ^{ext}, and hence ϕ vanishes,

$$n_0(E_f) = \int \frac{d\vec{k}}{4\pi^3} \frac{1}{\exp\left\{\beta\left(\frac{\hbar^2 k^2}{2m} - E_f\right)\right\} + 1}.$$
(4.20)

The value of the Fermi energy , E_f, appearing in (4.19) and (4.20) will be the same under the assumption that $\phi(\vec{r})$ is appreciable only in finite region of electron gas, outside of which the electron density is negligibly perturbed from its equilibrium value.

We combine (4.19) and (4.20) to write,

$$\rho^{ind}(\vec{r}) = -e\left\{n_0(E_f + e\phi(\vec{r})) - n_0(E_f)\right\}.$$
(4.21)

In the present case we assume that $e\phi(\vec{r})$ is small enough for (4.21) to be expanded to give in leading order

$$\rho^{ind}(\vec{r}) = -e^2 \frac{\partial n_0}{\partial E_f} \phi(\vec{r}).$$ (4.22)

Substituting this in (4.14) gives the Thomas-Fermi dielectric constant

$$\varepsilon(\vec{q}) = 1 + \frac{4\pi e^2}{q^2} \frac{\partial n_0}{\partial E_f}.$$ (4.23)

It is customary to define the Thomas-Fermi wave vector, Q, by

$$Q^2 = 4\pi e^2 \frac{\partial n}{\partial E_f},$$ (4.24)

so that

$$\varepsilon(\vec{q}) = 1 + \frac{Q^2}{q^2}.$$ (4.25)

In semiconductor media, it is convenient to insert an effective dielectric constant, ε_0, to take account of the effect of interband transition, the polarization of the ions, etc., in an *ad hoc* manner to find

$$Q^2 = \frac{4\pi e^2}{\varepsilon_0} \frac{\partial n}{\partial E_f}.$$ (4.26)

Q^{-1} is called " Screening length".

In general, the electron concentration corresponding to the Fermi energy E_f, $n(E_f)$ is written in the form :

$$n(E_f) = 2\int_{-\infty}^{\infty} \rho(E)f(E,E_f,T)dE, \qquad (4.27)$$

where $f(E, E_f, T)$ is the Fermi distribution function and $\rho(E)$ is the density of states. If we differentiate (4.27) with respect to E_f, we obtain

$$\frac{\partial n}{\partial E_f} = 2\int_{-\infty}^{\infty} \rho(E)\left(\frac{\partial f}{\partial E_f}\right)dE , \qquad (4.28)$$

since $\dfrac{\partial f}{\partial E_f} = -\dfrac{\partial f}{\partial E}$,and substituting (4.28) in (4.27) give the Thomas-Fermi

inverse screening length squared

$$Q^2 = 2\left(\frac{4\pi e^2}{\varepsilon_0}\right)\int_{-\infty}^{\infty} \rho(E)\left(-\frac{\partial f}{\partial E}\right)dE . \qquad (4.29)$$

Equation (4.26) and (4.29) are main results of the Thomas-Fermi approximation which we will use to derive and evaluate the diffusion-mobility ratio for n-type heavily doped semiconductors.

4.2 Heavily doped semiconductor

4.2.1 The model

Our model is a pure semiconductor represented by a single filled valence band separated from an empty conduction band by a band gap. The semiconductor is then doped with N_d attractive donor impurities so that shallow impurity states are formed just below the conduction band. As the doping increases the impurity levels form an impurity band and at higher concentrations this band broadens until it merges with the conduction band and becomes a band tail to the conduction band. The semiconductor is said[10] to be heavily doped when the conduction band has a band tail made up of impurity states. In gallium asenide (GaAs)[11] this requires a shallow donor concentration of $N_d > 10^{17}$ cm^{-3}. We assume that the impurity positions are random and uncorrelated in the lattice.

We shall also compensate the donor impurities by adding N_a acceptor impurities. In the model we include only the reduction in the number of electrons and the increase in the impurity potential due to the acceptor impurities. We do not take account of band tailing in the valence band. If the valence and conduction bands are well separated, tailing of the valence band should have little effect on a Fermi energy lying in the conduction band.

We ignore the electron-electron interaction in the model. Wolff[12] has shown that this is valid provided the interaction between the electron at $\bar{r}$ and impurity at $\bar{R}$ is represented by a screened coulomb potential. We will show later that screened

Coulomb potential agrees well with the Thomas-Fermi approximation, screened coulomb is

$$v(\vec{r} - \vec{R}) = -\frac{e^2}{\varepsilon_0 |\vec{r} - \vec{R}|} \exp\{-Q|\vec{r} - \vec{R}|\} \qquad (4.30)$$

and the conduction band is shifted by a small amount. The Hamiltonian describing each single electron is then

$$H = -\frac{\hbar^2}{2m^*} \nabla^2 + E_c^0 + E_0 + V(\vec{r}). \qquad (4.31)$$

Here E_c^0 is the energy of the bottom of the conduction band in the pure semiconductors, E_0 is the average potential of the impurities and added electrons

$$E_0 = \int d\vec{R}\, v(\vec{r} - \vec{R})$$

$$= \frac{4\pi e^2 (N_d + N_a)}{\varepsilon_0 Q^2}, \qquad (4.32)$$

and

$$V(\vec{r}) = \sum_i v(\vec{r} - \vec{R}) - E_0 \qquad (4.33)$$

is the fluctuation in the potential at $\vec{r}$ about the average. For randomly distributed, statistically independent impurities, we can show in sub-section 4.2.2 that the mean square fluctuation in $V(\vec{r})$ reduces to

$$\begin{aligned}
\xi_Q &\equiv \langle V(\vec{r})V(\vec{r}) \rangle_{\vec{R}} \\
&= (N_d + N_a) \int \frac{d\vec{R}}{\Omega} \left[v(\vec{r} - \vec{R}) \right]^2 \\
&= \frac{2\pi e^4}{Q \varepsilon_0^2} (N_d + N_a).
\end{aligned} \qquad (4.34)$$

The shifted conduction band edge in the impure crystals due to the impurities is

$$E_C = E_C^0 + E_0. \qquad (4.35)$$

To describe GaAs we take $\varepsilon_0 = 13.5$ and assume a parabolic conduction band having an effective mass $m^* = 0.072\ m_0$ (m_0 is electron mass)[13]. We consider $Z = \pm 1$ impurities, such as phosphorus(P) as the donor.

This model is identical to that used by Halparin and Lax[11] in their calculation of the density of states in the band tail region, and that used by Kane[1] in his calculation of the density of states which we will mention it again in sub-section 4.2.2,

and that used by Hwang[14] in his evaluation of E_f and Q. The model depends upon the validity of linear screening in the Thomas-Fermi approximation. If the Thomas-Fermi approximation does not hold, (4.30) is invalid and the concept of a screening length and must be abandoned in favor of more sophisticated descriptions of screening. The Thomas-Fermi approximation holds if variations in the impurity potential are small compared to the electron energy. In the present model this requires

$$\xi_Q^{1/2} \leq E_f - E_c, \tag{4.36}$$

and we take[12]

$$\xi_Q^{1/2} = E_f - E_c \tag{4.37}$$

as the limit of the present model. This will require large impurity concentrations (so that $E_f\text{-}E_c$ is large) and the electrons will always be "degenerate" so that Fermi statistics are required to describe the electron distribution.

4.2.2 Kane's density of states

The density of states for above model has been derived by several authors such as Sa-yakanit and Glyde[2] using the Feynman path integration, Halperin and Lax[11] using the minimum counting method, and Kane[1] using the semiclassical approach. Sa-yakanit and Glyde density of states is the most modern among them but it is very complicated to evaluate the density of states. The Kane density of states is easy to evaluate but it seems to be a rough density of states.

Sritrakool, Glyde and Sa-yakanit[15] has shown that the Fermi energy E_f and the electron screening length Q^{-1}, important parameters for evaluate the diffusivity-mobility ratio, have little different values when using different density of states to evaluate, especially when net carrier concentration is over 10^{18} cm^{-3} (for GaAs). So we will discuss about Kane's density of states in this section and use Kane's density of states to derive and evaluate the diffusivity-mobility ratio in next sub-section.

Kane (1963) has applied a semiclassical method to calculate the density of states for heavily doped semiconductors. The semiclassical approach assumes basically one approximation : the classical description of the electron wave packet. The potential fluctuations caused by charged impurities are assumed to be smooth in the sense that they change a little over the electron wave length. The electron only "feels" the potential of the point where it is located that a local density of states can be defined just as if the potential were constant. A local density of states is defined by

$$\rho_i(E - V(\vec{r})) = \frac{m^{*3/2}}{\sqrt{2}\pi^2\hbar^3}[E - V(\vec{r})]^{1/2} H(E - V(\vec{r})), \tag{4.38}$$

where $V(\vec{r})$ is the constant potential located at $\vec{r}$, m^* is electron effective mass and H is the Heaviside step function.

Then, the total density of states is simply

$$\rho(E) = \langle \rho_i(E - V(\vec{r})) \rangle_V$$

$$= \frac{m^{*3/2}}{\sqrt{2}\pi^2\hbar^3} \int [E - V]^{1/2} H(E - V) P(V) dV$$

$$= \frac{m^{*3/2}}{\sqrt{2}\pi^2\hbar^3} \int_{-\infty}^{E} [E - V]^{1/2} P(V) dV, \tag{4.39}$$

where $P(V)dV$ is the probability of finding the potential between V and $V+dV$. The calculation of the total density of states then reduces to the calculation of the distribution function for the potential $P(V)$.

An analytical, exact expression for $P(V)$ exists only on the condition that the potential at a certain point $\vec{r}$ can be written as a superposition of the influences of all impurities in a system with volume Ω. For, if the potential energy $V(\vec{r}, \{\vec{r}_i\})$ at $\vec{r}$, caused by a configuration of N impurities at position $\{\vec{r}_i\}$, can be written as a superposition

$$V(\vec{r}, \{\vec{r}_i\}) = \sum_{i=1}^{N} v(\vec{r} - \vec{r}_i) \tag{4.40}$$

where $v(\vec{r})$ is an arbitrary well-defined function. Assuming that the probability of finding an impurity at a point $\vec{r_i}$ is constant (and thus equals Ω^{-1})*, the probability for the potential energy to have the value V at position $\vec{r}$ is defined as

$$P(\vec{r},V) \;=\; \int\frac{d\vec{r_1}}{\Omega}\int\frac{d\vec{r_2}}{\Omega}\;\ldots\;\int\frac{d\vec{r_N}}{\Omega}\,\delta\big(V-V(\vec{r},\{\vec{r_i}\})\big). \tag{4.41}$$

Employing the identity

$$\delta(x-a) \;=\; \frac{1}{2\pi}\int\limits_{-\infty}^{\infty}e^{i(x-a)t}dt,$$

we can rewrite (4.41) as

$$P(\vec{r},V) \;=\; \frac{1}{2\pi}\int\limits_{-\infty}^{\infty}e^{iVt}f(t;\vec{r})dt \tag{4.42}$$

where

$$f(t;\vec{r}) \;=\; \left[\int\limits_{\Omega}\frac{d\vec{R}}{\Omega}\,e^{-iv(\vec{r}-\vec{R})t}\right]^{N}. \tag{4.43}$$

---

* The impurity is completely random.

Thermodynamically, the extensive properties of a structure do not change if the volume increases. Applying this principle, the distribution function $P(\vec{r}, V)$ becomes

$$P(V) = \lim_{\substack{\Omega \to \infty \\ N = \bar{N}\Omega}} \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{iVt} \left[1 + \frac{1}{\Omega} \int_{\Omega} d\vec{R} \left(e^{-iv(\vec{R})t} - 1 \right) \right]^N dt \qquad (4.44)$$

where $\bar{N}$ is impurity density. Moreover, $P(V)$ turns out to be independent of position $\vec{r}$, because the change of variables in Eq. (4.44) does not alter the integral if $\Omega \to \infty$. Suppose that

$$A = \int_{\Omega} d\vec{R} \left(\exp\left(-iv(\vec{R})t\right) - 1 \right). \qquad (4.45)$$

If $v(\vec{r})$ decreases sufficiently rapidly, then A rapidly approaches a constant value, even while the volume Ω keeps increasing. The following relationship then applies :

$$\lim_{\Omega \to \infty} \left[1 + \frac{A}{\Omega} \right]^{\bar{N}\Omega} = \exp(A\bar{N}),$$

and we finally obtain the exact result

$$P(V) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \exp\left[iVt + \bar{N} \int d\vec{R} \left(e^{-iv(\vec{R})t} - 1 \right) \right] dt. \qquad (4.46)$$

In the high-density limit (Gaussian model : $v \to 0$, $\overline{N} \to \infty$ and $\overline{N}v^2 = $ finite), $P(V)$ reduces to

$$P(V) = \frac{1}{2\pi} \int\limits_{-\infty}^{\infty} dt \exp\left[iVt - i\overline{N}t\int d\vec{R}\, v(\vec{R}) - \frac{\overline{N}t^2}{2}\int d\vec{R}\, v^2(\vec{R}) \right], \qquad (4.47)$$

where $\overline{N}\int d\vec{R}\, v(\vec{R})$ means average potential of the charged impurities, is denoted by E_0 , and $\overline{N}\int d\vec{R}\, v^2(\vec{R})$ is the mean square fluctuation in the potential of the charged impurities or fluctuation parameter[11] ,ξ_Q . So that

$$P(V) = \frac{1}{2\pi} \int\limits_{-\infty}^{\infty} dt \exp\left[iVt - iE_0t - \frac{\xi_Q}{2}t^2 \right]$$

$$= \frac{1}{\left(2\pi\xi_Q\right)^{1/2}} \exp\left[-\frac{(V - E_0)^2}{2\xi_Q} \right] \qquad (4.48)$$

This is the distribution function of the potential energy V for high-density limit.

In high-density limit (highly impure semiconductors), Kane treats the potential of impurity(v) as the screened Coulomb potential

$$v(\vec{r} - \vec{R}) = -\frac{e^2}{\varepsilon_0} \exp\left(-Q|\vec{r} - \vec{R}|\right), \qquad (4.49)$$

the potential agrees well with the Thomas-Fermi approximation used by Kane to construct the semiclassical density of states, as we show below.

From the Thomas-Fermi theory of screening (sub-section 4.1.2), we consider the case where the external potential is that of a point charge (only $Z = +1$ impurity) :

$$\phi^{ext}(\vec{r}) = \frac{e}{\varepsilon_0 |\vec{r}|}, \tag{4.50}$$

and its Fourier transform is

$$\phi^{ext}(\vec{q}) = \frac{4\pi e}{\varepsilon_0 q^2}. \tag{4.51}$$

Substituting (4.51) and (4.25) in (4.7), the total potential will then be

$$\phi(\vec{q}) = \frac{4\pi e}{\varepsilon_0 (q^2 + Q^2)}. \tag{4.52}$$

The Fourier transform can be inverted to give

$$\phi(\vec{r}) = \int \frac{d\vec{q}}{(2\pi)^3} \frac{4\pi e}{\varepsilon_0 (q^2 + Q^2)} \exp(i\vec{q}.\vec{r})$$

$$= \frac{e}{\varepsilon_0 |\vec{r}|} \exp\{-Q |\vec{r}|\}, \tag{4.53}$$

but the potential energy of electron at $\vec{r}$ due to an impurity at $\vec{R}$, $v(\vec{r}-\vec{R})$,

$$v(\vec{r}-\vec{R}) = -e\phi(\vec{r}-\vec{R})$$

$$= -\frac{e^2}{\varepsilon_0|\vec{r}-\vec{R}|}\exp\left\{-Q\left|\vec{r}-\vec{R}\right|\right\}, \qquad (4.54)$$

same as (4.49).

Constructing the density of states with a screened Coulomb potential by substituting (4.48) in (4.39) gives the Kane density of states

$$\rho(E) = \frac{m^{*3/2}}{2\pi^{5/2}\hbar^3\xi_Q^{1/2}} \int\limits_{-\infty}^{E} dV\,(E-V)^{1/2}\exp\left[-\frac{(V-E_0)^2}{2\xi_Q^{1/2}}\right] \qquad (4.55)$$

where

$$E_0 = -\frac{4\pi\bar{N}e^2}{\varepsilon_0 Q^2} \qquad (4.56)$$

$$\xi_Q = \frac{2\pi\bar{N}e^4}{\varepsilon_0^2 Q}. \qquad (4.57)$$

Equation (4.55) can be written in terms of the parabolic cylinder function $D_{-a-1/2}(z)$, which offers useful mathematical relations as

$$\rho(E) = \frac{m^{*3/2}}{4\pi^2\hbar^3}\xi_Q^{1/4}\exp\left\{-\frac{(E-E_0)^2}{4\xi_Q}\right\}D_{-3/2}\left(\frac{E_0-E}{\sqrt{\xi_Q}}\right), \quad (4.58)$$

where

$$D_{-a-1/2}(z) = \frac{1}{\Gamma(1/2+a)}\exp\left[-\frac{z^2}{4}\right]\int_0^\infty \exp\left\{-\frac{s^2}{2}-zs\right\}s^{a-1/2}ds$$

For general bottom of the conduction band edge in the pure semiconductor E_c^0 and the shifted conduction band edge in an impure semiconductor due to impurities E_c, (4.58) can be written as

$$\rho(E) = \frac{m^{*3/2}}{4\pi^2\hbar^3}\xi_Q^{1/4}\exp\left\{-\frac{(E-E_0-E_c^0)^2}{4\xi_Q}\right\}D_{-3/2}\left(\frac{E_0+E_c^0-E}{\sqrt{\xi_Q}}\right) \quad (4.59)$$

or

$$\rho(E) = \frac{m^{*3/2}}{4\pi^2\hbar^3}\xi_Q^{1/4}\exp\left\{-\frac{(E-E_c)^2}{4\xi_Q}\right\}D_{-3/2}\left(\frac{E_c-E}{\sqrt{\xi_Q}}\right) \quad (4.60)$$
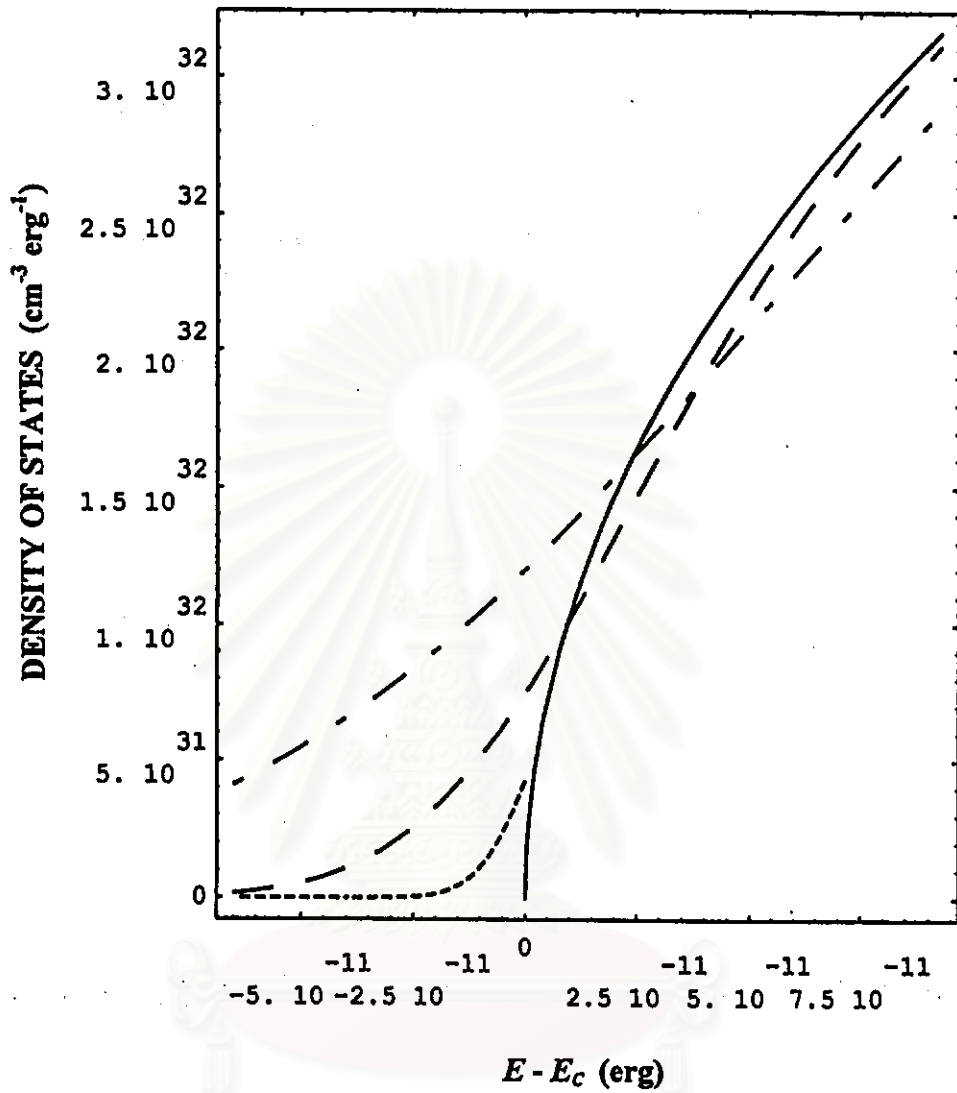
of which its asymptotes are

$$\rho(E) = \frac{m^{*3/2}}{\sqrt{2}\pi^2\hbar^3}(E-E_c)^{1/2} \quad \text{when} \quad \frac{(E-E_c)}{\sqrt{\xi_Q}} \gg 1$$

$$\rho(E) = \frac{m^{*3/2}}{4\pi^2\hbar^3}\frac{\xi_Q}{(E_c-E)^{3/2}}\exp\left[-\frac{(E-E_c)^2}{2\xi_Q}\right] \quad \text{when} \quad \frac{(E-E_c)}{\sqrt{\xi_Q}} \ll -1$$

Equation (4.58), (4.59) and (4.60) is Kane's density of states which we want to derive and evaluate the diffusivity-mobility ratio for n-type heavily doped semiconductor in next section.

<u>Figure 1</u> Kane's density of states at temperature $T = 10$K, without compensation ratio $(N_a/N_d = 0.0)$ for net carrier concentration $N_d - N_a = 1.000\text{x}10^{19}$ cm^{-3} (– —— – ——), $1.000\text{x}10^{18}$ cm^{-3} (— — ——), $5.000\text{x}10^{16}$ cm^{-3} (– – – – – –),   and for free particles (———)

4.3 The diffusivity-mobility ratio for n-type heavily doped semiconductors

In previous section the Thomas-Fermi approximation of screening and the generalized diffusivity-mobility ratio were known. In this section we will derive the diffusivity-mobility ratio for n-type heavily doped semiconductors in limit of the Thomas-Fermi approximation and compare our result with the empirical diffusivity-mobility ratio by Van Cong and Debiais in extremely high degenerate region.

4.3.1 The diffusivity-mobility ratio for n-type heavily doped semiconductors

The generalized diffusivity-mobility ratio, the ratio between the diffusion coefficient D and the majority-carrier mobility μ in n-type semiconductors, is known in the form (2.11)

$$\frac{D}{\mu} = \frac{n}{e}\left(\frac{dE_f}{dn}\right)_{T,V},\qquad (4.61)$$

where an E_f is measured from the bottom of the conduction band. To evaluate the value of the ratio D/μ, one needs to know how the Fermi energy depends on the electron concentration. Physically, when extra electrons are introduced to a system, the Fermi energy increases as a function of electron concentration. The number of electron concentration n is simply determined from the expression

$$n = 2\int_{-\infty}^{\infty} \rho(E)f(E,E_f,T)dE,$$ (4.62)

where $\rho(E)$ is the electron density of states of the system, when a single state is allowed in each energy level, and f is the Fermi distribution function. Inversely, the Fermi energy is dependent on the number of electron concentration through the relation in (4.62) and seems to be easy to determine.

However, the density of states is also a function of the electron concentration as the increase of the tail according to doping, for example. The doping enhances the screening of potential of the positive ions seen by an electron, the screening constant Q is related to the density of states through a simple equation in the Thomas-Fermi approximation as (4.29)

$$Q^2 = 2\left(\frac{4\pi e^2}{\varepsilon_0}\right)\int_{-\infty}^{\infty} \rho(E)\left(-\frac{\partial f}{\partial E}\right)dE.$$ (4.63)

From the Thomas-Fermi approximation of screening (sub-section 4.1.2), we know that the relation between Q and dn/dE_f (4.26) is

$$Q^2 = \frac{4\pi e^2}{\varepsilon_0}\frac{dn}{dE_f}.$$ (4.64)

Equation (4.61) with (4.63) and (4.64), we obtain the D/μ ratio in terms of density

of states as

$$\frac{D}{\mu} = \frac{n}{2e}\left[\int_{-\infty}^{\infty}\rho(E)\left(\frac{\partial f}{\partial E}\right)dE\right]^{-1}. \qquad (4.65)$$
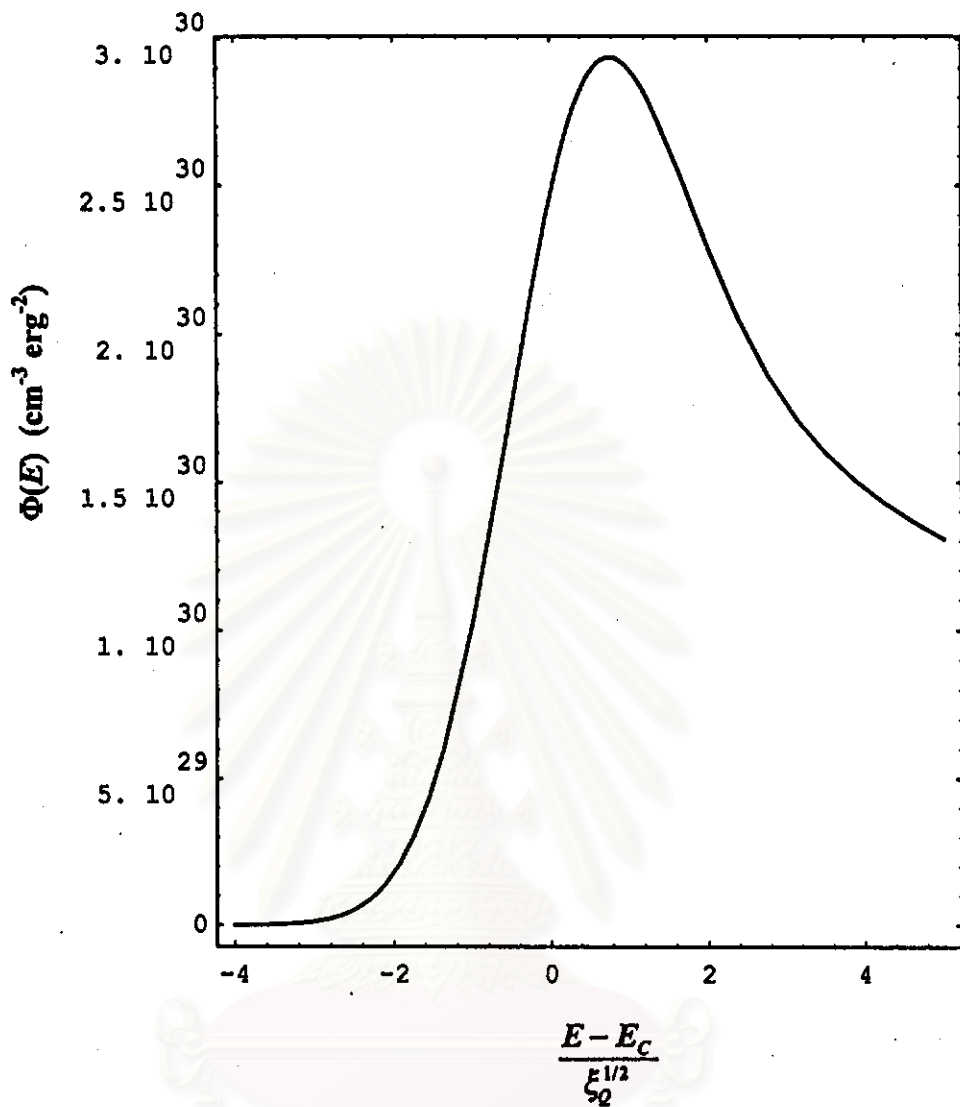
integrating by parts leads above equation to

$$\frac{D}{\mu} = \frac{n}{2e}\left[\int_{-\infty}^{\infty}\Phi(E)f(E,E_f,T)dE\right]^{-1}, \qquad (4.66)$$

where

$$\Phi(E) \equiv \frac{d\rho(E)}{dE}.$$

Figure 2 Derivative of Kane's density of states $\Phi(E)$ at temperature $T = 10K$, without compensation ratio $(N_a/N_d = 0.0)$ and net carrier concentration $N_d - N_a = 1.000 \times 10^{18} \text{cm}^{-3}$

By considering the characteristic of Φ versus E (Figure 2), we see that

i) as $E \to -\infty$: $\Phi \to 0$,

ii) as $E \to \infty$: $\Phi \to 0$,

which agree well with the Sommerfeld expansion[7] [Appendix]. Expansion of the integral in (4.66) leads to

$$\frac{D}{\mu} = \frac{n}{2e}\left[\int_{-\infty}^{E_f}\Phi(E)dE + \sum_{i=1}^{\infty}a_n(k_BT)^{2i}\frac{\partial^{2i-1}\Phi(E)}{\partial E^{2i-1}}\bigg|_{E=E_f}\right]^{-1}, \qquad (4.67)$$

or

$$\frac{D}{\mu} = \frac{n}{2e}\left[\rho(E)\big|_{E=E_f} + \sum_{i=1}^{\infty}a_i(k_BT)^{2i}\frac{\partial^{2i}\rho(E)}{\partial E^{2i}}\bigg|_{E=E_f}\right]^{-1}, \qquad (4.68)$$

where the coefficients a_i are

$$a_i = \left\{2 - \frac{1}{2^{2(ii)}}\right\}\varsigma(2i) , \qquad (4.69)$$

where $\varsigma(x)$ is the Reimann Zeta function. Some coefficients are $a_1 = 1.645$, $a_2 = 1.894$, $a_3 = 1.971$.

Equation (4.68) is the diffusivity-mobility ratio for n-type heavily doped semiconductors in limit of the Thomas-Fermi approximation or moderately degenerate region and higher.

Usually, the second term in parenthesis of (4.68) is very small, compared with the first term especially in extremely degenerate region (very high E_f). Then (4.68) becomes

$$\frac{D}{\mu} = \frac{n}{2e}\left(\frac{1}{\rho(E_f)}\right). \qquad (4.70)$$

In extremely degenerate region, the band tail density of states has same values as parabolic band density of states, $\rho_0(E)$:

$$\rho_0(E) = \frac{1}{4\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2} E^{1/2}, \qquad (4.71)$$

where E measured from the bottom edge of conduction band.

Combining (4.70) and (4.71) provides

$$\frac{D}{\mu} = \frac{n}{2e}\left[\frac{1}{4\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2} E_f^{1/2}\right]^{-1}. \qquad (4.72)$$

By comparing (4.72) with (4.61), we see that

$$\frac{dn}{dE_f} = 2\left(\frac{1}{4\pi^2}\right)\left(\frac{2m^*}{\hbar^2}\right)^{3/2} E_f^{1/2},$$

$$dn = 2\left(\frac{1}{4\pi^2}\right)\left(\frac{2m^*}{\hbar^2}\right)^{3/2} E_f^{1/2} dE_f. \tag{4.73}$$

Integrating both side of (4.73) gives

$$\int_{n_0}^{n} dn' = 2\left(\frac{1}{4\pi^2}\right)\left(\frac{2m^*}{\hbar^2}\right)^{3/2} \int_{0}^{E_f} E_f'^{1/2} dE_f'$$

$$n - n_0 = \frac{4}{3}\left(\frac{1}{4\pi^2}\right)\left(\frac{2m^*}{\hbar^2}\right)^{3/2} E_f^{3/2},$$

or

$$E_f = \frac{\hbar^2}{2m^*}\left[3\pi^2(n - n_0)\right]^{2/3}. \tag{4.74}$$

In extremely degenerate region, n is much larger than n_0, therefore $n - n_0 \approx n$ and

(4.74) becomes

$$E_f = \frac{\hbar^2}{2m^*}\left[3\pi^2 n\right]^{2/3}. \tag{4.75}$$

Substituting (4.75) in (4.72) gives

$$\frac{D}{\mu} = \frac{n}{2e}\left[\frac{1}{4\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\left(\frac{\hbar^2}{2m^*}\right)^{1/2}\left(3\pi^2 n\right)^{1/3}\right]^{-1}$$

$$= \frac{\pi\hbar^2}{em^*}\left(\frac{\pi}{3}\right)^{1/3}n^{2/3}, \tag{4.76}$$

or with the Van Cong and Dabiais's notation as of in Chapter III, (4.76) becomes

$$\frac{D}{\mu} = V_T\left(\frac{\pi}{6}\right)^{1/3}u^{2/3}, \tag{4.77}$$

which is identical to that derived by Van Cong and Dabiais result in (3.22).

Finally, we obtain the diffusivity-mobility ratio for n-type heavily doped semiconductors in the limit of the Thomas-Fermi approximation. In the next chapter, we will make use of this result to obtain the numerical results.

4.3.2 Numerical evaluation

In order to evaluate the diffusivity-mobility ratio for n-type heavily doped that we derive in previous section (4.68) at temperature T we need to know the Fermi energy, E_f, and the screening length Q^{-1} for a given net carrier concentration ($N_d - N_a$) and a compensation ratio (N_a/N_d).

Within the band model assumed in section 4.2, the net carrier concentration is

$$N_d - N_a = 2 \int_{-\infty}^{\infty} dE \, \rho_K(E) f\left(E, E_f, T\right), \qquad (4.78)$$

where $f(E, E_f, T)$ is the Fermi distribution function and $\rho_K(E)$ is Kane's density of states (4.58),

$$\rho_K(E) = \frac{m^{*3/2}}{4\pi^2 \hbar^3} \xi_Q^{1/4} \exp\left\{-\frac{(E - E_c)^2}{4\xi_Q}\right\} D_{-3/2}\left(\frac{E_c - E}{\sqrt{\xi_Q}}\right). \qquad (4.79)$$

This result is used to determine the Fermi energy E_f. In the Thomas-Fermi approximation the square of the inverse screening length (4.29) is

$$Q^2 = 2\left(\frac{4\pi e^2}{\varepsilon_0}\right) \int_{-\infty}^{\infty} dE \, \rho_K(E)\left(-\frac{\partial f}{\partial E}\right) \qquad (4.80)$$

Since the density of states $\rho_{_K}(E)$ depends upon Q through (4.57),

$$\xi_Q = \left(\frac{2\pi e^4}{Q\varepsilon_0^2}\right)(N_a + N_d).$$ (4.81)

Equation (4.78) and (4.80) must be solved iteratively until self consistent. To begin the iteration, we use an inverse screening length obtained using the degenerate parabolic band density of states $\rho_0(E)$:

$$\rho_0(E) = \frac{1}{4\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{3/2}\left(E - E_c\right)^{1/2},$$ (4.82)

to substitute in (4.80) and obtain

$$Q^2 = \frac{4m^*e^2}{\varepsilon_0\hbar^2}\left[\frac{3}{\pi}(N_d - N_a)\right]^{1/3}.$$ (4.83)

Since the final screening length obtained by (4.80) differs by only 10-20% from this initial screening length, the iteration then converges rapidly. In the integrands we replace the lower limit (-∞) by

$$E_{min} = E_C - 4\xi_Q^{1/2}$$ (4.84)

and the upper limit (+∞) by

$$E_{max} = E_f + 15k_B T \qquad (4.85)$$

which introduces an error of less than 0.01% in the integrations.

Within the Fermi energy, E_f, and the screening length, Q^{-1}, for a given net carrier concentration $(N_d - N_a)$ and a compensation ratio (N_a / N_d), we obtain a numerical result of the diffusivity-mobility ratio from (4.68)

$$\frac{D}{\mu} = \frac{(N_d - N_a)}{2e} \left[\rho_K(E)\Big|_{E=E_f} + \sum_{i=1}^{\infty} a_i (k_B T)^{2i} \frac{\partial^{2i} \rho_K(E)}{\partial E^{2i}}\Big|_{E=E_f} \right]^{-1} . \qquad (4.86)$$

In practice, the infinite-term summation is replaced by a two-term summation of with an error less than 0.001% in limit of the Thomas-Fermi approximation (4.36)

$$\xi_Q^{1/2} \leq E_f - E_c. \qquad (4.87)$$

The numerical evaluation process which we mention above, can be summarized into the flow chart in figure 3. Numerical results of the diffusivity-mobility ratio in the limit of the Thomas-Fermi approximation are shown in next chapter.

$$\text{START}$$

INPUT : N_d, N_a, N_a/N_d, T

$$E_{f_1} = \left[3\pi^2 \left(\frac{\hbar^2}{2m^*} \right)^{1/2} \left(N_d - N_a \right) \right]^{2/3}$$

$$Q_1 = \left[\frac{4m^*e^2}{\varepsilon_0 \hbar^2} \left(\frac{3}{\pi} \left(N_d - N_a \right) \right)^{1/3} \right]^{1/2}$$

$$\xi_Q = \frac{2\pi e^4}{Q_1 \varepsilon_0^2} \left(N_a + N_d \right)$$

$$Q_2 = \left[\frac{8\pi e^2}{\varepsilon_0} \int \rho_K(E, \xi_Q) \left(-\frac{\partial f(E, E_{f_1}, T)}{\partial E} \right) dE \right]^{1/2}$$

$Q_1 <= Q_2$ ← no — $Q_1 = Q_2$

↓ yes

Find E_{f_2} : $N_d - N_a = \int \rho_K(E, \xi_Q) f(E, E_{f_1}, T) dE$

$E_{f_2} = E_{f_1}$ — no → $E_{f_1} <= E_{f_2}$

↓ yes

OUTPUT : Q_2, E_{f_2}

CALC. : $\frac{D}{\mu} (N_d, N_a, E_{f_1}, Q_2, T)$

OUTPUT : $\frac{D}{\mu}$ as function of $N_d - N_a$
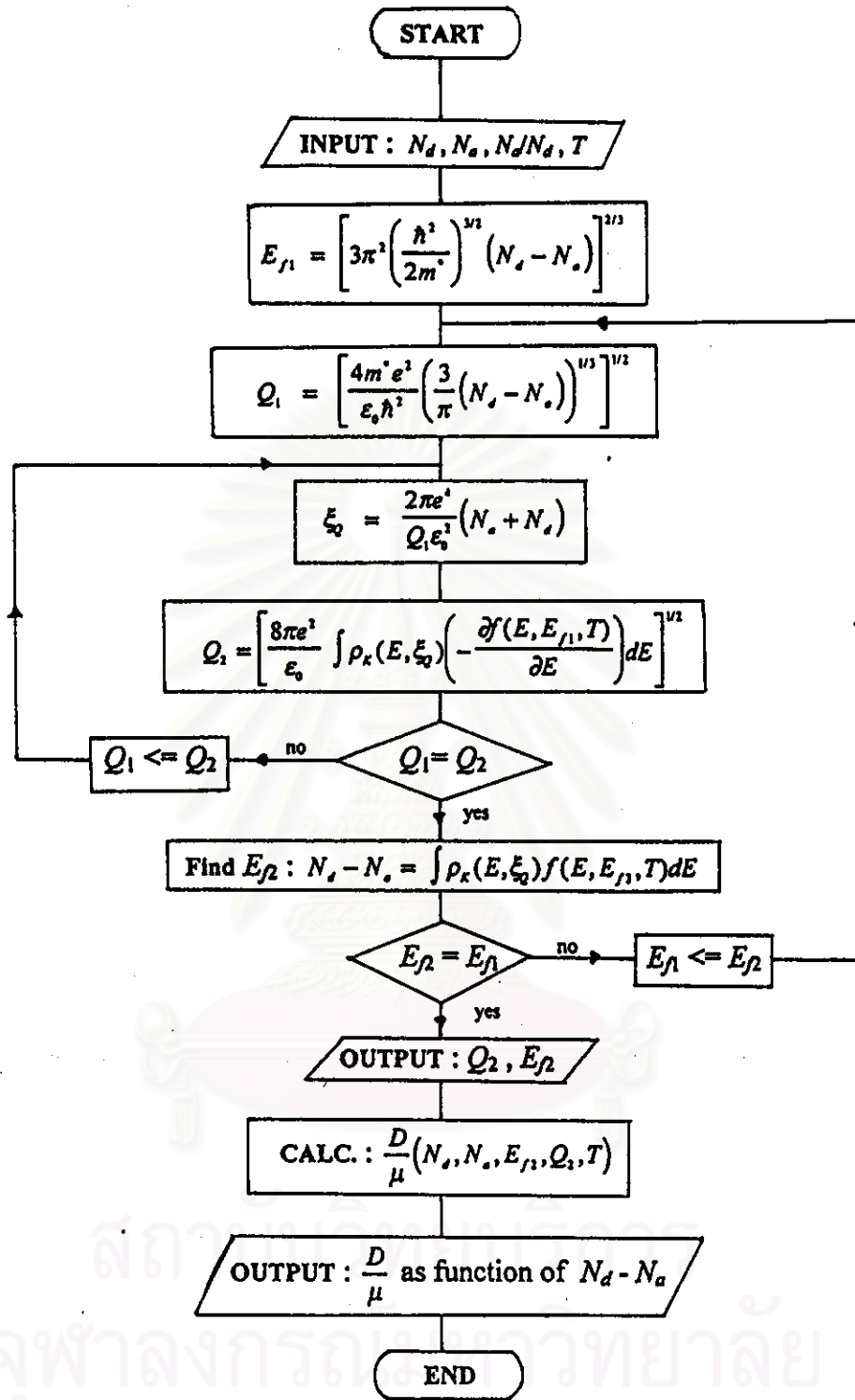
$$\text{END}$$

Figure 3 Flow chart of numerical evaluation of the diffusivity-mobility ratio.