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## Diffusion of Arsenic in Degenerate Silicon: a Quasi-Static Approach.

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RITUPARNA SHRIVASTAVA

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DIFFUSION OF ARSENIC IN DEGENERATE SILICON:

A QUASI-STATIC APPROACH

A Dissertation

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Louisiana State University and  
Agricultural and Mechanical College  
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## ABSTRACT

Diffusion under controlled conditions is one of the most important processes employed in the manufacture of semiconductor devices. The diffusion of group III and group V impurities in semiconductor material has been a subject of considerable work. It has been known for many years that diffusion in silicon at high concentrations, say  $10^{21} \text{ cm}^{-3}$ , produces impurity profiles that differ significantly from those predicted by a simple theory. This difficulty hinders the work of those engaged in the design of modern semiconductor devices, such as transistors, solar cells and integrated circuits, for which accurate process prediction is desirable.

The object of this research is to develop and study the models describing a constant source diffusion process which will accurately and efficiently predict the results of such a process. The effect of the internal electric field produced during the diffusion is analyzed using a quasi-static approximation for the holes and electrons. The use of both Fermi-Dirac and Maxwell-Boltzmann statistics is discussed. The assumption of charge neutrality is investigated under typical diffusion conditions. At relatively higher surface concentrations, in addition to the internal electric field, several other effects must be considered. In the present work, a model for arsenic diffusion in silicon is proposed which takes into account

the degeneracy of the carriers, partial ionization of the impurities, single acceptor level vacancies and the internal electric field.

The transport process for holes, electrons and impurities is described by the flux equations, the continuity equations and Gauss' law. Although simplifying assumptions are made, the resulting partial differential equations are highly nonlinear, and a numerical scheme must be used to solve the problem. An efficient computer program based on a quasi-linearization technique is written to obtain the impurity profiles from the processing data. Several other computer programs are used to investigate different models.

It is found that the internal electric field enhances diffusion at high concentrations. The electric field profiles are reminiscent of those obtained in a high-low junction. It is noted that the field varies almost linearly near the surface and then reaches a maximum value. Charge neutrality under typical diffusion conditions is found to be an excellent approximation. The results obtained using Fermi-Dirac statistics show that the use of classical statistics yields an underestimate of the impurity concentration values. At higher concentrations, incorporation of partial ionization, vacancies and degeneracy significantly affects the results obtained. There is a good agreement between the model and experimental

results based on neutron activation analysis. However, the impurity profiles strongly depend on the value of the intrinsic impurity diffusion coefficient.

## CHAPTER I

### INTRODUCTION

The term "diffusion", when applied to semiconductor device fabrication, is used loosely to describe impurity atom motion in a semiconductor at elevated temperatures. Diffusion under controlled conditions is one of the most important processes employed in the manufacture of semiconductor devices. In order to fabricate a device with a certain set of parameters, it is very important to be able to control the impurity diffusion profiles in the semiconductor wafer. The need for suitable models describing the diffusion phenomenon is evident.

In most practical situations, a constant source diffusion, a drive-in diffusion, or both are used. In the first case, surface concentration is held constant during the diffusion, whereas in the second case, the source is removed and redistribution takes place under the condition that the impurity atoms can neither enter nor leave the semiconductor wafer. In theory, it is possible to synthesize any given arbitrary profile compatible with the two-step process, by generating a proper control function [1]. However, in practice the direct profile resulting from the above two processes may be acceptable. We will mostly concern ourselves with the constant source diffusion process. In this process, the impurity atoms are introduced into a flowing inert gas, which deposits these atoms

on the surface of the semiconductor wafer. A desired surface concentration of the impurity atoms can be maintained. In practice, this value very often is equal to the solid solubility value. As the impurity atoms cross the surface and move into the semiconductor, some or most of them ionize depending on the concentration. If the motion of these ions were essentially the same as the motion of neutral particles, the flux  $f_c$  or the number of ions crossing a unit area in a unit time, will be given by Fick's law. For one-dimensional motion, and assuming parallel plane geometry,

$$f_c = -D_c \frac{\partial c(x,t)}{\partial x} \quad (1.1)$$

where  $D_c$  is the diffusion coefficient or diffusivity and  $c$  represents the concentration of ions. The ions also satisfy a continuity equation given by

$$\frac{\partial f_c}{\partial x} + \frac{\partial c}{\partial t} = G_c \quad (1.2)$$

where  $G_c$  is the net generation rate for ions. Assuming that all the impurity atoms ionize when they enter the surface, we can equate  $G_c$  to zero. Combining (1.1) and (1.2) then yields:

$$\frac{\partial c}{\partial t} = D_c \frac{\partial^2 c}{\partial x^2} . \quad (1.3)$$

This is called the simple diffusion equation. The solution to (1.3) for a semi-infinite solid under the constant source boundary conditions

$$c(0, t) = C_0 \quad (1.4a)$$

$$c(\infty, t) = 0 \quad (1.4b)$$

$$c(x, 0) = 0, \quad x > 0 \quad (1.4c)$$

is given by the complementary error function

$$c(x, t) = C_0 \operatorname{erfc}[x/(4D_1 t)^{1/2}] \quad (1.5)$$

where  $D_1$  is the value of  $D_c$  for the above diffusion step.

The boundary conditions for the drive-in diffusion are given by

$$c(x, 0) = c_1(x) \quad (1.6a)$$

$$\frac{\partial c(0, t)}{\partial x} = 0 \quad (1.6b)$$

$$c(\infty, t) = 0 . \quad (1.6c)$$

The solution to the diffusion equation in this case is [2]

$$c(x,t) = \frac{1}{2(\pi D_2 t)^{1/2}} \int_0^\infty c_1(\zeta) \left[ e^{-\frac{(x-\zeta)^2}{4D_2 t}} + e^{-\frac{(x+\zeta)^2}{4D_2 t}} \right] d\zeta \quad (1.7)$$

where  $D_2$  is the value of  $D_c$  for the drive-in cycle.

In the two-step diffusion process  $c_1(x)$  is given by (1.5). If the diffusion time for the first step  $t_1$  is such that  $D_1 t_1 \ll D_2 t$ , the delta function approximation for  $c_1(x)$  yields the Gaussian solution [3]

$$c(x,t) = \frac{2C_0}{\pi} \left( \frac{D_1 t_1}{D_2 t} \right)^{1/2} e^{-\frac{x^2}{4D_2 t}} \quad (1.8)$$

for the two-step diffusion profile.

It has been known for many years that the results of simple diffusion theory do not agree with experiment except at low surface concentrations [4]. This departure, to some extent, can be explained by the presence of an internal electric field which arises because of a mismatch in the diffusion coefficients of the impurity ions and the mobile carriers. For example, when arsenic atoms enter the solid, most of them ionize because of the high temperature, resulting in positive ions and electrons. The electrons tend to diffuse away from the ions due to a much higher diffusion coefficient. Since both species carry electrical

charge, an electric field develops which tends to retard the motion of electrons and enhance the motion of ions. The incorporation of this electric field in the model yields impurity density profiles which are closer to experimental results. However, the general differential equations governing field-aided diffusion are quite nonlinear and complex and a need for simple models soon becomes evident. Most of the models found in the literature assume local charge neutrality and are valid for nondegenerate conditions. In Chapter 2, the assumption of local charge neutrality has been examined with reference to a quasi-static approximation for both nondegenerate and degenerate statistics.

The field-aided diffusion theory described above, in itself, is inadequate to explain the experimental observations at relatively higher concentrations. At such high concentrations the effect of defects in the lattice becomes very important. Before considering the defects, it will be instructive to briefly discuss various mechanisms of diffusion in semiconductors [5]. Ring mechanism and direct interchange of neighboring atoms have been considered improbable. A "direct interstitial" mechanism has been suggested in which a lattice atom leaves its regular substitutional site and becomes an interstitial. One of its nearest neighboring substitutional atoms moves into the vacancy left behind by the first atom. Then the first atom, now at the interstitial position, moves into



the vacancy left behind by the second atom thus completing the cycle of indirect exchange. However, it can be argued that even such an interchange would be less likely than a vacancy mechanism. Defect-aided mechanisms are more probable in silicon and germanium. Most important of them are vacancy and interstitialcy (or indirect interstitial) mechanisms. In the vacancy mechanism the host atom is missing from its regular site and this enhances the impurity diffusion. In the interstitialcy mechanism, the interstitial atom chooses to move by pushing one of its nearest neighbors into another interstitial site and it itself takes up the substitutional site. Group III and Group V elements form strong covalent bonds with silicon and germanium atoms. This results in their existence being almost entirely in the substitutional form. A consequence of this is that they diffuse predominantly by either a vacancy or an interstitialcy mechanism. A definite statement about the mechanism, however, can not be made. A number of experimental techniques have demonstrated that vacancies and presumably interstitials may exist in different charge states. The effect of strong doping on self and impurity diffusion is closely tied to the acceptor and donor actions of the vacancies and interstitials.

An excellent review on diffusion mechanisms and point defects in Si and Ge can be found in [6]. It has become

customary to classify impurities as "slow" and "fast" diffusors. Diffusion coefficients of slow diffusors are 10-100 times higher than self diffusion coefficients. Fast diffusors usually diffuse several orders of magnitude faster than slow diffusors. Group III and Group V elements are typical representatives of slow diffusors. It is generally assumed that the diffusion mechanism involved in slow diffusors is a simple vacancy mechanism. A quantitative model for diffusion of these impurities was proposed by Swalin. His model seems to support vacancy mechanism in Ge and donor impurity diffusion via vacancies in Si. It however does not explain acceptor impurity diffusion in Si, for which Seeger and Chik have proposed the interstitialcy mechanism discussed before. An explanation in favor of donor impurity diffusion in Si, via vacancies, is that the Coulomb interaction between positively charged donors and negatively charged vacancies leads to an increased probability of finding a vacancy near a donor impurity, and therefore enhances the impurity diffusion.

A simple way to see how a vacancy may act as an acceptor is as follows [7]. There are four covalent bonds missing at the sight of a vacancy. This gives rise to a strong change in the valence electron distribution in the vicinity of the vacancy and leads to a lattice distortion. From a scattering theory point of view, it means that an atomic scatterer is missing in the lattice. This results

in the introduction of some bound states in the band gap. The vacancy may trap electrons from the valence band in these localized states. When a hole is introduced because of the electron making a transition to one of the localized states from the valence band, the vacancy becomes negatively charged because of the trapped electron and thus acts as an ionized p-type impurity. As discussed by Seeger and Chik, concentration of acceptor type defects is increased by n-type doping and decreased by p-type doping. Thus, diffusion via vacancies should be faster in n-doped material, and slower in p-doped material compared to the intrinsic material.

Evidence indicating that vacancies act as acceptors is found in the data obtained from irradiated Ge by Cleland, Crawford and Holmes [8]. In this study, the effect of  $\gamma$ -radiation on electrical properties of Ge was studied. Results indicate that exposure of n-type Ge to  $\gamma$ -rays decreases the extrinsic electron concentration. Valenta and Ramasastry [9] have explained the effect of heavy doping on self-diffusion of Ge by assuming that vacancies act as acceptors. Agreement for n-type data was fair, whereas p-type data did not agree that well. The discrepancy was not attributed to the above assumption, namely, that vacancies act as acceptors, and it was concluded that Ge self diffusion probably occurs via vacancies. The doping effect on impurity diffusion in Ge

is also in general agreement with vacancy model of diffusion. Because of the low concentration of point defects, it has not yet been possible to detect directly the presence of point defects in Si and Ge in thermal equilibrium at high temperatures.

Two classical models of the energy levels of vacancies and interstitials are that of James and Lark-Horowitz [10], and of Blount [11]. In the first model, interstitials act as donors and vacancies act as acceptors. In Blount's model on the other hand, interstitials and vacancies may act as both acceptors and donors. This is favored for the interstitialcy mechanism proposed by Seeger and Chik to explain the impurity diffusion of Group III and Group V elements in Si, whereas the fact that double negatively charged vacancies can exist is a point in favor of the James and Lark-Horowitz model.

With the above background in mind, the diffusion phenomenon will be discussed in the subsequent chapters. The object of the present research is to develop the models describing the diffusion phenomenon which include the effects of internal electric field, vacancies, partial ionization, and degeneracy of carriers. In Chapter 2, field-aided diffusion is discussed under degenerate and complete impurity ionization conditions. The assumption of local charge neutrality is investigated. In Chapter 3, Hu's theory of impurity diffusion [12] is applied to

arsenic diffusion in silicon under general conditions. Numerical computation of impurity profiles and results are discussed in Chapters 4 and 5, and the conclusions summarized in Chapter 6.

## CHAPTER 2

### FIELD-AIDED DIFFUSION

In an intrinsic semiconductor, at thermal equilibrium, holes and electrons are produced in equal numbers by thermal processes. When impurity atoms are introduced, they ionize and alter the concentration of majority carriers (e.g. electrons for an n-type impurity). As a result, the majority carrier concentration increases and due to recombination the minority carrier concentration decreases. The product  $pn$  remains constant at thermal equilibrium for a nondegenerate semiconductor. When the semiconductor is out of thermal equilibrium, it is necessary to consider the motions of electrons, holes, and impurity ions simultaneously, because the charge density at any point is a function of the concentrations of these species.

The analysis in the present work is restricted to the case of a constant band gap semiconductor at a constant temperature. It is also assumed that the impurities are singly ionized.

#### 2.1 Transport Equations for Nondegenerate Case

For a semi-infinite solid, a one-dimensional diffusion process for  $x \geq 0$ ,  $t \geq 0$  is defined by the flux equations, continuity equations, Poisson's equation, and appropriate boundary conditions.

The flux equations for an arbitrary carrier are given by

$$f_{\alpha} = - D_{\alpha} \frac{\partial \alpha}{\partial x} + Z_{\alpha} \mu_{\alpha} \alpha E \quad (2.1)$$

where  $\alpha$  represents the concentration of an arbitrary carrier ( $n$ ,  $p$  or  $c$  for electrons, holes or impurity ions, respectively),  $D_{\alpha}$  is the diffusion coefficient,  $\mu_{\alpha}$  is the mobility,  $E$  is the electric field, and  $Z_{\alpha}$  takes on the value  $+1$  or  $-1$  for a positive or negative carrier charge, respectively.

The continuity equation for the carrier  $\alpha$  is

$$\frac{\partial \alpha}{\partial t} = - \frac{\partial f_{\alpha}}{\partial x} + G_{\alpha} \quad (2.2)$$

where  $G_{\alpha}$  represents the net generation rate of the carrier.

Using the nondegenerate Einstein relation

$$\frac{D_{\alpha}}{\mu_{\alpha}} = \frac{kT}{e} \equiv V_T \quad (2.3)$$

and assuming 100% impurity ionization, which implies that

$$G_p = G_n \equiv G, \quad (2.4)$$

the general equations can be written as

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial x} \left[ D_p \frac{\partial p}{\partial x} - \frac{D_p p E}{V_T} \right] + G \quad (2.5a)$$

$$\frac{\partial n}{\partial t} = \frac{\partial}{\partial x} \left[ D_n \frac{\partial n}{\partial x} + \frac{D_n n E}{V_T} \right] + G \quad (2.5b)$$

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left[ D_c \frac{\partial c}{\partial x} - z_c \frac{D_c c E}{V_T} \right] . \quad (2.5c)$$

Poisson's equation yields

$$\frac{\partial E}{\partial x} = \frac{\rho}{\epsilon} = \frac{e}{\epsilon} (p - n + z_c c) \quad (2.6)$$

where  $\rho$  represents the charge density. Note that  $z_c = 1$  for donors and  $z_c = -1$  for acceptors. The permittivity  $\epsilon$  will be assumed constant.

The net generation rate  $G$  may be represented by the Shockley-Read-Hall model

$$G = - \frac{pn - n_i^2}{\tau_n (p + n_i) + \tau_p (n + n_i)} \quad (2.7)$$

where  $n_i$  is the intrinsic concentration of electrons and holes, and  $\tau_p$  and  $\tau_n$  are the lifetimes of holes and electrons, respectively.

The boundary conditions are governed by the kind of diffusion process. In most of the work, for simplicity, a constant source diffusion will be assumed in which case the boundary conditions are given by



$$c(x,0) = 0 \quad , \quad x > 0 \quad (2.8a)$$

$$p(x,0) = n(x,0) = n_i \quad , \quad x > 0 \quad (2.8b)$$

$$E(\infty, t) = 0 \quad (2.8c)$$

$$c(0, t) = C_0 \quad (2.8d)$$

$$\frac{\partial \alpha_{maj}(0, t)}{\partial x} = \frac{D_c}{D_{maj}} \frac{\partial c(0, t)}{\partial x} \quad (2.8e)$$

$$\frac{\partial \alpha_{min}(0, t)}{\partial x} = 0 \quad (2.8f)$$

where  $\alpha_{maj}$  and  $\alpha_{min}$  are majority and minority carrier concentrations, respectively.

## 2.2 Previous Work

The effect of the electric field on the transport process was first considered by Zaromb [13] and Smits [14]. Their work was based upon two major assumptions.

1. The material is charge-neutral at every point so that

$$\frac{\rho}{\epsilon} = p - n + Z_c c = 0 \quad (2.9)$$

2. It is assumed that  $pn = n_i^2$ . Strictly, this relation is only valid in thermal equilibrium for a nondegenerate semiconductor.

The electric field can then be expressed as

$$E = - z_c V_T \frac{1}{\sqrt{c^2 + 4n_i^2}} \frac{\partial c}{\partial x} . \quad (2.10)$$

An expression similar to (2.10) was derived by Kurtz and Yee [15] who neglected the effect of the minority current. They pointed out that an effective diffusion constant  $D_{\text{eff}}$  can be defined when (2.10) is used in the flux equation for the impurity atoms (2.1) to give

$$f_c = -D_{\text{eff}} \frac{\partial c}{\partial x} \quad (2.11)$$

where

$$D_{\text{eff}} = D_c \left( 1 + \frac{c}{\sqrt{c^2 + 4n_i^2}} \right) . \quad (2.12)$$

Substitution of (2.11) into the continuity equation yields

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left[ D_c \left( 1 + \frac{c}{\sqrt{c^2 + 4n_i^2}} \right) \frac{\partial c}{\partial x} \right] . \quad (2.13)$$

Lehovec and Slobodskoy [16] have obtained an approximate solution to the above equation for a constant source diffusion into an otherwise intrinsic semiconductor. They also provided the "corrections" to the surface concentration by extrapolating from the tail of the impurity distribution using a complementary error function.

Bordina et al. [17] have discussed the influence of the internal electric field by assuming that it may be taken as uniform. They then conclude that an effective doubling of the diffusion coefficient takes place in a region where  $c \gg n_i$ .

Vas'kin et al. [18] have treated impurity diffusion into a semiconductor uniformly doped with an impurity of the opposite type under the assumption that the local electric field can be represented by an average field defined in terms of a weighting function. Shaw and Wells [19] have analyzed the same problem without making the above assumption and have obtained numerical solutions for the impurity distributions. Klein and Beal [20] have discussed the case of simultaneous diffusion of oppositely charged impurities.

Nuyts and Van Overstraeten [21] have calculated the impurity diffusion profiles in silicon taking into account the diffusion of the base impurities. They have also discussed the use of degenerate statistics and partial impurity ionization although no computations have been

made incorporating these aspects. Hu and Schmidt [22] have also calculated constant source diffusion profiles, and have analyzed the effect of the internal electric field on a sequential diffusion process.

Quasi-static Approach. The general problem of the previous section was investigated by Perritt [23] and later by Widiger [24], without making the two major assumptions discussed earlier in this section. A quasi-static approximation was formulated under the following assumption.

In a semiconductor, even at diffusion temperatures, holes and electrons have a much larger mobility than the impurity ions. Thus the time required for an impurity ion distribution to change to a particular profile is many orders of magnitude larger than that required for the holes and electrons.  $D_p$  and  $D_n$  are approximately  $10^{13}$  times larger than  $D_c$ . The electrons and holes therefore readjust almost instantaneously, staying in a steady state determined by the impurity ion distribution. In thermodynamics this is referred to as "quasi-static equilibrium." The equations governing diffusion under quasi-static approximation were developed by Widiger who assumed the SRH model. A more general way to derive these equations is given in Appendix A. It is first assumed that

$$\frac{\partial p}{\partial t} = \frac{\partial n}{\partial t} = 0 \quad . \quad (2.14)$$

It can then be shown that regardless of the form of  $G$  in (2.5a) and (2.5b), and using only these two equations, we obtain

$$n = n_i \exp\left(\frac{\phi}{V_T}\right) \quad (2.15)$$

$$p = n_i \exp\left(-\frac{\phi}{V_T}\right) \quad (2.16)$$

which, of course, implies that

$$pn = n_i^2 \quad .$$

The general problem under quasi-static approximation thus reduces to

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left[ D_c \frac{\partial c}{\partial x} - \frac{z_c c D_c}{V_T} E \right] \quad (2.17)$$

$$\frac{\partial^2 \phi}{\partial x^2} = \frac{e}{\epsilon} [n - p - z_c c] \quad (2.18)$$

where

$$E = - \frac{\partial \phi}{\partial x} \quad . \quad (2.19)$$

Note that electrostatic potential  $\phi$  has been assumed to be zero at  $x \rightarrow \infty$  for convenience, where the material has

been chosen to be intrinsic. It may also be noted that using (2.15) and (2.16), (2.18) can be written as

$$\frac{\partial^2 \phi}{\partial x^2} = \frac{e}{\epsilon} [2n_i \sinh(\frac{\phi}{V_T}) - z_c c] . \quad (2.20)$$

The boundary conditions for the above problem for a constant source diffusion are

$$c(0,t) = C_0 \quad (2.21a)$$

$$\frac{\partial \phi(0,t)}{\partial x} = 0 \quad (2.21b)$$

$$c(\infty,t) = 0 \quad (2.21c)$$

$$\phi(\infty,t) = 0 \quad (2.21d)$$

$$c(x,0) = 0, \quad x > 0 . \quad (2.21e)$$

It is seen that as a consequence of the law of mass action  $pn = n_i^2$ , the generation term  $G$  becomes zero if SRH model of (2.7) is assumed. This fact, however, is not required in the above model.

The quasi-static problem has been investigated and impurity profiles calculated using numerical techniques for a constant source diffusion [24], drive-in diffusion [25] and two-step diffusion processes [26].

It is interesting to note that if local charge neutrality is assumed in Poisson's equation, i.e.  $\frac{\partial^2 \phi}{\partial x^2} = 0$ , then

$$\phi = V_T \sinh^{-1} \left( -\frac{c z_c}{2n_i} \right) . \quad (2.22)$$

Thus,

$$E = - \frac{\partial \phi}{\partial x} = \frac{- V_T z_c}{\sqrt{c^2 + 4n_i^2}} \frac{\partial c}{\partial x} . \quad (2.23)$$

Substituting (2.23) into (2.17) yields

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} (D_{\text{eff}} \frac{\partial c}{\partial x}) \quad (2.24)$$

where

$$D_{\text{eff}} = D_c \left( 1 + \frac{c}{\sqrt{c^2 + 4n_i^2}} \right) . \quad (2.25)$$

This result has been obtained previously in (2.11) and (2.12).

Some important points may be noted at this stage. As is evident by (2.15) and (2.16), the law of mass action  $pn = n_i^2$  still holds during the diffusion, although strictly speaking the system is not in thermal equilibrium. This is a consequence of the assumptions made in quasi-static approximation. In the charge neutrality approximation, the

term  $\frac{\partial^2 \phi}{\partial x^2}$  has been neglected only in Poisson's equation. It is easy to see (Section 2.4) that if this term is also neglected in the transport equation, the two equations decouple and the simple diffusion equation is obtained. As pointed out earlier, all the above results are valid only under nondegenerate conditions. Finally it may be noted that (2.24) is in such a form that for a constant source diffusion the variables can be separated, as was shown by Shaw and Wells (Section 4.5). It appears that (2.24) is not separable for drive-in diffusion boundary conditions. An alternative formulation of the charge neutrality approximation of (2.24) in terms of  $\phi$  (instead of  $c$ ) is discussed in Section 2.4.

### 2.3 Transport Equations for Degenerate Case

In this section the transport equations for the degenerate case will be discussed. Holes and electrons in this case are described by Fermi-Dirac statistics and instead of the classical Einstein relation, its generalized form must be used. For concreteness, a donor type diffusion will be assumed.

The flux equations are still given by [27]

$$f_p = -D_p \frac{\partial p}{\partial x} + \mu_p p E \quad (2.26a)$$



$$f_n = - D_n \frac{\partial n}{\partial x} - \mu_n n E \quad (2.26b)$$

$$f_c = - D_c \frac{\partial c}{\partial x} + \mu_c c E . \quad (2.26c)$$

The continuity equation for impurity ions with 100% ionization is

$$\frac{\partial c}{\partial t} + \frac{\partial f_c}{\partial x} = 0 . \quad (2.27)$$

At this stage we make the following two assumptions.

1. The flux for minority carriers (holes) is zero,

$$f_p = 0 . \quad (2.28)$$

Note that the continuity equation for holes then implies

$$\frac{\partial p}{\partial t} = G_p .$$

Since holes readjust almost instantaneously, this implies

$\frac{\partial p}{\partial t} = G_p = 0$ . This, however, need not be assumed for the derivation that follows.

2. The flux for the impurity ions equals the flux for the majority carriers (electrons),

$$f_c = f_n . \quad (2.29)$$

Again, using the continuity equations for impurity ions and electrons, this implies that  $\frac{\partial (n-c)}{\partial t} = G_n$ . If quasi-static conditions were assumed it would imply  $\frac{\partial c}{\partial t} = -G_n$ .

It will be shown later that the above two assumptions imply that the quasi-Fermi levels for holes and electrons are equal.

The first assumption, using (2.26a), yields

$$\frac{1}{p} \frac{\partial p}{\partial x} = \frac{\mu_p}{D_p} E = - \frac{\mu_p}{D_p} \frac{\partial \phi}{\partial x} .$$

Integrating, we have

$$\phi(x) = - \int_x^\infty \frac{\partial \phi}{\partial x} dx = \int_x^\infty \frac{D_p}{\mu_p} \frac{1}{p} \frac{\partial p}{\partial x} dx \quad (2.30)$$

where  $\phi(\infty) = 0$  has been chosen for convenience. For a parabolic density of states, the generalized Einstein relation gives

$$\frac{D_p}{\mu_p} = \frac{kT}{e} \frac{F_{1/2}(\eta_p)}{F_{-1/2}(\eta_p)} \quad (2.31)$$

with

$$\eta_p(x) \equiv \frac{E_v(x) - E_{fp}(x)}{kT} ,$$

where  $E_v(x)$  is the top edge of the valence band and  $E_{fp}$  is the quasi-Fermi level for holes.

Also,

$$p = N_v F_{1/2}(\eta_p) . \quad (2.32)$$

Therefore,

$$\frac{dp}{d\eta_p} = N_v F_{-1/2}(\eta_p) . \quad (2.33)$$

Dividing (2.32) by (2.33) and substituting in (2.31) we obtain

$$\frac{D_p}{\mu_p} = \frac{kT_p}{e} \frac{d\eta_p}{dp} .$$

Using this, (2.30) yields

$$\phi(x) = \int_x^\infty \frac{kT}{e} \frac{d\eta_p}{dp} \frac{\partial p}{\partial x} dx = \frac{kT}{e} [\eta_p(\infty) - \eta_p]$$

where

$$\eta_p(\infty) = \frac{E_v(\infty) - E_f}{kT} = - \frac{E_g}{kT} - \eta_i$$

with

$$\eta_i \equiv \frac{E_f - E_c(\infty)}{kT} . \quad (2.34)$$

Note that thermal equilibrium conditions have been assumed at  $x \rightarrow \infty$ .  $E_g$  and  $E_c(x)$  represent the band gap and the bottom edge of the conduction band, respectively. Thus,

$$\eta_p = \eta_p(\infty) - \frac{e\phi}{kT} = -\frac{E_g}{kT} - \eta_i - \frac{e\phi}{kT} \quad (2.35)$$

which gives

$$p = N_v F_{1/2} \left( -\frac{e\phi}{kT} - \frac{E_g}{kT} - \eta_i \right). \quad (2.36)$$

Turning to the second approximation, we have

$$-D_c \frac{\partial c}{\partial x} + \mu_c cE = -D_n \frac{\partial n}{\partial x} - \mu_n nE. \quad (2.37)$$

Now, at typical diffusion temperatures,  $\mu_n \gg \mu_c$  and  $n \approx c$  so that  $\mu_n nE \gg \mu_c cE$ . Also, Poisson's equation gives

$$c = n - p - \frac{\epsilon}{e} \frac{\partial^2 \phi}{\partial x^2}. \quad (2.38)$$

Thus, (2.37) becomes

$$-D_c \frac{\partial n}{\partial x} + D_c \frac{\partial p}{\partial x} + D_c \frac{\epsilon}{e} \frac{\partial^3 \phi}{\partial x^3} = -D_n \frac{\partial n}{\partial x} + \mu_n n \frac{\partial \phi}{\partial x}. \quad (2.39)$$

The first term in (2.39) drops out because  $D_n \gg D_c$ . Using (2.32) and (2.35) we can write

$$\frac{\partial p}{\partial x} = \frac{-ep}{kT} \frac{F^{-1/2}(\eta_p)}{F^{1/2}(\eta_p)} \frac{\partial \phi}{\partial x} \approx - \frac{ep}{kT} \frac{\partial \phi}{\partial x} ,$$

since  $\eta_p$  is a large negative quantity. Substituting in (2.39) we obtain,

$$- \frac{\partial n}{\partial x} + \frac{\mu_n}{D_n} n \frac{\partial \phi}{\partial x} + \frac{\mu_c}{D_n} p \frac{\partial \phi}{\partial x} = \frac{D_c}{D_n} \frac{\epsilon}{e} \frac{\partial^3 \phi}{\partial x^3}$$

where  $\frac{D_c}{\mu_c} = \frac{kT}{e}$  has been used. Observing that  $\mu_n n \gg \mu_c p$  the above equation simplifies to

$$\frac{\mu_n}{D_n} n \frac{\partial \phi}{\partial x} - \frac{\partial n}{\partial x} = \frac{D_c}{D_n} \frac{\epsilon}{e} \left( \frac{\partial^3 \phi}{\partial x^3} \right) . \quad (2.40)$$

Now, considering the quantity on the r.h.s., it is noted that  $D_c \ll D_n$ , and if it is assumed that  $\frac{\partial^3 \phi}{\partial x^3}$  is not very large, the r.h.s. can be neglected in comparison to other terms. Physically, this means that the gradient of the charge density should not be extremely large. Thus, we obtain

$$\frac{\partial \phi}{\partial x} = \frac{D_n}{\mu_n} \frac{1}{n} \frac{\partial n}{\partial x}$$

or,

$$\phi(x) = \int_{-\infty}^x \frac{D_n}{\mu_n} \frac{1}{n} \frac{\partial n}{\partial x} dx . \quad (2.41)$$

Using the generalized Einstein relation

$$\frac{D_n}{\mu_n} = \frac{kT}{e} \frac{F_{1/2}(\eta)}{F_{-1/2}(\eta)}$$

where

$$\eta(x) \equiv \frac{E_{fn}(x) - E_c(x)}{kT} ,$$

and

$$n = N_c F_{1/2}(\eta) , \quad (2.42)$$

we can integrate the r.h.s. of (2.41) to obtain

$$\eta = \frac{e\phi}{kT} + \eta_i \quad (2.43)$$

which gives

$$n = N_c F_{1/2} \left( \frac{e\phi}{kT} + \eta_i \right) . \quad (2.44)$$

It may be noted that (2.35) and (2.43) imply that

$$\eta_p = -\eta - \frac{E_g}{kT}$$

or,

$$E_{fp} = E_{fn} .$$

This result is not surprising because (2.41) could have been written directly if the thermal equilibrium conditions were assumed at the outset. Present analysis, however, gives a better insight of the approximations involved.

Substituting (2.36) and (2.44) back into the Poisson's equation (2.38), and combining the flux and the continuity equations we obtain

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left[ D_c \frac{\partial c}{\partial x} + \mu_c c \frac{\partial \phi}{\partial x} \right] \quad (2.45)$$

$$\begin{aligned} \frac{\partial^2 \phi}{\partial x^2} = \frac{e}{\epsilon} \left[ N_c F_{1/2} \left( \frac{\phi}{V_T} + \eta_i \right) - N_v F_{1/2} \left( -\frac{\phi}{V_T} - \frac{E_g}{kT} - \eta_i \right) \right. \\ \left. - c \right] . \end{aligned} \quad (2.46)$$

It is noted that under typical diffusion conditions the argument of the second Fermi function in (2.46), which represents the minority carriers, is a large negative quantity and hence the Fermi function can be approximated by an exponential function; thus

$$\begin{aligned} N_v F_{1/2} \left( -\frac{\phi}{V_T} - \frac{E_g}{kT} - \eta_i \right) &\approx N_v \exp \left( -\frac{E_g}{kT} - \eta_i \right) \exp \left( -\frac{\phi}{V_T} \right) \\ &= n_i \exp \left( -\frac{\phi}{V_T} \right) \end{aligned}$$

where

$$n_i = N_v F_{1/2} \left( -\frac{E_g}{kT} - \eta_i \right) \approx N_v \exp \left( -\frac{E_g}{kT} - \eta_i \right) \quad (2.47)$$

has been used. Instead of (2.46), we may then use

$$\frac{\partial^2 \phi}{\partial x^2} = \frac{e}{\epsilon} [N_c F_{1/2} \left( \frac{\phi}{V_T} + \eta_i \right) - n_i \exp \left( -\frac{\phi}{V_T} \right) - c] \quad (2.48)$$

Note that if the first term is also expressed by Maxwell-Boltzmann statistics (nondegenerate case), we obtain

$$\begin{aligned} N_c F_{1/2} \left( \frac{\phi}{V_T} + \eta_i \right) &\approx N_c \exp \left( \frac{\phi}{V_T} \right) \exp(\eta_i) \\ &= n_i \exp \left( \frac{\phi}{V_T} \right) \end{aligned}$$

where

$$n_i = N_c F_{1/2}(\eta_i) \approx N_c \exp(\eta_i)$$

has been used. For nondegenerate conditions, therefore, (2.48) reduces to

$$\frac{\partial^2 \phi}{\partial x^2} = \frac{e}{\epsilon} [2n_i \sinh \left( \frac{\phi}{V_T} \right) - c]$$



which is the same as (2.20) of the previous section.

The boundary conditions and numerical solution to (2.45) and (2.48) will be discussed in Chapter 4.

We now consider the problem of finding  $N_c$ ,  $N_v$  and  $n_i$ . The effective density of states  $N_c$  and  $N_v$  are given by

$$N_c = 2 \left( \frac{2\pi kT m_n^*}{h^2} \right)^{3/2} \quad (2.49a)$$

$$N_v = 2 \left( \frac{2\pi kT m_p^*}{h^2} \right)^{3/2} \quad (2.49b)$$

where  $m_n^*$  and  $m_p^*$  are density of states effective masses of electrons and holes, respectively. In general, knowledge of  $m_n^*$  and  $m_p^*$  at typical diffusion temperatures is poor, although it is possible to extrapolate from the results obtained at lower temperatures [28]. A way to circumvent the problem is to avoid the direct use of  $m_n^*$  and  $m_p^*$  in (2.49).

For an intrinsic material,

$$n_i = N_c F_{1/2}(\eta_i) . \quad (2.50)$$

Data for the intrinsic carrier concentration  $n_i(T)$  is known experimentally [29]. It is easy to show that

$$E_f = \frac{1}{2} [E_c(\infty) + E_v(\infty)] + \frac{1}{2} kT \ln \left( \frac{N_v}{N_c} \right) \quad (2.51)$$

since the material is intrinsic as  $x \rightarrow \infty$ . Using (2.34) and (2.51), the value of  $\eta_i$  in (2.50) may be computed as

$$\eta_i = - \frac{E_g}{2kT} + \frac{3}{4} \ln \left( \frac{m_p^*}{m_n^*} \right) . \quad (2.52)$$

The ratio of effective masses,  $m_p^*/m_n^*$ , is a relatively weak function of temperature [30] and therefore  $N_c$  computed using (2.50) should give a better value than that using (2.49a). Data for  $E_g(T)$  used in (2.52) is also known experimentally [31].

#### 2.4 Degenerate Case Under Charge Neutrality

The degenerate quasi-static formulation for a donor type impurity diffusion yields (2.45) and (2.48), repeated here for convenience.

$$\frac{\partial c}{\partial t} = \frac{\partial}{\partial x} \left[ D_c \frac{\partial c}{\partial x} + \mu_c c \frac{\partial \phi}{\partial x} \right] \quad (2.53)$$

$$\frac{\partial^2 \phi}{\partial x^2} = \frac{e}{\epsilon} \left[ N_c F_{1/2} \left( \frac{\phi}{V_T} + \eta_i \right) - n_i \exp\left(-\frac{\phi}{V_T}\right) - c \right] \quad (2.54)$$

If it is assumed that  $\frac{\partial^2 \phi}{\partial x^2} = 0$ , i.e.  $\rho(x) = 0$ , everywhere in the semiconductor, then

$$E = - \frac{\partial \phi}{\partial x} = \text{constant}$$

and, because of the boundary conditions

$$E(\infty, t) = 0$$

$$\phi(\infty, t) = 0 ,$$

we obtain

$$E(x, t) = 0$$

$$\phi(x, t) = 0 .$$

Thus (2.53) and (2.54) decouple and the classical diffusion equation

$$\frac{\partial c}{\partial t} = D_c \frac{\partial^2 c}{\partial x^2}$$

is obtained.

In this section, instead of assuming that  $\frac{\partial^2 \phi}{\partial x^2} = 0$  in both (2.53) and (2.54), we neglect it only in Poisson's equation, i.e. we assume that  $\frac{\partial^2 \phi}{\partial x^2} \ll n, p$  or  $c$ . The equations under charge neutrality thus become

$$\frac{\partial c}{\partial t} = D_c \frac{\partial^2 c}{\partial x^2} + \mu_c c \frac{\partial^2 \phi}{\partial x^2} + \mu_c \frac{\partial c}{\partial x} \frac{\partial \phi}{\partial x} \quad (2.55)$$

$$c = N_c F_{1/2} \left( \frac{\phi}{V_T} + \eta_i \right) - n_i \exp\left(-\frac{\phi}{V_T}\right). \quad (2.56)$$

Unlike the nondegenerate case of Section 2.2,  $E$  here can not be expressed entirely in terms of  $c$ . Nevertheless, it is possible to obtain a single equation in  $\phi$ . Differentiating  $c$  from (2.56) and substituting in (2.55), we obtain

$$\frac{\partial \phi}{\partial t} = \frac{D_c}{V_T} f_1(\phi) \left( \frac{\partial \phi}{\partial x} \right)^2 + D_c f_2(\phi) \left( \frac{\partial^2 \phi}{\partial x^2} \right) \quad (2.57)$$

where

$$f_1(\phi) \equiv \frac{F_{-3/2} \left( \frac{\phi}{V_T} + \eta_i \right) + F_{-1/2} \left( \frac{\phi}{V_T} + \eta_i \right)}{F_{-1/2} \left( \frac{\phi}{V_T} + \eta_i \right) + F_{1/2}(\eta_i) \exp\left(-\frac{\phi}{V_T}\right)} \quad (2.58a)$$

and

$$f_2(\phi) \equiv \frac{F_{-1/2} \left( \frac{\phi}{V_T} + \eta_i \right) + F_{1/2} \left( \frac{\phi}{V_T} + \eta_i \right)}{F_{-1/2} \left( \frac{\phi}{V_T} + \eta_i \right) + F_{1/2}(\eta_i) \exp\left(-\frac{\phi}{V_T}\right)}. \quad (2.58b)$$

Now, if a normalization

$$\hat{\phi} = \frac{\phi}{V_T} \quad (2.59)$$

is used, (2.57) becomes

$$\frac{\partial \hat{\phi}}{\partial t} = D_c [f_1(\hat{\phi}) \left(\frac{\partial \hat{\phi}}{\partial x}\right)^2 + f_2(\hat{\phi}) \left(\frac{\partial^2 \hat{\phi}}{\partial x^2}\right)] \quad (2.60)$$

where  $f_1(\hat{\phi})$  and  $f_2(\hat{\phi})$  are the functions defined by (2.58a) and (2.58b) with  $\phi/V_T$  replaced by  $\hat{\phi}$ .

Boundary Conditions. Considering a constant source diffusion, the boundary conditions are given by

$$c(0, t) = C_0 \quad (2.61a)$$

$$c(\infty, t) = 0 \quad (2.61b)$$

$$c(x, 0) = 0, \quad x > 0. \quad (2.61c)$$

The boundary conditions in terms of  $\hat{\phi}$  are easily obtained as

$$\hat{\phi}(0, t) = \phi_0 \quad (2.62a)$$

$$\hat{\phi}(\infty, t) = 0 \quad (2.62b)$$

$$\hat{\phi}(x, 0) = 0, \quad x > 0 \quad (2.62c)$$

where  $\phi_0$  is computed by solving the implicit algebraic equation

$$C_0 = N_c F_{1/2}(\phi_0 + \eta_i) - n_i \exp(-\phi_0). \quad (2.63)$$

Transformation. It will be shown in Section 4.5 that the partial differential equation of the form (2.60) is separable for the constant source boundary conditions given above. Thus, just like the nondegenerate case of Section 2.2, the degenerate case also yields an equation which is separable although the dependent variable now is  $\phi$  instead of  $c$ . The electric field here can not be expressed entirely in terms of  $c$  but may be easily computed as

$$E = - \frac{\partial \phi}{\partial x} . \quad (2.64)$$

Reduction of the Equation for Nondegenerate Conditions. For nondegenerate case, all the Fermi functions reduce to exponential functions and (2.57) reduces to

$$\frac{\partial \phi}{\partial t} = \left[ \frac{2}{1 + \exp(-\frac{2\phi}{V_T})} \right] \left[ \frac{D_c}{V_T} \left( \frac{\partial \phi}{\partial x} \right)^2 + D_c \left( \frac{\partial^2 \phi}{\partial x^2} \right) \right] . \quad (2.65)$$

This equation in terms of  $\phi$  is an alternative to the charge neutrality formulation in terms of  $c$  discussed earlier in Section 2.2.

## 2.5 Discussion

In this Chapter impurity diffusion into an intrinsic semiconductor was discussed under nondegenerate and degenerate conditions. Formulations resulting from the

assumption of local charge neutrality were presented. In each of the cases the diffusion model is described by either a single or a set of differential equations. The numerical procedures to solve these equations are discussed in Chapter 4. In Chapter 5 numerical results are presented and the formulations compared to each other. It is found that under typical diffusion conditions, local charge neutrality turns out to be a good approximation. This provides the basis for the model to be discussed in the next Chapter which includes the effect of vacancies.

## CHAPTER 3

### DIFFUSION VIA VACANCIES

The models for field-aided diffusion discussed in Chapter 2, although applicable to both acceptor and donor type impurities, yield results which do not agree with experiment at higher concentrations. When defects such as vacancies and interstitials are considered, it becomes necessary to specify the kind of impurities. In silicon, vacancies are believed to be responsible for donor type impurity diffusion, whereas interstitialcy mechanism is favored for acceptor type impurities [6]. In this Chapter, diffusion of arsenic in silicon is discussed and a vacancy mechanism is assumed.

#### 3.1 Previous Work

Several models for arsenic diffusion in silicon have been proposed. Hu [12] has considered an impurity-vacancy-semiconductor system. The flux equations have been systematically derived from thermodynamical considerations. Local charge neutrality has been assumed in the theory. Analysis without this assumption becomes very complicated, and does not seem to have been tried in the general case. However, based on the discussion from Chapter 2, it may be expected that local charge neutrality should be an excellent assumption even in the present case. Prior to



the publication of the above theory, using some other arguments, Hu and Schmidt [22] had analyzed As diffusion in Si. The equations used there were later justified by Hu. Nevertheless, there was some arbitrariness in the computations of Hu and Schmidt because of a factor  $\beta$ , which was assumed to be 100. As discussed by Nuyts and Van Overstraeten [32], the above value of  $\beta$  is unrealistic. Also, the analysis assumed nondegenerate conditions and complete impurity ionization, although the general theory of impurity diffusion proposed by Hu is not restricted to these conditions. Hu and Schmidt have pointed out that the validity of their model breaks down at high surface concentrations because there is no limit to the enhancement effect due to vacancies. It should be interesting to find out if the same result is obtained when partial ionization is taken into account and Fermi-Dirac statistics are used.

In the model proposed by Chiu and Ghosh [33], two energy levels have been attributed to the vacancies in an attempt to explain the decrease in the diffusion coefficient of As in Si at very high concentrations. They have reported excellent agreement between the theory and experiment except for short diffusion times. In their analysis, however, as many as four constants were matched numerically, having assumed that the impurity diffusion coefficient ratio in extrinsic to nearly intrinsic silicon is given by

$$\frac{D}{D_i} = fgh$$

where  $f$ ,  $g$ , and  $h$  are contributions due to vacancies, cluster mechanism and internal electric field, respectively. The analysis again assumes nondegenerate conditions and complete impurity ionization. The cluster mechanism mentioned above needs some explanation. In order to explain the retardation of diffusion observed experimentally at higher concentrations, it has been postulated that As atoms start forming clusters as the concentration goes up. Two models have been proposed. The As-complex considered by Fair and Weber [34] consists of two As atoms, whereas in Hu's cluster model [35], it consists of four As atoms. For chemical reasons, only one such complex may dominate in a certain temperature range. However, there is still an uncertainty as to which model actually applies. Hu's model gives a good fit to the experimental vapor pressure data. Fair and Weber have claimed that their model gives better results at shorter diffusion times compared to Chiu and Ghosh who have used Hu's cluster model. It should be pointed out that Fair and Weber have included the influence of partial impurity ionization through an empirical equation. Also, in addition to using nondegenerate equations, they have approximated the electric field by

$$E \approx \frac{kT}{e} \frac{1}{c} \frac{\partial c}{\partial x} .$$

As can be seen from (2.23), the above equation is valid only for  $c \gg 2n_i$ , and at typical diffusion temperatures, this inequality is easily violated.

Nuyts and Van Overstraeten [32] have applied Hu's diffusion model to the diffusion of phosphorus in silicon. They also restricted their analysis to nondegenerate conditions and assumed complete ionization. Contrary to the comment made earlier in the Chapter that interstitialcy mechanism is favored for acceptor type impurities, they assumed vacancy mechanism to be valid for simultaneous diffusion of boron in silicon.

As the impurity concentration becomes higher and higher, the discrete impurity energy levels separate out and start forming energy bands. This is, of course, a consequence of Pauli's exclusion principle. Under such conditions, strictly speaking, it is not sufficient just to replace Maxwell-Boltzmann statistics by Fermi-Dirac statistics and neglect the impurity band formation. Two of the theories dealing with these impurity bands have been proposed by Kane [36] and Morgan [37]. Jain and Van Overstraeten [38] have used these models and have analyzed the diffusion problem by writing the overall diffusion coefficient as

$$D_{As} = D_{iAs} D_{ef} D_{ev} D_{cf}$$

where the factors on the right hand side correspond to the intrinsic As diffusion coefficient, electric field, vacancies and cluster formation (using Hu's cluster model), respectively. They have claimed a good agreement between the theory and experiment.

Of all the above models, Hu's diffusion model has a very strong point in favor of it, in that it evolves in a very systematic and general way from the fundamentals of thermodynamics. The generality of the results does not seem to have been utilized completely. In this Chapter, As diffusion in Si is analyzed using Hu's theory. The partial ionization of the impurity atoms is taken into account, and Fermi-Dirac statistics are used to describe the carriers.

### 3.2 The Diffusion Model

The following major assumptions are made at various stages in the development of the model.

1. The temperature during the diffusion is held constant.
2. Vacancies act as single level acceptors.
3. Local charge neutrality is assumed.
4. Vacancies have very little effect on the Fermi level. Conversely, the Fermi level determines the concentration of vacancies.
5. Fermi-Dirac statistics are used to describe the carrier densities. However, the formation of impurity

bands is ignored. Constant band gap and electron affinity are assumed.

6. In order to better understand the influence of carrier degeneracy and partial ionization, cluster formation of As atoms is not considered.

7. Vacancy production due to plastic deformation is neglected.

8. Quasi-thermal equilibrium is assumed so that  $E_{fn} \approx E_f$  and  $E_{fp} \approx E_f$ .

Under these assumptions, according to Hu's theory [12], we have

$$D_c = D_c^* \frac{v}{v^*} \quad (3.1)$$

$$D_v = D_v^* \quad (3.2)$$

where  $D_c$  represents the impurity diffusion coefficient and  $D_c^*$  is its value at infinite dilution of impurities with vacancy at its thermal equilibrium concentration.  $D_v$ ,  $D_v^*$ ,  $v$  and  $v^*$  are the corresponding diffusion coefficients and concentrations for vacancies. The flux equations are given by

$$f_c = -D_c^* \frac{v}{v^*} \left( 1 + \frac{\partial \ln \gamma_c}{\partial \ln c} \right) \frac{\partial c}{\partial x} \quad (3.3)$$

$$f_v = -D_v^* \frac{v}{c} \frac{\partial \ln \gamma_v}{\partial \ln c} \frac{\partial c}{\partial x} - D_v^* \frac{\partial v}{\partial x} \quad (3.4)$$

where  $\gamma_c$  and  $\gamma_v$  are the activity coefficients given by

$$\gamma_c = \frac{1+\zeta^*}{1+\zeta} \quad (3.5)$$

$$\gamma_v = \frac{1+\xi^*}{1+\xi} , \quad (3.6)$$

where  $\zeta$ ,  $\xi$ ,  $\zeta^*$  and  $\xi^*$  are defined by

$$\zeta = g_c^{-1} \exp\left(\frac{E_D - E_f}{kT}\right) \quad (3.7)$$

$$\xi = g_v \exp\left(\frac{E_f - E_v}{kT}\right) \quad (3.8)$$

$$\zeta^* = g_c^{-1} \exp\left(\frac{E_D - E_i}{kT}\right) \quad (3.9)$$

$$\xi^* = g_v \exp\left(\frac{E_i - E_v}{kT}\right) . \quad (3.10)$$

In writing (3.1)-(3.4), it has been assumed that the concentration of impurity-vacancy pairs is much smaller than the vacancy concentration. The impurity concentration has also been assumed to be small compared to the concentration of the host lattice atoms. In the above equations,  $E_f$ ,  $E_D$ , and  $E_v$  represent the Fermi level, donor energy level, and vacancy energy level, respectively.  $E_i$  represents the value of the Fermi level which would yield equal concentrations of holes and electrons. Also,  $g_c$  and  $g_v$  are degeneracy factors for the donor and vacancy levels. Thus,

$$\gamma_c = \frac{1+\zeta^*}{1 + g_c^{-1} \exp(\frac{E_D - E_f}{kT})} . \quad (3.11)$$

Differentiation w.r.t.  $x$  gives

$$\frac{\partial \ln \gamma_c}{\partial x} = [1 + g_c \exp(\frac{E_f - E_D}{kT})]^{-1} \frac{\partial \eta}{\partial x} \quad (3.12)$$

where

$$\eta \equiv \frac{E_f - E_c}{kT} . \quad (3.13)$$

If

$$g_c \exp(\frac{E_f - E_D}{kT}) \ll 1 ,$$

then (3.12) can be approximated by

$$\frac{\partial \ln \gamma_c}{\partial x} \approx \frac{\partial \eta}{\partial x} . \quad (3.14)$$

It will be shown later that the term  $\frac{\partial \eta}{\partial x}$  is proportional to the electric field. From (3.12) and (3.3) it is evident that as the Fermi level goes above  $E_D$ , the term involving the electric field becomes less significant. At 1200 °C, the above inequality is well satisfied for  $E_D - E_f \geq 0.38$  eV.

For donors  $\xi \gg 1$ , and (3.6) can be written as

$$\gamma_v = \frac{1 + g_v \exp(\eta_i + \epsilon_v)}{g_v \exp(\eta + \epsilon_v)} \quad (3.15)$$

where

$$\epsilon_v \equiv \frac{E_c - E_v}{kT}$$

and

$$\eta_i = \frac{E_f - E_c(\infty)}{kT} .$$

Note that at typical diffusion temperatures  $E_g$  is about 0.8 eV for Si and  $E_v = E_c - 0.4$  eV. Therefore, nothing can be said about the magnitude of  $\xi^*$ .

In computing the flux of total impurities  $f_c$ , the theory has taken into account the fact that a certain fraction of donor atoms may remain neutral, some may be charged positively and some of these may form pairs with the charged and neutral vacancies. Within the semiconductor, there is no generation of the total impurities. The continuity equation thus yields

$$\frac{\partial c}{\partial t} + \frac{\partial f_c}{\partial x} = 0 . \quad (3.16)$$

Substitution of (3.3) in (3.16) gives



$$\frac{\partial c}{\partial t} = \frac{D_c^*}{v^*} \frac{\partial}{\partial x} \left[ v \left( \frac{\partial c}{\partial x} + c \frac{\partial \eta}{\partial x} \right) \right] \quad (3.17)$$

where (3.14) has been used. Note that  $v^*$  is independent of  $x$ .

The continuity equation for vacancies is

$$\frac{\partial v}{\partial t} + \frac{\partial f_v}{\partial x} = G_v(x, t) \quad (3.18)$$

In general,  $G_v$  may not be zero. This term may be caused, for example, by plastic deformation. A mismatch in the size of diffusing impurities and the host lattice atoms is a major cause of dislocations. Substitution of (3.4) into (3.18) yields

$$\frac{\partial v}{\partial t} = G_v(x, t) + \frac{\partial}{\partial x} \left[ D_v^* v \frac{\partial \ln \gamma_v}{\partial x} + D_v^* \frac{\partial v}{\partial x} \right] . \quad (3.19)$$

As discussed by Hu and also by Nuyts and Van Overstraeten [32], quasi-equilibrium condition for vacancies under typical diffusion conditions is a good approximation. Thus, assuming  $\frac{\partial v}{\partial t} \approx 0$ , (3.19) yields

$$\frac{\partial}{\partial x} \left[ D_v^* v \frac{\partial \ln \gamma_v}{\partial x} + D_v^* \frac{\partial v}{\partial x} \right] = -G_v(x) .$$

Integrating both sides from  $x$  to  $\infty$ , and noting that as  $x \rightarrow \infty$ ,  $v \rightarrow v^*$  i.e.  $\frac{\partial v}{\partial x} \rightarrow 0$ , and  $\gamma_v \rightarrow 1$ , we obtain

$$D_V^* v \frac{\partial \ln(v \gamma_V)}{\partial x} = \int_x^\infty G_V(x) dx .$$

Integrating once again,

$$v = \gamma_V^{-1} [v^* - \int_x^\infty \frac{\gamma_V}{D_V^*} dx \int_x^\infty G_V(\zeta) d\zeta] . \quad (3.20)$$

Note that  $\gamma_V < 1$ , and  $D_V^*$  is large [32]. The mismatch in the radii of As and Si atoms is very small resulting in a small generation term  $G_V$ . Thus, if the integral on the r.h.s. can be neglected, we simply have

$$v \approx \frac{v^*}{\gamma_V} . \quad (3.21)$$

Substitution of (3.21) into (3.17) yields

$$\frac{\partial c}{\partial t} = D_c^* \frac{\partial}{\partial x} [\gamma_V^{-1} (\frac{\partial c}{\partial x} + c \frac{\partial \eta}{\partial x})] . \quad (3.22)$$

### 3.3 Computation of the Fermi Level

The unknown  $\eta$  appearing in (3.22) can be evaluated using the condition of local charge neutrality. Then, (3.22) with suitable boundary conditions describes the transport problem. Local charge neutrality implies

$$n - p - c^+ + v^- = 0 \quad (3.23)$$

where  $c^+$  and  $v^-$  are the ionized donor atom and charged vacancy concentrations, respectively, with  $v^-$  given by [12]

$$\begin{aligned} v^- &= v \frac{\xi}{1+\xi} \\ &= \frac{v}{1 + g_v^{-1} \exp(-\eta - \epsilon_v)} \end{aligned} \quad (3.24)$$

Since  $\xi \gg 1$ ,  $v^- \approx v$ . However, this concentration itself is so small compared to other terms in (3.23) that it can be safely neglected [12].

The electron and hole concentrations are given by

$$n = N_c F_{1/2}(\eta) \quad (3.25)$$

and

$$p = N_v F_{1/2}(-\eta - \epsilon_g) \quad (3.26)$$

where  $\epsilon_g$  is the normalized band gap. For donor diffusion,

$$(-\eta - \epsilon_g) \ll -1$$

and

$$p \approx N_v \exp(-\eta - \epsilon_g) \quad (3.27)$$

For partial ionization, the ionized donor concentration is given by [12]

$$c^+ = \frac{c}{1 + g_c \exp(\eta + \frac{E_d}{kT})} \quad (3.28)$$

where  $E_d = E_c - E_D$  is the ionization energy. Note that for sufficiently negative values of  $\eta$ ,  $c^+ \approx c$  and we approach the 100% ionization case.

Substituting (3.25), (3.27) and (3.28) into (3.23) with  $g_c = 2$  we obtain

$$N_c F_{1/2}(\eta) - N_v \exp(-\eta - \epsilon_g) - \frac{c}{1 + 2\exp(\eta + \epsilon_d)} = 0 \quad (3.29)$$

Thus, (3.29) can be used to evaluate  $\eta$ .

### 3.4 Summary of the Problem

We must solve the partial differential equation (3.22) where  $\eta$  is obtained using (3.29). The values of  $N_c$  and  $N_v$  are found, as in Section 2.3, by using the equations

$$N_c = \frac{n_i}{F_{1/2}(\eta_i)} \quad (3.30)$$

$$N_v = n_i \exp(\eta_i + \epsilon_g) \quad (3.31)$$

Also,  $\gamma_v$  and  $n$  are given by (3.15) and (3.13).

For a constant source diffusion the boundary conditions are

$$c(0,t) = C_0$$

$$c(\infty,t) = 0$$

$$c(x,0) = 0, \quad x > 0. \quad (3.32)$$

These will be transformed in terms of suitable variables at a later stage.

### 3.5 Form of Impurity Flux With and Without Vacancies

Using (3.3) and (3.14), the impurity flux with vacancies can be expressed as

$$f_c = -D_c^* \frac{v}{v} \left[ \frac{\partial c}{\partial x} + c \frac{\partial \eta}{\partial x} \right] \quad (3.33)$$

When the vacancies are in quasi-equilibrium, using (3.21),

$$f_c = - \frac{D_c^*}{\gamma_v} \left[ \frac{\partial c}{\partial x} + c \frac{\partial \eta}{\partial x} \right].$$

Now,

$$\begin{aligned}
\frac{\partial \eta}{\partial x} &= \frac{\partial}{\partial x} \left( \frac{E_f - E_c}{kT} \right) \\
&= - \frac{1}{kT} \frac{\partial E_c}{\partial x} = - \frac{e}{kT} E
\end{aligned}$$

where  $E$  is the electric field. Thus, we obtain

$$\begin{aligned}
f_c &= - \frac{D_c^*}{\gamma_v} \left[ \frac{\partial c}{\partial x} - \frac{e}{kT} cE \right] \\
&= \frac{1}{\gamma_v} \left[ -D_c^* \frac{\partial c}{\partial x} + \mu_c^* cE \right] \tag{3.34}
\end{aligned}$$

where  $\mu_c^* = \frac{eD_c^*}{kT}$  has been used. Comparing (2.26c) and (3.34) we see that the forms of the flux equation are similar except for the factor  $1/\gamma_v$ . This can also be viewed as a change in the impurity diffusion coefficient which now becomes  $\frac{D_c^*}{\gamma_v}$ . In other words, the impurity diffusion coefficient is now proportional to the vacancy concentration  $v$ . At low donor concentrations  $\gamma_v \rightarrow 1$ , and (3.34) reduces to (2.26c).

### 3.6 Transformation of the Equations

The equations summarized in Section 3.4 can be transformed into a simpler form. It is possible to substitute for the derivatives of  $c$  in (3.22) using (3.29). An equation entirely in terms of the dependent variable  $\eta$  is then obtained. Noting that

$$\xi^* = g_v \exp(\eta_i + \epsilon_v) ,$$

(3.22) can be written as

$$\begin{aligned} \frac{\partial c}{\partial t} = & \left( \frac{D_c^* \xi^*}{1 + \xi^*} \right) \exp(\eta - \eta_i) \left[ 2 \frac{\partial c}{\partial x} \frac{\partial \eta}{\partial x} + c \left( \frac{\partial \eta}{\partial x} \right)^2 \right. \\ & \left. + \frac{\partial^2 c}{\partial x^2} + c \frac{\partial^2 \eta}{\partial x^2} \right] \end{aligned} \quad (3.35)$$

where (3.15) has been used. Also, (3.29) gives

$$c = [1 + 2 \exp(\eta + \epsilon_d)] [N_c F_{1/2}(\eta) - N_v \exp(-\eta - \epsilon_g)] . \quad (3.36)$$

Differentiation of (3.36) yields the following expressions:

$$\frac{\partial c}{\partial x} = \frac{\partial \eta}{\partial x} \phi_1(\eta) \quad (3.37)$$

where

$$\begin{aligned} \phi_1(\eta) \equiv & N_c F_{-1/2}(\eta) + N_v \exp(-\eta - \epsilon_g) + 2 N_c \exp(\eta + \epsilon_d) \\ & \times \{ F_{1/2}(\eta) + F_{-1/2}(\eta) \} , \end{aligned} \quad (3.38)$$

$$\frac{\partial c}{\partial t} = \frac{\partial \eta}{\partial t} \phi_1(\eta) \quad (3.39)$$

and

$$\frac{\partial^2 c}{\partial x^2} = \frac{\partial^2 \eta}{\partial x^2} \phi_1(\eta) + \left(\frac{\partial \eta}{\partial x}\right)^2 \phi_2(\eta) \quad (3.40)$$

where

$$\begin{aligned} \phi_2(\eta) \equiv & N_c F_{-3/2}(\eta) - N_v \exp(-\eta - \epsilon_g) + 2N_c \exp(\eta + \epsilon_d) \\ & \times \{F_{1/2}(\eta) + 2F_{-1/2}(\eta) + F_{-3/2}(\eta)\} . \end{aligned} \quad (3.41)$$

Now, substituting (3.37), (3.39), and (3.40) in (3.35), after some lengthy manipulation, we obtain

$$\frac{\partial \eta}{\partial t} = D \exp(\eta - \eta_i) \left[ \left(\frac{\partial \eta}{\partial x}\right)^2 \frac{\phi_3(\eta)}{\phi_1(\eta)} + \left(\frac{\partial^2 \eta}{\partial x^2}\right) \frac{\phi_4(\eta)}{\phi_1(\eta)} \right] \quad (3.42)$$

where

$$\begin{aligned} \phi_3(\eta) \equiv & N_c F_{1/2}(\eta) + 2N_c F_{-1/2}(\eta) + N_c F_{-3/2}(\eta) \\ & + 2\exp(\eta + \epsilon_d) \{4 N_c F_{1/2}(\eta) + 4 N_c F_{-1/2}(\eta) \\ & + N_c F_{-3/2}(\eta) - N_v \exp(-\eta - \epsilon_g)\} \end{aligned} \quad (3.43)$$



$$\begin{aligned}
\phi_4(\eta) &\equiv N_c F_{1/2}(\eta) + N_c F_{-1/2}(\eta) + 2\exp(\eta + \epsilon_d) \\
&\times \{2N_c F_{1/2}(\eta) + N_c F_{-1/2}(\eta) - N_v \exp(-\eta - \epsilon_g)\}
\end{aligned}
\tag{3.44}$$

and

$$D \equiv \frac{D_c^* \xi^*}{1 + \xi^*} . \tag{3.45}$$

At this point, it is convenient to make a transformation of the dependent variable,

$$\eta = \psi + \eta_i , \tag{3.46}$$

so that the new variable  $\psi$  is defined by

$$\psi \equiv \frac{E_f - E_i}{kT} . \tag{3.47}$$

With this transformation (3.42) becomes

$$\frac{\partial \psi}{\partial t} = D \left[ \left( \frac{\partial \psi}{\partial x} \right)^2 f_1(\psi) + \left( \frac{\partial^2 \psi}{\partial x^2} \right) f_2(\psi) \right] \tag{3.48}$$

where

$$f_1(\psi) \equiv \exp(\psi) \frac{\phi_3(\psi+\eta_i)}{\phi_1(\psi+\eta_i)} \quad (3.49)$$

and

$$f_2(\psi) \equiv \exp(\psi) \frac{\phi_4(\psi+\eta_i)}{\phi_1(\psi+\eta_i)} \quad (3.50)$$

Thus, the problem has been reduced to solving (3.48).

The boundary conditions for the constant source diffusion, given in Section 3.4, can be easily written in terms of  $\psi$  as

$$\psi(0, t) = \psi_0 \quad (3.51a)$$

$$\psi(\infty, t) = 0 \quad (3.51b)$$

$$\psi(x, 0) = 0, \quad x > 0 \quad (3.51c)$$

where  $\psi_0$  is computed by solving the equation

$$\begin{aligned} C_0 - [1 + 2\exp(\psi_0 + \eta_i + \epsilon_d)] [N_c F_{1/2}(\psi_0 + \eta_i) \\ - N_v \exp(-\psi_0 - \eta_i - \epsilon_g)] = 0, \end{aligned} \quad (3.52)$$

which follows directly from (3.36).

### 3.7 Discussion

It can be noted that the partial differential equation (3.48), and the boundary conditions (3.51), are of the same form as those obtained in Section 2.4 except that instead of the variable  $\hat{\phi}$ , we now have  $\psi$ . Therefore, the numerical solution to (3.48) can be found exactly in the same manner. As shown in Section 4.5, a transformation of the variables can be used to separate the variables. The resulting ordinary differential equation can be solved efficiently by using a numerical technique. The results are discussed in Chapter 5.

## CHAPTER 4

### NUMERICAL ANALYSIS

The models discussed in the previous chapters result in a set of partial differential equations. These equations are highly nonlinear, and it may be extremely difficult, if not impossible, to find a closed form solution. A numerical solution is the only viable alternative. There exist a number of methods to solve a boundary value problem [39]. In the present case, a quasi-linearization technique is used. The partial differential equations are first transformed into ordinary differential equations by discretizing the time step. The process then consists of reducing the set of ODE to successive approximate sets of linear equations which can be solved more easily using an iteration scheme. A desired accuracy can be reached by repeating the process of linearization.

In this Chapter, a general method for solving coupled nonlinear ODE is first presented. The treatment closely follows that of Widiger [24]. The procedure is then applied to individual cases discussed in the previous chapters.

#### 4.1 Discretization of Independent variables

To facilitate the numerical techniques, the independent variables have to be discretized, thereby yielding sets of

difference equations. The variables in the present case are  $t_i$  and  $x_j$ , defined by

$$t_i = (i-1)\Delta t + t_0, \quad i = 1, \dots, n$$

$$x_j = (j-1)\Delta x \quad j = 1, \dots, m$$

where  $\Delta t$  and  $\Delta x$  are chosen to be fixed for simplicity. The discretization of  $t$  transforms the PDE into an ODE at a certain time step. The abruptness of the initial condition at the surface can be dealt with by assuming a non-zero starting time  $t_0$ .

The time derivative is approximated by a two-point implicit scheme,

$$\frac{\partial f(t_i)}{\partial t} \approx \frac{f(t_i) - f(t_{i-1})}{\Delta t} .$$

The procedure then is as follows. Once time  $t$  is discretized, the PDE is transformed into an ODE at a time  $t_i$ . If the solution to the ODE is known at time  $t_{i-1}$ , the ODE can be solved to yield the solution at time  $t_i$ . Beginning with  $i=1$ , the above step is performed for each time increment, until the desired final time is reached. The solution of the ODE is discussed in the next Section.

## 4.2 General Quasi-linearization Technique

The quasi-linearization technique is based on Newton's approximating procedure for finding the roots of an arbitrary function. Given a function  $f(x)$ , it is desired to find the roots  $x_r$  of the equation

$$f(x) = 0 \quad . \quad (4.1)$$

An initial guess  $x^0$  to the correct value of the root is made. Thus

$$f(x^0 + \Delta x) = 0 \quad (4.2)$$

where

$$x_r = x^0 + \Delta x \quad .$$

Expanding (4.2) by a Taylor series about  $x^0$ , we obtain

$$f(x^0) + f'(x^0)\Delta x + \frac{1}{2} f''(x^0)\Delta x^2 + \dots = 0$$

The above equation is to be solved for  $\Delta x$  to determine the true root. The problem can be simplified by truncating the series after the linear term; then

$$f(x^0) + f'(x^0)\Delta x \approx f(x^0 + \Delta x) = 0 \quad .$$

The approximate solution to  $\Delta x$ , denoted by  $\Delta x^1$ , can then be found by solving

$$f(x^0) + f'(x^0)\Delta x^1 = 0 ,$$

thus yielding a better approximation to  $x_r$  as

$$x^1 = x^0 + \Delta x^1 = x^0 - \frac{f(x^0)}{f'(x^0)} . \quad (4.3)$$

One can now start with  $x^0$  as the initial guess and find  $x^1$  which is closer to the true root. The process can then be repeated with  $x^{i+1}$  substituted in place of  $x^i$  in the next iteration until the desired accuracy is achieved.

This process, of course, is not guaranteed to work. The function must satisfy certain properties and the initial guess must be sufficiently close to the desired root. However, if the function has only one root and the iteration procedure converges, the true root will be approached.

Consider now the problem

$$\begin{aligned} f_1(y_1, \dots, y_n, y_1', \dots, y_n', y_1'', \dots, y_n'', x) &= 0 \\ \vdots \\ f_n(y_1, \dots, y_n, y_1', \dots, y_n', y_1'', \dots, y_n'', x) &= 0 \end{aligned} \quad (4.4)$$

or, expressed in matrix notation,

$$f(y, y', y'', x) = 0 \quad (4.5)$$

The primes indicate derivatives with respect to  $x$ , and  $f_i$  represents a known, algebraic function of its arguments. Thus (4.4) is, in general, a set of ordinary, coupled, nonlinear differential equations with dependent variables  $y_1, \dots, y_n$  and independent variable  $x$ . The solution for  $y$  is desired. An initial guess,  $y^0$ , is first made. A set of linear equations with a dependent variable  $\Delta y^1$  can be derived by expanding (4.4) as a power series in terms of the dependent variables and their derivatives about the initial guess  $y^0$ . The resulting equations truncated after the linear term yield for the  $i$ 'th equation,

$$f_i^0 + \sum_{j=1}^n \frac{\partial f_i^0}{\partial y_j''} \Delta y_j^{1''} + \sum_{j=1}^n \frac{\partial f_i^0}{\partial y_j'} \Delta y_j^{1'} + \sum_{j=1}^n \frac{\partial f_i^0}{\partial y_j} \Delta y_j^1 = 0 \quad (4.6)$$

where  $f_i^0$  represents the value of  $f_i$  evaluated at the initial guess  $y^0$ . In matrix notation, the equations can be written as

$$A^0 \Delta y^{1''} + B^0 \Delta y^{1'} + C^0 \Delta y^1 = D^0 \quad (4.7)$$

where



$$A^0 = \begin{bmatrix} \frac{\partial f_1^0}{\partial y_1^n} & \cdots & \frac{\partial f_1^0}{\partial y_n^n} \\ \vdots & & \\ \frac{\partial f_n^0}{\partial y_1^n} & \cdots & \frac{\partial f_n^0}{\partial y_n^n} \end{bmatrix} \quad (4.8a)$$

$$B^0 = \begin{bmatrix} \frac{\partial f_1^0}{\partial y_1^r} & \cdots & \frac{\partial f_1^0}{\partial y_n^r} \\ \vdots & & \\ \frac{\partial f_n^0}{\partial y_1^r} & \cdots & \frac{\partial f_n^0}{\partial y_n^r} \end{bmatrix} \quad (4.8b)$$

$$C^0 = \begin{bmatrix} \frac{\partial f_1^0}{\partial y_1} & \cdots & \frac{\partial f_1^0}{\partial y_n} \\ \vdots & & \\ \frac{\partial f_n^0}{\partial y_1} & \cdots & \frac{\partial f_n^0}{\partial y_n} \end{bmatrix} \quad (4.8c)$$

and

$$D^0 = \begin{bmatrix} -f_1^0 \\ \vdots \\ -f_n^0 \end{bmatrix} = -f^0. \quad (4.8d)$$

The set (4.7) is a set of coupled, linear, ordinary differential equations, which when solved, yields  $\Delta y^1$ . Once  $\Delta y^1$  is known, the improved initial guess is given by

$$y^1 = y^0 + \Delta y^1. \quad (4.9)$$

It has been assumed for the time being that the boundary conditions have been taken care of in a similar fashion. They will be dealt with explicitly later on.

It should be pointed out that  $f$  is a known function, and hence all of its partial derivatives in (4.8) are known. Thus  $A^0$ ,  $B^0$ ,  $C^0$  and  $D^0$  are all known functions of  $y^0$ ,  $y^{0'}$ , and  $y^{0''}$ . It is therefore simple, in principle, to solve (4.7). Once  $y^1$  is found as in (4.9), the above procedure can be repeated with all the zero superscripts replaced by one superscripts. The process can be repeated until the desired accuracy is attained.

For  $i$ 'th iteration, (4.7) can be written as

$$A^i \frac{d^2 \Delta y^{i+1}}{dx^2} + B^i \frac{d \Delta y^{i+1}}{dx} + C^i \Delta y^{i+1} = D^i \quad (4.10)$$

The derivatives involved in  $A^i$ ,  $B^i$ ,  $C^i$  and  $D^i$  are evaluated at each point using a five-point polynomial approximation scheme. As mentioned before, the variable  $x$  has been discretized. To find the derivatives of  $\Delta y^{i+1}$ , the following three-point approximations are used.

$$\frac{dq_k}{dx} = \frac{q_{k+1} - q_{k-1}}{2\Delta x} \quad (4.11)$$

$$\frac{d^2 q_k}{dx^2} = \frac{q_{k+1} - 2q_k + q_{k-1}}{\Delta x^2} \quad (4.12)$$

Here,  $k$  denotes the discretization index of the  $x$  coordinate. Using (4.11), (4.12) in (4.10) we obtain

$$A_k^i \frac{\Delta y_{k+1}^{i+1} - 2\Delta y_k^{i+1} + \Delta y_{k-1}^{i+1}}{\Delta x^2} + B_k^i \frac{\Delta y_{k+1}^{i+1} - \Delta y_{k-1}^{i+1}}{2\Delta x} + C_k^i \Delta y_k^{i+1} = D_k^i \quad (4.13)$$

Simplification of the above equation yields

$$\alpha_k^i \Delta y_{k+1}^{i+1} + \beta_k^i \Delta y_k^{i+1} + \gamma_k^i \Delta y_{k-1}^{i+1} = D_k^i \quad (4.14)$$

where

$$\alpha_k^i = \frac{1}{\Delta x^2} A_k^i + \frac{1}{2\Delta x} B_k^i \quad (4.15a)$$

$$\beta_k^i = -\frac{2}{\Delta x^2} A_k^i + C_k^i \quad (4.15b)$$

$$\gamma_k^i = \frac{1}{\Delta x^2} A_k^i - \frac{1}{2\Delta x} B_k^i \quad (4.15c)$$

If the solution to (4.14) is assumed to have a form

$$\Delta y_k^{i+1} = g_k^i - h_k^i \Delta y_{k+1}^{i+1} \quad (4.16)$$

then the substitution for  $\Delta y_{k-1}^{i+1}$  in (4.14) gives

$$\alpha_k^i \Delta y_{k+1}^{i+1} + (\beta_k^i - \gamma_k^i h_{k-1}^i) \Delta y_k^{i+1} + \gamma_k^i g_{k-1}^i = D_k^i$$

Repeated substitution yields

$$[\alpha_k^i - (\beta_k^i - \gamma_k^i h_{k-1}^i) h_k^i] \Delta y_{k+1}^{i+1}$$

$$+ [(\beta_k^i - \gamma_k^i h_{k-1}^i) g_k^i + \gamma_k^i g_{k-1}^i - D_k^i] = 0$$

Since  $\Delta y_{k+1}^{i+1}$  is finite, this equation is easily satisfied by letting each term in the brackets to be zero. Then,

$$h_k^i = (\beta_k^i - \gamma_k^i h_{k-1}^i)^{-1} \alpha_k^i \quad (4.17)$$

$$g_k^i = (\beta_k^i - \gamma_k^i h_{k-1}^i)^{-1} (D_k^i - \gamma_k^i g_{k-1}^i) . \quad (4.18)$$

Thus, if  $h_k^i$  and  $g_k^i$  are known for a particular  $x_k$ , they can be found for the next  $x_{k+1}$  by using (4.17) and (4.18).

Note that  $k$  is the position index whereas  $i$  is the iteration index. For a particular time step, and for a given  $i$ , computations are done for all  $k$ . The iteration index  $i$  is then changed till a desired convergence is reached. The time index is next changed and the entire process repeated until the final time is reached.

### 4.3 Quasi-static Problem

The problem stated in Section 2.3 can be simplified by normalization of the variables. Let  $\hat{x}$ ,  $\hat{t}$ ,  $\hat{c}$  and  $\hat{\phi}$  represent the normalized variables. Then a normalization scheme is as follows.

$$\begin{aligned} c &= n_i \hat{c} \\ \phi &= V_T \hat{\phi} \\ x &= \sqrt{\frac{\epsilon V_T}{e n_i}} \hat{x} \\ t &= \frac{\epsilon V_T}{e D_c n_i} \hat{t} \end{aligned} \tag{4.19}$$

With these substitutions, and defining

$$\beta = \frac{C_0}{n_i} , \tag{4.20}$$

the quasi-static equations for the degenerate case become

$$\frac{\partial \hat{c}}{\partial \hat{t}} = \frac{\partial}{\partial \hat{x}} \left( \frac{\partial \hat{c}}{\partial \hat{x}} + \hat{c} \frac{\partial \hat{\phi}}{\partial \hat{x}} \right) \tag{4.21a}$$

$$\frac{\partial^2 \hat{\phi}}{\partial \hat{x}^2} = \frac{F_{1/2}(\hat{\phi} + \eta_i)}{F_{1/2}(\eta_i)} - \exp(-\hat{\phi}) - \hat{c} . \tag{4.21b}$$

For notational simplicity the normalized variables will be denoted by  $c$ ,  $\phi$ ,  $x$  and  $t$  in Sections 4.3 and 4.4.

With the discretization of the time coordinate (4.21) becomes

$$\frac{d^2\phi}{dx^2} - \frac{F_{1/2}(\phi+\eta_i)}{F_{1/2}(\eta_i)} + \exp(-\phi) + c = 0 \quad (4.22a)$$

$$\frac{d}{dx} \left( \frac{dc}{dx} + c \frac{d\phi}{dx} \right) - \frac{c-N}{\Delta t} = 0 \quad (4.22b)$$

where the notation

$$c = c(x, t_i)$$

$$\phi = \phi(x, t_i)$$

$$N = c(x, t_{i-1})$$

has been used.

Now the function  $f$  can be written as

$$f = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix} = \begin{bmatrix} \frac{d^2\phi}{dx^2} - \frac{F_{1/2}(\phi+\eta_i)}{F_{1/2}(\eta_i)} + \exp(-\phi) + c \\ \frac{d^2c}{dx^2} + c \frac{d^2\phi}{dx^2} + \frac{dc}{dx} \frac{d\phi}{dx} - \frac{c}{\Delta t} + \frac{N}{\Delta t} \end{bmatrix} \quad (4.23)$$

$$y = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} \phi \\ c \end{bmatrix} . \quad (4.24)$$

For the nondegenerate case [24], the second term in the expression for  $f_1$  becomes  $\exp(\phi)$  instead of  $F_{1/2}(\phi+\eta_i)/F_{1/2}(\eta_i)$ . Corresponding changes for this case can be easily made in the expressions below. For the vector  $f$  above, the matrices  $A^i$ ,  $B^i$ ,  $C^i$  and  $D^i$  are given by

$$A^i = \begin{bmatrix} \frac{\partial f_1}{\partial \phi''} & \frac{\partial f_1}{\partial c''} \\ \frac{\partial f_2}{\partial \phi''} & \frac{\partial f_2}{\partial c''} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ c & 1 \end{bmatrix} \quad (4.25a)$$

$$B^i = \begin{bmatrix} \frac{\partial f_1}{\partial \phi'} & \frac{\partial f_1}{\partial c'} \\ \frac{\partial f_2}{\partial \phi'} & \frac{\partial f_2}{\partial c'} \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ \frac{dc}{dx} & \frac{d\phi}{dx} \end{bmatrix} \quad (4.25b)$$

$$C^i = \begin{bmatrix} \frac{\partial f_1}{\partial \phi} & \frac{\partial f_1}{\partial c} \\ \frac{\partial f_2}{\partial \phi} & \frac{\partial f_2}{\partial c} \end{bmatrix} = \begin{bmatrix} -\frac{F_{-1/2}(\phi+\eta_i)}{F_{1/2}(\eta_i)} - \exp(-\phi) & 1 \\ 0 & \frac{d^2\phi}{dx^2} - \frac{1}{\Delta t} \end{bmatrix}$$

$$(4.25c)$$

$$D^i = \begin{bmatrix} -f_1 \\ -f_2 \end{bmatrix} = \begin{bmatrix} -\frac{d^2\phi}{dx^2} + \frac{F_{1/2}(\phi+\eta_i)}{F_{1/2}(\eta_i)} - \exp(-\phi) - c \\ -\frac{d^2c}{dx^2} - c \frac{d^2\phi}{dx^2} - \frac{dc}{dx} \frac{d\phi}{dx} + \frac{c}{\Delta t} - \frac{N}{\Delta t} \end{bmatrix}$$

(4.25d)

where for simplicity, superscripts  $i$  have been suppressed in  $\phi$  and  $c$ .

The flow diagram of the numerical method is shown in Fig. 4.1.

#### 4.4 Boundary Conditions

Normalized boundary conditions for the constant source diffusion are

$$c(0, t) = \beta$$

$$\frac{\partial \phi(0, t)}{\partial x} = 0$$

$$c(\infty, t) = 0$$

$$\phi(\infty, t) = 0$$

$$c(x, 0) = 0, \quad x > 0. \quad (4.26)$$



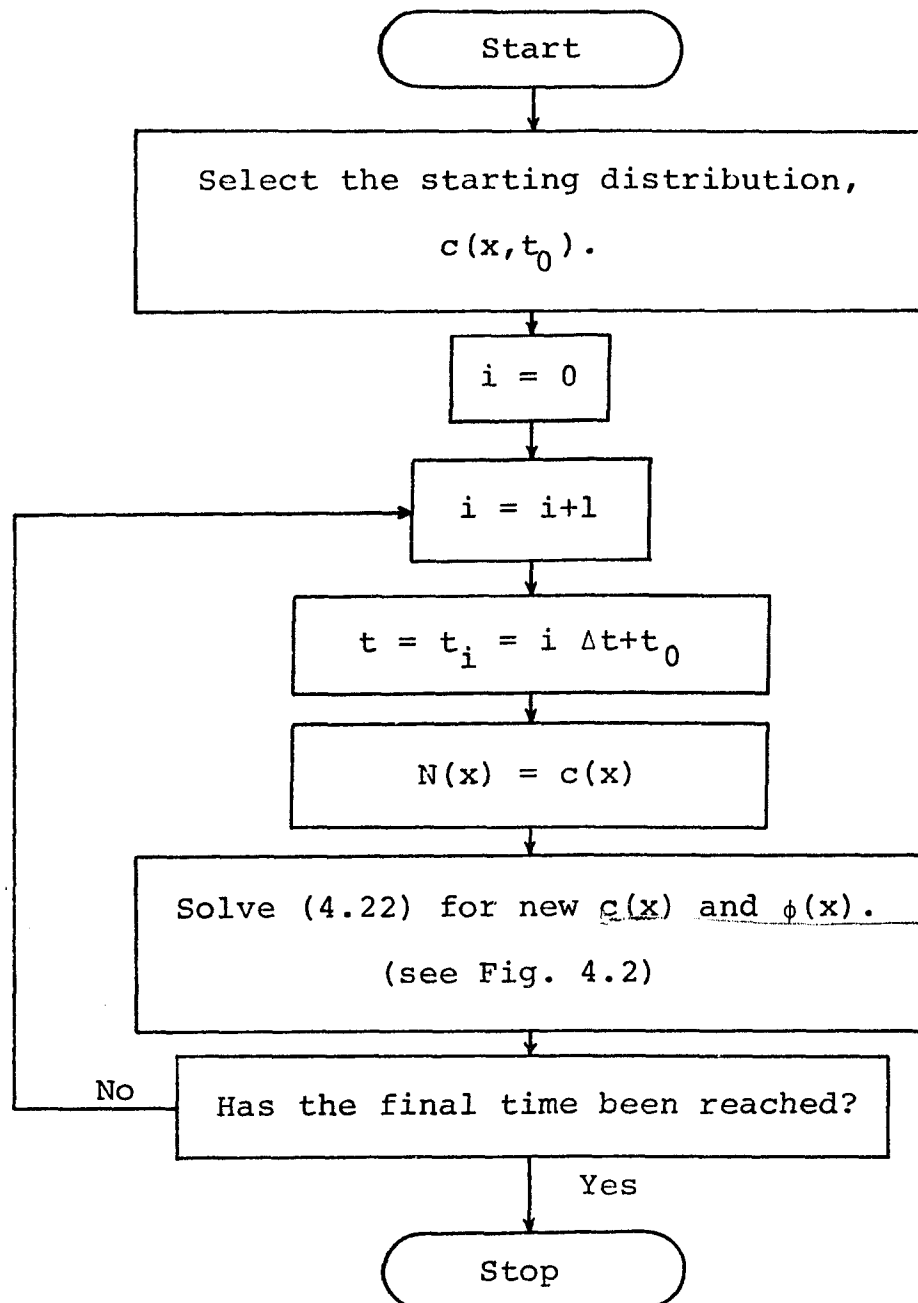


FIGURE 4.1. Flow Diagram of the Numerical Method

Notice that the only parameter in the above conditions, other than the dependent and the independent variables, is the normalized surface concentration  $\beta$ . A series of solutions over a range of  $\beta$  will, therefore, give a general solution to the quasi-static problem.

After the time is discretized, the boundary conditions for the ordinary differential equations become

$$c(0) = \beta$$

$$\frac{d\phi(0)}{dx} = 0$$

$$c(\infty) = 0$$

$$\phi(\infty) = 0 . \quad (4.27)$$

These boundary conditions can be satisfied in the  $i$ 'th iteration by requiring that

$$\Delta c^{i+1}(0) = \beta - c^i(0)$$

$$\frac{d\Delta\phi^{i+1}(0)}{dx} = - \frac{d\phi^i(0)}{dx}$$

$$\Delta c^{i+1}(\infty) = - c^i(\infty)$$

$$\Delta\phi^{i+1}(\infty) = -\phi^i(\infty) . \quad (4.28)$$

If the initial guess is picked such that

$$c^0(0) = \beta$$

$$c^0(\infty) = 0$$

$$\phi^0(\infty) = 0$$

then the desired boundary conditions can be met by merely requiring that

$$\Delta c^{i+1}(0) = 0$$

$$\frac{d\Delta\phi^{i+1}(0)}{dx} = - \frac{d\phi^i(0)}{dx}$$

$$\Delta c^{i+1}(\infty) = 0$$

$$\Delta\phi^{i+1}(\infty) = 0 \quad . \quad (4.29)$$

Numerically, it is impractical to extend the x-coordinate to infinity. Therefore, a distance L is chosen which is large enough to approximate infinity and the boundary conditions are applied at x=L. If the distance L corresponds to the m'th point, the boundary conditions become

$$\Delta c_1^{i+1} = 0$$

$$\frac{\Delta \phi_2^{i+1} - \Delta \phi_1^{i+1}}{\Delta x} = - \frac{d\phi_1^i}{dx}$$

$$\Delta c_m^{i+1} = 0$$

$$\Delta \phi_m^{i+1} = 0 . \quad (4.30)$$

Note that the quantity  $\frac{d\phi_1^i}{dx}$  has already been determined while finding the matrices A, B, C and D.

The procedure for solving (4.10) is as follows. If it is selected that

$$h_1^i = \begin{bmatrix} -1 & 0 \\ 0 & 0 \end{bmatrix} \quad (4.31a)$$

and

$$g_1^i = \begin{bmatrix} \Delta x \frac{d\phi_1^i}{dx} \\ 0 \end{bmatrix} \quad (4.31b)$$

then  $\Delta y_1^{i+1}$  given by (4.16) will satisfy the surface boundary conditions of (4.30). Using (4.17) and (4.18)  $h_k^i$  and  $g_k^i$  can then be generated for  $k = 2, \dots, m$ . Choosing

$$\Delta y_m^{i+1} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \quad (4.32)$$

will satisfy the boundary conditions at  $x=L$ , given by (4.30), and (4.16) will generate  $\Delta y_k^{i+1}$  for  $k = m-1, \dots, 1$ .

The technique for numerically solving the problem described here is summarized in the block diagram given in Fig. 4.2. In the actual program many of the functions represented in the block diagram have been combined for better computational efficiency.

The normalized boundary conditions for drive-in diffusion are given by

$$\frac{\partial c(0,t)}{\partial x} = 0$$

$$\frac{\partial \phi(0,t)}{\partial x} = 0$$

$$c(\infty, t) = 0$$

$$\phi(\infty, t) = 0$$

$$c(x, 0) = N_0(x) , \quad x > 0 \tag{4.33}$$

where  $N_0(x)$  is the normalized starting distribution for the drive-in diffusion. Note that the first boundary condition is obtained because the flux of the impurity atoms at  $x=0$  is zero. Thus,

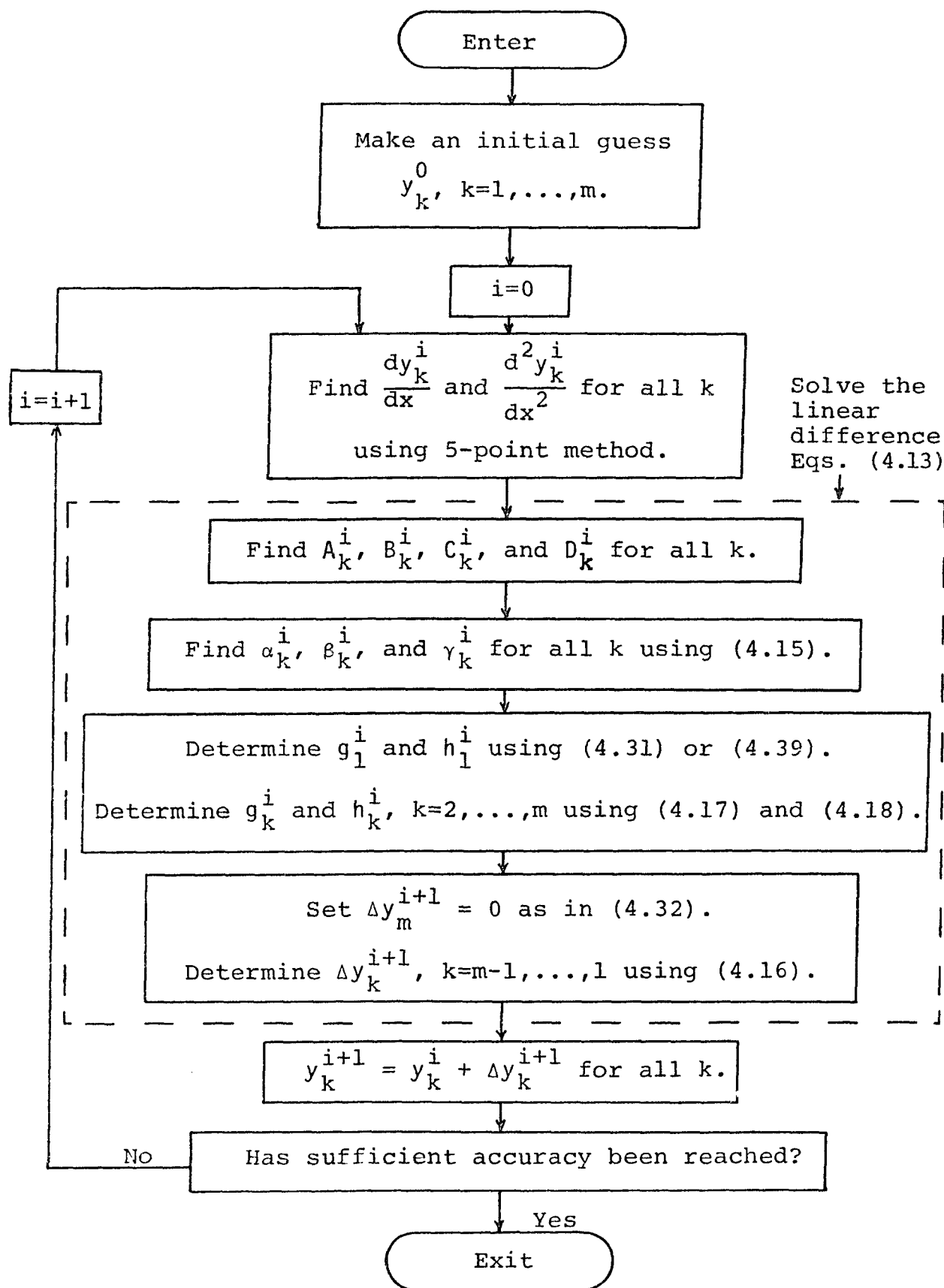


FIGURE 4.2. Flow Diagram of the Iteration Procedure

$$D_c \frac{\partial c(0,t)}{\partial x} - \mu_c cE(0,t) = 0 . \quad (4.34)$$

The semiconductor material as a whole may be assumed to be charge neutral. The total charge  $Q$  per unit area is given by

$$\begin{aligned} Q &= \int_0^{\infty} \rho \, dx \\ &= \epsilon \int_0^{\infty} \frac{\partial E}{\partial x} \, dx \\ &= \epsilon [E(\infty, t) - E(0, t)] . \end{aligned}$$

Equating  $Q$  to zero and noting that  $E(\infty, t) = 0$ , we have

$$E(0, t) = 0 . \quad (4.35)$$

Thus (4.34) yields the first boundary condition.

Proceeding as we did earlier in the Section, instead of (4.28), we now obtain

$$\begin{aligned} \frac{d\Delta c^{i+1}(0)}{dx} &= - \frac{dc^i(0)}{dx} \\ \frac{d\Delta \phi^{i+1}(0)}{dx} &= - \frac{d\phi^i(0)}{dx} \end{aligned}$$

$$\Delta c^{i+1}(\infty) = -c^i(\infty)$$

$$\Delta \phi^{i+1}(\infty) = -\phi^i(\infty) . \quad (4.36)$$

If the initial guess is picked such that

$$c^0(\infty) = 0$$

$$\phi^0(\infty) = 0 ,$$

then the desired boundary conditions will be met by merely requiring that

$$\frac{d\Delta c^{i+1}(0)}{dx} = - \frac{dc^i(0)}{dx}$$

$$\frac{d\Delta \phi^{i+1}(0)}{dx} = - \frac{d\phi^i(0)}{dx}$$

$$\Delta c^{i+1}(\infty) = 0$$

$$\Delta \phi^{i+1}(\infty) = 0 . \quad (4.37)$$

Instead of (4.30), in this case, we now have

$$\frac{\Delta c_2^{i+1} - \Delta c_1^{i+1}}{\Delta x} = - \frac{dc_1^i}{dx}$$



$$\frac{\Delta\phi_2^{i+1} - \Delta\phi_1^{i+1}}{\Delta x} = - \frac{d\phi_1^i}{dx}$$

$$\Delta c_m^{i+1} = 0$$

$$\Delta\phi_m^{i+1} = 0 \quad . \quad (4.38)$$

Therefore, (4.31) become

$$h_1^i = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix} \quad (4.39a)$$

$$g_1^i = \begin{bmatrix} \Delta x \frac{d\phi_1^i}{dx} \\ \Delta x \frac{dc_1^i}{dx} \end{bmatrix} \quad . \quad (4.39b)$$

Note that (4.32) remains the same.

#### 4.5 Quasi-linearization Technique for a Scalar Equation

As discussed in Sections 2.4 and 3.6, the partial differential equations describing the diffusion process can be written in a general form

$$\frac{\partial \phi}{\partial t} = D \left[ f_1(\phi) \left( \frac{\partial \phi}{\partial x} \right)^2 + f_2(\phi) \frac{\partial^2 \phi}{\partial x^2} \right] \quad (4.40)$$

where  $f_1(\phi)$  and  $f_2(\phi)$  take different forms. The boundary conditions are of the form

$$\phi(0, t) = \phi_0$$

$$\phi(\infty, t) = 0$$

$$\phi(x, 0) = 0, \quad x > 0. \quad (4.41)$$

A transformation of independent variables  $(x, t) \rightarrow (y, \tau)$ , similar to the one suggested by Shaw and Wells [19], is chosen so that

$$y = \frac{x}{\sqrt{4Dt}}$$

$$\tau = t. \quad (4.42)$$

The dependent variable in terms of these new independent variables then becomes

$$\phi(x, t) = v[y(x, t), \tau(x, t)]. \quad (4.43)$$

Note that the variable  $v$  used here is not to be confused with vacancy concentration, a notation used in Chapter 3.

Now,

$$\begin{aligned} \frac{\partial \phi}{\partial x} &= \frac{\partial v}{\partial y} \frac{\partial y}{\partial x} + \frac{\partial v}{\partial \tau} \frac{\partial \tau}{\partial x} \\ &= \frac{1}{\sqrt{4D\tau}} \frac{\partial v}{\partial y} \end{aligned} \quad (4.44)$$

Similarly,

$$\begin{aligned}\frac{\partial^2 \phi}{\partial x^2} &= \frac{\partial}{\partial y} \left[ \frac{1}{\sqrt{4D\tau}} \frac{\partial v}{\partial y} \right] \frac{\partial y}{\partial x} \\ &= \frac{1}{4D\tau} \frac{\partial^2 v}{\partial y^2}\end{aligned}\tag{4.45}$$

and

$$\begin{aligned}\frac{\partial \phi}{\partial t} &= \frac{\partial v}{\partial y} \frac{\partial y}{\partial t} + \frac{\partial v}{\partial \tau} \frac{\partial \tau}{\partial t} \\ &= -\frac{y}{2\tau} \frac{\partial v}{\partial y} + \frac{\partial v}{\partial \tau}\end{aligned}\tag{4.46}$$

Substituting these in (4.40) we obtain

$$4\tau \frac{\partial v}{\partial \tau} = 2y \frac{\partial v}{\partial y} + f_1(v) \left(\frac{\partial v}{\partial y}\right)^2 + f_2(v) \frac{\partial^2 v}{\partial y^2}\tag{4.47}$$

and the boundary conditions become

$$v(0, \tau) = \phi_0$$

$$v(\infty, \tau) = 0 .\tag{4.48}$$

Notice that the last two conditions in (4.41) reduce to a single condition in (4.48).

Because of the form of the equation and the boundary conditions, it is easy to show that  $v$  is independent of  $\tau$ , in which case (4.47) reduces to

$$2y \frac{dv}{dy} + f_1(v) \left(\frac{dv}{dy}\right)^2 + f_2(v) \frac{d^2v}{dy^2} = 0 , \quad (4.49)$$

with

$$v(0) = \phi_0$$

$$v(\infty) = 0 . \quad (4.50)$$

Notice that the only parameter in the above problem is  $\phi_0$ . Thus, solutions  $v(y)$  known for all possible values of  $\phi_0$  constitute a general solution to the problem. Once  $v(y)$  has been computed using a numerical procedure,  $\phi(x,t)$  can be obtained for a given  $x$  and  $t$  by using

$$\phi(x,t) = v\left(\frac{x}{\sqrt{4Dt}}\right) . \quad (4.51)$$

A simple way to find  $\phi(x,t)$  from  $v(y)$  is to interpolate  $\phi(x,t)$  according to the equation  $x = \sqrt{4Dt} y$ .

The quasi-linearization technique discussed in Section 4.2 can be used directly to solve (4.49). Since only one equation is involved, the matrices and vectors reduce to scalars. The  $y$  coordinate is uniformly

discretized and the final point  $m$ , corresponding to a distance  $L$  sufficiently large to adequately represent infinity, is chosen.

Let  $i$  denote the iteration number and  $k$  the point in the  $y$  direction. Applying the definitions of Section 4.2, we have

$$f(v'', v', v, y) = 2y \frac{dv}{dy} + f_1(v) \left(\frac{dv}{dy}\right)^2 + f_2(v) \left(\frac{d^2v}{dy^2}\right) \quad (4.52)$$

and

$$A = \frac{\partial f}{\partial v''} = f_2(v) \quad (4.53a)$$

$$B = \frac{\partial f}{\partial v'} = 2y + 2f_1(v) \quad (4.53b)$$

$$C = \frac{\partial f}{\partial v} = \left(\frac{d^2v}{dy^2}\right) \left(\frac{df_2}{dv}\right) + \left(\frac{dv}{dy}\right)^2 \left(\frac{df_1}{dv}\right) \quad (4.53c)$$

$$D = -f = -2y \frac{dv}{dy} - f_1(v) \left(\frac{dv}{dy}\right)^2 - f_2(v) \frac{d^2v}{dy^2} . \quad (4.53d)$$

For simplicity, superscripts and subscripts have been omitted in the above expressions; e.g.  $A$  actually is  $A_k^i$ ,  $v$  actually is  $v_k^i$ , etc. Also,  $\frac{\partial f_1}{\partial v}$  and  $\frac{\partial f_2}{\partial v}$ , which occur in the expression for  $C$ , are found by analytic differentiation.

Note that for different problems only the quantities A, B, C and D need be changed. The rest of the procedure described here remains unaltered. This, of course, assumes that the problem and the boundary conditions are in the given form. Applying the results of Section 4.3,

$$\Delta v_k^{i+1} = g_k^i - h_k^i \Delta v_{k+1}^{i+1} \quad (4.54)$$

where

$$g_k^i = \frac{D_k^i - \gamma_k^i g_{k-1}^i}{\beta_k^i - \gamma_k^i h_{k-1}^i} \quad (4.55a)$$

and

$$h_k^i = \frac{\alpha_k^i}{\beta_k^i - \gamma_k^i h_{k-1}^i} \quad (4.55b)$$

where

$$\alpha_k^i = \frac{A_k^i}{(\Delta y)^2} + \frac{B_k^i}{2\Delta y} \quad (4.56a)$$

$$\beta_k^i = -\frac{2A_k^i}{(\Delta y)^2} + C_k^i \quad (4.56b)$$

$$\gamma_k^i = \frac{A_k^i}{(\Delta y)^2} - \frac{B_k^i}{2\Delta y} . \quad (4.56c)$$

The boundary conditions chosen for difference variables are

$$h_1^i = g_1^i = 0 \quad (4.57a)$$

and

$$\Delta v_m^{i+1} = 0 . \quad (4.57b)$$

This assumes that the initial guess is constrained to satisfy the boundary conditions.

The computation procedure is the same as that shown in Fig. 4.2 except that various expressions are replaced by the ones above. An initial guess  $v_k^0$  for all  $k$  is made, the correction  $\Delta v_k^{i+1}$  is found, and the new initial guess

$$v_k^1 = v_k^0 + \Delta v_k^1 , \quad (4.58)$$

is used to restart the procedure which is repeated until sufficient accuracy is obtained.

#### 4.6 Application to the Charge Neutrality Approximation

The method discussed in the last section can now be applied to solve the equations of Section 2.4. We have

$$f_1(v) = \frac{F_{-3/2}(v+\eta_i) + F_{-1/2}(v+\eta_i)}{F_{-1/2}(v+\eta_i) + F_{1/2}(\eta_i)\exp(-v)} \equiv \frac{\lambda_1(v)}{\lambda_2(v)} \quad (4.59)$$

and

$$f_2(v) = \frac{F_{-1/2}(v+\eta_i) + F_{1/2}(v+\eta_i)}{F_{-1/2}(v+\eta_i) + F_{1/2}(\eta_i)\exp(-v)} \equiv \frac{\lambda_3(v)}{\lambda_2(v)} \quad (4.60)$$

where  $\lambda_1$ ,  $\lambda_3$  and  $\lambda_2$  represent the numerators and denominators of  $f_1(v)$  and  $f_2(v)$ , respectively. Thus,

$$\frac{df_1}{dv} = [\lambda_2(v) \frac{d\lambda_1}{dv} - \lambda_1(v) \frac{d\lambda_2}{dv}] [\lambda_2(v)]^{-2} \quad (4.61)$$

$$\frac{df_2}{dv} = [\lambda_2(v) \frac{d\lambda_3}{dv} - \lambda_3(v) \frac{d\lambda_2}{dv}] [\lambda_2(v)]^{-2} \quad (4.62)$$

where

$$\frac{d\lambda_1}{dv} = F_{-5/2}(v+\eta_i) + F_{-3/2}(v+\eta_i) \quad (4.63a)$$

$$\frac{d\lambda_2}{dv} = F_{-3/2}(v+\eta_i) - F_{1/2}(\eta_i)\exp(-v) \quad (4.63b)$$

$$\frac{d\lambda_3}{dv} = F_{-3/2}(v+\eta_i) + F_{-1/2}(v+\eta_i) \quad (4.63c)$$

The quantities A, B, C and D are now known and the procedure of the previous section can be applied.

#### 4.7 Application to Vacancy-aided Diffusion

The diffusion process in this case is defined by the equation



$$\frac{\partial \psi}{\partial t} = D \left[ \left( \frac{\partial \psi}{\partial x} \right)^2 f_1(\psi) + \left( \frac{\partial^2 \psi}{\partial x^2} \right) f_2(\psi) \right] \quad (4.64)$$

where  $D$ ,  $f_1$  and  $f_2$  are given in Section 3.6.

The lengthy form of  $f_1$  and  $f_2$  makes the expressions for  $A$ ,  $B$ ,  $C$  and  $D$  rather cumbersome, although, in principle, it is simple to find them. In order to evaluate these quantities, we need to evaluate  $\frac{\partial f_1}{\partial \psi}$  and  $\frac{\partial f_2}{\partial \psi}$ . After some manipulation, these are given by

$$\frac{\partial f_1}{\partial \psi} = f_1(\psi) + \exp(\psi) \frac{\phi_5(\psi+\eta_i)}{\phi_1(\psi+\eta_i)} - \exp(\psi) \frac{\phi_3(\psi+\eta_i)\phi_6(\psi+\eta_i)}{[\phi_1(\psi+\eta_i)]^2} \quad (4.65)$$

$$\frac{\partial f_2}{\partial \psi} = f_2(\psi) + \exp(\psi) \frac{\phi_7(\psi+\eta_i)}{\phi_1(\psi+\eta_i)} - \exp(\psi) \frac{\phi_4(\psi+\eta_i)\phi_8(\psi+\eta_i)}{\phi_1(\psi+\eta_i)} \quad (4.66)$$

where

$$\begin{aligned} \phi_5(\lambda) \equiv & N_c [F_{-1/2}(\lambda) + 2F_{-3/2}(\lambda) + F_{-5/2}(\lambda) \\ & + 2 \exp(\lambda+\epsilon_d) \{4F_{1/2}(\lambda) + 8F_{-1/2}(\lambda) \\ & + 5F_{-3/2}(\lambda) + F_{-5/2}(\lambda)\}] \end{aligned} \quad (4.67a)$$

$$\begin{aligned} \phi_6(\lambda) &\equiv N_c F_{-3/2}(\lambda) - N_v \exp(-\lambda - \epsilon_g) + 2N_c \exp(\lambda + \epsilon_d) \\ &\times \{F_{1/2}(\lambda) + 2F_{-1/2}(\lambda) + F_{-3/2}(\lambda)\} \end{aligned} \quad (4.67b)$$

$$\begin{aligned} \phi_7(\lambda) &\equiv N_c [F_{-1/2}(\lambda) + F_{-3/2}(\lambda) + 2\exp(\lambda + \epsilon_d) \\ &\times \{2F_{1/2}(\lambda) + 3F_{-1/2}(\lambda) + F_{-3/2}(\lambda)\}] \end{aligned} \quad (4.67c)$$

$$\begin{aligned} \phi_8(\lambda) &\equiv N_c F_{-3/2}(\lambda) - N_v \exp(-\lambda - \epsilon_g) + 2N_c \exp(\lambda + \epsilon_d) \\ &\times \{F_{1/2}(\lambda) + 2F_{-1/2}(\lambda) + F_{-3/2}(\lambda)\} . \end{aligned} \quad (4.67d)$$

Thus A, B, C and D are known, and the numerical procedure of Section 4.5 can be used.

#### 4.8 Computation of the Boundary Condition

We now consider the computation of  $\psi_0$  for a given  $C_0$  by using (3.52). The Newton-Raphson method for finding the roots of a nonlinear algebraic equation can be used. However, we need a starting guess for  $\psi_0$  which is sufficiently close to the true root. One way to find this starting guess is to consider the equation for the non-degenerate case and complete ionization, in which case (3.52) reduces to

$$C_0 - \{N_c \exp(\psi_0^1 + \eta_i) - N_v \exp(-\psi_0^1 - \eta_i - \epsilon_g)\} = 0$$

or,

$$\psi_0^1 = \sinh^{-1} \left( \frac{C_0}{2n_i} \right) = \sinh^{-1} (\beta/2) \quad (4.68)$$

where the superscript on  $\psi_0$  denotes the initial guess.

The true root can now be obtained by following the iteration procedure

$$\psi_0^{i+1} = \psi_0^i - \frac{F(\psi_0^i)}{F'(\psi_0^i)} \quad (4.69)$$

where

$$F(\psi_0) = [1 + 2\exp(\psi_0 + \eta_i + \epsilon_d)] \left[ \frac{F_{1/2}(\psi_0 + \eta_i)}{F_{1/2}(\eta_i)} - \exp(-\psi_0) \right]^{-\beta} \quad (4.70)$$

and

$$F'(\psi_0) = \exp(-\psi_0) + \frac{F_{-1/2}(\psi_0 + \eta_i)}{F_{1/2}(\eta_i)} + \frac{2\exp(\psi_0 + \eta_i + \epsilon_d)}{F_{1/2}(\eta_i)} \\ \times [F_{1/2}(\psi_0 + \eta_i) + F_{-1/2}(\psi_0 + \eta_i)] \quad (4.71)$$

#### 4.9 Discussion

The results obtained using the numerical techniques presented in this Chapter are discussed in Chapter 5. To compare the results of vacancy-aided diffusion using Fermi-Dirac statistics to those obtained using Maxwell-

Boltzmann statistics, the simplest approach is to replace the Fermi integral subroutine by one where an exponential function is used in place of the Fermi functions. For computations with complete ionization,  $\epsilon_d$  may be replaced by a negative quantity of large magnitude, effectively negating the effect of the partial ionization term.

## CHAPTER 5

### RESULTS

The formulations described in the previous chapters, for convenience, are abbreviated here as follows: quasi-static (Section 2.3) as QS, charge neutrality (Section 2.4) as CN, and vacancy-aided (Section 3.2) as VA. In this Chapter, numerical results using the techniques discussed earlier are presented for the case of a constant source diffusion of As in Si.

As indicated earlier,  $n_i$  is calculated from the data in [29] using

$$n_i = 7.766 \times 10^{15} \exp(5.528269 \times 10^{-3} T) \quad (5.1)$$

where the units are  $\text{cm}^{-3}$  and  $T$  is in  $^{\circ}\text{K}$ . The above expression is valid in the temperature range of 900-1200  $^{\circ}\text{C}$ . For the intrinsic diffusion coefficient of As in Si several empirical expressions have been suggested [40, 33, 41]. Masters and Fairfield have suggested the expression

$$D_C^* = 60 \exp(-4.2/kT) \quad (5.2)$$

Chiu and Ghosh have proposed

$$D_C^* = 24 \exp(-4.0833/kT) \quad (5.3)$$

whereas Kennedy and Murley have given

$$D_C^* = 2870 \exp(-4.5725/kT) . \quad (5.4)$$

The units of  $D_C^*$  and  $kT$  in the above expressions are  $\text{cm}^2/\text{sec}$  and eV, respectively. The band gap for Si in eV is given by [31]

$$E_g = 1.205 - 2.8 \times 10^{-4} T . \quad (5.5)$$

The ratio of effective masses is assumed to be temperature independent [30],

$$\frac{m_p^*}{m_n^*} = \left( \frac{0.67818}{1.19250} \right)^{2/3} . \quad (5.6)$$

Using (2.52) then yields

$$\eta_i = -6.98956 \times 10^3 T^{-1} + 1.34193 . \quad (5.7)$$

Other physical constants used are:

$$T = 1050 \text{ } ^\circ\text{C}$$

$$k = 8.62 \times 10^{-5} \text{ eV}/^\circ\text{K}$$

$$e = 1.602 \times 10^{-19} \text{ coulomb}$$

$$\epsilon = 11.7 \epsilon_0 = 1.0359 \times 10^{-12} \text{ farad/cm} .$$

The maximum value of the surface concentration used is  $C_0 = 1.6 \times 10^{21} \text{ cm}^{-3}$ , which represents the solid solubility value at the diffusion temperature. The values of  $E_d$  and  $(E_c - E_v)$  are nominally assumed to be 0.05 and 0.4 eV, respectively.

The profiles resulting from the QS approximation using FD and MB statistics are shown in Fig. 5.1 for various diffusion times. An average value from (5.2) and (5.3) of  $D_c^* = 6.44 \times 10^{-15} \text{ cm}^2/\text{sec}$  has been used. The complementary error function profiles, which represent the correct solution for  $E=0$ , are also shown. It is observed that the internal electric field enhances diffusion at high concentrations. It is also seen that the use of MB statistics, instead of FD statistics, gives an underestimate of the impurity density values, typical error being about 4% near the surface and 50% deep in the material. It was found that at low concentrations, use of either statistics yields the same result, which is not unexpected, since all the Fermi functions reduce to exponential functions. The electric field plots for the QS approximation with MB statistics are shown in Fig. 5.2. These profiles are reminiscent of those obtained in a high-low junction. It may be noted that the field varies almost linearly near the surface and then reaches a maximum value. This maximum value decreases as the diffusion time increases. Similar profiles are obtained

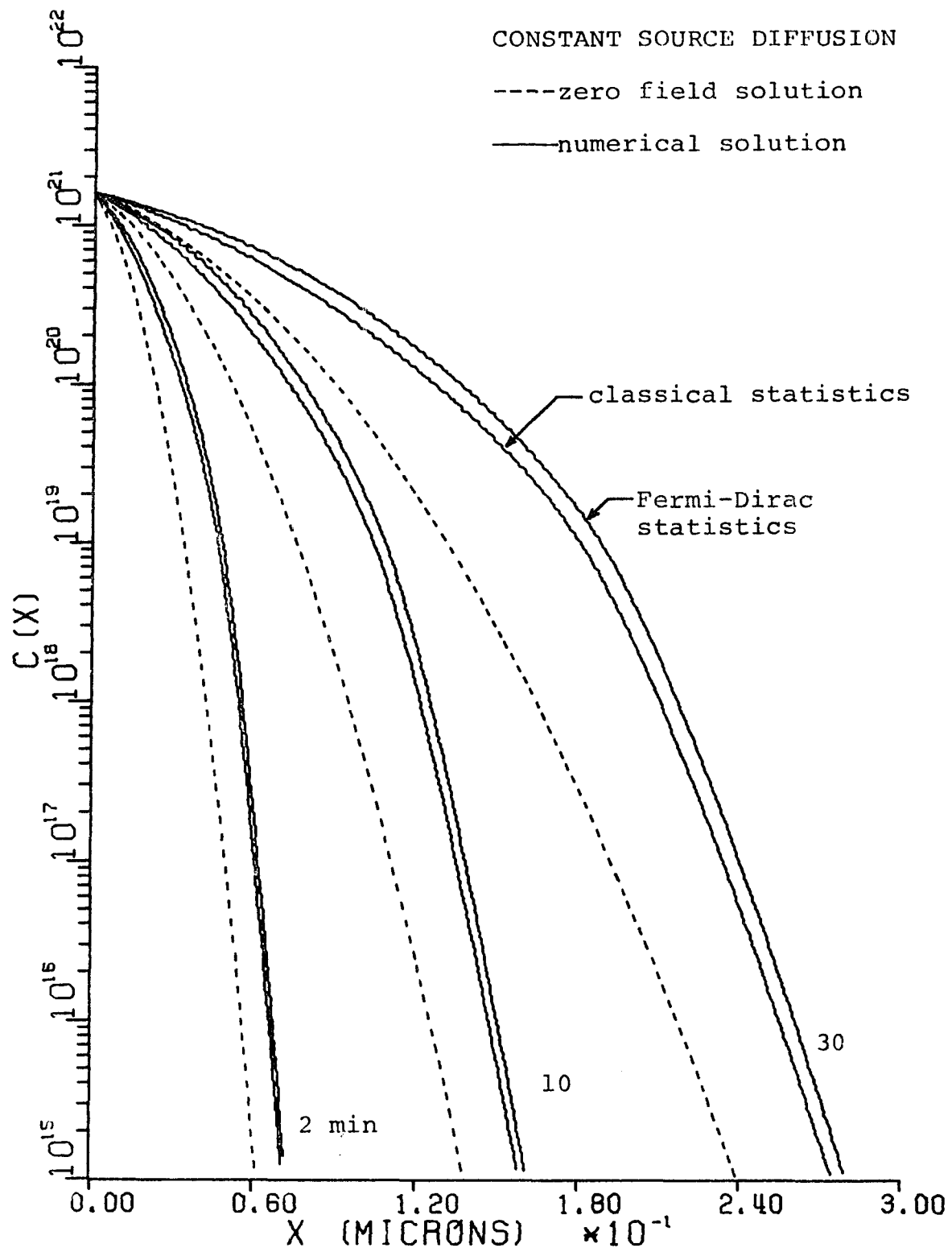


FIGURE 5.1. Impurity Profiles of Arsenic in Silicon Using the Quasi-static Model



when FD statistics are used.

The solution of the CN approximation was compared to the QS approximation. When the impurity density profiles were plotted on the log scale of Fig. 5.1, no significant difference was observed between QS and CN results. The electric field obtained from the CN model with MB statistics was also found to be insignificantly different from that shown in Fig. 5.2. It is concluded from the above analysis that charge neutrality is an excellent approximation for describing a typical diffusion process. The CN model is simpler and computationally very efficient compared to the QS model. It can, therefore, be used conveniently to find the effect of the internal electric field.

The effect of vacancies can be analyzed by comparing the results of VA model to those of the CN model as shown in Fig. 5.3. It is evident that at high concentrations vacancies substantially enhance impurity diffusion. The profiles show a region of relatively slowly varying density followed by a region where it drops suddenly. The intrinsic diffusion coefficient used has been obtained using (5.2) for both models for a consistent comparison. Note that the VA model includes the effect of partial ionization in addition to the use of FD statistics.

As indicated in Chapter 3, Hu and Schmidt [22] have computed the results of As diffusion in Si. They have

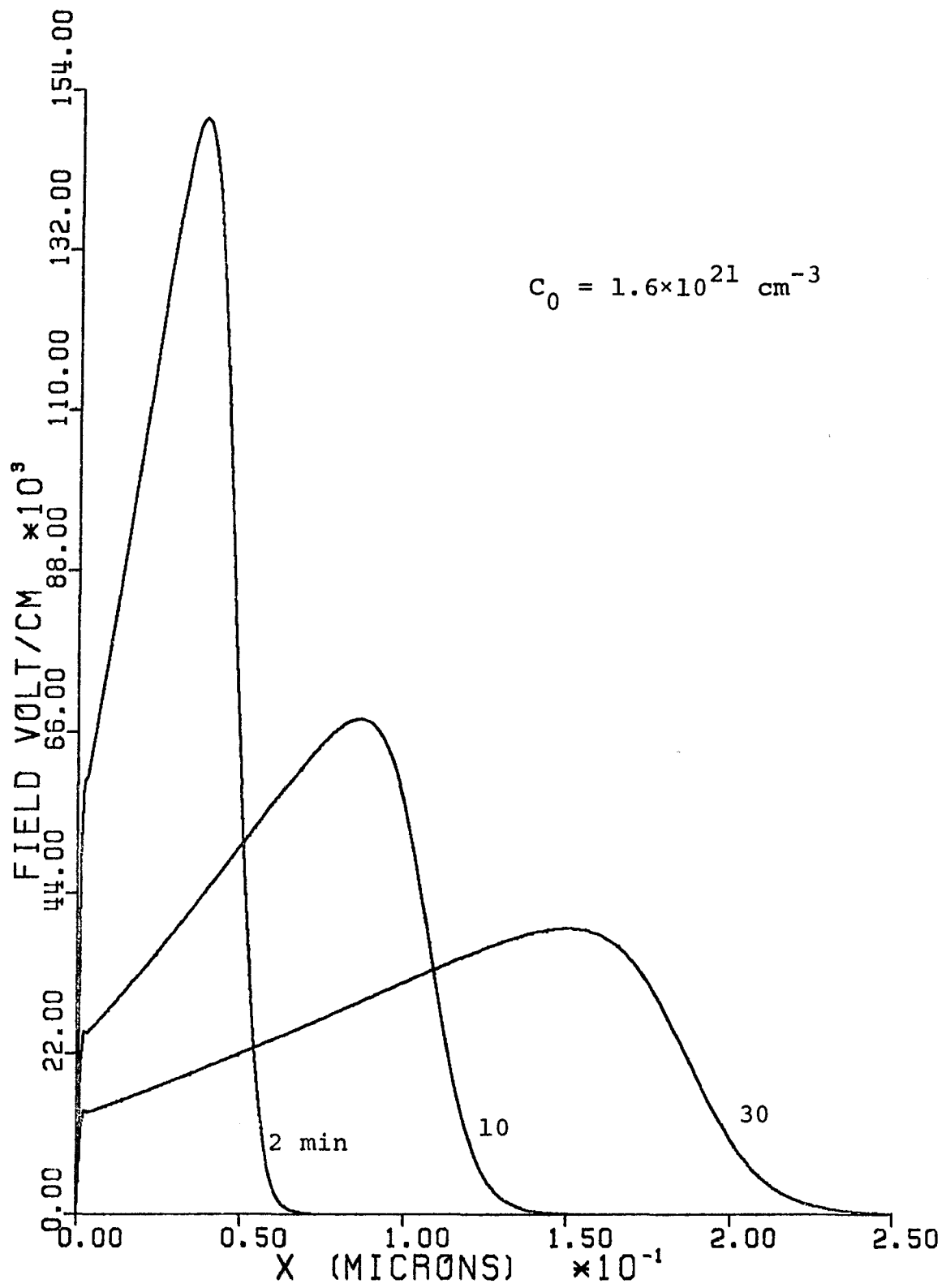


FIGURE 5.2. Electric Field for the Constant Source Diffusion

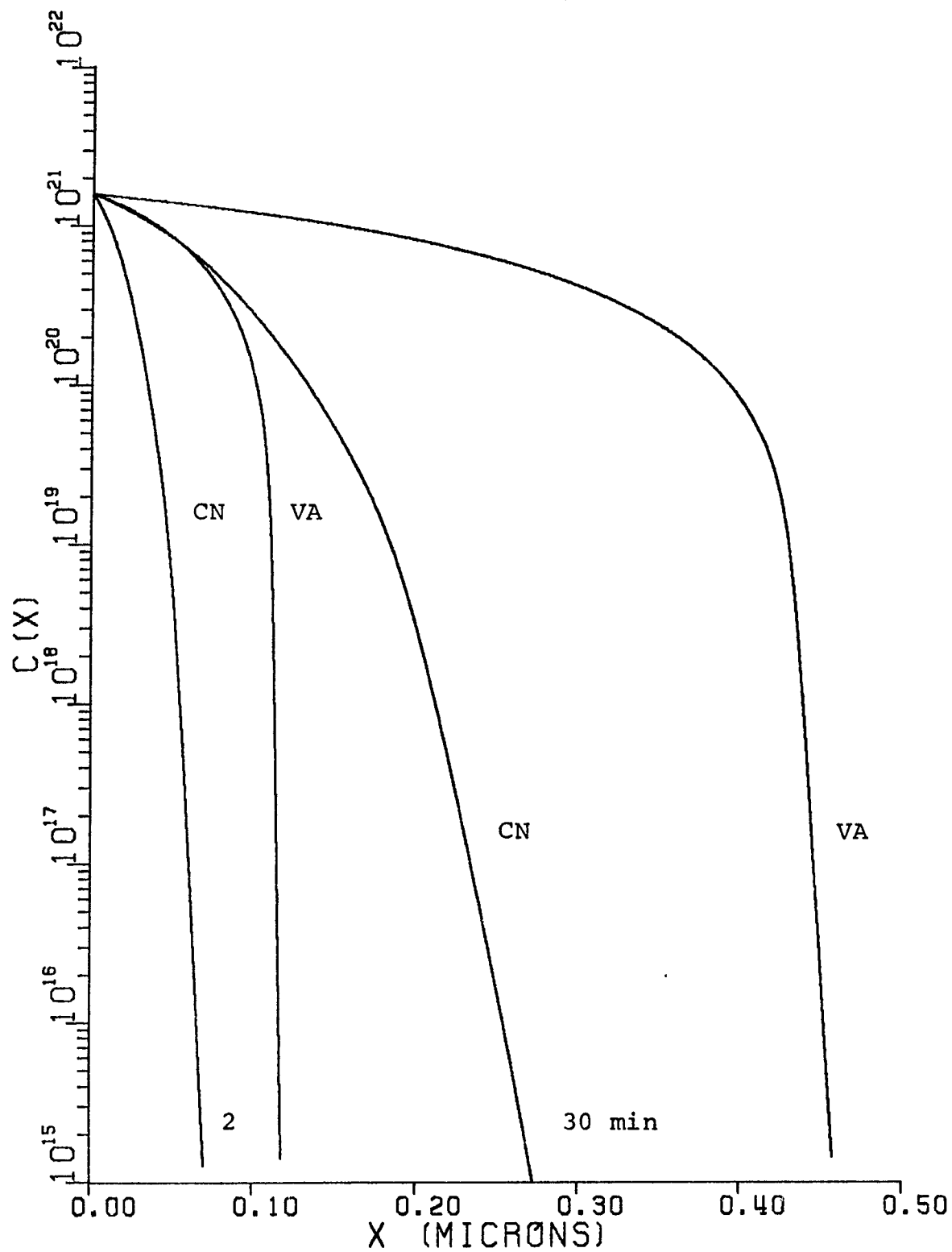


FIGURE 5.3. Comparison of Results Using Charge Neutrality and Vacancy-aided Models for High Surface Concentration

used MB statistics and have assumed complete ionization. Also, a factor  $\beta$  was assumed to be 100 which is only a rough approximation [32]. In Fig. 5.4, profiles obtained using the VA model are shown for the following cases: FD statistics with partial ionization, MB statistics with partial ionization, FD statistics with complete ionization and MB statistics with complete ionization. The last case is similar to that considered by Hu and Schmidt. It is evident that at high concentrations the assumption of complete ionization introduces very large errors. Hu and Schmidt have indicated that the validity of their physical model breaks down at high concentrations because there is no limit to the enhancement effect due to vacancies. It is seen here that with the incorporation of partial ionization, the VA model continues to remain valid. Note that as in the case of the QS model, use of MB statistics yields an underestimate of the impurity density. At relatively low surface concentrations, e.g.,  $C_0 = 10^{19} \text{ cm}^{-3}$ , the use of either statistics and ionization conditions does not make any significant difference.

At low concentrations, the effect of the electric field becomes less significant and the CN model yields results which are very close to the complementary error function profiles as shown in Fig. 5.5. As pointed out in Section 3.5, the form of the impurity flux with vacancies reduces to that of the QS case at near intrinsic conditions.

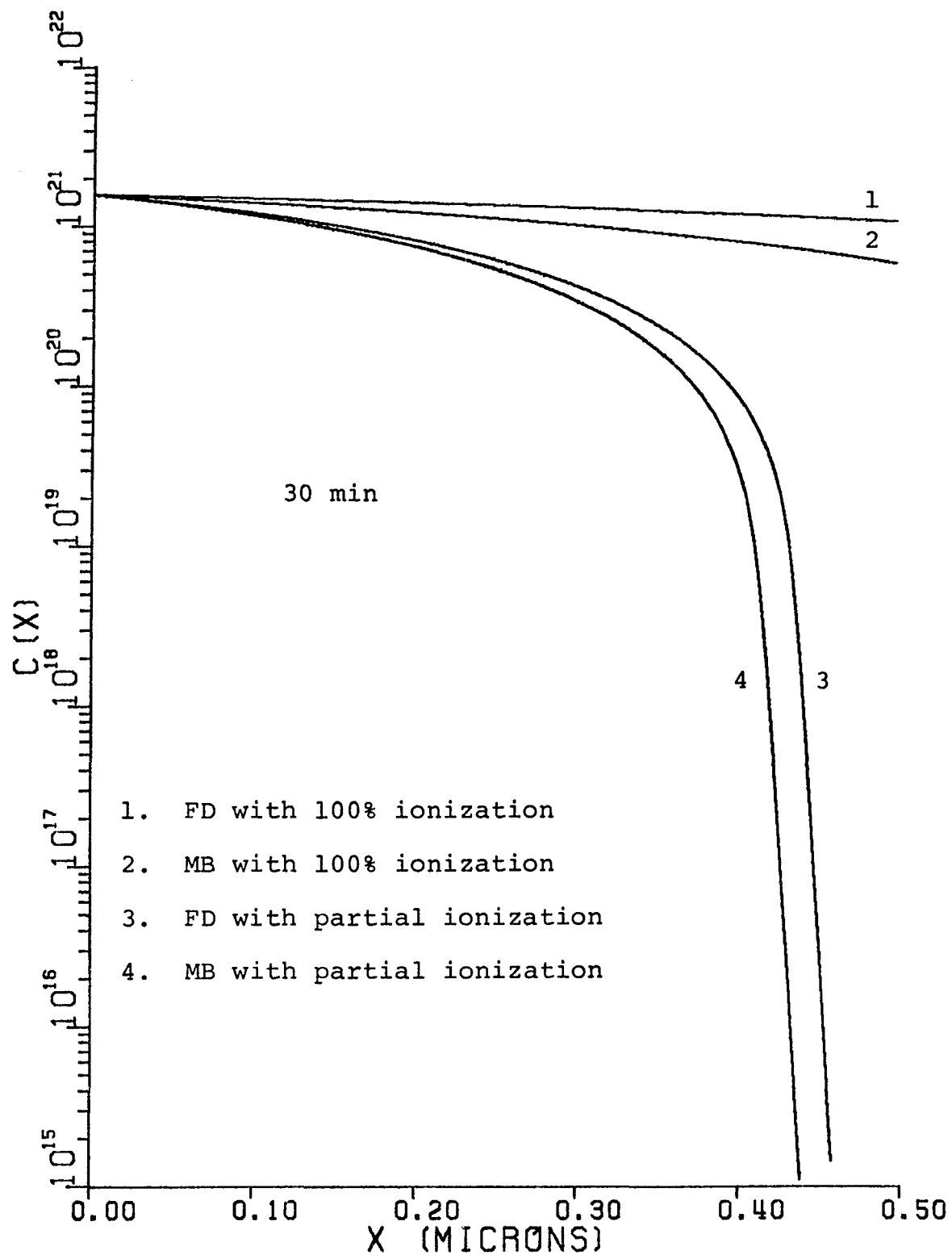


FIGURE 5.4. Effect of Statistics and Ionization on Impurity Concentration Using the Vacancy-aided Model

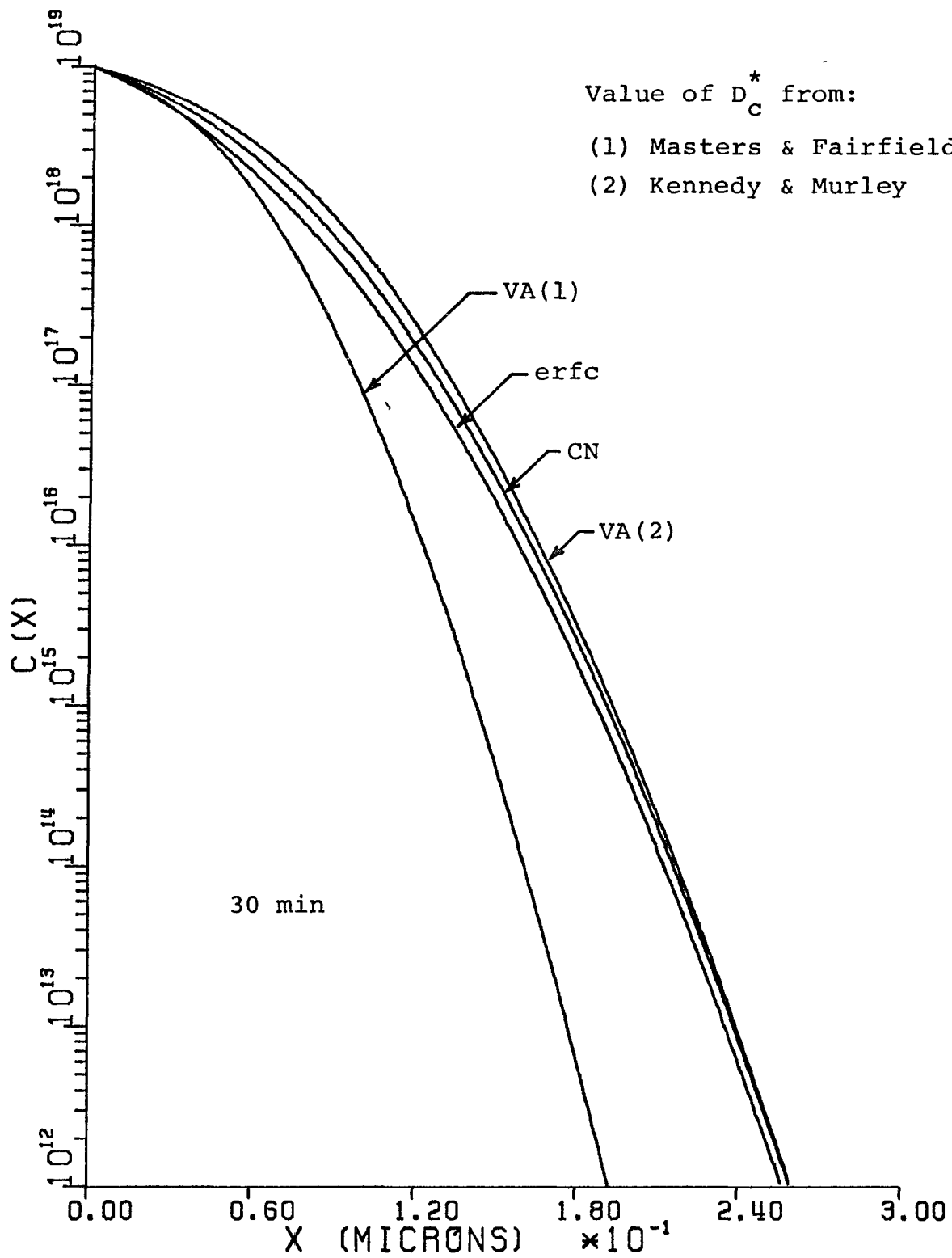


FIGURE 5.5. Impurity Profiles for Low Surface Concentration Using Charge Neutrality, Vacancy-aided and Zero Field Models

However, in the VA model, it was assumed that  $\xi \gg 1$ , and therefore, strictly speaking, the model is not valid at low concentrations. The range of validity of the model can not be determined at present because, as is evident from Fig. 5.5, the impurity profiles strongly depend on the value of the intrinsic diffusion coefficient used.

Comparison between the experimental results [33] and the calculated profiles using the vacancy-aided model for various values of  $D_c^*$  and the vacancy levels is shown in Fig. 5.6. Note that good agreement exists for the case 3. It was found that the results were relatively insensitive to the variations in donor ionization level.

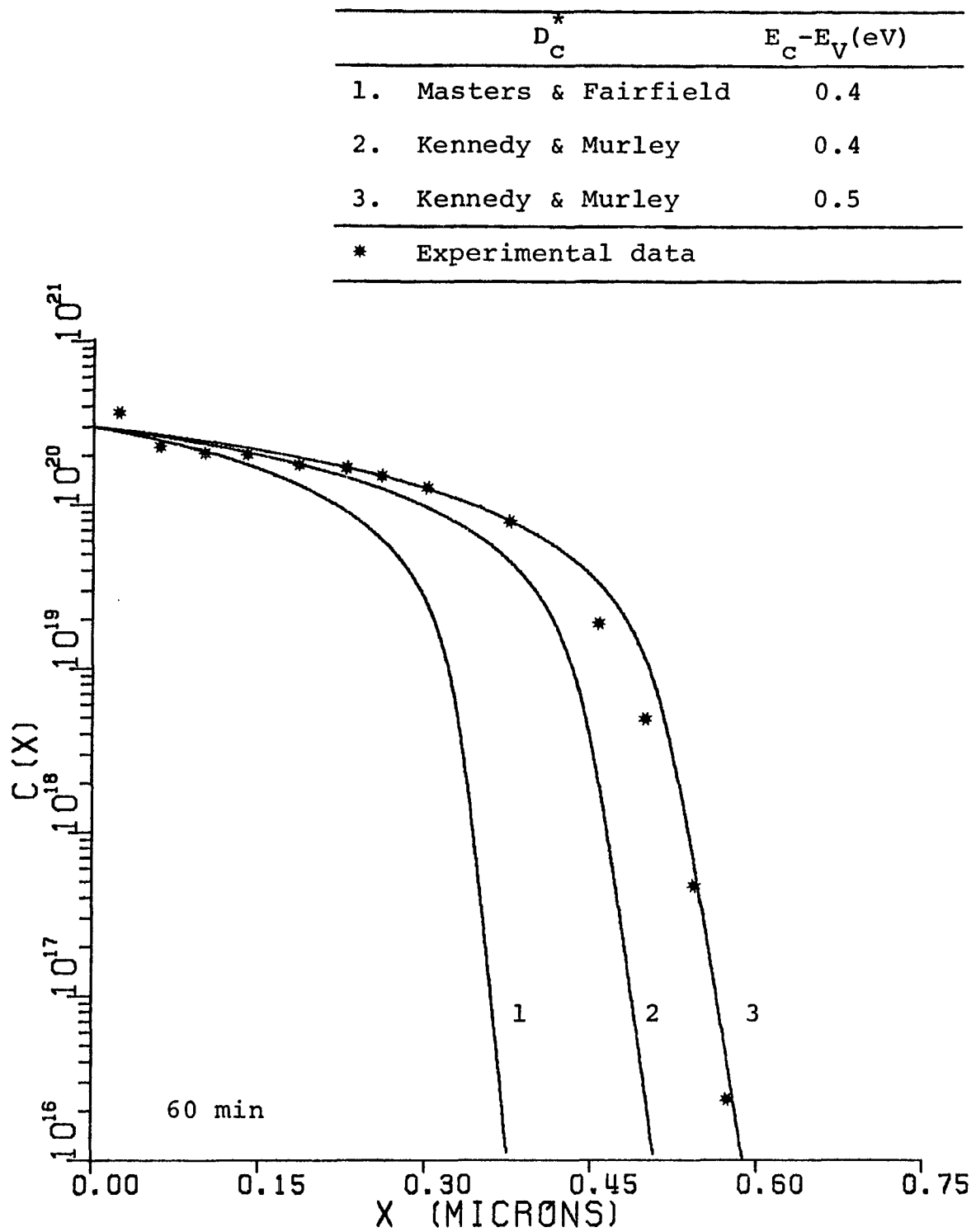


FIGURE 5.6. Comparison Between Experimental Data and Calculated Profiles Using Vacancy-aided Model



## CHAPTER 6

### CONCLUSIONS

The object of this study has been to develop and analyze various models describing the diffusion phenomenon. The effects of internal electric field, degeneracy of carriers, partial ionization and vacancies have been considered. Because of the complexity of the models involved, numerical techniques had to be used to obtain the solutions of the differential equations describing the transport process.

Previous analysis [24] has shown that the assumption of quasi-static equilibrium for holes and electrons in describing a diffusion process is valid. In the present research, formulations considering quasi-static equilibrium and charge neutrality have been examined for degenerate conditions. A vacancy-aided model has been proposed for arsenic diffusion in silicon. A constant source diffusion has been assumed.

The major contributions of this research may be summarized as follows.

1. The quasi-static model used to analyze the effect of internal electric field was extended to degenerate conditions by using the Fermi-Dirac statistics. It was concluded that the use of classical statistics yields an underestimate of the impurity density values. While this

error is significant at high surface concentrations, at low concentrations the use of classical statistics was considered to be a good approximation. The impurity density profiles were computed by numerically solving the partial differential equations governing diffusion. Due to enormous computation times, a need for simpler models was felt.

2. The assumption of local charge neutrality was examined for the degenerate case. It was concluded that charge neutrality is an excellent assumption to describe impurity diffusion under typical conditions. It was found that due to considerable simplification of the problem for a constant source diffusion, the resulting equations can be solved very efficiently on a digital computer. Whereas it takes hours of CPU time for the quasi-static model, it only takes a few minutes for the charge neutrality model.

3. The results from Hu's diffusion theory [12] were applied to arsenic diffusion in silicon under general conditions. The effects of vacancies, electric field and partial ionization of impurities were included and Fermi-Dirac statistics were used to describe the carriers. Quasi-equilibrium for vacancies and local charge neutrality were assumed. It was shown that using a transformation of variables, the problem can be simplified considerably for a constant source diffusion. The numerical solution can thus be obtained very efficiently. The results show very

significant enhancement of diffusion at high surface concentrations when compared to those obtained using the charge neutrality model. At such concentrations, the partial ionization was found to have a very large effect on the density values. The use of classical statistics was found to yield an underestimate of the impurity density values as in the case of quasi-static model.

It was noted that the impurity flux equation in the vacancy-aided model has the same form as that in the quasi-static model provided that  $D_C^* \gamma_V^{-1}$  is used in place of  $D_C^*$ . For low concentrations,  $\gamma_V \rightarrow 1$ . However, the equation numerically solved in the model, strictly speaking, is not valid at low concentrations due to an assumption made to simplify the problem at high concentrations. The charge neutrality model, nevertheless, is valid and can be used in such a case.

4. The results obtained using the vacancy-aided model were compared to the experimental data. It was found that using certain suggested values of the intrinsic diffusion coefficient and the energy levels, gives good agreement between the model and experiment. However, the results obtained strongly depend on these values.

Recommendations for further research are as follows.

1. It was pointed out that the vacancy-aided model suggested here may be in error at low concentrations because it was assumed that  $\xi \gg 1$ . This assumption was

made to simplify the model, and to avoid unnecessary computations at higher concentrations. The derivations can be modified by relaxing the above assumption so that the vacancy-aided model approaches the charge neutrality model at low concentrations.

2. Further research is needed to determine the correct values of the vacancy and donor levels, and the intrinsic diffusion coefficient of arsenic in silicon.

3. The vacancy-aided model should be re-examined in view of the cluster formation of As-atoms at high concentrations.

4. The model in the present work was applied to the case of a constant source diffusion. It should also be analyzed for a drive-in diffusion.

5. The model should be re-examined for application to diffusion of phosphorus and boron in silicon [42-46].

6. The problem of diffusion into a doped semiconductor should be considered.

7. Due to gas-solid interaction at the surface, further examination may show the surface boundary condition to be dependent on the flux and concentration. In such a case, the assumption of a constant surface boundary condition is no longer valid and the problem must be solved in a different way.

In the research presented here an attempt has been made to enhance the basic understanding of the diffusion

process. Such basic research may lead to improvement in device performance through optimization of device parameters.

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## APPENDIX A

### NONDEGENERATE QUASI-STATIC FORMULATION

Under nondegenerate conditions and assuming 100% ionization, the equations governing the holes and electrons are given by

$$\frac{\partial p}{\partial t} = \frac{\partial}{\partial x} \left[ D_p \frac{\partial p}{\partial x} + \frac{D_p p}{V_T} \frac{\partial \phi}{\partial x} \right] + G \quad (\text{A.1})$$

$$\frac{\partial n}{\partial t} = \frac{\partial}{\partial x} \left[ D_n \frac{\partial n}{\partial x} - \frac{D_n n}{V_T} \frac{\partial \phi}{\partial x} \right] + G . \quad (\text{A.2})$$

No assumptions are made regarding the form of the generation term  $G$ . According to the quasi-static approximation, we set  $\dot{p} = \dot{n} = 0$  in the above equations. Eliminating  $G$  then yields

$$\frac{\partial}{\partial x} \left[ D_p \frac{\partial p}{\partial x} + \frac{D_p p}{V_T} \frac{\partial \phi}{\partial x} \right] = \frac{\partial}{\partial x} \left[ D_n \frac{\partial n}{\partial x} - \frac{D_n n}{V_T} \frac{\partial \phi}{\partial x} \right] . \quad (\text{A.3})$$

Integrating both sides from  $x$  to  $\infty$  and noting that  $\frac{\partial p}{\partial x}$ ,  $\frac{\partial n}{\partial x}$ , and  $\frac{\partial \phi}{\partial x}$  approach zero as  $x \rightarrow \infty$ , we obtain

$$\frac{\partial \phi}{\partial x} = V_T \left[ \frac{D_n \frac{\partial n}{\partial x} - D_p \frac{\partial p}{\partial x}}{D_n n + D_p p} \right] . \quad (\text{A.4})$$

We note that

$$\frac{\partial (pn)}{\partial x} = p \frac{\partial n}{\partial x} + n \frac{\partial p}{\partial x} , \quad (\text{A.5})$$

so that

$$\frac{\partial n}{\partial x} = \frac{1}{p} \frac{\partial (pn)}{\partial x} - \frac{n}{p} \frac{\partial p}{\partial x} \quad (\text{A.6})$$

or,

$$\frac{\partial p}{\partial x} = \frac{1}{n} \frac{\partial (pn)}{\partial x} - \frac{p}{n} \frac{\partial n}{\partial x} . \quad (\text{A.7})$$

Using (A.6) and (A.7), we can write (A.4) in two equivalent forms:

$$\frac{\partial \phi}{\partial x} = V_T \left[ \frac{D_n}{p(D_n n + D_p p)} \frac{\partial (pn)}{\partial x} - \frac{1}{p} \frac{\partial p}{\partial x} \right] \quad (\text{A.8})$$

$$= V_T \left[ \frac{1}{n} \frac{\partial n}{\partial x} - \frac{D_p}{n(D_n n + D_p p)} \frac{\partial (pn)}{\partial x} \right] . \quad (\text{A.9})$$

Consider the form (A.9). If it is assumed that  $pn$  is a slowly varying function of  $x$  so that

$$\left| \frac{\partial n}{\partial x} \right| \gg \left| \frac{D_p}{D_n n + D_p p} \frac{\partial (pn)}{\partial x} \right| , \quad (\text{A.10})$$

we may directly integrate the resulting equation to obtain

$$n = n_i \exp\left(\frac{\phi}{V_T}\right) , \quad (\text{A.11})$$

where it has been assumed that as  $x \rightarrow \infty$ ,  $\phi \rightarrow 0$ , and  $n \rightarrow n_i$ .

Similarly, it can be seen from (A.8) that if

$$\left| \frac{dp}{dx} \right| \gg \left| \frac{D_p}{D_n n + D_p p} \frac{\partial (pn)}{\partial x} \right| , \quad (\text{A.12})$$

we can integrate the equation to obtain

$$p = n_i \exp\left(-\frac{\phi}{V_T}\right) . \quad (\text{A.13})$$

From (A.11) and (A.13), it follows that

$$pn = n_i^2 . \quad (\text{A.15})$$

Substituting (A.11) and (A.13) into Poisson's equation we obtain

$$\frac{\partial^2 \phi}{\partial x^2} = \frac{e}{\epsilon} [2n_i \sinh\left(\frac{\phi}{V_T}\right) - c] . \quad (\text{A.16})$$

Looking back at the inequalities (A.10) and (A.12), we note that at typical diffusion temperatures,

$$\frac{D_p}{D_n n + D_p p} \approx \frac{1}{n+p} \approx 10^{-19} ,$$



and the inequalities are justified if  $p_n$  is a slowly varying function of  $x$ . It is not necessary to assume that  $p_n$  is a constant although it is evident from (A.8) and (A.9) that it forms a self-consistent solution.

It may also be noted that if instead of the inequalities, we assume  $n \gg p$ , so that  $D_n n \gg D_p p$ , we still obtain (A.11) and (A.13). However, at typical diffusion temperatures the inequality  $n \gg p$  is violated over some range of  $x$  and this constitutes a higher level of approximation than is really needed.

# APPENDIX B

## COMPUTATION OF THE FERMI INTEGRALS

The Fermi integrals or Fermi functions arise in the carrier density expressions when a parabolic density of states is assumed. The Fermi integral of order  $j$  is defined as

$$F_j(\eta) = \frac{1}{\Gamma(j+1)} \int_0^\infty \frac{x^j dx}{\exp(x-\eta)+1} . \quad (B.1)$$

where  $\Gamma(n)$  is the Gamma function with the properties

$$\begin{aligned} \Gamma(n) &= (n-1)\Gamma(n-1), \quad n \geq 1 \\ \Gamma(1) &= 1 \\ \Gamma(1/2) &= \sqrt{\pi} \end{aligned} \quad (B.2)$$

Gamma function with negative arguments can be avoided by using [47]

$$\Gamma(z) = \frac{\pi}{\sin(\pi z)} \frac{1}{\Gamma(1-z)} . \quad (B.3)$$

In the present work, the functions  $F_{1/2}(\eta)$ ,  $F_{-1/2}(\eta)$ ,  $F_{-3/2}(\eta)$  and  $F_{-5/2}(\eta)$  are required. Some of these are tabulated [48-50]. An excellent discussion on approximations of the Fermi functions can be found in [47]. However, these approximations, though useful in analytical work, are not accurate enough for the present work over

the entire range of the argument. Brient and Wilson [51] have made accurate computations of these functions by directly integrating the expressions numerically. For the functions  $F_j(\eta)$ ,  $j = 1/2$  and  $-1/2$ , the integrals are obtained in sections using Simpson's rule with 32 points per segment with the lower limit equal to  $\epsilon=d$ , where  $d$  is chosen so that

$$\int_0^d \frac{x^j dx}{\exp(j-\eta)+1} \approx \frac{1}{1+\exp(-\eta)} \frac{d^{j+1}}{(j+1)} \leq 10^{-5} . \quad (\text{B.4})$$

Each succeeding section is taken as a region equal in length to all previous regions combined, i.e.,  $d$  to  $2d$ ,  $2d$  to  $4d$  etc., until the upper limit of  $2^n d$  for  $n$  regions is reached such that  $2^n d > \eta + 70$  for  $j=1/2$ , and  $2^n d > \eta + 50$  for  $j = -1/2$ . The resultant sum of sectional integrations is then accurate to five parts in  $10^7$ .

The derivatives of Fermi integrals are given by

$$\frac{dF_j(\eta)}{d\eta} = F_{j-1}(\eta) \quad (\text{B.5})$$

Writing the integrals explicitly,

$$F_{1/2}(\eta) = \frac{2}{\sqrt{\pi}} \int_0^\infty \frac{\sqrt{x} dx}{\exp(x-\eta)+1} \quad (\text{B.6a})$$

$$F_{-1/2}(\eta) = \frac{1}{\sqrt{\pi}} \int_0^\infty \frac{x^{-1/2} dx}{\exp(x-\eta)+1} \quad (\text{B.6b})$$

$$F_{-3/2}(\eta) = \frac{-1}{2\sqrt{\pi}} \int_0^{\infty} \frac{x^{-3/2} dx}{\exp(x-\eta)+1} \quad (\text{B.6c})$$

and

$$F_{-5/2}(\eta) = \frac{3}{4\sqrt{\pi}} \int_0^{\infty} \frac{x^{-5/2} dx}{\exp(x-\eta)+1} . \quad (\text{B.6d})$$

Although the algorithm given by Brient and Wilson is very accurate, it is computationally very expensive to use in an iteration procedure.

Battocletti [52] has proposed a series of polynomial approximations for the Fermi integrals of order 1/2. For arguments less than zero and for large positive arguments analytic expressions can be used [47, 48]. In the range of arguments from -1 to 12, Battocletti's proposed approximations yield an rms relative error of less than 1 in  $10^6$  for the function  $F_{1/2}(x)$ . The polynomials are easily differentiated. Battocletti's algorithm is as follows.

1. For  $x < -12.5$ :

$$F_{1/2}(x) = \exp(x)$$

$$F_{-1/2}(x) = \exp(x)$$

$$F_{-3/2}(x) = \exp(x)$$

$$F_{-5/2}(x) = \exp(x) .$$

2. For  $-12.5 \leq x \leq -2.0$ :

$$F_{1/2}(x) = \sum_{r=1}^{\infty} \frac{(-1)^{r+1} \exp(rx)}{r^{3/2}} \quad (\text{use six terms})$$

$$F_{-1/2}(x) = \sum_{r=1}^{\infty} \frac{(-1)^{r+1} \exp(rx)}{\sqrt{r}} \quad (\text{use six terms})$$

$$F_{-3/2}(x) = \sum_{r=1}^{\infty} (-1)^{r+1} \sqrt{r} \exp(rx) \quad (\text{use eight terms})$$

$$F_{-5/2}(x) = \sum_{r=1}^{\infty} (-1)^{r+1} r\sqrt{r} \exp(rx) \quad (\text{use eight terms}).$$

3. For  $-2.0 < x \leq 0.0$ :

$$F_{1/2}(x) = \exp(x) + \sum_{n=0}^6 a_n \exp[(n+2)x]$$

$$F_{-1/2}(x) = \exp(x) + \sum_{n=0}^6 a_n (n+2) \exp[(n+2)x]$$

$$F_{-3/2}(x) = \exp(x) + \sum_{n=0}^6 a_n (n+2)^2 \exp[(n+2)x]$$

$$F_{-5/2}(x) = \exp(x) + \sum_{n=0}^6 a_n (n+2)^3 \exp[(n+2)x]$$

where

$$a_0 = -0.35353667$$

$$a_1 = 0.19210895$$

$$a_2 = -0.12236525$$

$$\begin{aligned}
a_3 &= 0.78991718 \times 10^{-1} \\
a_4 &= -0.43441957 \times 10^{-1} \\
a_5 &= 0.16320377 \times 10^{-1} \\
a_6 &= -0.29297496 \times 10^{-2} .
\end{aligned}$$

4. For  $0.0 < x \leq 3.0$ :

$$F_{1/2}(x) = \sum_{n=0}^7 b_n x^n$$

$$F_{-1/2}(x) = \sum_{n=1}^7 b_n n x^{(n-1)}$$

$$F_{-3/2}(x) = \sum_{n=2}^7 b_n n(n-1) x^{(n-2)}$$

$$F_{-5/2}(x) = \sum_{n=3}^7 b_n n(n-1)(n-2) x^{(n-3)}$$

where

$$\begin{aligned}
b_0 &= 0.76514805 \\
b_1 &= 0.60491025 \\
b_2 &= 0.18990505 \\
b_3 &= 0.20131714 \times 10^{-1} \\
b_4 &= -0.39688853 \times 10^{-2} \\
b_5 &= -0.76558999 \times 10^{-3} \\
b_6 &= 0.30807837 \times 10^{-3} \\
b_7 &= -0.28395599 \times 10^{-4} .
\end{aligned}$$

5. For  $3.0 < x \leq 6.0$ :

$$F_{1/2}(x) = 0.75225278 x^{3/2} \sum_{n=0}^5 \frac{c_n}{x^{2n}}$$

$$F_{-1/2}(x) = 0.75225278 x^{1/2} \sum_{n=0}^5 \left(\frac{3}{2} - 2n\right) \frac{c_n}{x^{2n}}$$

$$F_{-3/2}(x) = 0.75225278 x^{-1/2} \sum_{n=0}^5 \left(\frac{3}{2} - 2n\right) \left(\frac{1}{2} - 2n\right) c_n \\ \times \frac{1}{x^{2n}}$$

$$F_{-5/2}(x) = 0.75225278 x^{-3/2} \sum_{n=0}^5 \left(\frac{3}{2} - 2n\right) \left(2n - \frac{1}{2}\right) \\ \times \left(2n + \frac{1}{2}\right) c_n \frac{1}{x^{2n}}$$

where

$$c_0 = 1.0002404$$

$$c_1 = 1.1981922$$

$$c_2 = 2.9838285$$

$$c_3 = -24.984495$$

$$c_4 = 96.877279$$

$$c_5 = -156.23522 .$$

6. For  $6.0 < x \leq 12$ :

The equations are the same as in 5 above except that

the summation is 0 through 4 i.e.  $\sum_{n=0}^4$ , and

$$c_0 = 1.0000313$$

$$c_1 = 1.2248008$$

$$c_2 = 1.8177898$$

$$c_3 = -5.0849956$$

$$c_4 = -3.2409718 .$$

7. For  $x > 12.0$ :

The equations are the same as in 5 above with

$$c_0 = 1.0$$

$$c_1 = 1.2337005$$

$$c_2 = 1.0654119$$

$$c_3 = 9.7015185$$

$$c_4 = 242.71502$$

$$c_5 = 11865.691 .$$

In the actual program, the computations have been done more efficiently, e.g.,

$$\begin{aligned} f(x) &= e^x + a_0 e^{2x} + a_1 e^{3x} + a_2 e^{4x} + a_3 e^{5x} + a_4 e^{6x} \\ &\quad + a_5 e^{7x} + a_6 e^{8x} \\ &= e^x (1 + e^x (a_0 + e^x (a_1 + e^x (a_2 + e^x (a_3 + e^x (a_4 + e^x (a_5 + a_6 e^x))))))) \end{aligned}$$



The second form above is more efficient than the first one, since at the expense of one more multiplication, seven less computations for raising  $e$  to a power are made. This subroutine is called millions of times and even a small saving here will reflect in the overall computation time.

Computed values using Battocletti's algorithm were compared with Brient and Wilson's scheme and excellent agreement was found.

## APPENDIX C

### PROGRAM INFORMATION

The computer programs used to obtain the results reported in Chapter 5 are written in FORTRAN-IV and were run on an IBM OS/360 computer system. Typical CPU time required to run the quasi-static program with diffusion time of 30 minutes and starting condition at 2 minutes is about 2 hours. This, of course, depends on the values of  $\Delta x$  and  $\Delta t$  used in the computation. Typical values are  $\Delta x = 0.001\mu$  and  $\Delta t = 0.5s$ . The CPU times required for the charge neutrality and the vacancy-aided models are of the order of few minutes.

A brief description of the "input data" is given below. Wherever necessary, comments have been added in the program to make them self-explanatory. The source deck listing of the various programs follows the input data given below.

#### Quasi-static Program

CPUST	CPU segmentation time, in minutes
CXEO	Surface concentration, in $\text{cm}^{-3}$
TEMP	Temperature, in $^{\circ}\text{C}$
DSUBC	Diffusion constant, in $\text{cm}^2 \text{ sec}^{-1}$
TO	Starting time, in sec
Z	= 1 for donors
	= -1 for acceptors

TSTOP	Diffusion time, in sec
CKC	Convergence factor (accuracy check)
DX1	Distance increment, in micron
DT1	Time increment, in sec
CSTOP	Value of concentration below which all the values are equated to zero, in $\text{cm}^{-3}$
CCHK	Value of concentration below which the accuracy check is not applied, in $\text{cm}^{-3}$

#### Charge Neutrality Program

CXEO	Surface concentration, in $\text{cm}^{-3}$
TEMP	Temperature, in $^{\circ}\text{C}$
DSUBC	Diffusion constant, in $\text{cm}^2 \text{ sec}^{-1}$
TO	Diffusion time, in sec
DX1	Distance increment at which the solution is desired, in micron
CKC	Convergence factor
Z	= 1 for donors = -1 for acceptors
ALPHA	Information to be printed out on the output

#### Vacancy-aided Program

CXEO	Surface concentration, in $\text{cm}^{-3}$
TEMP	Temperature, in $^{\circ}\text{C}$
TO	Diffusion time, in sec
DX1	Distance increment at which the solution is

desired, in micron

CKC      Convergence factor

ALPHA    Information to be printed out on the output





```

      NPM1=NP-1
      NPM2=NP-2
      N100=(NP+60)/100
      N101=N100+1
C
C
C
C
*****
***** PRINTOUT OF TITLE PAGE *****
      PRINT 600
      IF(Z.EQ.1.D0) PRINT 630
      IF(Z.EQ.-1.D0) PRINT 631
      PRINT 602,CXEC
      PRINT 614,IRESET,KRESET
      IF(ITRUNC.EQ.1) PRINT 618
      IF(ITRUNC.EQ.0) PRINT 619
      PRINT 603,NP
      PRINT 613
      PRINT 601,TEMP,NSUBI,DSUEC,BETA,XL,DX1,DT1
      PRINT 620,EK,ECHARGE,EPSICN
      PRINT 621,CKC,CSTOP,CCHK,TO,TSTOP,DTPRNT,DTPUN,DTTAP
      READ(5,625) ALPHA
      PRINT 626,ALPHA
      PRINT 213
C
600 FORMAT(/5X,'QUASI-STATIC ANALYSIS PROGRAM FOR FIELD-AIDED DIFFUSION'//10X,
10N'////)
601 FORMAT(/5X,'PHYSICAL CONDITIONS-'/10X,'TEMP = ',F13.1,' DEG C',/10X,
10X,'NSUBI = ',1PD13.4,' PER CC'/10X,'DSUBC = ',1PD13.4,' CM*CM',/10X,
2M/SEC'/10X,'BETA = ',0PF13.2/10X,'LENGTH = ',F13.5,' MICRONS',/10X,
30X,'DX = ',F13.5,' MICRONS'/10X,'DT = ',F13.3,' SEC')
603 FORMAT(5X,'TOTAL NUMBER OF PCINTS = ',I4)
613 FORMAT(5X,'CONVERGENCE CHECK--IF ON ANY ITERATION THE RELATIVE CHANGE OF C AND V IS LESS THAN CKC',/24X,'PROGRAM PROCEEDS TO THE NEXT TIME STEP')
614 FORMAT(5X,'DECK QS1 VERSION 3'/5X,
10X,'NO. OF PCINTS USED IN LOOKAHEAD = ',I4,', 1 UNTIL K.GT.',I6)
618 FORMAT(5X,'TRUNCATED RUN')
619 FORMAT(5X,'INITIAL RUN')
620 FORMAT(/5X,'PHYSICAL CONSTANTS USED-'/10X,'BK = ',1PD13.4,' JOULES/DEG K'/10X,
10X,'ECHARGE = ',1PD13.4,' COUL'/10X,'EPSILON = ',1PD13.4,' F/CM')
621 FORMAT(/5X,'CONTROL CONSTANTS USED-'/10X,'CKC = ',1PD13.4,' PER CC'/10X,
10X,'CSTOP = ',1PD13.4,' SEC'/10X,'CCHK = ',1PD13.4,' PER CC'/10X,
20X,'TSTART = ',0PF13.3,' SEC'/10X,'TSTOP = ',F13.3,' SEC'/10X,
30X,'DTPRNT = ',F13.3/10X,'DTPUN = ',F13.3/10X,
40X,'DTTAP = ',F13.3)

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630 FORMAT(5X,'DIFFUSION OF DONOR IMPURITY IONS IN SILICON')
631 FORMAT(5X,'DIFFUSION OF ACCEPTOR IMPURITY IONS IN SILICON')
602 FORMAT(5X,'SURFACE CONCENTRATION C(0,T) = ',1E13.5)
625 FORMAT(18A4/18A4)
626 FORMAT(///1X,18A4//1X,18A4)

C
T=TC
K=0
ITER=0
DELTA=DT1

*****

C
STARTING CONDITIONS FOR C(X) AND V(X)
MODEL -- RHO IS CONSTANT, P(X)*N(X)=NSUBI*NSUBI AND
C(X) MUCH MUCH GREATER THAN RHO/(1.6E-19 COUL.)

C
IMPURITY ATOM DISTRIBUTION CO(X)
COMPLEMENTARY ERROR FUNCTION ASSUMED

C
XX=DSQRT(4.D0*DSUBC*T)*1.D4
DO 4 I=2,NFM1
CO(I)=BETA*LERFC(X(I)/XX)
IF(CO(I).LT.CSTCFN) GO TO 5
4 ISTOP=I
5 ISTOP1=ISTOP+1
DO 6 I=ISTOP1,NFM1
CO(I)=0.D0
6 CO(I)=0.D0

C
POTENTIAL FUNCTION V(X)

C
DO 9 I=2,ISTOP
CD2=CC(I)*0.5D0
VO(I)=CD2+DLG((CD2+DSQRT(CD2**2+1.D0))*DEXP(-CD2))
9 CONTINUE
DO 14 I=ISTOP1,NFM1
14 VO(I)=0.D0

C
*****
BOUNDARY CONDITIONS FOR C(X) AND V(X) FOR ALL TIME
*****
VALUES AT X = 0
MODEL--DV/LX=C AND C(0,T)=CONSTANT

C
CO(1)=BETA
VC(1)=VC(2)
C

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C      A2=Z*V0(I)*VNORM
21 PRINT 303,I,X(I),A1,A2
000022280
000022290
000022300
000022310
000022320
000022330
000022340
000022350
000022360
000022370
000022380
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000022700
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000022730
000022740

C      FORMAT(5X,'STARTING DISTRIBUTIONS',/6X,'TIME =',F9.2,' SEC. OR'
650 'F10.3',/6X,'MIN',/6X,'DX =',F13.8,'MICRONS',/
651 'FORMAT',/5X,'X(MICRONS)',/5X,'C(X)',/10X,'V(X)',/
652 'FORMAT',/6X,'NUMBER OF TIME STEPS',/16)
653 'FORMAT',/6X,'NUMBER OF ITERATIONS',/16)
654 'FORMAT',/6X,'CCMELEMENTARY ERROR FUNCTION USED FOR STARTING DISTRIB
UTIONS',/
C      ***** ESTIMATED DISTRIBUTIONS AT END OF FIRST TIME STEP *****
C      DO 12 I=1,NP
C      V(I)=VC(I)
C      C(I)=CO(I)
C      *****
C      27 K=K+1
C      T=T+DELTAT
C      IF(T.GT.TSTOE) GO TO 999
C      IT100=T*10000.D0+C.1D0
C      DT=DELTAT/TNORM
C      TAU=T/TNORM
C      INDX=0
C      J=0
C      26 J=J+1
C      ITER=ITER+1
C      JFLAG=0
C      CALL DESDER(C,DC,DEC,DX,LASTI)
C      CALL DESDER(V,EV,EVC,DX,LASTI)
C      ***** CALC. CF IMPROVEMENTS *****
C      CALL DELTA(C,V,DC,EV,DEC,DELTA,DELTA,CO,DX,DT,LASTI,
1 ETAI,ETA1)
C      ***** FORM NEW C(X) AND V(X) AND CHECK CONVERGENCE *****
C      DO 34 I=1,LSTIM1
C      IX=I
C      CORRCD=DABS(DELTAC(I))

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      A5=DEXP(-Z*V(I))*CNCFM
      F1=V(I)+ETAI
      CALL FERMI(F1,FHALF,1)
      A6=(FHALF/ETAI)*CNCFM
      A7=Z*(C(I)+DEXP(-V(I)))-FHALF/ETAI)*CNCFM
      A8=-Z*DV(I)*CNCFM
70  PRINT 303,I,X(I),A1,A2,A3,A4,A5,A6,A7,A8
C
79  CONTINUE
      IF(MOD(IT100,IDTFUN).NE.0) GC TO 86
C
85  TMIN=T/60,D0
      WRITE(7,900) LASTI,TMIN,EX1
      DO 850 I=1, LASTI
      F1=V(I)+ETAI
      CALL FERMI(F1,FHALF,1)
      CHARGE(I)=Z*(C(I)+DEXP(-V(I)))-FHALF/ETAI)*CNCFM
      FIELD(I)=-Z*DV(I)*CNCFM
85C  DELTAC(I)=C(I)*CNCFM
      WRITE(7,901) {DELTAC(I)} I=1, LASTI
      WRITE(7,901) {FIELD(I)} I=1, LASTI
      WRITE(7,901) {CHARGE(I)} I=1, LASTI
C
86  CONTINUE
C
      IF(K.LE.KRESET) GOTO 76
      CALL RESET(V,VC,NP)
      CALL RESET(C,CC,NP)
      GOTO 87
76  CONTINUE
      DO 77 I=1,NP
      VC(I)=V(I)
77  CO(I)=C(I)
87  CONTINUE
C
      CALL KICK(ICFU)
      IF(MOD(IT100,IDTAP).NE.0.AND.ICPU.LE.ICPUST) GOTO 75
C
      WRITE(7,951) K,T,ITER,ISTOP,LASTI
      WRITE(7,950) {CO(I)} I=1, LASTI
      WRITE(8,951) K,T,ITER,ISTOP,LASTI
      WRITE(8,950) {CC(I),VO(I),I=1, LASTI)
      STOP
C
75  GO TO 27
C
999  CCNTINUE

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SUBROUTINE RESET(Y, YC, NP)
IMPLICIT REAL*8 (A-H, O-Z)
DIMENSION Y(1), YC(1)
IF (ICH.NE.2) GOTO 10
DO 100 I=1, NE
YNEW=Y(I)+Y(I)-YC(I)
YO(I)=Y(I)
100 Y(I)=YNEW
RETURN
10 CONTINUE
DO 200 I=1, NE
200 YO(I)=Y(I)
RETURN
ENTRY SETRES (IRESET)
ICH=IRESET
RETURN
END

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SUBROUTINE DELTA(C,V,DC,DV,DEC,EDV,DELTAC,DELTAV,CO,
1 DX,DT,NP,FTAI,FFTAI)
1 IMPLICIT REAL*8(A-H,C-Z)
REAL*8 N,NINV
DIMENSION C(1),V(1),DC(1),DV(1),DEC(1),DDV(1),DELTAC(1),
1 DELTAV(1),CO(1)
DIMENSION A(4),B(4),CC(4),AL(4),BE(4),GA(4),H(4),D(2),G(2)
C
DXLI=1.D0/{DX+DX}
DXSI=1.D0/{DX+DX}
DTI=1.D0/D1
NPM1=NP-1
C
C ZERO B. C.
G(1)=EX*DV(1)
G(2)=0.D0
H(1)=-1.D0
H(2)=0.D0
H(3)=0.D0
H(4)=0.D0
C
C LOOP TO DETERMINE G AND H
DO 10 I=1,NP
IF(I.EQ.1) GOTO 9
C INITIAL VALUES
F1=V(1)+FTAI
CALL FERMI(F1,FHALF,1)
CALL FERMI(F1,FMINUS,2)
FFI=DEXP(-V(I))
C LINEAR MATRICES
A(1)=DXSI
A(2)=C(I)*DXSI
A(3)=0.D0
A(4)=DXSI
B(1)=0.D0
B(2)=DC(I)*DXDI
B(3)=0.D0
B(4)=DV(I)*LXDI
CC(1)=-FMINUS/FFTAI-FFI
CC(2)=0.D0
CC(3)=1.D0
CC(4)=DDV(I)-DTI
D(1)=-{DDV(1)-FHALF/FFTAI+FFI+C(I)}
D(2)=-{DDC(I)+DC(I)*DV(I)+C(I)*DBV(I)-(C(I)-CO(I))*DTI}
C DISCRETIZED MATRICES

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DO 8 J=1,4
  AL{J}=A{J}+E{J}
  BE{J}=CC{J}-A{J}-A{J}
8 GA{J}=A{J}-B{J}
C CHARACTERISTIC MATRIX
  CALL MM2(GA,H,B,4,-1)
  CALL MA{BE,B,4,-1}
  CALL MINV2(E)
C NEW
  CALL MM2(E,AL,H,2)
  CALL MM2(GA,G,A,1)
  CALL MA{D,A,A,2,-1}
  G{1}=B{1}*A{1}+E{3}*A{2}
  G{2}=E{4}*A{2}
  IF(DABS{B(2)}.GT.(1.D-30).CR.DABS(A(1)).GT.(1.D-30))
1  G{2}=G{2}+E{2}*A{1}
C SAVE IN ARRAYS
9 CONTINUE
  DV{I}=H{1}
  IF(DABS{H(2)}.LT.(1.D-39)) H{2}=0.D0
  DC{I}=H{2}
  DDV{I}=H{3}
  DDC{I}=H{4}
  DELTAV{I}=G{1}
  DELTAC{I}=G{2}
10 CONTINUE
C INFINITE B. C.
  DELTAV{I}=0.D0
  DELTAC{I}=0.D0
C LOOP TO DETERMINE N AND C
  DO 20 I=1,NPM1
    K=NP-I
    KP1=K+1
C
    DELTAV{K}=DELTAV{K}-DV{K}*DELTAV{KP1}-DDV{K}*DELTAC{KP1}
    IF(DABS{DELTAV{K)}.LT.(1.D-39)) DELTAV{K}=0.D0
    DELTAC{K}=DELTAC{K}-DC{K}*DELTAV{KP1}-DDC{K}*DELTAC{KP1}
    IF(DABS{DELTAC{K)}.LT.(1.D-39)) DELTAC{K}=0.D0
20 CONTINUE
C
  RETURN
END

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      SUBROUTINE MA(A,B,C,N,NS)
      REAL*8 A,B,C
      DIMENSION A(1),E(1),C(1)
      IF(NS) 10,20,30
10  CONTINUE
      DO 15 I=1,N
15  C(I)=A(I)-B(I)
      RETURN
20  CONTINUE
      DO 25 I=1,N
25  C(I)=-A(I)
      RETURN
30  CONTINUE
      DO 35 I=1,N
35  C(I)=A(I)+B(I)
      RETURN
      END

```

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SUBROUTINE MINV2(A)
REAL*8 A,B,D,DI
DIMENSION A(4),B(4)
B(1)=A(4)
B(2)=-A(2)
B(3)=-A(3)
B(4)=A(1)
C=A(1)*A(4)-A(2)*A(3)
DI=1./C/D
DO 20 J=1,4
20 A(J)=B(J)*DI
RETURN
END

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```

SUBROUTINE MM2(A,B,C,N)
REAL*8 A,B,C
DIMENSION A(1),E(1),C(1)
C(1)=A(1)*B(1)+A(3)*E(2)
C(2)=A(2)*B(1)+A(4)*E(2)
IF(N.EQ.1) GOTO 1
C(3)=A(1)*B(3)+A(3)*E(4)
C(4)=A(2)*B(3)+A(4)*E(4)
1 RETURN
END

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SUBROUTINE DFSDER (Y, LY, CDY, DX, NP)
IMPLICIT REAL*8 (A-H,O-Z)
DIMENSION Y(1), LY(1), DDY(1)
NPM1=NP-1
NPM2=NP-2
NPM3=NP-3
NPM4=NP-4
C1=1.D0/(12.D0*DX)
C2=1.D0/(12.D0*DX)
DO 300 I=3,NPM2
  DY(I)=C1*(Y(I-1)-Y(I+1))-Y(I+2)
  DDY(I)=C2*(Y(I-1)+Y(I+1))-30.D0*Y(I)-Y(I+2)
  DDY(I)=35.D0*Y(1)-104.D0*Y(2)+114.D0*Y(3)-56.D0*Y(4)
  DDY(I)=1.D0*Y(5)*C2
  DDY(2)=11.D0*Y(1)-20.D0*Y(2)+6.D0*Y(3)+4.D0*Y(4)-Y(5))*C2
  DDY(NPM1)=(-Y(NPM4))*C2
  DDY(NPM1)+11.D0*Y(NPM4)
  DDY(NPM1)=11.D0*Y(NPM3)+114.D0*Y(NPM2)
  DDY(NPM1)+35.D0*Y(NPM1)+35.D0*Y(NPM1)*C2
  DDY(1)=(-25.D0*Y(1)+48.D0*Y(2)-36.D0*Y(3)+16.D0*Y(4)
  DDY(2)=(-3.D0*Y(5))*C1
  DDY(2)=(-3.D0*Y(1)-10.D0*Y(2)+18.D0*Y(3)-6.D0*Y(4)+Y(5))*C1
  DDY(NPM1)=(-Y(NPM4))+6.C1
  DDY(NPM1)+3.D0*Y(NPM4)
  DDY(NPM1)=3.D0*Y(NPM4)-16.D0*Y(NPM3)+36.D0*Y(NPM2)
  DDY(NPM1)=48.D0*Y(NPM1)+25.D0*Y(NPM1)*C1
RETURN
END

```

```

C THIS SUBROUTINE FERMI(X,FHALFX,IXX)
IMPLICIT REAL*8(A-H,C-Z)
DIMENSION C(10)
IF (X.LT.-12.5D0.CR.X.GT.-2.D0) GO TO 10
IF (IXX.EQ.2) GO TO 20
SUM=0.D0
A=1.D0
DO 30 I=1,6
B=I*1.D0
CC=A*DEXP(B*X)/(B*DSQRT(E))
SUM=SUM+CC
IF (DABS(CC).LT.1.D-30) GO TO 40
A=A*(-1.D0)
30 CONTINUE
40 FHALFX=SUM
20 SUM=0.D0
A=1.D0
DO 50 I=1,8
B=I*1.D0
CC=A*DEXP(B*X)/DSQRT(B)
SUM=SUM+CC
IF (DABS(CC).LT.1.D-30) GO TO 60
A=A*(-1.D0)
50 CONTINUE
60 FHALFX=SUM
10 IF (X.LT.-12.5D0.CR.X.GT.0.D0) GO TO 70
XE=DEXP(X)
IF (IXX.EQ.2) GO TC 8C
FHALFX=XE*(1.D0+XE*(-0.35353667D0+XE*(0.19210895D0+
1 XE*(-0.12236525D0+XE*(0.78991718D-1+XE*(-0.43441957D-1+XE*
2 (0.16320377D-1-0.29297496D-2*XE))))))
80 FHALFX=XE*(1.D0+XE*(-0.70707334D0+XE*(0.57632685D0+XE*
1 (-0.489461D0+XE*(0.39455859D0+XE*(-0.260651742D0+XE*
2 (0.14242639D0-0.234379568D-1*XE))))))
70 IF (X.LT.-12.5D0.CR.X.GT.3.D0) GO TO 90
IF (IXX.EQ.2) GO TC 10D
FHALFX=0.76514805D0+X*(0.60491025D0+X*(0.18990505D0+X*(
1 0.20131714D-1+X*(-0.34688853D-2+X*(-0.76558999D-3+X*
2 (0.30807837D-3-0.26395559D-4*X))))))
100 FHALFX=0.60491025D0+X*(0.3798101D0+X*(0.060395142D0+X*
1 (-1.58755412D-2+X*(-3.82794995D-3+X*(1.84847022D-3-1.98769193D-4*
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2 X))))))
RETURN
90 IF(X.GT.3.D0)GC TC 110
  FHALFX=DEXP(X)
  RETURN
110 IF(X.GT.6.D0)GC TO 120
  N=5
  C{1}=1.002404D0
  C{2}=1.19819222D0
  C{3}=2.98382285D0
  C{4}=-24.984495D0
  C{5}=96.877279D0
  C{6}=-156.23522D0
  GC TO 130
120 IF(X.GT.12.D0)GC TO 140
  N=4
  C{1}=1.0000313EC
  C{2}=1.2248008D0
  C{3}=1.8177898D0
  C{4}=-5.0849956EC
  C{5}=-3.2409718D0
  GO TO 130
140 N=5
  C{1}=1.D0
  C{2}=1.2337005D0
  C{3}=1.0654119D0
  C{4}=9.7015185D0
  C{5}=242.71502D0
  C{6}=11865.691D0
  IF(1X.EQ.2)GC TC 150
  TEMP=0.75225278D0*X*DSQRT(X)
  SUM=0.D0
  BYX2=1.D0/(X*X)
  DO 160 I=1,N
    SUM=BYX2*(SUM+C{N-I+2})
    FHALFX=TEMP*(C(1)+SUM)
    RETURN
150 TEMP=0.75225278D0*DSQRT(X)
  SUM=0.D0
  BYX2=1.D0/(X*X)
  DO 170 I=1,N
    SUM=BYX2*(SUM+C{N-I+2}*(1.5D0-C(1)+SUM))
    FHALFX=TEMP*(1.5D0-C(1)+SUM)
    RETURN
170
END

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```

```

C THIS PROGRAM COMPUTES THE RESULT OF THE TRANSPORT PROBLEM UNDER
C LCCAL CHARGE NEUTRALITY CONDITIONS USING QUASI-LINEARIZATION.
C ***** DEGENERATE CASE *****
C

```

```

      IMPLICIT REAL*8 (A-H,O-Z)
      REAL*8 N, NSUBI
      REAL*4 ALPHA
      DIMENSION C(2000), DC(2000), DDC(2000), Y(2000)
      DIMENSION DLTAC(2000), ALPHA(36), X(2000)
      DIMENSION Y1(2000), WCRK(2000), ARG(10), VAL(10), C1(2000)
      NMAX=2000

```

```

C
C READ INPUT DATA
C

```

```

      READ(5,952) CXEC, TEMF, DSUBC, TO
      READ(5,952) DX1, CKC, CSTOP, Z
      READ(5,625) ALPHA

```

```

C
C COMPUTE VARIOUS QUANTITIES.
C

```

```

      BK=1.381D-23
      ECHRG=1.602D-19
      VNCRM=BK*(TEMP+273.15D0)/ECHRG
      NSUBI=7.766D15*DEXP(5.528269D-3*(TEMP+273.15D0))
      ETAI=-6.989559165D3/(TEMP+273.15D0)+1.341932688D0
      CALL FERMI(ETAI, FETAI, 1)
      BETA=CXEC/NSUBI

```

```

C
C WRITE OUT THE VARIOUS QUANTITIES.
C

```

```

      WRITE(6,100) TEMF, CXEC, DSUBC
100  FORMAT(1X, 'TEMP= ', F13.1/1X, 'SURFACE CONC.= ', 1PD13.4/
      1 1X, 'DSUBC= ', 1PD13.4)
      WRITE(6,101) IC, DX1
101  FORMAT(1X, 'TIME= ', F13.3/1X, 'DX1= ', F13.5)
      WRITE(6,102) BETA, NSUBI
102  FORMAT(1X, 'BETA= ', F13.5/1X, 'NSUBI= ', 1PD13.4)

```

```

C
C THE PARAMETER DY1 CORRESPONDS TO NORMALIZED DX1.
C

```

```

      LY1=DX1/(2.D0*DSQRT(DSUBC*TO))*1.D-4
      DY=0.01D0
      CSICPN=CSTOP/NSUBI
      VSTOP=1.D-31
      VSICPN=VSTOP/VNCRM
      CCHK=VSICPN*1.D05

```

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00000100
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00000433

```

```

C      Y(1)=C.DO
C THE INITIAL GUESS AND Y ARE DETERMINED
C
C      DO 12 I=2,NMAX
12  Y(I)=Y(I-1)+DY
C      DO 1 I=2,NMAX
      IF (CXEQ.LE.1.D20) CD2=C.5DO*BETA*DERFC (.707DO*Y(I))
      IF (CXEQ.GT.1.D20) CD2=C.5DO*BETA*DERFC (.500DO*Y(I))
      C(I)=CD2+DLOG((CD2+DSQRT(CD2**2+1.DO))*DEXP(-CD2))
      IF (C(I).LT.VSTOPN) GO TO 2
1  CONTINUE
C
C C(I) HAS ALSO BEEN USED TO REPRESENT THE POTENTIAL.
C
C      2 ISTOP=I
      FIRSTI=ISTOP-10
      WRITE(6,995) ISTOP
      LASTI=ISTOP+10
      IF (LASTI.GT.NMAX) LASTI=NMAX
      LSTIM1=LASTI-1
      DO 9 I=ISTOP,NMAX
9  C(I)=C.DO
C
C COMPUTE VBETA AT THE SURFACE ASSUMING NON-DEG. CCNDITION.
C
C      VBETA=BETA*C.5DO
      VBETA=VBETA+DLOG((VBETA+DSQRT(VBETA**2+1.DO))*DEXP(-VBETA))
C
C COMPUTE THE TRUE BOUNDARY CONDITION FOR DEG. CONDITIONS.
C
C      300 CONTINUE
      F1=VBETA+ETAI
      CALL FERMI(F1,F2,1)
      CALL FERMI(F1,F3,2)
      F4=F2/FETAI-DEXP(-VBETA)-BETA
      F5=F3/FETAI+DEXP(-VBETA)
      VBETA1=VBETA
      VBETA=VBETA-F4/F5
      IF (DABS((VBETA1-VBETA)/VBETA).LT.1.D-3) GO TO 301
      GO TO 300
301 C(1)=VBETA
      VBETA1=VBETA*VNOEM
      WRITE(6,310) VBETA1
310 FORMAT('1X','F10=' ,D15.7)
C
C      K=C

```

```

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```



```

C
C BEGINNING OF ITERATION ICCF
C
C   5 K=K+1
C
C COMPUTE DERIVATIVES AND DELTA C
C
C   CALL DFSDER(C,DC,DDC,DY,IASTI)
C   CALL DELTA(C,DC,DDC,DLTAC,Y,DY,IASTI,ETAI,FETAI)
C
C CHECK CONVERGENCE.
C
C   JF=0
C   DO 4 I=2,ISTIM1
C     C(I)=C(I)+DLTAC(I)
C     CAES=DABS(C(I))
C     ERROR=DABS(DLTAC(I)/C(I))
C     IF(C(I).LT.VSTOPN) GC TC 7
C     IF(ERROR.GT.CKC.AND.CAES.GT.CCHK) JF=1
C   4 CONTINUE
C   7 ISTOP=I
C     LASTI=ISTOP+10
C     IF(LASTI.GT.NMAX) LASTI=NMAX
C     LSTIM1=LASTI-1
C     DO 14 I=ISTOP,NMAX
C   14 C(I)=0.D0
C
C     IF(JF.EQ.1) GOTO 5
C
C END OF THE ITERATION LOOP.
C
C   WRITE(6,222)
C   222 FORMAT('X','OUT OF THE MAIN LOOP')
C
C FOLLOWING DO LOOP MAKES A MESH WITH SEPERATION DY1.
C
C   DO 20 I=1,NMAX
C   20 Y1(I)=DY1*(I-1)
C
C INTERPOLATE THE CORRESPONDING VALUES.
C
C   NDIM=8
C   DO 21 I=1,NMAX
C     CALL DATSG(Y1(I),Y,C,WORK,1000,1,ARG,VAL,NDIM)
C     CALL DACFI(Y1(I),ARG,VAL,C1(I),NDIM,CKC,IER)
C     IF(C1(I).LT.VSTOPN) GC TO 30
C   21 CONTINUE

```

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```

30	ISTOP=I	00001230
	LASTI=ISTOP+1	00001240
	IF (LASTI.GT.NMAX) LASTI=NMAX	00001250
	DO 31 I=ISTOP, LASTI	00001260
31	C1(I)=0.00	00001270
	DO 22 I=1, LASTI	00001280
	WRITE(6,954) Y(I), C(I), Y1(I), C1(I)	00001290
954	FORMAT(1X, F9.5, 2X, E15.6, 2X, F9.5, 2X, D15.6)	00001300
22	C(I)=C1(I)	00001310
C		00001340
	DO 11 I=1, LASTI	00001350
	F1=C(I)+ETAI	00001351
	CALL FERMI(F1, F2, 1)	00001352
	EC(I)=F2/FETAI-DEXP(-C(I))	00001353
11	CONTINUE	00001370
	KST=0	00001380
	CNCRN=NSUBI	00001420
	VNORM=BK*(TEMP+273.15DC)/ECHRG	00001430
	WRITE(6,970)	00001440
970	FORMAT(5X//1X, 80(1H*)/5X, 'X(I)', 12X, 'C(X)', 10X, 'V(X)'/	00001450
1	1X, 80(1H*)//)	00001460
	DO 200 I=1, LASTI	00001470
	EDC(I)=DC(I)*CNORM	00001480
	A2=Z*C(I)*VNCRN	00001490
	X(I)=DX1*(I-1)	00001500
	WRITE(6,960) X(I), EDC(I), A2	00001510
960	FORMAT(1X, F9.5, 1PD15.6)	00001520
200	CONTINUE	00001530
	WRITE(6,961)	00001540
961	FORMAT(1X)	00001550
C		00001551
C	WRITE RESULTS ON FILE 8	00001560
C	OUTPUT FORMAT IS SUITABLE FOR TRUNCATION STEP IN QS1.	00001570
		00001571
	WRITE(6,951) KST, TO, KST, ISTOP, LASTI	00001580
	WRITE(8,951) KST, TO, KST, ISTOP, LASTI	00001590
	WRITE(8,950) (DC(I), C(I), I=1, LASTI)	00001600
	WRITE(6,950) (DC(I), C(I), I=1, LASTI)	00001610
	IMIN=IC/60.D0	00001620
	DO 888 I=1, LASTI	00001630
888	C(I)=-Z*C(I)*VNCRN	00001640
	DX1=DX1*1.D-4	00001650
	CALL DFSDER(C, DC, WORK, DX1, LASTI)	00001660
	DX1=DX1*1.D4	00001691
	WRITE(7,900) LASTI, TMIN, DX1	00001700
900	FORMAT(I4, F10.2, 1PD20.10)	00001710
	WRITE(7,901) (DC(I), I=1, LASTI)	00001711

```

      WRITE(7,901) (DC(I),I=1,LASTI)
      WRITE(6,901) (DC(I),I=1,LASTI)
901  FORMAT(1P8E10.3)
      STCF
C
995  FORMAT(1X,'NUMBER OF PCINTS= ',I5)
950  FORMAT(2(1X,D25.18))
951  FORMAT(1X,I11,1X,D25.18,1X,I11,1X,I12,1X,I7)
952  FORMAT(4E10.3)
953  FORMAT(4I10)
625  FORMAT(18A4/18A4)
      END

```

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```

C	SUBROUTINE DELTA(C,DC,DDC,DLTAC,Y,DY,NP,ETAI,FETAI)	00001840
C	THIS SUBROUTINE FORMS THE DELTAC'S USING THE QUASI-	00001850
C	LINEARIZATION METHOD	00001860
	IMPLICIT REAL*8 (A-H,O-Z)	00001870
	REAL*8 INV	00001880
	DIMENSION C(1),DC(1),DDC(1),DLTAC(1),Y(1)	00001890
	DYDI=0.5DC/DY	00001900
	DYSI=1.DC/(DY*DY)	00001910
	DC(1)=0.D	00001920
	DDC(1)=0.DC	00001930
C		00001940
C	DETERMINE INITIAL QUANTITIES	00001950
C		00001960
	DC 1: I=2,NP	00001970
	V1=C(I)+ETAI	00001980
	CALL FERMI(V1,F1,1)	00001981
	CALL FERMI(V1,F2,2)	00001982
	CALL FERMI(V1,F3,3)	00001983
	CALL FERMI(V1,F4,4)	00001984
	DE=DEXP(-C(I))	00001985
	F5=F2+FETAI*DE	00001986
	F6=1.DC/(F5*F5)	00001987
	F7=F3-FETAI*DE	00001988
C		00001989
C	COMPUTE A, B, C, AND D	00002060
C		00002070
	A=(F2+F1)/F5	00002080
	B=2.DC*Y(I)+2.DC*DC(I)*(F3+F2)/F5	00002090
	CC=DDC(I)*F6*(F5*(F3+F2)-(F2+F1)*F7)+DC(I)*DC(I)*F6*(F5*(F4+F3)-	00002100
	1*(F3+F2)*F7)	00002110
	D=-2.DC*Y(I)*DC(I)-A*DDC(I)-(F3+F2)*DC(I)*DC(I)/F5	00002111
	AM=A*DYSI	00002120
	BM=B*DYDI	00002150
C		00002160
C	COMPUTE AL, EE, AND GA	00002170
C		00002180
	AL=AM+BM	00002190
	EE=-AM-AM+CC	00002200
	GA=AM-BM	00002210
C		00002220
C	COMPUTE G AND H	00002230
C		00002240
	S=1.DC/(BE-GA*DDC(I-1))	00002250
	DDC(I)=AL*S	00002260
	DC(I)=(D-GA*DC(I-1))*S	00002270
C		00002280
		00002290

```

      10 CONTINUE
C
C  COMPUTE DELTAC
      DLTAC(NF)=0.D0
      DO 20 I=2,NF
        II=NF-I+1
        DLTAC(II)=DC(II)-DDC(II)*DLTAC(II+1)
      20 CONTINUE
C
      RETURN
C
      END

```

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00002400
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```

	SUBROUTINE DFSDER (Y,DY,DDY,DX,NP)	00002420
C	THIS SUBROUTINE NUMERICALLY COMPUTES THE FIRST AND	00002430
C	SECOND DERIVATIVES BY FITTING A POLYNOMIAL	00002440
C	OVER 5 ECINIS	00002450
	IMPLICIT REAL*8 (A-F,O-Z)	00002460
	DIMENSION Y(1),DY(1),DDY(1)	00002470
	NPM1=NP-1	00002480
	NPM2=NP-2	00002490
	NPM3=NP-3	00002500
	NPM4=NP-4	00002510
	C1=1.D0/(12.D0*DX)	00002520
	C2=1.D0/(12.D0*DX*DX)	00002530
C		00002540
C	DETERMINING FOR ECINIS 3 TO N-2	00002550
C		00002560
	DO 300 I=3,NPM2	00002570
	DY(I)=C1*(Y(I-2)-8.D0*(Y(I-1)-Y(I+1))-Y(I+2))	00002580
	300 DDY(I)=C2*(-Y(I-2)+16.D0*(Y(I-1)+Y(I+1))-30.D0*Y(I)-Y(I+2))	00002590
C		00002600
C	DETERMINING FOR THE ECINIS 1, 2, N-1, AND N	00002610
	DDY(1)=(35.D0*Y(1)-104.D0*Y(2)+114.D0*Y(3)-56.D0*Y(4)	00002620
	+11.D0*Y(5))*C2	00002630
	DDY(2)=(11.D0*Y(1)-20.D0*Y(2)+6.D0*Y(3)+4.D0*Y(4)-Y(5))*C2	00002640
	DDY(NPM1)=(-Y(NPM4)+4.D0*Y(NPM3)+6.D0*Y(NPM2)-20.D0*Y(NPM1)	00002650
	+11.D0*Y(NP))*C2	00002660
	DDY(NP)=(11.D0*Y(NPM4)-56.D0*Y(NPM3)+114.D0*Y(NPM2)	00002670
	-104.D0*Y(NPM1)+35.D0*Y(NP))*C2	00002680
	DY(1)=(-25.D0*Y(1)+48.D0*Y(2)-36.D0*Y(3)+16.D0*Y(4)	00002690
	-3.D0*Y(5))*C1	00002700
	DY(2)=(-3.D0*Y(1)-10.D0*Y(2)+18.D0*Y(3)-6.D0*Y(4)+Y(5))*C1	00002710
	DY(NPM1)=(-Y(NPM4)+6.D0*Y(NPM3)-18.D0*Y(NPM2)+10.D0*Y(NPM1)	00002720
	+3.D0*Y(NP))*C1	00002730
	DY(NP)=(3.D0*Y(NPM4)-16.D0*Y(NPM3)+36.D0*Y(NPM2)	00002740
	-48.D0*Y(NPM1)+25.D0*Y(NP))*C1	00002750
C		00002760
	RETURN	00002770
	END	00002780

```

SUBROUTINE FERMI(X,FHALFX,IXX)
C THIS SUBROUTINE IS BASED ON FATTOLLETTI'S ALGORITHM.
IMPLICIT REAL*8(A-H,O-Z)
DIMENSION C(10)
IF(X.LT.-12.5D0.OR.X.GT.-2.D0)GO TO 10
  IF(IXX.EQ.2)GO TO 20
  IF(IXX.EQ.3)GO TO 180
  IF(IXX.EQ.4)GO TO 190
  SUM=0.D0
  A=1.D0
  DO 30 I=1,6
    B=I*1.D0
    CC=A*DEXP(B*X)/(B*DSQRT(B))
    SUM=SUM+CC
    IF(DABS(CC).LT.1.D-30)GO TO 40
    A=A*(-1.D0)
  30 CONTINUE
  40 FHALFX=SUM
  RETURN
  20 SUM=0.D0
  A=1.D0
  DO 50 I=1,8
    B=I*1.D0
    CC=A*DEXP(B*X)/DSQRT(B)
    SUM=SUM+CC
    IF(DABS(CC).LT.1.D-30)GO TO 60
    A=A*(-1.D0)
  50 CONTINUE
  60 FHALFX=SUM
  RETURN
  180 SUM=0.D0
  A=1.D0
  DO 200 I=1,10
    B=I*1.D0
    CC=A*DEXP(B*X)*DSQRT(B)
    SUM=SUM+CC
    IF(DABS(CC).LT.1.D-30)GO TO 210
    A=A*(-1.D0)
  200 CONTINUE
  210 FHALFX=SUM
  RETURN
  190 SUM=0.D0
  A=1.D0
  DO 220 I=1,12
    B=I*1.D0
    CC=A*DEXP(B*X)*B*DSQRT(B)
    SUM=SUM+CC

```

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00005690
00005700
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```

IF (DAES(GC).LT.1.D-30) GO TO 230
A=A*(-1.D0)
230 CONTINUE
FHALFX=SUM
RETURN
10 IF(X.LT.-12.5D0.CR.X.GT.0.D0)GO TO 70
XE=DEXF(X)
IF(IXX.EQ.2)GC TC 8
IF(IXX.EQ.3)GC TC 240
IF(IXX.EQ.4)GC TC 250
FHALFX=XE*(1.D0+XE*(-0.35353667D0+XE*(0.19210895D0+
1 XE*(-0.122336525D0+XE*(0.78991718D-1+XE*(-0.43441957D-1+XE*
2 (0.16320377D-1-0.29297496D-2*XE))))))
RETURN
80 FHALFX=XE*(1.D0+XE*(-(0.70707334D0+XE*(0.57632685D0+XE*
1 (-0.489461D0+XE*(0.39495859D0+XE*(-0.260651742D0+XE*
2 (0.114242635D0-0.234379968D-1*XE))))))
RETURN
240 FHALFX=XE*(1.D0+XE*(-1.41414668D0+XE*(1.72898055D0+
1 XE*(-1.957844D0+XE*(1.97479295D0+XE*(-1.563910452D0+
2 XE*(0.799698473D0-XE*(0.1875039744D0))))))
RETURN
250 FHALFX=XE*(1.D0+XE*(-2.82829336D0+XE*(5.18694165D0+
1 XE*(-7.831376D0+XE*(9.87396475D0+XE*(-9.383462712D0+
2 XE*(5.597889311D0-XE*(1.500031795D0))))))
RETURN
70 IF(X.LT.-12.5D0.CR.X.GT.3.D0)GC TO 9C
IF(IXX.EQ.2)GC TC 100
IF(IXX.EQ.3)GC TC 260
IF(IXX.EQ.4)GC TC 270
FHALFX=XE*(0.76514805D0+XE*(1.60491025D0+X*(0.18990505D0+X*(
1 (0.20131714D-1+X*(-0.39688853D-2+X*(-0.76558999D-3+X*
2 (0.3007637D-3-0.28395599D-4*X))))))
RETURN
100 FHALFX=XE*(0.60491025D0+X*(0.3798101D0+X*(0.060395142D0+X*
1 (-1.58755412D-2+X*(-3.82794995D-3+X*(1.84847022D-3-1.98769193D-4*
2 X))))))
RETURN
260 FHALFX=XE*(0.3798101D0+X*(0.120790284D0+X*(-4.76266236D-2+
1 X*(-1.53117998D-2+X*(9.2423511D-3-X*1.192615158D-3))))
RETURN
270 FHALFX=XE*(0.100790284+X*(-3.52532472D-2+X*(-4.59353994D-2+
1 X*(3.69694044D-2-X*5.96307579D-3)))
RETURN
00 IF(X.GT.3.D0)GC TC 110
FHALFX=DEXF(X)
RETURN
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11- IF(X.GI.6.DC)GO TO 120
    C(1)=1.0002404DC
    C(2)=1.1981922DC
    C(3)=2.2408285DC
    C(4)=-2.2408285DC
    C(5)=96.877279DC
    C(6)=-19.22522DC
    TC=19.22522DC
120 IF(X.GI.12.DC)GO TO 140
    N=4
    C(1)=1.000313DC
    C(2)=1.2248008DC
    C(3)=1.28177898DC
    C(4)=-5.0849956DC
    C(5)=-3.2439718DC
    TC=19.22522DC
140 N=5
    C(1)=1.00037005DC
    C(2)=1.22654119DC
    C(3)=9.7015195DC
    C(4)=24.2265.691DC
    C(5)=11865.2)GC TC 150
    IF(IXX.EQ.3)GC TC 280
    IF(IXX.EQ.4)GC TC 290
    IF(TMP=0.DC)
      SUM=0.DC
      BYX2=1.DC/(X*X)
      DO 160 I=1,N
        SUM=BYX2*(SUM+C(N-I+2))
      FHALFX=TEMP*(C(1)+SUM)
      RETURN
150 TEMP=0.75225278DC*DSQRT(X)
    SUM=0.DC
    BYX2=1.DC/(X*X)
    DO 170 I=1,N
      SUM=BYX2*(SUM+C(N-I+2))*(1.5DC-2.DC*(N-I+1)))
    FHALFX=TEMP*(1.5DC*C(1)+SUM)
    RETURN
280 TEMP=0.75225278DC/DSQRT(X)
    SUM=0.DC
    BYX2=1.DC/(X*X)
    DO 300 I=1,N
      SUM=BYX2*(SUM+C(N-I+2))*(1.5DC-2.DC*(N-I+1))*(0.5DC-
1

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      FHALFX=TEMP*(0.75DC*C(1)+SUM)
      RETURN
290  TEMP=0.75225278DC/(X*DSQRT(X))
      SUM=0.DC
      BYX2=1.DC/(X*X)
      DC 310  I=1,N
310  SUM=BYX2*(SUM+C(N-I+2)*(1.5DC-2.DC*(N-I+1))*(2.DC*
1  (N-I+1)-0.5DC)*(2.DC*(N-I+1)+0.5DC))
      FHALFX=TEMP*(-0.375DC*C(1)+SUM)
      RETURN
      END

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C THIS IS A PROGRAM TO SOLVE THE PRE-DEP PROBLEM OF DIFFUSION IN
C A SEMICONDUCTOR - IMPURITY-VACANCY SYSTEM USING A QUASI-LINEARIZATION
C METHOD.
C
C IMPLICIT REAL*8 (A-H,C-Z)
C REAL*8 NSUBI
C REAL*4 ALFHA
C DIMENSION V(2000), EV(2000), DDV(2000), Y(2000)
C DIMENSION DLTAV(2000), ALFHA(36), X(2000)
C DIMENSION Y1(2000), WORK(2000), ARG(10), VAL(10), C(2000)
C
C NMAX=2000
C
C READ IN THE DIFFUSION PARAMETERS.
C
C READ(5,900) CXEC,TEMP,TC
C 900 FORMAT(4D10.0)
C READ(5,900) DX1,AFROXL,CKC
C 901 FORMAT(18A4/18A4)
C
C COMPUTE VARIOUS QUANTITIES FOR ARSENIC DIFFUSION IN SILICON.
C
C EA=0.05D0
C ESUBV=0.4D0
C BK=8.620D-5
C EKT=BK*(TEMP+273.15D0)
C DSTAR=60.D0*DEXE*(-4.2D0/EKT)
C NSUBI=7.706D15*DEXE*(5.528269D-3*(TEMP+273.15D0))
C ESUBG=1.205D0-2.EF-4*(TEMP+273.15D0)
C FTAI=-6.989559165D3/(TEMP+273.15D0)+1.341932688D0
C VSUBC=FTAI
C CALL FERMI(ETAI,FTAI,1)
C XNC=NSUBI/FTAI
C XNV=NSUBI*DEXE(ETAI+ESUBG/EKT)
C GV=2.D0
C EAFAR=EA/EKT
C XISTAR=GV*DEXE(VSUBC+ESUBV/EKT)
C DSUBC=DSTAR*XISTAR/(1.E0+XISTAR)
C FETA=CXEC/NSUBI
C FGNM=ESUBG/EKT
C TMIN=TC/60.D0
C CXCM=DX1*1.D-4
C
C WRITE OUT THE VARIOUS QUANTITIES.
C

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00000100
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00000220
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	WRITE(6,800)	00000440
800	FORMAT(1H1)	00000450
	WRITE(6,801) CXEC,TEMP,IC	00000460
	WRITE(6,802) NSUBI,XNC,XNV,DSUBC	00000470
	WRITE(6,803) ESUBG,VSUBC,XISTAR	00000480
801	FORMAT(/1X,'SURFACE CCNC.(/CC.)=',1PD13.4/1X,'TEMP (DEG C)=' ,	00000490
	11PD13.4/1X,'DIFF. TIME (SEC.)=',1PD13.4)	00000500
802	FORMAT(1X,'NSUBI (/CC.)=',1PD13.4/1X,'NC (/CC.)=',1PD13.4/	00000510
	11X,'NV (/CC.)=',1PD13.4/1X,'DSUBC (CM**2/SEC)=' ,1PD13.4)	00000520
803	FORMAT(1X,'BAND GAP (EV)=' ,F13.5/1X,'VSUBC=' ,1PD13.4/	00000530
	11X,'XISTAR=' ,1PD13.4)	00000540
C		00000550
C	COMPUTE DY1 CORRESPONDING TO THE REQUIRED DIFFUSION TIME.	00000551
C		00000560
	DY1=DX1/(2.D0*DSQRT(DSUBC*TO))*1.D-4	00000570
	DY=0.01D0	00000580
	IF(EA.LT.-1.D0.AND.CXEC.GT.1.D20) DY=0.05D0	00000581
	VSTOPN=1.D-15	00000590
	VCHK=VSTOPN*1.D05	00000600
C		00000610
C	COMPUTE THE STARTING GUESS FOR V(I). ASSUME ERFC STARTING CONDITION	00000611
C	FOR THE IMPURITY DENSITY AND THEN FIND V(I) ASSUMING NON-DEGENERATE	00000612
C	CONDITION AND COMPLETE IONIZATION.	00000613
		00000620
	M=NMAX	00000621
	IF(EA.LE.-1.D0.AND.CXEC.GT.1.D20) M=1500	00000622
	Y(1)=0.D0	00000630
	DO 10 I=2,NMAX	00000640
10	Y(I)=Y(I-1)+DY	00000650
	DO 11 I=2,M	00000660
	IF(CXEC.LE.1.D20) CD2=0.5D0*BETA*DERFC(0.5D0*Y(I))	00000670
	IF(CXEC.GT.1.D20) CD2=0.5D0*BETA*DERFC(0.100D0*Y(I))	00000671
	IF(EA.LT.-1.D0.AND.CXEC.GT.1.D20) CD2=0.5D0*BETA	00000672
	V(I)=CD2+DLOG((CD2+DSQRT(CD2*CD2+1.D0))*DEXP(-CD2))	00000680
	IF(V(I).LT.VSTOPN) GO TO 12	00000690
11	CONTINUE	00000700
12	ISTOP=I	00000710
	FIRSTI=ISTOP-10	00000720
	WRITE(6,804) ISTOP	00000730
804	FORMAT(1X,'NC. OF PCINIS=' ,I5)	00000740
	LASTI=ISTOP+10	00000750
	IF(LASTI.GT.NMAX) LASTI=NMAX	00000760
	LASTIM=LASTI-1	00000770
	DO 13 I=ISTOP,NMAX	00000780
13	V(I)=0.D0	00000790
C		00000791
C	COMPUTE VBETA AT THE SURFACE ASSUMING NON-DEG. CONDITION AND COMPLETE	00000792

```

C IONIZATION.
C
C      VBETA=0.5DC*BETA
C      VBETA=VBETA+DLG((VEETA+DSQRT(VBETA*VBETA+1.D0))*DEXP(-VBETA))
C
C COMPUTE THE TRUE VALUE OF THE BOUNDARY CONDITION VBETA AT THE SURFACE
C BY ITERATION FOR DEGENERATE CONDITIONS AND INCOMPLETE IONIZATION.
C
C 14 CONTINUE
C    Q1=VEETA+VSUBO
C    Q2=VBETA+VSUBO+EABAR
C    CALL FERMI(Q1,F1,1)
C    CALL FERMI(Q1,F2,2)
C    F3=2.D0*DEXP(Q2)
C    F4=DEXP(-VEETA)
C    F5=(1.D0+F3)*(F1/FETAI-F4)-BETA
C    F6=F2/FETAI+F4+F3*(F1+F2)/FETAI
C    VBETA1=VBETA
C    VBETA=VBETA-F5/F6
C    IF(DABS((VBETA1-VBETA)/VBETA).LT.1.D-3) GO TO 15
C    GO TO 14
C 15 V(1)=VBETA
C    WRITE(6,805) VBETA
C 805 FORMAT(1X,'VBETA=',1PD15.5)
C
C      K=1
C
C BEGIN ITERATION LOOP.
C
C 20 K=K+1
C
C COMPUTE DERIVATIVES OF V AND THE CORRECTIONS DLTAV.
C
C    CALL DESDER(V,DV,DDV,DY,IASTI)
C    CALL DELTA(V,DV,DDV,DLTAV,Y,DY,IASTI,VSUBO,XNC,XNV,
C    1EABAR,EGNM)
C
C CHECK CONVERGENCE.
C
C    JF=0
C    DO 21 I=2,ISTIM1
C      V(I)=V(I)+DLTAV(I)
C      ABDL=DABS(V(I))
C      ERROR=DABS(DLTAV(I)/V(I))
C      IF(V(I).LT.VSTOPN) GO TO 22
C      IF(ERROR.GT.CKC.AND.ABDL.GT.VCHK) JF=1

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00001080
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21 CONTINUE
22 ISTOP=I
   LASTI=ISTOP+1
   IF (LASTI.GT.NMAX) LASTI=NMAX
   LSTIM1=LASTI-1
   DO 23 I=ISTOP,NMAX
23  V(I)=0.D0
   IF (JF.FQ.1) GO TO 20
C
C  END OF THE ITERATION LOOP.
C
   WRITE(6,806)
806  FORMAT(1X,'OUT OF THE MAIN LOOP')
C
C  FORM A MESH CORRESPONDING TO DY1.
C
   DO 26 I=1,NMAX
26  Y1(I)=DY1*(I-1)
C
C  INTERPOLATE THE CORRESPONDING V(I) VALUES.
C
   NDIM=8
   DO 27 I=1,NMAX
   CALL DATSG(Y1(I),Y,V,WORK,NMAX,1,ARG,VAL,NDIM)
   CALL DACFI(Y1(I),ARG,VAL,C(I),NDIM,CRC,IER)
   IF (C(I).LT.VSTOPN) GO TO 28
27  CONTINUE
28  ISTOP=I
   LASTI=ISTOP+1
   IF (LASTI.GT.NMAX) LASTI=NMAX
   DO 29 I=ISTOP,LASTI
29  C(I)=0.D0
   DO 30 I=1,LASTI
   WRITE(6,808) Y1(I),V(I),Y1(I),C(I)
808  FORMAT(1X,F9.5,2X,D15.6,2X,F9.5,2X,D15.6)
30  V(I)=C(I)
C
C  COMPUTE THE ELECTRIC FIELD.
C
   CALL DESDER(V,DV,DDV,DXCM,LASTI)
   DO 32 I=1,LASTI
32  DDV(I)=-BKT*DV(I)
C
C  COMPUTE C(I) VALUES CORRESPONDING TO V(I). PRINT AND PUNCH IN A
C  PROPER FORMAT.
C
   DO 31 I=1,LASTI

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000001370
000001400
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000001491
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000001504
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000001512
000001520
000001530

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00001600
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00001640
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00001670
00001680
00001690
00001700

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X(I)=DX1*(I-1)
O1=V(I)+VSUBO
CALL FERM1(O1,F1,1)
C(I)=(1.D+2.DC*DEXP(O1+FAVARP))*(XNC*F1-NSUBI*DEXP(-V(I)))
WRITE(6,819)X(I),C(I),V(I),DDV(I)
FORMAT(1X,F9.5,3(1PD15.6,4X))
CONTINUE
WRITE(7,817)LASTI,TMIN,DX1
FORMAT(14,F1.2,1PD20.10)
WRITE(7,811)C(I),I=1, LASTI)
WRITE(7,812)LASTI,TMIN,DX1
WRITE(7,811)DDV(I),I=1, LASTI)
FORMAT(1PD8D1.3)
WRITE(6,800)
WRITE(6,811)C(I),I=1, LASTI)
WRITE(6,811)DDV(I),I=1, LASTI)
STOP
END

```

811

817

819

819

```

SUBROUTINE DELTA(C,EC,DDC,DLTAC,Y,DY,NP,ETAI,XNC,XNV,
1  XBAR,EGM)
  IMPLICIT REAL*8(A-H,O-Z)
  REAL*8 INVP
  DIMENSION C(1),DC(1),DEC(1),DLTAC(1),Y(1)
  DYDI=2.5D0/DY
  DYSI=1.D0/(DY*DY)
  DC(1)=:D
  DDC(1)=:D
20001630
20001640
20001650
20001660
20001670
20001680
20001690
20001700
20001710
20001720
20001730
20001740
20001750
20001760
20001770
20001780
20001790
20001800
20001810
20001820
20001830
20001840
20001850
20001852
20001860
20001870
20001890
20001900
20001910
20001920
20001930
20001940
20001950
20001970
20001980
20002000
20002010
20002020
20002030
20002040
20002050
20002060
20002070

  COMPUTE VARIOUS QUANTITIES TO BE USED LATER.
30001720
30001730
30001740
30001750
30001760
30001770
30001780
30001790
30001800
30001810
30001820
30001830
30001840
30001850
30001852
30001860
30001870
30001890
30001900
30001910
30001920
30001930
30001940
30001950
30001970
30001980
30002000
30002010
30002020
30002030
30002040
30002050
30002060
30002070

  DO 1 I=2,NP
    V1=C(I)+ETAI+BARAR
    V2=C(I)+ETAI+EGNM
    V3=-C(I)-ETAI-EGNM
    CALL FERMI(V1,F1,1)
    CALL FERMI(V1,F2,2)
    CALL FERMI(V1,F3,3)
    CALL FERMI(V1,F5,4)
    F4=DEXP(C(I))
    F6=DEXP(V2)
    F7=DEXP(V3)
    R=XNV/XNC
40001840
40001850
40001852
40001860
40001870
40001890
40001900
40001910
40001920
40001930
40001940
40001950
40001970
40001980
40002000
40002010
40002020
40002030
40002040
40002050
40002060
40002070

    COMPUTE THE FUNCTIONS F1(ETA) AND F2(ETA), AND THEIR DERIVATIVES
    APPEARING IN THE NUMERICAL PROCEDURE.
50001840
50001850
50001852
50001860
50001870
50001890
50001900
50001910
50001920
50001930
50001940
50001950
50001970
50001980
50002000
50002010
50002020
50002030
50002040
50002050
50002060
50002070

    XN1=F1+2.D0*F2+2.D0*F6*(4.D0*F1+4.D0*F2+2.F3-R*F7)
    XD1=F2+5*F7+2.D0*F6*(F1+F2)
    XN2=F1+F2+2.D0*F6*(2.D0*F1+F2)-2.D0*F*DEXP(FARAR-EGNM)
    XD2=F2+2*F7+2.D0*F6*(F1+F2)
    F1V=F4*XN1/XD1
    F2V=F4*XN2/XD2
    DF1V=F1V+(F4/XD1)*(F2+2.D0*F3+F5+2.D0*F6*(4.D0*F1+8.D0*F3
    +F5))- (F4*XN1/(XD1*(F3-R*F7+2.D0*F6*(F1+2.D0*F2+F3))
    DF2V=F2V+(F4/XD2)*(F2+F3+2.D0*F6*(2.D0*F1+3.D0*F2+F3))-
    1 (F4*XN2/(XD2*XN2))*(F3-R*F7+2.D0*F6*(F1+2.D0*F2+F3))
60001920
60001930
60001940
60001950
60001970
60001980
60002000
60002010
60002020
60002030
60002040
60002050
60002060
60002070

    COMPUTE THE QUANTITIES A, B, C AND D.
70002010
70002020
70002030
70002040
70002050
70002060
70002070

    A=F2V
    B=2.D0*V(I)+2.D0*F1V*DC(I)
    CC=DF1V*DC(I)*DC(I)+DF2V*DDC(I)
    R=-F1V*DC(I)*DC(I)-F2V*DDC(I)-2.D0*Y(I)*DC(I)
80002010
80002020
80002030
80002040
80002050
80002060
80002070

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```

      AM=A*DYSI
      BM=B*DYDI
CC  COMPUTE ALPHA, BETA AND GAMMA.
CC
      AL=AM+BM
      BF=-AM-AM+CC
      GA=AM-PM
CC  COMPUTE G AND H.
CC
      S=1.DC/(BE-GA*DFC(I-1))
      DDC(I)=AL*S
      DC(I)=(D-GA*DC(I-1))*S
CC
      1C CONTINUE
CC  COMPUTE THE CORRECTION TERMS.
CC
      DLTAC(NP)=C.DC
      DO 2C I=2,NP
      II=NP-I+1
      DLTAC(II)=DC(II)-DDC(II)*DLTAC(II+1)
      2C CONTINUE
      RETURN
      END

```

```

      SUBROUTINE DESDER (Y,DY,DDY,DX,NP)
C THIS SUBROUTINE NUMERICALLY COMPUTES THE FIRST AND
C SECOND DERIVATIVES BY FITTING A POLYNOMIAL
C OVER 5 POINTS
      IMPLICIT REAL*8 (A-H,O-Z)
      DIMENSION Y(1),DY(1),DDY(1)
      NPM1=NP-1
      NPM2=NP-2
      NPM3=NP-3
      NPM4=NP-4
      C1=1.D0/(12.D0*DX)
      C2=1.D0/(12.D0*DX*DX)
C
C DETERMINING FOR POINTS 3 TO N-2
      DO 300 I=3,NPM2
        DY(I)=C1*(Y(I-2)-8.D0*(Y(I-1)-Y(I+1))-Y(I+2))
        DDY(I)=C2*(-Y(I-2)+16.D0*(Y(I-1)+Y(I+1))-30.D0*Y(I)-Y(I+2))
      300
C DETERMINING FOR THE POINTS 1, 2, N-1, AND N
      DDY(1)=(35.D0*Y(1)-104.D0*Y(2)+114.D0*Y(3)-56.D0*Y(4)
1      +11.D0*Y(5))*C2
      DDY(2)=(11.D0*Y(1)-20.D0*Y(2)+6.D0*Y(3)+4.D0*Y(4)-Y(5))*C2
      DDY(NPM1)=(-Y(NPM4)+4.D0*Y(NPM3)+6.D0*Y(NPM2)-20.D0*Y(NPM1)
1      +11.D0*Y(NP))*C2
      DDY(NP)=(11.D0*Y(NPM4)-56.D0*Y(NPM3)+114.D0*Y(NPM2)
1      -104.D0*Y(NPM1)+35.D0*Y(NP))*C2
      DY(1)=(-25.D0*Y(1)+48.D0*Y(2)-36.D0*Y(3)+16.D0*Y(4)
1      -3.D0*Y(5))*C1
      DY(2)=(-3.D0*Y(1)-10.D0*Y(2)+18.D0*Y(3)-6.D0*Y(4)+Y(5))*C1
      DY(NPM1)=(-Y(NPM4)+6.D0*Y(NPM3)-18.D0*Y(NPM2)+10.D0*Y(NPM1)
1      +3.D0*Y(NP))*C1
      DY(NP)=(3.D0*Y(NPM4)-16.D0*Y(NPM3)+36.D0*Y(NPM2)
1      -48.D0*Y(NPM1)+25.D0*Y(NP))*C1
C
      RETURN
      END

```

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```

```

C THIS SUBROUTINE IS BASED ON RATTOCLETTI'S ALGORITHM.
SUBROUTINE FERM(X,FHALFX,IXX)
IMPLICIT REAL*8(A-H,C-Z)
DIMENSION C(12)
IF(X.LT.-12.5D0.OR.X.GT.-2.D0)GO TO 10
IF(IXX.EQ.2)GO TO 20
IF(IXX.EQ.3)GO TO 180
IF(IXX.EQ.4)GO TO 190
SUM=0.D0
A=1.D0
DO I=1,6
B=I*I.D0
CC=A*DEXP(B*X)/(B*DSORT(B))
SUM=SUM+CC
IF(DABS(CC).LT.1.D-30)GO TO 40
A=A*(-1.D0)
CONTINUE
FHALFX=SUM
RETURN
SUM=0.D0
A=1.D0
DO I=1,8
B=I*I.D0
CC=A*DEXP(B*X)/DSORT(B)
SUM=SUM+CC
IF(DABS(CC).LT.1.D-30)GO TO 60
A=A*(-1.D0)
CONTINUE
FHALFX=SUM
RETURN
SUM=0.D0
A=1.D0
DO I=1,12
B=I*I.D0
CC=A*DEXP(B*X)*DSORT(B)
SUM=SUM+CC
IF(DABS(CC).LT.1.D-30)GO TO 210
A=A*(-1.D0)
CONTINUE
FHALFX=SUM
RETURN
SUM=0.D0
A=1.D0
DO I=1,12
B=I*I.D0
CC=A*DEXP(B*X)*B*DSORT(B)
SUM=SUM+CC

```

```

IF (PARS(CC).LI.1.D-30) GO TO 230
A=A*(-1.D)
CONTE=INTE
FHALFX=SUM
RETURN
1 IF (X.LI.-12.5DC.OR.X.GT.0.D) GO TO 70
XE=DEXP(X)
IF (IXX.EQ.2) GO TO 80
IF (IXX.EQ.3) GO TO 240
IF (IXX.EQ.4) GO TO 250
FHALFX=XE*(1.DC+XE*(0.35353667D0+XE*(0.10210895D0+
1 XE*(-0.122336525D0+XE*(0.78991718D-1+XE*(-0.43441957D-1+XE*
2 (-0.16320377D-1-0.29297406D-2*XE))))))
RETURN
80 FHALFX=XE*(1.DC+XE*(-0.77737334D0+XE*(0.57632685D0+XE*
1 (-0.439461D0+XE*(0.39495859D0+XE*(-0.260651742D0+XE*
2 (-0.114242639D0-0.234379968D-1*XE))))))
RETURN
240 FHALFX=XE*(1.DC+XE*(-1.41414668D0+XE*(1.72898055D0+
1 XE*(-1.957844D0+XE*(1.97479295D0+XE*(-1.563910452D0+
2 XE*(0.799698473D0-XE*(0.187533974D0))))))
RETURN
250 FHALFX=XE*(1.DC+XE*(-2.82829336D0+XE*(5.18694165D0+
1 XE*(-7.831376D0+XE*(9.87396475D0+XE*(-9.383462712D0+
2 XE*(5.597889311D0-XE*(1.500331795D0))))))
RETURN
70 IF (X.LI.-12.5DC.OR.X.GT.3.D) GO TO 90
IF (IXX.EQ.2) GO TO 100
IF (IXX.EQ.3) GO TO 260
IF (IXX.EQ.4) GO TO 270
FHALFX=0.76514805D0+X*(0.60491025D0+X*(0.18999505D0+X*(
1 0.20131714D-1+X*(-0.38688953D-2+X*(-0.76558999D-3+X*
2 (-0.333817837D-3-0.28395509D-4*X))))))
RETURN
100 FHALFX=0.60491025D0+X*(0.3798101D0+X*(0.060395142D0+X*
1 (-1.58755412D-2+X*(-0.82794995D-3+X*(1.84847022D-3-1.98769193D-4*
2 X))))))
RETURN
260 FHALFX=0.3798101D0+X*(0.120790284D0+X*(-4.76266236D-2+
1 X*(-1.53117998D-2+X*(9.2423511D-3-X*1.192615158D-3))))
RETURN
270 FHALFX=0.120790284D0+X*(-9.52532472D-2+X*(-4.593553094D-2+
1 X*(3.69694044D-2-X*5.9637579D-3)))
RETURN
90 IF (X.GT.3.D) GO TO 110
FHALFX=DEXP(X)
RETURN

```

11	IF (X.GT.6.D0) GO TO 12	00003630
	N=5	00003640
	C(1)=1.0002404D0	00003650
	C(2)=1.1981922D0	00003660
	C(3)=2.9828285D0	00003670
	C(4)=-24.084495D0	00003680
	C(5)=96.877279D0	00003690
	C(6)=-156.23522D0	00003700
	GO TO 13	00003710
12	IF (X.GT.12.D0) GO TO 14	00003720
	N=4	00003730
	C(1)=1.0000313D0	00003740
	C(2)=1.2248008D0	00003750
	C(3)=1.8177898D0	00003760
	C(4)=-5.1849956D0	00003770
	C(5)=-3.2409718D0	00003780
	GO TO 13	00003790
14	N=5	00003800
	C(1)=1.D0	00003810
	C(2)=1.2337005D0	00003820
	C(3)=1.0654119D0	00003830
	C(4)=9.7015185D0	00003840
	C(5)=242.71502D0	00003850
	C(6)=11865.691D0	00003860
13	IF (IXX.EQ.2) GO TO 15	00003870
	IF (IXX.EQ.3) GO TO 28	00003880
	IF (IXX.EQ.4) GO TO 29	00003890
	TEMP=.75225278D0*X*DSQRT(X)	00003900
	SUM=.D0	00003910
	BYX2=1.D0/(X*X)	00003920
	DO 16 I=1,N	00003930
16	SUM=BYX2*(SUM+C(N-I+2))	00003940
	FHALFX=TEMP*(C(1)+SUM)	00003950
	RETURN	00003960
15	TEMP=.75225278D0*DSQRT(X)	00003970
	SUM=.D0	00003980
	BYX2=1.D0/(X*X)	00003990
	DO 17 I=1,N	00004000
17	SUM=BYX2*(SUM+C(N-I+2)*(1.5D0-2.D0*(N-I+1)))	00004010
	FHALFX=TEMP*(1.5D0*C(1)+SUM)	00004020
	RETURN	00004030
28	TEMP=.75225278D0/DSQRT(X)	00004040
	SUM=.D0	00004050
	BYX2=1.D0/(X*X)	00004060
	DO 3 I=1,N	00004070
3	SUM=BYX2*(SUM+C(N-I+2)*(1.5D0-2.D0*(N-I+1))*(0.5D0	00004080
	1-2.D0*(N-I+1)))	00004090

```

      FHAFX=TEMP*(1.75D0*C(1)+SUM)
      RETURN
290  TEMP=(.75225278D0/(X*DSQRT(X)))
      SUM=1.D0
      BYX2=1.D0/(X*X)
      DO 310 I=1,N
310  SUM=BYX2*(SUM+C(N-I+2)*(1.5D0-2.D0*(N-I+1))*(2.D0*
1  (N-I+1)-1.5D0)*(2.D0*(N-I+1)+1.5D0))
      FHAFX=TEMP*(-1.375D0*C(1)+SUM)
      RETURN
      END

```

```

00004100
00004110
00004120
00004130
00004140
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00004190
00004200

```

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## VITA

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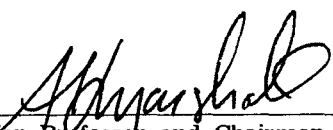
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Major Field: Electrical Engineering

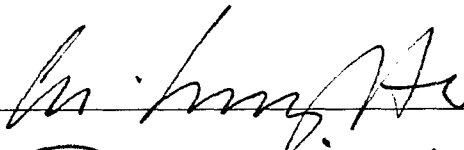
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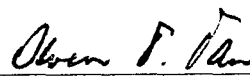
  
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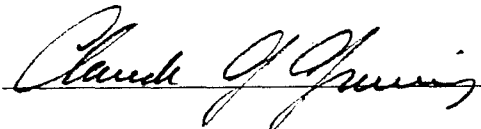
  
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Date of Examination:

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