

"THE NUMERICAL ANALYSIS OF THE ELECTRICAL PROPERTIES OF PN
JUNCTION DEVICES IN NON-EQUILIBRIUM CONDITIONS"

by

VOJISLAV ARANDJELOVIC, Dipl.Ing.

a Thesis submitted for the Degree of
DOCTOR OF PHILOSOPHY
of the
UNIVERSITY OF LONDON

Department of Electrical Engineering,
Imperial College of Science and Technology,
January 1969

ABSTRACT

An investigation of the methods for solving the problem of steady-state current flow in semiconductor junction devices is performed.

A systematic examination of the analytical approaches for solving the problem showed that a comprehensive solution could not be obtained by analytical means. Stiffness of the original system of equations also precludes the application of integrating routines of general type.

By deriving suitable integral representations for the diffusion-drift equations and Poisson's equation an iterative, variable step size method for solving junction equations is formulated. The method, which reduces to generating a sequence of initial value problems, is applied to the structure of a uniform-base transistor.

A method for direct solution of two-point boundary value problems of class M, combined with the integral representations obtained for diffusion-drift equations, is found sufficiently powerful to formulate a general numerical algorithm for solving the junction transport equations. Suitable choice of junction variables in the basic system permits formulating efficient algorithms for treating arbitrary structures under arbitrary bias conditions.

The solutions calculated for a diffused junction diode demonstrate the ability of the method to handle high reverse voltages. In another application of the method the cut-off frequency for transcon-

ductance of a special MOS structure is analyzed.

The method is further extended to include the analysis of the steady-state transport processes in junction transistors. A detailed numerical study of the d.c. and a.c. properties of a double-diffused transistor structure is performed.

ACKNOWLEDGEMENTS

The author wishes to express his deep gratitude to his supervisor Mr. J. J. Sparkes of the Department of Electrical Engineering Science of University of Essex, Colchester for his encouragement and guidance during the course of this work. He also wishes to thank Dr. R. Spence of the Electrical Engineering Department, Imperial College, London for his interest and help during the course of this work. Thanks are also due to his many colleagues in the Electronics Laboratory, in particular J. M. Garduno, L. Houselander, G. Selby, Mr. Vehovec and his old colleagues Drs. H. Y. Chow, E. J. Purslow and P. D. van der Puije for many interesting discussions and criticisms.

Partial financial support of this work by Institut za nuklearne nauke "Boris Kidric" - Vinca, Yugoslavia is gratefully acknowledged. Interest of Mr. K. J. S. Cave of Allen Clark Research Centre, The Plessey Company Limited, Caswell and subsequent help by The Plessey Company Limited allowed this work to be completed.

TABLE OF CONTENTS

TITLE	1
ABSTRACT	2
ACKNOWLEDGEMENTS	4
TABLE OF CONTENTS	5
LIST OF SYMBOLS	9
 CHAPTER 1 <u>CARRIER TRANSPORT IN SEMICONDUCTOR JUNCTIONS</u>	 16
1.1 Introduction	16
1.2 Formulation of the problem	17
1.3 On the nature of the transport coefficients	20
1.3.1 Mobility as a function of semiconductor structure	20
1.3.2 Carrier mobilities in high electric fields	24
1.3.3 Diffusion coefficient	26
1.4 Recombination processes	27
1.5 Aim of the thesis	29
1.6 Statement of originality	30
 CHAPTER 2 <u>ANALYTICAL THEORIES OF TRANSPORT PROCESSES IN P-N JUNCTIONS: A SURVEY</u>	 32
2.1 Introduction	32
2.2 Steady-state analysis	33
2.2.1 Thermal equilibrium	34
2.2.2 Analysis of neutral regions	35
2.2.3 Low-level diffusion currents	36
2.2.3.1 Uniformly doped neutral regions	36
2.2.3.2 Non-uniform doping	39
2.2.4 High current densities	40
2.2.4.1 Diffusion-dominated models	41
2.2.4.2 Hybrid models	43
2.2.4.3 Field-dominated models	46

2.2.4.3.1	Thin junctions	46
2.2.4.3.2	Long-base junctions	47
2.2.4.3.3	Long p-i-n structures	48
2.2.5	Recombination currents	50
2.2.6	Properties of the transition region	51
2.2.6.1	Space charge capacitance	53
2.2.7	Reverse breakdown	56
2.3	Transient analysis	57
2.3.1	Forward transient	58
2.3.2	Reverse transient	59
2.4	Conclusions	61
CHAPTER 3	<u>NUMERICAL TREATMENT OF P-N JUNCTION TRANSPORT EQUATIONS</u>	63
3.1	Introduction	63
3.2	Preliminary integrations	65
3.2.1	The electrostatic field equation	66
3.3	Auxiliary variable	69
3.4	Local iteration loop	71
3.5	The over-all iteration loop	74
CHAPTER 4	<u>NUMERICAL ANALYSIS OF UNIFORM-BASE TRANSISTOR STRUCTURES</u>	78
4.1	Introduction	78
4.2	Strategy of the method	78
4.3	Self-consistent behaviour of the solutions in a p^+ collector	79
4.3.1	Iterative calculation of solutions	83
4.3.2	The near-base section of the collector	88
4.4	The numerical analysis of the base	89
4.4.1	The electron-depleted base section, next to the collector	89
4.4.2	The low-field mid-base section	90
4.4.3	The negative-field base section, next to the emitter	94
4.5	The p^+ emitter region	99

4.6	The complete solutions for a particular pnp structure	102
4.7	Conclusions	108
CHAPTER 5 <u>GENERAL ITERATIVE SCHEME FOR NUMERICAL TREATMENT OF SEMICONDUCTOR JUNCTION STRUCTURES</u>		109
5.1	Introduction	109
5.2	Outline of the method	110
5.2.1	The treatment of the charge carrier densities and the current densities	111
5.2.2	Treatment of Poisson's equation	113
5.2.2.1	Formation of the matrix T	116
5.2.2.2	The discretization formula	119
5.2.3	The iterative procedure	119
5.2.4	Convergence of the iterative procedure	120
5.3	Modifications of the analytical formulation	124
5.3.1	Choice of a suitable reference point	125
5.3.2	Shifting of the potential origin	127
CHAPTER 6 <u>APPLICATION OF THE GENERAL ITERATIVE SCHEME FOR NUMERICAL ANALYSIS OF SINGLE JUNCTION STRUCTURES</u>		130
6.1	Introduction	130
6.2	The numerical solutions of a diffused junction diode	131
6.2.1	The internal distributions	132
6.2.2	The terminal characteristics	137
6.3	Selected one-dimensional calculations of MOS structures	143
6.3.1	Input capacitance and transconductance of MOST's	143
6.3.2	Graded channel MOST structures	146
6.4	Accuracy of the results	151
CHAPTER 7 <u>THE NUMERICAL ANALYSIS OF DOUBLE-DIFFUSED TRANSISTOR STRUCTURES</u>		152
7.1	Introduction	152
7.2	The elements of the analysis	153
7.3	Doping profile of the analysed transistor	154

7.4	The boundary conditions	155
7.5	The expressions for the charge carrier densities and constant current densities	158
7.5.1	Emitter domain, $0 \leq x \leq x_m$	159
7.5.2	Collector domain, $x_m \leq x \leq L$	159
7.5.3	Terminal current densities	160
7.6	The electrostatic potential and iteration loop	161
7.7	Modifications pertaining to reverse collector biases	162
7.8	Limitations in the collector domain analysis	165
7.9	The numerical results for the structure of Fig.7.1	166
7.9.1	The internal distributions	167
7.9.2	Terminal characteristics of the device	172
CHAPTER 8	<u>CONCLUSIONS</u>	187
8.1	General conclusions	187
8.2	Further research	189
8.2.1	Further applications of the developed numerical technique	189
8.2.2	Generalizations of the present numerical technique	190
Appendix 1		194
Appendix 2		195
Appendix 3		199
Appendix 4		200
Appendix 5		202
Appendix 6		203
Appendix 7		206
Appendix 8		210
Appendix 9		213
REFERENCES		233

LIST OF SYMBOLS

a	a constant; also the column vector defined in section 5.2.2
A	a coefficient; also cross-sectional area of a junction
b	ratio of electron and hole mobilities
B	matrix of constant coefficients defined in section 5.2.2
B_o	a constant
c	a coefficient
C	per-unit-area junction capacitance
C_{CB}	per-unit-area output capacitance of transistors
C_{EB}	per-unit-area input capacitance of transistors
C_g	total gate capacitance
C_s	per unit-area capacitance of the surface space charge region
C_o	per-unit-area capacitance of the oxide layer
d	length of an intrinsic semiconductor domain
d_n	length of an n-type neutral semiconductor domain
d_p	length of a p-type neutral semiconductor domain
D_n	diffusion coefficient of electrons
D_p	diffusion coefficient of holes
e	auxiliary variable
e_r	error bound for electrostatic potential calculations
e_o	current value of the auxiliary variable
E	electrostatic field
$\bar{E}$	mean value of the electrostatic field in an interval δx
E_b	electrostatic field at breakdown
E_{drift}	limiting value of the electrostatic field in a uniformly doped collector region
E_j	electrostatic field at the metallurgical junction in equilibrium
E_{jc}	electrostatic field at the collector metallurgical junction in equilibrium
E_{je}	electrostatic field at the emitter metallurgical junction in equilibrium
E_L	lower bound for the electrostatic field in a p^+ collector region

E_{L1}	lower bound for the electrostatic field in a p^+ emitter region
E_t	electrostatic field at a point in a p^+ collector
f	general notation for a function; also the column vector defined in section 5.2.2
f_n	n-th component of the vector f
f_T	cut-off frequency for transconductance of MOST's; also gain-bandwidth product of junction transistors
F	local space charge as function of position and electrostatic potential
F_o	a constant
g	generation rate; also $g(x) = \frac{\partial F}{\partial u}$ in section 5.2.2
g_{ch}	channel conductance of MOST's
g_m	transconductance
g_o	common-base output conductance of junction transistors
h	integration step
H	a constant
I_D	drain current
I_T	inverse of the matrix T
J	current density; also matrix of constant coefficients defined in section 5.2.2
J_B	total current density at the base contact
J_C	total current density at the collector contact
J_E	total current density at the emitter contact
J_f	forward transient current density
J_n	electron current density
J_{no}	constant electron current density
J_p	hole current density
J_{pc}	collector-controlled constant hole current density
J_{pe}	emitter-controlled constant current density
J_{po}	constant hole current density
J_r	reverse transient current density
J_{rg}	generation-recombination current density

J_s	saturation current density
K	vector composed of the remaining terms of Poisson's equation at interior mesh points of an one-dimensional mesh
l	depth of the substrate of MOST's
L	high-level diffusion length; also total length of a structure
L_c	length of a uniformly doped collector
L_{ch}	length of the channel in MOST's
L_e	length of a uniformly doped emitter
L_m	a constant
L_n	diffusion length of electrons in a p-type region
L_p	diffusion length of holes in an n-type region
M	total number of discrete steps defined for the numerical treatment of Poisson's equation
n	electron density
n_{b2}	electron density at the plane $E=0$ in the base of a pnp transistor
n_e	excess minority carrier density in a semiconductor
n_i	intrinsic carrier concentration
n_j	electron density at the metallurgical junction in equilibrium
n_{no}	electron density in an n-type neutral material in equilibrium
n_p	electron density distribution in the near-base section of a p^+ emitter
n_{po}	electron density in a p-type neutral material in equilibrium
n_o	electron density in a near-intrinsic material in equilibrium
n_l	electron density related to the energy level of traps
N	net impurity concentration
N_a	concentration of acceptor impurities
N_c	effective density of states in the conduction band

N_d	concentration of donor impurities
N_s	surface concentration
N_v	effective density of states in the valence band
N_o	total number of impurities per-unit-area
p	hole density
p_{b2}	hole density at the plane $E=0$ in the base of a pnp transistor
p_{high}	upper limit for p_{b2}
p_j	hole density at the metallurgical junction in equilibrium
p_{jc}	hole density at the collector metallurgical junction in equilibrium
p_{je}	hole density at the emitter metallurgical junction in equilibrium
p_{low}	lower limit for p_{b2}
p_{min}	minimum hole density in the base of a pnp transistor
p_{no}	hole density in an n-type material in equilibrium
p_{po}	hole density in a p-type material in equilibrium
p_U	upper bound for the hole density distribution in a p^+ collector
p_{U1}	upper bound for the hole density distribution in a p^+ emitter
p_t	hole density at a point in a p^+ collector
p_o	hole density in a near-intrinsic material in equilibrium
p_l	hole density related to the energy level of traps
q	electronic charge
Q	matrix
Q_g	total per-unit-area charge on the gate of MOST's
Q_n	per-unit-area electron charge in the channel of MOST's
Q_s	per-unit-area charge in the semiconductor
r	normalized time; also recombination rate
r_f	normalized time of forward conduction
r_a	normalized recovery time of a junction
R_e	matrix

R_m	a constant
S	matrix
S_o	a coefficient
S_n	surface recombination velocity for electrons
S_p	surface recombination velocity for holes
t	time; also running variable in integrals
T	temperature in $^{\circ}\text{K}$; also tridiagonal matrix associated with the numerical treatment of Poisson's equation
u	electrostatic potential
$u^{(o)}$	a potential guess
$u^{(1)}$	an improved potential distribution
u_{rk}	k-th intermediate potential reference in a reverse biased junction
u_{xx}	second partial derivative of $u(x,y)$ in the x-direction
U	recombination rate
U_n	recombination rate in an n-type material
U_p	recombination rate in a p-type material
v	drift velocity of carriers
V	total voltage across a junction
V_a	applied junction voltage
V_b	voltage across barrier region at high currents
V_{CB}	collector-base applied voltage
V_D	drain voltage
V_{EB}	emitter-base applied voltage
V_g	gate voltage
V_m	near-contact voltage drop in diode base
V_n	voltage across neutral semiconductor
V_s	semiconductor surface potential
V_T	Boltzmann voltage, kT/q
V_o	"built-in" voltage
V_{oc}	collector-base "built-in" voltage
V_{oe}	emitter-base "built-in" voltage
V_l	a coefficient
w	junction depletion region width
w_b	metallurgical base width

w_n	n-side depletion region width of a junction
w_p	p-side depletion region width of a junction
w_c	energy level at conduction band edge
w_t	energy level of traps
w_v	energy level at valence band edge
x	distance
x'	length of a self-consistent behaviour of electrostatic field distribution in a p^+ collector
x''	length of a self-consistent behaviour of hole density distribution in a p^+ collector
x_{bl}	position of the point in the base where $p=p_{\min}, E=E_{c2}$
x_{b2}	position of the point $E=0$ in the base
x_{cc}	position of the collector contact
x_{cmj}	position of the collector metallurgical junction
x_{ec}	position of the emitter contact
x_{emj}	position of the emitter metallurgical junction
x_i	penetration of the gate voltage in the substrate of MOST's
x_m	position of the potential reference point
x_{mj}	position of the metallurgical junction
x_n	interior mesh point defined for the numerical treatment of Poisson's equation
x'_1	length of a self-consistent behaviour of hole density distribution in a p^+ emitter
y	general notation for a dependent variable; also a coordinate in two-dimensional systems
Y_m	a constant
z	vector
Z	width of the substrate of MOST's
α_i	i-th coefficient associated with the difference equation for solving Poisson's equation
β_i	i-th coefficient associated with the difference equation for solving Poisson's equation
$\beta_{\max}$	maximum current gain
δE_m	maximum permissible error in computing electrostatic field

δu	potential correction
$\delta u_{\max}$	maximum permissible error in computing potential function
δu_p	potential correction in the x-direction
δu_t	potential correction in the y-direction
δx	small increment in position coordinate
ϵ	dielectric constant
λ	normalized distance; also running variable in integrals
μ	mobility
μ_c	mobility due to Coulomb scattering
μ_I	mobility due to Coulomb scattering on ionized impurities
μ_L	mobility due to lattice scattering
$\mu_{\max}$	a constant
$\mu_{\min}$	a constant
μ_n	electron mobility
μ_p	hole mobility
ρ	local space charge
τ	high level lifetime = $\tau_{po} + \tau_{no}$
τ_{no}	lifetime of electrons in a highly p-type material
τ_{po}	lifetime of holes in a highly n-type material
ω	angular frequency

CHAPTER 1

CARRIER TRANSPORT IN SEMICONDUCTOR JUNCTIONS1.1 Introduction

Since the discovery of the transistor action in 1948, a vast amount of research has been done on properties of semiconductor materials and devices. A great deal of this activity has been devoted to study of p-n junctions, since on their properties most of semiconductor devices are based.

Even though the system of equations describing the fundamental electronic transport properties in semiconductors is very well established, the theories for the behaviour of p-n junctions are numerous. This is a consequence of the equally numerous assumptions that have been applied in these theories in order to facilitate the analysis.

In this chapter the problem of carrier transport in non-degenerate semiconductors is stated in its original form. Then, the refinements which remove some of the restrictions implied by the original formulation are introduced into the basic model in order to extend its validity to the device structures of contemporary technical importance.

1.2 Formulation of the problem

The fundamental equations in the analysis of current flow in semiconductor devices are those which describe the motion of carriers in semiconductors under the combined influence of external fields and of deviations from thermal equilibrium densities of carriers. The mobile charge carriers, holes and electrons, are subject to drift under electric fields and to diffusion in the presence of concentration gradients. The corresponding flow densities, produced by the simultaneous action of a small electric field and a small concentration gradient are given by the relations generally referred to as diffusion-drift equations*

$$J_p = q \mu_p p E - q D_p \text{grad} p, \quad (1.1)$$

$$J_n = q \mu_n n E + q D_n \text{grad} n. \quad (1.2)$$

The concepts of drift and diffusion represent approximations of the physical case and do not have meaning unless the thermal velocity of carriers is large compared with their drift velocity and the probability of recombination in a mean free time between collisions is small. (Semiconductor models have been proposed which do not require the use of those concepts and hence evolve from a different mathematical model^{2,3,4}.)

* The displacement currents $\frac{\partial E}{\partial t}$ can be neglected up to signal frequencies comparable with the inverse of the dielectric relaxation time and are not considered in the theory of junction devices, e.g. in near intrinsic germanium the frequency limit is 15GHz or 700GHz in 1 Ω cm Ge.

Further description of the transport behaviour of electrons and holes in the semiconductors under non-equilibrium conditions is furnished by the equations of continuity for each type of carrier

$$\frac{\partial p}{\partial t} = (g-r) - 1/q \operatorname{div} J_p, \quad (1.3)$$

$$\frac{\partial n}{\partial t} = (g-r) + 1/q \operatorname{div} J_n. \quad (1.4)$$

The equations (1.3) and (1.4) simply state that in a given volume element, the time rate of change in the number of charge carriers of a given type arises either from a difference between the rates of generation and recombination of these carriers, or from a difference between the currents of the corresponding particles entering and leaving that volume, or else due to both of these effects.

Since the diffusion-drift equations include the electric field, in addition to the carrier densities and currents, to arrive at a complete description of the problem another equation is required. This is obtained with the help of one of the Maxwell's equations, i.e. Poisson's equation which relates the carrier concentrations to the electrostatic field

$$\operatorname{div} E = \rho/\epsilon. \quad (1.5)$$

In (1.5) local charge density, ρ , is assumed to consist of two components: charge residing on the mobile charge carriers, electrons and holes, and charge located on the immobile donor and acceptor ions. The situations in which all donors and acceptors are substantially fully ionized, which occurs at normal temperatures in most semiconductor

devices, are assumed throughout this work. Thus

$$\rho = q(p - n + N_d - N_a). \quad (1.6)$$

Strictly speaking the charge associated with the localized energy states should be included in (1.6), and its rate of change in (1.3) and (1.4). But the population of these levels is usually very small and adjusts very quickly to the changes in p and n (the decay of injected carriers is considered to be adiabatically slow compared to the adjustment in these states). Consequently, it is generally accepted that in the usual electronic devices these effects are not important enough to be included in the basic equations.

The electric field is treated as an electrostatic one which is consistent with the frequency limit introduced by neglecting the dielectric currents in (1.1) and (1.2). Therefore

$$E = - \text{grad} u. \quad (1.7)$$

This is also consistent with the circumstance that the effects of magnetic fields, with none applied, are in general quite negligible.

All developments in the theory of semiconductor devices are based upon the system of equations (1.1)-(1.5)*. Therefore it is the

* The set of fundamental equations can be alternatively expressed in terms of the quasi-Fermi potentials³², in which case separate relationships between these potentials, electrostatic potential, and the carrier densities, based on the relevant statistical considerations (Boltzmann statistics, in non-degenerate materials), must be established. In this work, however, the equations (1.1)-(1.5), as formulated originally by Van Roosbroeck¹⁸ are treated.

fundamental problem to solve the equations (1.1)-(1.5) for a given geometry, doping, and applied bias.

1.3 On the nature of the transport coefficients

To describe the movement of the charge carriers in an electric field, the concept of mobility relating drift velocity of carriers to the field under whose influence they drift is introduced

$$v = \mu E. \quad (1.8)$$

The equation (1.8) can be used as the definition of drift mobility. (Strictly speaking μ is a tensor, but because of the small dimensions of the studied systems, the scalar approximation is a very good one).

1.3.1 Mobility as a function of semiconductor structure

The magnitude of the mobility depends upon the nature and density of scattering centres present in a semiconductor specimen and of the average thermal velocity of the carriers. Scattering mechanisms responsible for determining carrier mobility are brought about by anything which causes a deviation from perfect periodicity of the lattice potential. The list of mechanisms includes

- 1 - the thermal vibration of atoms;
- 2 - Coulomb potential of ionized impurity atoms;
- 3 - Coulomb potential of current carriers themselves;

- 4 - neutral impurity atoms;
- 5 - various lattice defects (dislocations, interstitial atoms, etc.).

The first mechanism is dominant in high resistivity materials. The second and third may cause a considerable reduction in mobility in low resistivity samples. The fourth mechanism can be important in materials with high degree of compensation. Scattering by lattice imperfections is usually unimportant. For transistor-grade material scattering by the first three mechanisms is of importance.

The explanation by Prince^{14,15} of the measurements of germanium and silicon samples with different concentrations of impurities, based on the expressions derived by Conwell and Weisskopf¹⁷, involves a rather large value for the effective mass of holes. By postulating also that majority carriers constitute scattering centres identical with impurity atoms in so far as scattering mechanism is concerned, it was possible to fit the experimental data by the formula

$$\mu_I = 2^{7/2} \pi^{-3/2} q^{-3} m_h^{-1/2} \epsilon^2 (kT)^{3/2} [N_I \ln(1 + (3kT\epsilon q^{-2} N_I^{-1/3})^2)]^{-1}, \quad (1.9)$$

where $m_h = 3m_0$ is the assumed effective mass of holes, and $N_I = N_d + n \approx 2N_d$ in n-type semiconductor stands for the concentration of scattering centers.

If μ_L is the mobility that results from the lattice scattering, the total effect of both scattering mechanisms can be estimated by adding the reciprocals²¹

$$1/\mu = 1/\mu_I + 1/\mu_L. \quad (1.10)$$

The calculations in which the difference between the scattering mechanisms is considered¹⁹ result in the formula for the total mobility

$$\mu = \mu_L [1 + \zeta^2 (C_1 \zeta \cos \zeta + S_1 \zeta \sin \zeta - \frac{\pi}{2} \sin \zeta)], \quad (1.11)$$

in which

$$\zeta = (\mu_L / \mu_c)^{\frac{1}{2}}. \quad (1.12)$$

The mobility μ_c in (1.12) is due to both Coulomb scattering mechanisms.

A useful formula for numerical calculations of mobility using (1.11) and (1.12) is²⁰

$$\mu_L / \mu_c = K_1 N_r \ln(1 + K_2 N_r^{-2/3}) + K_3 P_r \ln(1 + K_4 P_r^{-2/3}), \quad (1.13)$$

where $N_r = N_I 10^{-18}$, $P_r = n_e 10^{-18}$ (N_I and n_e in cm^{-3}), and the coefficients K_i for the case of majority and minority carrier mobility are given in Table 1.

Table 1

	K_1	K_2	K_3	K_4
majority	.745	76.	.5166	132.6
minority	1.490	47.1	.5166	132.6

As an example the equations (1.11) - (1.13) are used to compute the mobility of minority carriers, holes in n-type germanium. The results, shown in Fig. 1.1, indicate that a considerable reduction of the mobility (or diffusivity) is caused by the impurity densities quite

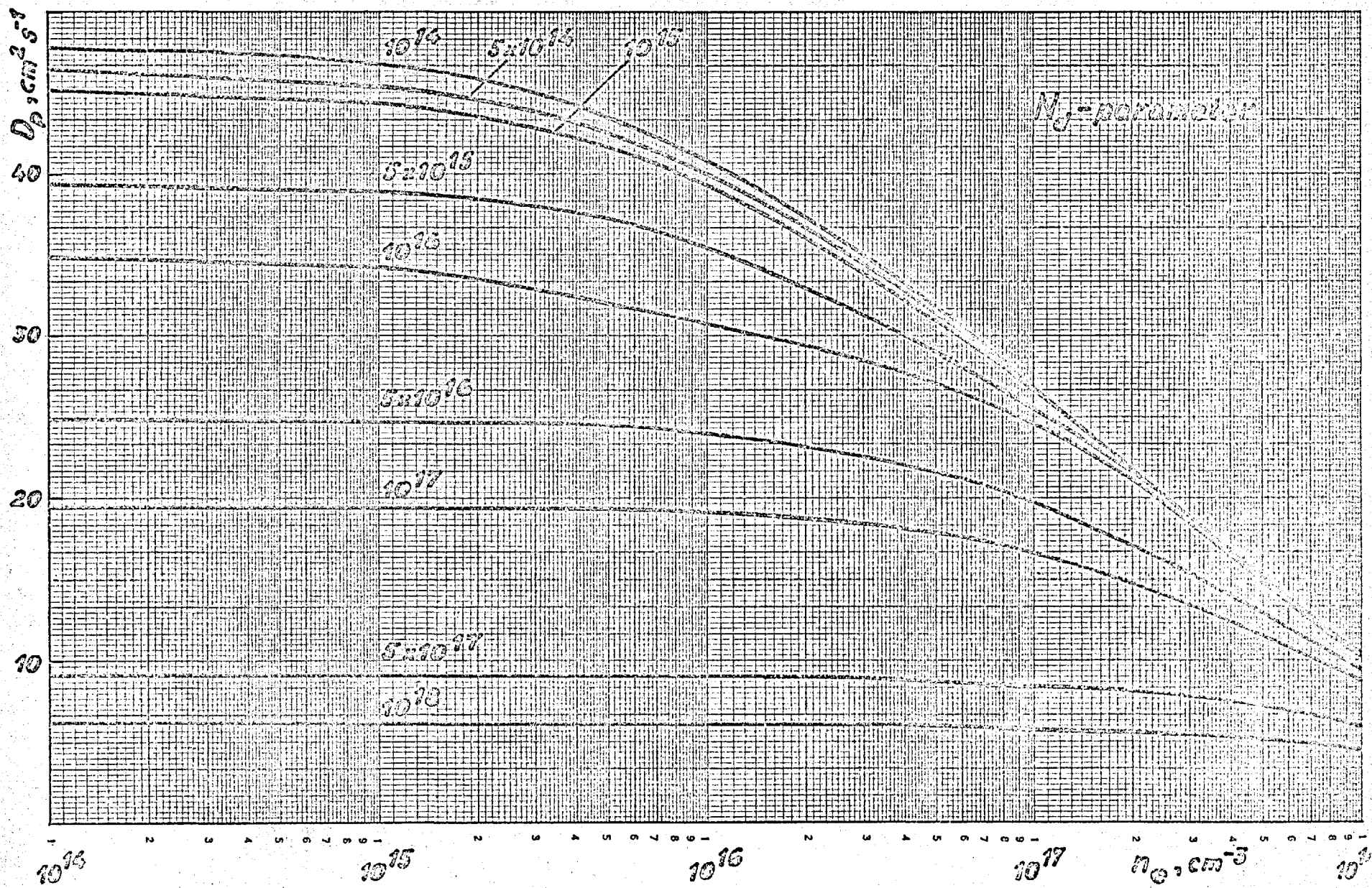


Fig. 1.1

common in junction device practice (for numerical details see Appendix 1).

1.3.2 Carrier mobilities in high electric fields

When the electric field in the semiconductor is increased beyond a certain critical value, the carriers acquire drift velocities of an order of magnitude comparable with that of their average thermal velocity. The influence of that field can no longer be considered as a small perturbation of their random thermal motion. The mobility itself becomes then a function of the electric field⁶, thus losing much of its physical significance.

High-field mobility measurements^{5,8} indicate that there can be observed three characteristic ranges in the relation mobility vs. field. First is a low-field range, over which the mobility is constant and Ohm's law, as defined by (1.8), is valid. Second is a nonlinear range where the mobility is approximately proportional to the square root of the field. At still higher fields the carrier velocity reaches a constant saturation value, and the mobility must vary as E^{-1} . Gunn's measurements⁹ extend to sufficiently high values of the electric field to indicate the existence of the fourth range, before avalanche multiplication, where the mobility is proportional to $E^{-.866}$. Recent investigations of the high-field phenomena in silicon¹⁰ do not confirm Gunn's results at very high fields, but rather fall in line with those reported by Ryder⁸ and Prior⁵.

The combined influence of both doping and high electric fields

could be estimated through an expression of the form

$$\mu(N, E) = \mu(N) f(E), \quad (1.14)$$

where $\mu(N)$ denotes the functional dependence of mobility upon doping, given by (1.12), and $f(E)$ is given by

$$f(E) = \begin{cases} 1, & E \leq E_{c1}, \\ (E_{c1}/E)^{\frac{1}{2}}, & E_{c1} < E \leq E_{c2}, \\ (E_{c1} E_{c2})^{\frac{1}{2}}/E, & E_{c2} < E. \end{cases} \quad (1.15)$$

The experimental values of E_{c1} and E_{c2} quoted in the literature^{5,8} are given in Table 2a.

Table 2a

	E_{c1} (V/cm)	E_{c2} (V/cm)
electrons in Ge	900	3,400
holes in Ge	1,400	8,000
electrons in Si	2,500	10,600
holes in Si	7,500	-

The empirical fit of Irvin's data¹¹ by Caughy and Thomas¹³, combined with the high-field approximations of Norris and Gibbons¹⁰, results in an expression for the mobility in silicon which is suitable

for the implementation on a digital computer

$$\mu(N, E) = \left(\frac{\mu_{\max} - \mu_{\min}}{1 + (N/N_{\text{ref}})^{\alpha}} + \mu_{\min} \right) \frac{1}{1 + (E/E_c)^{\beta})^{1/\beta}} \quad (1.15a)$$

The values of the empirical parameters in (1.15a) are given in Table 2b.

Table 2b

	$\mu_{\max}$	$\mu_{\min}$	N_{ref}	α	E_c	β
holes	495.	47.7	$6.3 \cdot 10^{16}$	0.76	19.5	1
electrons	1330.	65.0	$8.5 \cdot 10^{16}$	0.72	8.0	2

(μ 's in cm^2/Vs , N_{ref} in cm^{-3} , and E_c in kV/cm).

1.3.3 Diffusion coefficient

The diffusion coefficients of carriers are closely related to the mobilities because the same scattering mechanisms impede the motion of the carriers in drift and diffusion. Under the assumptions which made the equations (1.1) and (1.2) valid, these are interrelated through the so-called Einstein relation

$$\frac{D}{\mu} = \frac{kT}{q} \quad (1.16)$$

From the fact that the mobilities decrease with the electric field, it could be expected that the high field scattering of the carriers becomes remarkably effective in comparison with that in the thermal equilibrium state. From the viewpoint of diffusion effects, it has been suggested¹²

that the diffusion coefficients grow to very large values in such conditions, because the rate of randomization of the carriers increases. However, an experimental evidence supporting this suggestion is not available and the common practice is that the diffusion coefficients are inferred from the mobilities through (1.16).

1.4 Recombination processes

Whenever there is a deviation from the equilibrium carrier densities in a crystal a generation or recombination process arises to adjust the carrier densities to their equilibrium values. These processes affect the transport of the charge carriers through the continuity equations (1.3) and (1.4).

In general, two principal mechanisms control the recombination processes observed in semiconductors. The first is a direct transition of electrons and holes between the conduction and valence bands. This is the intrinsic, radiative recombination process. The second mechanism for recombination requires the presence of localized energy states in the forbidden gap of the semiconductor. The presence of such states increases considerably the rate of recombination of electrons and holes. Impurities and imperfections within the semiconductor introduce these kinds of states, with the net effect of decreasing the lifetime of excess carriers. From the experimental results it is generally accepted¹⁰⁷ that in germanium and silicon, recombination takes

place principally through trapping or recombination centres, and that direct transitions between the conduction and valence bands account for only small proportion of the recombination taking place.

The rate of recombination for non-equilibrium but steady-state conditions in a semiconductor having a small density of recombination centres situated approximately half-way across the forbidden energy gap is found to be^{25,26}

$$U = - \frac{pn - n_i^2}{\tau_{po}(n+n_1) + \tau_{no}(p+p_1)} , \quad (1.17)$$

where

$$p_1 = N_v \exp(W_v - W_t)/kT ,$$

$$n_1 = N_c \exp(W_t - W_c)/kT .$$

In a p-type material, with $p \gg p_1, n_1$, and n_i , the equation (1.17) reduces to

$$U_p = - \frac{n - n_p}{\tau_{no}} , \quad (1.17a)$$

while in an n-type material, with $n \gg p_1, n_1$, and n_i ,

$$U_n = - \frac{p - p_n}{\tau_{po}} . \quad (1.17b)$$

The equations (1.17a,b) are the familiar linear recombination laws which constitute good approximation to (1.17) when the excess minority carrier density is much smaller than the equilibrium carrier density.

Very often, recombination centres occurring at the surface of a semiconductor are more effective, than those in the bulk, in eliminating the charge carriers from the transport processes. The

phenomenon can be characterized by surface recombination velocity³²

such that

$$\begin{aligned} J_p &= S_p(p - p_o), \\ J_n &= S_n(n - n_o), \end{aligned} \quad (1.18a)$$

where J_p and J_n are the recombination currents flowing perpendicularly "into" the surface.

The inclusion of these surface effects into analysis of carrier transport would necessitate a multi-dimensional treatment. Alternatively, if the surface and bulk effects are interpreted through an equivalent lifetime, this multi-dimensional treatment could be avoided. In general, unless specifically desired, the precautions are taken to eliminate the effects of these surface states.

1.5 Aim of the thesis

Direct application of the general relations (1.1) and (1.2) for an analysis of the transport processes in semiconductor devices could be justified only in very few cases of practical interest. The physical conditions originally postulated to be responsible for much of what takes place in the interior of a typical semiconductor junction structure are not very representative of the conditions that may exist in the contemporary structures. Profound changes in the impurity content quite common in diffused junction structures, and an almost complete

absence of the field-free regions in such systems preclude an application of (1.1) and (1.2), without the refinements pertinent to the variations of the transport coefficients with doping and the electric field. (The availability of computers is no solution to the problem unless the physical equations are formulated beyond dispute).

The main aim of this thesis is to obtain the general solutions for the model defined by (1.1) - (1.5) and auxiliary relations (1.6), (1.7) and (1.12) - (1.16) which will be applicable to arbitrary doping profiles and arbitrary bias conditions.

The existing analytical techniques are examined, but the solution of the problem is attempted by numerical means. Two fundamental assumptions will restrict the validity of the solutions obtained by the present analysis. These are:

- (i) the numerical analysis of one-dimensional structures will be performed; and
- (ii) the analysis will concentrate on the steady-state properties of the analysed systems.

1.6 Statement of originality

Since the commencement of the present work a great deal of research has been done on similar problems to those treated in this thesis. Except where references have been made to the work of others, the results and conclusions presented here were obtained independently by the author.

An analysis of existing analytical models for current flow in semiconductor junctions has revealed the possibilities of analytical techniques. It became clear that only the application of numerical methods could provide more details regarding the behaviour of junction devices.

The original contributions in this thesis are:

(a) The treatment of diffusion-drift equations. This leads to the relations suitable for generating convergent numerical algorithms for solving junction transport equations;

(b) An approximate integral of Poisson's equation (exact for the case of a uniform doping) which permitted formulation of an one-step variable step-length integration method for the junction equations;

(c) The one-current solutions for uniformly doped transistor structures obtained by generating a suitable sequence of the initial value problems;

(d) The general iterative algorithm for numerical solution of junction equations, developed through the application of methods for direct solution of two-point boundary value-problems;

(e) The set of complete steady-state solutions, including high reverse biases, for a diffused junction diode;

(f) A method for improving the cut-off frequency for transconductance of a class of MOS structures;

(g) The set of complete steady-state solutions for a double-diffused planar transistor structure which includes realistic values of the collector bias.

CHAPTER 2

ANALYTICAL THEORIES OF TRANSPORT PROCESSESIN P-N JUNCTIONS: A SURVEY2.1 Introduction

A knowledge of the geometrical and structural properties of a p-n junction, together with its recombination characteristics should, in principle, be sufficient for predicting its behaviour under specified operating conditions. Unfortunately, with all these features known, it appears to be prohibitively difficult to obtain any exact predictions since the general solutions of the basic system (1.1)-(1.5) * do not seem to be obtainable by analytical means. A rigorous analytical treatment of this system has not been reported. Instead, a variety of alternative, but not necessarily justifiable, approaches have been made to simplify the basic equations and thus facilitate the analysis. Each approach, however, has introduced a new set of uncertainties concerning the analytical limitations arising from the use of simplifying assumptions.

There is a considerable wealth of information regarding the theories of behaviour of p-n junctions. An effort is made in this

* In this and all subsequent references to the basic system, the one-dimensional form of equations (1.1)-(1.5) is implied.

chapter to embody into a single entity the material covering all these theories and to assess their significance. Although the primary objective of the present effort is to classify the steady-state theories, a brief coverage of the theories of transients in p-n junctions is included towards the end of the chapter.

2.2 Steady-state Analysis

Under steady-state conditions the time-dependent terms $\frac{\partial p}{\partial t}$ and $\frac{\partial n}{\partial t}$ vanish in (1.3) and (1.4). Although this simplifies the fundamental system, in that it now includes only ordinary differential equations, the corresponding general solutions are still not expressible in terms of the known analytical functions. Therefore, any attempt to arrive at a solution of the problem in an analytical manner must rely on a set of additional physical approximations of the general case.

Except in very few cases where different reductions of the basic system were possible, Shockley's original strategy³² of defining the space charge and neutral regions within a junction structure has been universally accepted³³. Duly simplified transport equations are then applied to each of the regions separately. The complete solution is obtained by matching the boundary conditions.

2.2.1 Thermal equilibrium

At equilibrium the exponential relations between the electrostatic potential and the carrier densities follow from (1.1) and (1.2). With the help of (1.5) the potential and carrier distributions are expressible as explicit functions of position only in the intrinsic domain of the so-called p-i and n-i structures^{27,28, 103,118}. Otherwise the problem of solving for these equilibrium distributions can at best be reduced to one-dimensional numerical integration^{27,28,29}. As an exception, it is possible, applying analytical techniques, to solve exactly for the equilibrium junction variables at the metallurgical junction of a uniformly doped abrupt structure.

If the electrostatic field and the space charge are negligible far out in the bulk, from (1.1), (1.2) and (1.5) the following equilibrium carrier densities are obtained

$$n_{no} = \frac{1}{2} N_d \left[1 + (1 + 4 n_i^2 / N_d^2)^{\frac{1}{2}} \right], p_{no} = n_i^2 / n_{no}, \quad (2.1a)$$

and

$$p_{po} = \frac{1}{2} N_a \left[1 + (1 + 4 n_i^2 / N_a^2)^{\frac{1}{2}} \right], n_{po} = n_i^2 / p_{po}, \quad (2.1b)$$

Since $J_p = J_n = 0$, a combination of (1.1), (1.2) and (1.5) can be integrated once to give

$$E^2 = \frac{2qV_T}{\epsilon} \left(p - p_{no} + n - n_{no} - N_d \ln \frac{n}{n_{no}} \right) \quad (2.2a)$$

and

$$E^2 = \frac{2qV_T}{\epsilon} \left(p - p_{po} + n - n_{po} - N_a \ln \frac{p}{p_{po}} \right), \quad (2.2b)$$

within the n- and the p-region, respectively. The requirement for continuity of the electrostatic field at the interface between the two regions results in an equation which can be solved for either p_j or n_j (hole or electron-density at the metallurgical junction), e.g.

$$n_j = \exp \left[(N_a \ln n_{po} + N_d \ln n_{no} + p_{po} + n_{po} - p_{no} - n_{no}) / (N_a + N_d) \right] \quad (2.3)$$

and consequently

$$p_j = n_i^2 / n_j, \quad (2.4)$$

$$E_j = \left[\frac{2qV_T}{\epsilon} (p_j - p_{no} + n_j - n_{no} - N_d \ln \frac{n_j}{n_{no}}) \right]^{\frac{1}{2}}. \quad (2.5)$$

With the above three values known, the two uniform sides of a junction at equilibrium can be treated independently.

Because of the difficulties associated with integrating (1.5), it is not possible to obtain any preliminary results concerning the equilibrium solutions of an arbitrarily graded junction. The only alternative to an application of numerical methods for computing these solutions is the development of the equivalent series representations for the junction variables¹⁰⁴.

2.2.2 Analysis of neutral regions

The classical Shockley's assumption of the existence of neutral semiconductor regions on both sides of an impurity transition, sufficiently far away from it, provided a corner stone for many theoretical developments concerning the behaviour of p-n junctions.

Whenever the contributions from these regions dominate the properties of a junction structure, the corresponding analysis is greatly facilitated by the fact that the equation (1.5) of the fundamental system simplifies to

$$p - n + N = 0. \quad (2.6)$$

2.2.3 Low-level diffusion currents

Under the conditions of low injections the simplification (2.6) applies because the majority carrier densities in the neutral regions remain substantially unaltered by injection. Moreover, since $n \ll p \cong N_a$ in the p-region and $p \ll n \cong N_d$ in the n-region, the transport coefficients and lifetimes are also independent of injection.

2.2.3.1 Uniformly doped neutral regions

If the impurity density is uniform throughout, the drift terms in the diffusion-drift equations are negligible compared to their diffusion counterparts. The basic equations, in addition to (2.6), are thus reduced to

$$J_p = -q D_p \frac{dp}{dx}, \quad (2.7)$$

$$J_n = q D_n \frac{dn}{dx}, \quad (2.8)$$

$$\frac{dJ_p}{dx} + \frac{p - p_{no}}{\tau_{po}} = 0, \quad (2.9)$$

$$\frac{dJ_n}{dx} - \frac{n-n_{po}}{\tau_{no}} = 0. \quad (2.10)$$

Two second order linear differential equations, one for each type of charge carrier, result from this simplified system. Further implication of the low-level assumption is that the total voltage drop occurs across the space charge region, giving the boundary conditions for the injected carriers *

$$p = p_{no} \exp(q V_a / kT), \quad (2.11a)$$

$$n = n_{po} \exp(q V_a / kT), \quad (2.11b)$$

at the interfaces between the space charge region and the neutral regions.

Also

$$p = p_{no} \text{ as } x \rightarrow +\infty, \quad (2.11c)$$

$$n = n_{po} \text{ as } x \rightarrow -\infty. \quad (2.11d)$$

As a result the familiar junction equation follows

$$J = J_s (\exp(q V_a / kT) - 1). \quad (2.12)$$

The parameter J_s , the so-called saturation current density, governs the totality of junction properties (geometry, material, boundary conditions). In general, a consideration must be given to the carrier transport properties of the metal-semiconductor contacts. The concept of surface recombination velocity, introduced by (1.18), may be used to replace

* These are the low-level forms of the more generally defined boundary conditions at these interfaces^{111, 114}.

the boundary conditions at infinity, (2.11c, d). Then, for the arbitrary lengths of the neutral regions, d_p and d_n , and the arbitrary recombination velocities at the respective contacts, S_p and S_n , the saturation current density J_s is^{35,53,106}

$$J_s = \frac{qD_p p_{no}}{L_p} \frac{\text{ch}(\frac{d_n}{L_p}) + \frac{D_p}{S_p L_p} \text{sh}(\frac{d_n}{L_p})}{\text{sh}(\frac{d_n}{L_p}) + \frac{D_p}{S_p L_p} \text{ch}(\frac{d_n}{L_p})} + \frac{qD_n n_{po}}{L_n} \frac{\text{ch}(\frac{d_p}{L_n}) + \frac{D_n}{S_n L_n} \text{sh}(\frac{d_p}{L_n})}{\text{sh}(\frac{d_p}{L_n}) + \frac{D_n}{S_n L_n} \text{ch}(\frac{d_p}{L_n})}. \quad (2.13)$$

Different special cases of (2.13) are given in Table 3.

The validity of the exponential relation (2.12) is little disputed for germanium structures at current levels sufficiently small that the step-function approximations for the majority carrier densities³⁴

Table 3

S_p, S_n - arbitrary $\frac{d_{p,n}}{L_{p,n}}$ - small	$J_s = \frac{qD_p p_{no}}{d_n} \frac{1}{1 + \frac{D_p}{S_p d_n}} + \frac{qD_n n_{po}}{d_p} \frac{1}{1 + \frac{D_n}{S_n d_p}}$
S_p, S_n - infinite $\frac{d_{p,n}}{L_{p,n}}$ - arbitrary	$J_s = qD_p \frac{p_{no}}{L_p} \text{cth}(\frac{d_n}{L_p}) + qD_n \frac{n_{po}}{L_n} \text{cth}(\frac{d_p}{L_n})$
S_p, S_n - infinite $\frac{d_{p,n}}{L_{p,n}}$ - small	$J_s = qD_p p_{no}/d_n + qD_n n_{po}/d_p$
$\frac{d_{p,n}}{L_{p,n}}$ - infinite	$J_s = qD_p p_{no}/L_p + qD_n n_{po}/L_n$

could be considered reasonable. The position is less clear cut with the silicon structures where the diffusion of minority carriers is not the dominant process at small injections⁴⁰. It should also be noted that, in general, unless the linear recombination laws are used in the continuity equations (2.9) and (2.10) an analytical solution like (2.12) could not be obtained¹²⁴.

2.2.3.2 Non-uniform doping

Calculations of the non-uniform neutral regions are more difficult because of the impurity variations. In spite of this added complication, some calculations, unrelated to any particular impurity profile, are possible if the low-level assumptions are further specialized to eliminate the recombination terms from the model (2.6)-(2.10).

The structure of special interest is the asymmetrical narrow-base junction, similar to the emitter-base junctions in diffused transistors. If a p+n type structure is considered, then $J_n \approx 0$ and the built-in field in the n-base is

$$E \approx -\frac{1}{N} \frac{dN}{dx}, \quad (2.14)$$

since $n \approx N \gg p$. With the Boltzmann boundary conditions (2.11a, b) and the ideal ohmic contacts, the exponential relation between an applied voltage V_a and the current density J , like (2.12), follows. Here,

however, J_s is^{16,122}.

$$J_s = qn_i^2 \left(\frac{D_p}{\int_0^{d_n} N dx} + \frac{D_n}{\int_{-d_p}^0 N dx} \right), \quad (2.15)$$

i.e. the average impurity concentrations of the two neutral regions are responsible for the total current through the junction.

2.2.4 High current densities

When the density of injected carriers becomes comparable to the equilibrium majority carrier density in either of the neutral regions, the high-current conditions arise. Many quantities become interdependent and further assumptions must be introduced to avoid excessive mathematical difficulties in handling the differential equations.

The available models for analyzing the high-current phenomena fall into three groups¹²⁶: diffusion-dominated, hybrid, and field-dominated models. Although each of these three models puts the emphasis on different physical processes, they all share certain common assumptions. These are:

(i) Under high-injection conditions the densities of the mobile charge carriers are nearly equal, i.e.

$$p \cong n. \quad (2.16)$$

In fact from (2.6) $p \cong n - N$, but because $p, n \gg N$ (2.16) follows ((2.6) may thus be called the weak form of (2.16));

(ii) High-level recombination is linear in p and n , i.e.

$$U = \frac{p}{\tau} = \frac{n}{\tau}, \quad (2.17)$$

where $\tau = \tau_{po} + \tau_{no}$ is high-level lifetime. This follows from (1.17) since $p, n \gg n_i, p_i, n_i$;

(iii) The transport coefficients remain unaffected by high-injections.

The validity of (2.17) is usually not questioned since the pn product does increase at high forward biases¹²⁹ and (1.17) asymptotically approaches (2.17). The space charge neutrality assumption, however, has a more profound effect on the solutions¹⁸ and is more often a subject of appraisal^{47,48,127,131}. The third assumption, although very crude⁷, is not much criticized. The advantages of operating with constant transport coefficients seem to outweigh the significance of the errors that this assumption brings in the solutions. (The speculations concerning doubling of the diffusion coefficients at high levels¹²⁸ are related to entirely different assumptions.)

2.2.4.1 Diffusion-dominated models

In diffusion-dominated models the injected densities of carriers are determined primarily by diffusion process, rather than by the applied field. (Therefore, except for the different boundary conditions, the complete low-level theory of uniformly doped junctions is based on this type of model).

The complete differential equation for the hole density in an

n-base is

$$\frac{d^2 p}{dx^2} + \frac{1}{V_T} \left(p \frac{dE}{dx} + E \frac{dp}{dx} \right) - \frac{p - p_{no}}{L^2} = 0. \quad (2.18)$$

In a neutral, field-free semiconductor the second and the third term in (2.18) disappear. The familiar linear differential equation for holes results³⁶. Now, L is the high-level diffusion length,

$$L = [2\tau D_n / (D_n + D_p)]^{1/2}.$$

If the pn product through, and at the edges of, the barrier region is expressed as⁴⁰

$$pn = n_i^2 \exp(V_b/V_T), \quad (2.19)$$

V_b must be interpreted to include the voltage associated with the field that holds the majority carriers as well as the voltage that appears across the barrier region, but excluding ohmic drops. The near equality of majority and minority carriers results in the high-level Boltzmann boundary condition

$$p = n_i \exp(V_b/2V_T), \quad x = 0. \quad (2.20a)$$

Also

$$p \rightarrow p_{no} \text{ as } x \rightarrow \infty, \quad (2.20b)$$

giving the well known result for the hole current density in a p+n structure³⁶

$$J_p = \frac{2qd_n n_i}{\tau} \exp(V_b/2V_T). \quad (2.21)$$

The low-level conditions are maintained within the highly doped side

and the total current density also includes the electron component calculated by (2.12). With different geometries certain modifications of the multiplying factor in (2.21) are obtained, but the same exponential dependence is preserved^{37,45}.

The complete omission of the electric field from this analysis lead to the concept at an effective diffusion coefficient¹²⁸. From (1.1), (1.2) and (2.16), neglecting J_n ,

$$J_p = -q(2D_p) \left(\frac{dp}{dx} \right)_{x=0} \quad (2.22)$$

This apparent doubling of the diffusion coefficient is easily interpreted in terms of the neglected drift-current components which under these conditions become comparable to the classical diffusion currents⁴².

2.2.4.2 Hybrid models

The hybrid models account for the electric field which arises as a result of the majority carrier modulation on the high resistivity side of a junction. The injected densities are still treated as primarily determined by the diffusion process. The field enters in to give the current, after the carrier densities have been fixed in terms of diffusion and the boundary conditions.

The field terms are neglected in (2.18), but they are retained in (1.1) and (1.2). With an ohmic contact situated at the end ($x=d_n$) of the n-neutral region of a p+n structure, and the voltage across the

junction barrier V_b , the current density is^{38,44,46}.

$$J = \frac{2 p_{no} \text{cth} \left(\frac{d_n}{L} \right)}{L} D_p \left(1 + \frac{p(O)}{p(O) + N_d} \right) (\exp(V_b/V_T) - 1). \quad (2.23)$$

From (1.1) and (1.2) the field in this region is

$$E = \frac{J}{q \mu_p ((b+1)p + bN_d)} - V_T \frac{b-1}{(b+1)p + bN_d} \frac{dp}{dx}, \quad (2.24)$$

producing the voltage drop across the bulk semiconductor region

$$V_n = \frac{JY}{q(b+1)\mu_p} - V_T \frac{b-1}{b+1} \ln \frac{(b+1)p(d_n) + bN_d}{(b+1)p(O) + bN_d}, \quad (2.25)$$

where

$$Y = \int_0^{d_n} \frac{b+1}{(b+1)p + bN_d} dx.$$

The total voltage or the V-I characteristic is now

$$V = V_b + V_n, \quad (2.26)$$

with V_b and V_n given by (2.23) and (2.25) respectively. The next step in generalizing (2.26) is the introduction of an arbitrary recombination velocity at the metal-semiconductor contact. The relations between the voltages and currents remain the same as in (2.23) and (2.25) except for the slight modifications of the multiplying coefficients^{39,43,51}.

High current densities could give rise to a significant voltage drop in the vicinity of the semiconductor-metal contact. The introduction of the effective recombination velocities at the edge of this

near-contact space charge region, $x=d'_n$ ($d'_n < d_n$), has been suggested⁵². This modifies (2.26) in that it now includes the voltage drop across this near contact region, V_m . In general, the limiting V-I characteristic is of the type⁵²

$$J = J_c \exp(V/c V_T), \quad (2.27)$$

where the parameters J_c and c are

	J_c	c
d'_n/L - small	$2qD_p(p_{no}N_d)^{1/2}/d'_n$	2
d'_n/L - large	$qD_p^2N_d \exp(2d'_n/L)/(4L^2S_p'(b+1))$	$bch(d'_n/L)/(b+1)$

and

$$S'_p = \frac{S_p \exp(V_m/V_T)}{1 + \frac{S_p}{D_p} \int_{d'_n}^{d_n} \exp\left(-\int_{d'_n}^x \frac{Edt}{V_T}\right) dx}.$$

At moderate levels the volume recombination dominates the conduction process. Further increase in current density leads to an enhancement of carrier recombination at the contact, with an asymptotic characteristic^{52,55} $I \propto V^2$.

2.2.4.3 Field-dominated models

The term "field-dominated" means that the densities of injected carriers are determined primarily by the applied field rather than by diffusion processes.

The conditions associated with this type of model could arise in several different structures. These are discussed in turn.

2.2.4.3.1 Thin junctions

The assumption (i) is further strengthened by adding the condition

$$\frac{dp}{dx} = \frac{dn}{dx} . \quad (2.28)$$

In the assumption (ii) rather large values for τ are assumed, which amounts to neglecting the recombination in the bulk, i.e. $U \cong 0$. (Conceptually this implies that, if the conductivity of a semiconductor region is to be significantly increased by injection of the charge carriers, the injected carriers should be able to penetrate most of the region before recombining^{45,46,56}).

With these additional simplifications a combination of the basic equations can be integrated, giving the relations between the current densities, electric field, electrostatic potential and carrier densities⁵⁶. The unique solution of the problem is obtained by fixing the carrier densities at the external contacts to their equilibrium values and relating them via Boltzmann factor at the edges of the space charge region. In the limit, when the diffusion barrier height disappears, the

current-voltage characteristic is

$$J = S^2(V-V_0)^2, \quad (2.29)$$

where V_0 is the "built-in" voltage and S^2 is a coefficient dependent upon the physical parameters of the junction. The character at this square-law dependence is identical with the asymptotic square characteristic obtained for the short pin structures^{52,55}.

2.2.4.3.2 Long-base junctions

The complete differential equation for the hole density (2.18), modified by using the weak form of (2.16) and (2.24), is

$$\frac{d^2 p}{dx^2} - \frac{JN_d}{2D_p(2p+N_d)((b+1)p+N_d b)} \frac{dp}{dx} + \frac{N_d(b-1)}{(2p+N_d)((b+1)p+N_d b)} \left(\frac{dp}{dx}\right)^2 - \frac{p-p_{no}}{L^2} = 0. \quad (2.30)$$

The analysis of the second and third terms in (2.30) shows⁴⁹ that after a distance x_1 , defined by

$$\frac{L N_d J}{qD_p(2p(x_1)+N_d)((b+1)p+N_d b)} = 1, \quad (2.31)$$

the second term is no longer negligibly small. Thus, if $p \gg N_d$, in $x > x_1$ (2.30) takes the form

$$\frac{d^2 p}{dx^2} - \frac{1}{L_i} \frac{dp}{dx} - \frac{p-p_{no}}{L^2} = 0, \quad (2.32)$$

where

$$\frac{1}{L_i} = \frac{1}{d_n - x_1} \int_{x_1}^{d_n} \frac{JN_d dx}{qD_p(2p+N_d)((b+1)p+N_d b)}. \quad (2.33)$$

With the Boltzmann boundary condition at the edge of the space charge region, $x=0$, and an ohmic contact at $x=d_n$, the asymptotic V-I characteristic (dominated by the voltage drop across x_1-d_n) is^{49,50}

$$J = \frac{qN_d L(b+1)\mu_p}{2V_T d_n^2} v^2. \quad (2.34)$$

2.2.4.3.3 Long p-i-n structures

In a near-intrinsic semiconductor, long compared to a diffusion length, the field-driven current regimes arise under the so-called double-injection conditions^{41,57}. Now $N \approx 0$ and n and p in (2.16) stand for the injected carrier densities.

From the complete differential equations for the carrier densities, (2.18) and its electron counterpart, it follows that

$$\frac{d}{dx}((p+n)E) - (n_0 - p_0) \frac{dE}{dx} + \frac{d^2}{dx^2}(p+n)V_T = \frac{(b+1)n}{\mu_n} = \frac{(b+1)p}{\mu_p}, \quad (2.35)$$

where the total charge carrier densities are expressed as the sums of the equilibrium, p_0 and n_0 , and the injected densities, p and n . The discussed diffusion models ignore the first two terms on the left-hand side of (2.35) and the field terms in (1.1) and (1.2). The hybrid models omit the field terms in (2.35) and later use (1.1) and (1.2) to compute $E(x)$. The field-driven current regimes are calculated neglecting the third term in (2.35) as well as the diffusion terms in (1.1) and (1.2). (The diffusion components are generally significant near the contacts,

but in a sample which is many diffusion lengths long the field terms are dominant over most of the sample).

By introducing the average value of the injected carriers $\bar{n}$ and the average electric field in the sample V/d , the total current density can be approximated by⁵⁷

$$J \cong q(b+1)\mu_p \bar{n} V/d, \quad (2.36)$$

since at high injections $p=n \gg p_0, n_0$.

In view of (2.16), in a reasonably extrinsic sample $|p-n| < |p_0 - n_0|$. From (2.35) is then^{57,130}

$$\bar{n} = \frac{\mu_n (n_0 - p_0) \tau}{b+1} \frac{V}{d^2}, \quad (2.37)$$

giving the final result

$$J = q \tau \mu_n \mu_p (n_0 - p_0) \frac{V^2}{d^3}. \quad (2.38)$$

It should be noted that this square-law regime is of different character to the asymptotic square-law regimes obtained with the hybrid models. At extremely high injections the V-I characteristic of long p-i-n structures goes over to a cube-law⁶¹.

The existence of the square-law V-I characteristic in many different structures gave the basis for speculating with the coefficients A and V_1 of the generalized relation^{58,59}

$$V = A(J)^{\frac{1}{2}} + V_1. \quad (2.39)$$

However, the expressions obtained for A and V_1 could not be interpreted in terms of the physical parameters of a junction.

2.2.5 Recombination currents

Measurements on actual diodes generally result, oppositely to (2.12), in a non-saturating current at moderate and large reverse biases (still not involving the process of multiplication). Also at small forward biases the current increases more slowly than that predicted by (2.12). These departures from the ideal theory, observable in silicon at room temperature⁶⁴ and in germanium at lower temperatures^{65,66}, are attributed to charge generation in the space charge region.

In the space charge region of a reversely biased p-n junction both types of carriers are rapidly swept out, giving the net generation rate (equation (1.17))

$$U = \frac{n_i^2}{p_1 \tau_{no} + n_1 \tau_{po}} \quad (2.40)$$

The reverse current due to this generation process is

$$J_{rg} = \frac{qn_i^2 w}{p_1 \tau_{no} + n_1 \tau_{po}} \quad (2.41)$$

Since w increases with reverse bias there is no true reverse saturation of current for the case where the space charge generation dominates reverse current.*

* For germanium at room temperature n_i is large enough for the saturation current of (2.12) to be dominant. However, at lower temperatures, and in silicon at room temperature, n_i is considerably smaller so that the current density of (2.41) plays a dominant role in determining the junction current.

At forward biases, when p and n exceed n_i , p_1 , and n_1 significantly, the upper limit for the current due to recombination in the space charge region is

$$J_{rg} = \frac{qn_i w}{\tau_{no} + \tau_{po}} \exp(V_a/2V_T). \quad (2.42)$$

An approximate expression for the generation-recombination current, which fits the limits (2.41) and (2.42) is⁶⁸

$$J_{rg} = \frac{qn_i^2 w (\exp(V_a/V_T) - 1)}{n_1 \tau_{po} + p_1 \tau_{no} + (\tau_{po} + \tau_{no}) n_i \exp(qV_a/2V_T)}. \quad (2.43)$$

Alternatively, J_{rg} can be computed approximately by postulating the potential distribution across the space charge layer in accordance with the impurity profile of the junction^{64,67,69}.

The total current density is given by the sum of (2.12) and (2.43). As the forward bias is increased the diffusion currents into the neutral regions increase faster than the recombination current in the barrier layer until the diffusion and recombination of carriers in the neutral regions becomes the essential conduction mechanism.

2.2.6 Properties of the transition region

The most common approximation in the analysis of the region of transition from p to n material is that of the space charge, or depletion, layer. The depletion layer concept is based upon an assumption that the electrostatic charge density is everywhere equal to the density of ionized impurity atoms; therefore the space charge region is

completely depleted of mobile holes and electrons.

This assumption eliminates from Poisson's equation the distribution terms for the mobile charge carriers, and thereby reduces the problem of analyzing the electrostatic potential distribution to a mathematically tractable differential equation. Since the form of the space charge distribution is assumed at the outset, Poisson's equation has the simple form

$$-\frac{d^2u}{dx^2} = \frac{dE}{dx} = q/\epsilon N(x). \quad (2.44)$$

Charge neutrality occurs when mobile charge carriers attain the spatial distribution required to reduce to zero the total charge, i.e.

$$N(x) = 2n_i \sinh(u(x)), \quad (2.45)$$

or upon differentiation

$$E(x) = V_T (4n_i^2 + N(x)^2)^{-\frac{1}{2}} \frac{dN(x)}{dx}. \quad (2.46)$$

Equation (2.46) gives the electrostatic field distribution within the neutral semiconductor due to an impurity distribution $N(x)$.

In the depletion region the electrostatic field is

$$E(x) = \frac{q}{\epsilon} \int N(x) dx + E_0. \quad (2.47)$$

The field values at the depletion layer boundaries are given by (2.46), thus

$$V_T ((4n_i^2 + N(x)^2)^{-\frac{1}{2}} \frac{dN(x)}{dx}) \Big|_{w_p}^{w_n} = \frac{q}{\epsilon} \int_{w_p}^{w_n} N(x) dx. \quad (2.48)$$

Upon assuming a given n-side depletion region width w_n , (2.48) provides a means of establishing w_p and thereby the total depletion region width.

Second integration of the impurity atom distribution yields the total junction potential

$$V = \frac{q}{\epsilon} \int_{w_p}^{w_n} dx \int_{w_p}^x N(t) dt = \frac{q}{\epsilon} \int_{w_p}^{w_n} xN(x) dx + E_o(w_n - w_p) + V_o. \quad (2.49)$$

The potential defined by (2.49) is conveniently represented as a sum of the "built-in" voltage V_o , resulting from the equilibrium distribution of uncompensated impurity atoms, and the voltage which results from an external biasing source. From (2.45) the "built-in" voltage is

$$V_o = V_T \ln \frac{(N(w_p) + (N^2(w_p) + 4n_i^2)^{1/2})(N(w_n) + (N^2(w_n) + 4n_i^2)^{1/2})}{4n_i^2}, \quad (2.50)$$

which for reasonably extrinsic semiconductors reduces to the familiar formula

$$V_o = V_T \ln \frac{N(w_p)N(w_n)}{n_i^2}. \quad (2.51)$$

2.2.6.1 Space-charge capacitance

The interrelation between the depletion layer width and an externally applied bias through (2.48) and (2.49) indicates that there is a voltage dependent charge associated with the depletion layer. It is thus possible to introduce the concept of the space-charge capacitance

$$C = \left| \frac{dQ}{dV} \right|, \quad (2.52)$$

where Q is the result of carrying out the integration in (2.47) from the

metallurgical junction up to one of the depletion layer edges, and V is the voltage given by (2.49).

This part of the total junction capacitance is dominant at reverse and small forward voltages. At moderate and high injections the contribution, to the total capacitance, of the component which arises due to storage of the minority carriers in the neutral regions prevails¹⁰⁹. It was initially derived for the simplest cases of abrupt and linearly graded junctions³², and later generalized to an arbitrary impurity profile^{78,79,80}, that the a.c. per-unit-area capacitance defined by (2.52) is the same as the capacitance of metal plates spaced apart by the depletion layer width with the semiconductor as dielectric material.

In view of the significance of the impurity diffusion process in making p-n junction devices, the Gaussian and complementary error functions (assumed to result from the diffusion processes¹³²) have received a considerable attention. The efforts are made in both, numerical⁷¹⁻⁷⁷ and analytical⁷⁷ treatments of the simplified Poisson's equation to show that a diffused structure can be approximated by the combination of the properties attributed to a step- and a linearly graded junction.

Complete depletion of the mobile charge carriers and consequently absence of any current flow give a high degree of mathematical simplicity, but introduce serious limitations to the applicability of the results obtained by this type of analysis. Theoretical improvements of the depletion layer analysis are attempted by introducing an approximate

contribution of the mobile charge carriers to the properties of the transition region^{70,109,110,112}. The junction current is still neglected and the mobile charge carrier distributions are obtained from an assumed potential distribution in the transition layer, analogously to the approximate analysis of the generation-recombination currents^{64,67,69}. The results of this analysis at medium and large reverse voltages showed^{133,134} that determination of the junction barrier height on the basis of the capacitance measurements could be significantly in error if the measurements are interpreted in terms of the simple depletion theory.

At moderate and high forward biases, or in reverse biased junctions in the presence of collected current, the current densities could be considerable and the space charge layer becomes densely populated with the mobile charge carriers. Several attempts to analyze the conditions that exist in the transition region of a junction under non-zero current conditions have been made^{81,82,116,117}. All of them, however, had to rely on various other simplifying assumptions, thus producing the results which are more qualitative than accurate. A comprehensive solution of the problem requires a full treatment of the basic system.

2.2.7 Reverse breakdown

The voltage saturated reverse characteristic, reverse breakdown, of a p-n junction, which occurs when the electric field in a junction becomes too large, can not be explained on the basis of the currents derived so far.

The physical phenomena which can give rise to reverse breakdown are either the effect of avalanche multiplication or Zener effect. Zener breakdown results when the electric field in the space charge region is sufficiently high to cause direct excitations from the valence to the conduction band. Avalanche breakdown occurs when the charge carriers acquire sufficient kinetic energy between collisions to cause ionizing collisions. Since the hole and electron produced by such a collision each have a finite probability of making a further ionizing collision, this type of breakdown is usually referred to as avalanche multiplication.

Zener breakdown occurs in very highly doped junctions where the space charge layer is too narrow for avalanche multiplication to occur. The mechanism of carrier multiplication requires significantly less electric fields and it occurs in wider, consequently less heavily doped, junctions. In most p-n junction devices the breakdown is caused by the avalanche effect.

The subject of reverse breakdown is a separate field of study beyond the scope of this work. The only quantity relevant to the present analysis is the electric field at which the carrier multiplication becomes pronounced, E_b . Its relation to the doping density is

calculated by^{86,87}

$$E_b = \left(H \frac{8\pi q}{\epsilon} N^{1-a} \right)^{\frac{1}{2}}, \quad (2.53)$$

where the empirically derived constants H and a , for germanium and silicon, are given in Table 4.

Table 4

	H	a
G_e	10^{13}	0.725
S_i	3.10^{13}	0.750

The electric fields associated with the solutions of the basic system (or any of its simplified forms) must not exceed the limit defined by (2.53).

2.3 Transient analysis

The study of transient behaviour of p-n junctions deals with the time dependent charge carrier densities, voltages and currents. Hence, the basic system (1.1)-(1.5) remains complete and must be treated as a set of partial differential equations.

Two principal phenomena are of interest: the forward and reverse transients. The analyses of both of these rely upon the simplifications very similar to those discussed in connection with the

steady-state analysis. This is shown in the next two sections of this chapter.

2.3.1 Forward transient

Under the low-level conditions specified by (2.6)-(2.10), the time dependent hole density in a neutral n-region of a highly asymmetrical junction is

$$\frac{\partial^2 p}{\partial \lambda^2} - p = \frac{\partial p}{\partial r}, \quad (2.54)$$

where $\lambda = x/L_p$ and $r = t/\tau_p$ are the normalized distance and time.

Using (2.12) as the final condition after the application of a constant current step J_p , the solution of (2.54), subject to the conditions

$$p(\lambda, 0) = 0, \quad (2.55a)$$

$$p(\infty, r) = 0, \quad (2.55b)$$

$$p(0, \infty) = p_n (\exp(V/V_T) - 1), \quad (2.55c)$$

$$J_f = - \frac{qD_p}{L_p} \left(\frac{\partial p}{\partial \lambda} \right)_{\lambda=0}, \quad (2.55d)$$

is^{83,88}

$$p(\lambda, r) = p(0, \infty) S(\lambda, r), \quad (2.56)$$

where

$$S(\lambda, r) = -\text{sh}(\lambda) \text{erfc}\left(\frac{\lambda}{2r^{1/2}} - r^{1/2}\right). \quad (2.57)$$

The transient V-I characteristic is obtained by representing the total voltage as the sum of the junction voltage and the ohmic drop

across the bulk (analogously to the high-level steady-state hybrid models), i.e.

$$V(r) = V_T \ln(1 + \frac{J_f}{J_s} \operatorname{erf}(r^{1/2})) + J_f R_o (1 - \frac{L}{d_n} \ln(1 + \frac{(b+1) \operatorname{erf}(r^{1/2})}{p_{no} + b n_{no}})), \quad (2.58)$$

where $R_o = 1 / (A_{ip} (b n_{no} + p_{no}))$.

The more general case of switching at an arbitrary current level was tackled numerically by Kano and Reich⁸⁹. However, they facilitated the analysis by assuming the previously discussed high-level neutrality conditions, eqns.(2.16) and (2.28). Nevertheless, it was possible to observe from their solutions, that an essentially capacitive low-level behaviour of a junction⁸⁸ becomes inductive at high-current forward switching^{89,135}.

2.3.2 Reverse transient

The phenomena of carrier injection and consequent conductivity modulation make it possible for a large reverse current to flow after a junction is switched from forward to reverse bias⁹⁰⁻⁹³. The complete transient is usually separated into two phases: constant current phase during which the reverse current is limited by the external resistance, and the decay phase when the current reduces at the rate determined by the minority carrier lifetime and the junction geometry.

The assumptions defining the low-level conditions are again the stepping stones for the analysis.

After a finite forward conduction, r_f , the initial condition for the hole density is

$$p(\lambda, 0) = \frac{J_f L_p}{qD_p} S(\lambda, r_f). \quad (2.59a)$$

The boundary conditions are

$$p(\infty, r) = 0, \quad (2.59b)$$

$$p(0, r) = p_{no} (\exp(V/V_T) - 1), \quad (2.59c)$$

$$J_{ro} = \frac{qD_p}{L_p} \left(\frac{\partial p}{\partial \lambda} \right)_{\lambda=0}. \quad (2.59d)$$

At the end of the recovery phase, $r=r_a$,

$$V(r_a) = 0. \quad (2.59e)$$

During the recovery phase the junction voltage is^{84,85,94}

$$V(r) = V_T \ln \left(1 + \frac{J_f}{J_s} \operatorname{erf} \left((r_f + r)^{\frac{1}{2}} \right) - \frac{J_f}{J_s} \left(1 + \frac{J_{ro}}{J_f} \right) \operatorname{erf} \left(r^{\frac{1}{2}} \right) \right). \quad (2.60)$$

If $r_f \rightarrow \infty$ (2.60) reduces to the familiar result obtained in the analysis of the reverse switching after a stationary forward conduction⁹⁵⁻⁹⁹

$$\operatorname{erf}(r_a) = \frac{1}{1 + J_{ro}/J_f}. \quad (2.61)$$

During the current decay phase the V-I characteristic is much more complicated^{94,136}. If the additional simplification $p(0, r) = 0$ is introduced, the current density as a function of time is¹⁰⁰

$$J(r) = J_f \left(\frac{J_{ro}}{J_f} + \frac{2}{\pi} (S_1(r_f + r_a, r) - (1 + J_{ro}/J_f) S_1(r_f, r)) \right), \quad (2.62)$$

where

$$S_1(r_1, r_2) = \int_0^{(r_1/r_2)^{\frac{1}{2}}} \frac{\exp(-r_1(y^2 + 1))}{y^2 + 1} dy. \quad (2.63)$$

Numerical evaluation of S_1 is possible in terms of the relatively rapidly convergent series¹⁰⁰.

A treatment of the reverse transients in graded junctions is further complicated by the presence of the field terms in the governing equations. The models implying pure diffusion are obviously inadequate.

The available solutions^{101,102} have been restricted to the exponential type grading. By postulating that the electric field in (1.1) and (1.2) comes exclusively from the impurity grading, the time dependent equation (2.54) is enlarged by adding the corresponding constant field term. The solutions are then obtained, subject to the usual assumptions concerning the low-levels and highly asymmetrical doping.

2.4 Conclusions

Analytical models for charge carrier transport in semiconductor junctions have been analyzed. A classification of each available model has been carried out by estimating its degree of applicability with respect to the set of governing equations formulated in chapter 1.

There are two essentially different types of model, one neglecting space charge and the other exclusively concerned with it. The

interrelations between models of one type have been clarified.

The most successful and the most widespread is the low-level neutral model. It is asymptotic on the low-current side where the disturbance of the equilibrium is very small. The range of its validity on the high-current side is uncertain. A generalization of the model to cover a full current range is impossible without a change in the basic philosophy of the approach.

The position is far less clear cut at high-currents, where there exists a multitude of models. Each of them accounts for a specific set of observations, but does not reflect the physical processes embraced in the basic model. Since simplifying assumptions must be made at the outset of any high-current analysis, it does not seem possible to extend any of these models to an all-embracing (high- and low-current) neutral model.

As in the case of the low-level neutral model, the space charge model is current-limited. Its extensions into the high current range are heuristic and do not provide a sound basis for any significant generalizations.

The analyses of transients in p-n junctions suffer from the identical drawbacks of the steady-state case. The theoretical possibility that the general steady state solution could be obtained as a special case of the general transient solution is thus very remote indeed.

CHAPTER 3

NUMERICAL TREATMENT OF P-N JUNCTIONTRANSPORT EQUATIONS3.1 Introduction

Analytical treatments of equations (1.1)-(1.5) were analyzed in Chapter 2. It was shown that, under certain conditions, an analytical approach can give some useful results, but a general solution of the problem cannot be obtained using known analytical functions.

Numerical methods, with the aid of digital computers, represent an alternative approach to the problem. Several types of numerical solutions are available at present. In many of them, however, there are serious limitations due to the various approximations applied to the fundamental equations. The drawbacks which reduce the generality of these solutions could be summarized as follows: space charge neutrality, constant mobilities, and linear recombination with a constant lifetime of injected carriers were introduced by Lieb et al.⁶², Kano and Reich⁸⁹, and Van der Maesen et al.¹³¹; space charge neutrality and constant mobilities were assumed by Fulkerson and Nussbaum¹¹³; linear recombination and constant mobilities enter in Nussbaum's⁶³ model; Sanchez computes his solutions¹³⁷ assuming constant mobilities. The iterative procedure proposed by Gummel¹⁰⁵ is free of these drawbacks. The linearized Poisson's equation with the expressions for the quasi-

Fermi potentials supplies the information equivalent to the solution of the problem as formulated by equations (1.1)-(1.5). The reverse transformations convert the computed quasi-potentials to the physical variables defined in Chapter 1. However, for a large potential variation, like the one that exists in a reverse biased junction, Gummel's formulation encounters the computation of very large, and very small, exponential functions which invariably leads to numerical difficulties. A straightforward correspondence between the physical phenomena in the interior of a device and the physical variables in (1.1)-(1.5) makes highly attractive a formulation of an algorithm for direct computation of these variables. Such an algorithm^{138,139} is described in this chapter.

Before proceeding further, it should be pointed out that the numerical treatment of the equations (1.1)-(1.5) involves additional difficulties, since with these equations, the solutions obtained applying direct numerical procedures, such as Runge-Kutta or predictor-corrector methods, diverge rapidly from the desired solutions³⁰. An illustration of this property of the basic equations, which is called stiffness, is given in Appendix 2. By performing some preliminary integrations in the basic system, and introducing an auxiliary variable this additional difficulty is partly overcome in the following method.

3.2 Preliminary integrations

It is convenient to rewrite the equations (1.1) and (1.2) in the form

$$\frac{dp}{dx} - \frac{pE}{V_T} + \frac{J_p}{qD_p} = 0, \quad (3.1)$$

$$\frac{dn}{dx} + \frac{nE}{V_T} - \frac{J_n}{qD_n} = 0. \quad (3.2)$$

Note that (3.1) and (3.2) could be considered to be first order linear differential equations for p and n respectively, with the nonconstant coefficients $\frac{E}{V_T}$, $\frac{J_p}{qD_p}$, and $\frac{J_n}{qD_n}$.

The first order equation of the type

$$y' + f(x)y + q(x) = 0 \quad (3.3)$$

has the general solution¹

$$y = \exp\left(-\int f(x)dx\right)\left(y_0 - \int q(x)\exp\left(\int f(x)dx\right)dx\right), \quad (3.4)$$

where y_0 denotes an arbitrary constant. Equation (3.4) is a valid solution of (3.1) and (3.2) if the nonconstant coefficients $\frac{E}{V_T}$, $\frac{J_p}{qD_p}$, and $\frac{J_n}{qD_n}$ are some explicit functions of the independent variable x . For the purpose of the numerical computations this is indeed the case*, and the solutions for (3.1) and (3.2) can be written readily as

* Any numerical integration routine can be replaced by Taylor series representation of the corresponding functions, thereby treating them as explicit functions of the independent variable.

$$p(x) = \exp\left(\int \frac{E}{V_T} dt\right) \left(A - \int \frac{\exp\left(-\int \frac{E}{V_T} dt\right)}{qD_p(t)} J_p dt\right), \quad (3.5)$$

$$n(x) = \exp\left(-\int \frac{E}{V_T} dt\right) \left(B + \int \frac{\exp\left(\int \frac{E}{V_T} dt\right)}{qD_n(t)} J_n dt\right), \quad (3.6)$$

The integrations which are not under the exp sign must be performed numerically since the functions J_p/qD_p and J_n/qD_n are not known explicitly. The variation of the diffusivities with doping and the electrostatic field, discussed in Chapter 1, is expressed in (3.5) and (3.6) by writing D_p and D_n as the functions of the independent variable. The values of the integration constants, A and B, depend upon the reference potential level, and in any particular case they have to be determined in conjunction with Poisson's equation or some equivalent expression governing the potential distribution.

The mobile charge carrier densities are thus expressed in terms of the diffusivities, the electrostatic field (or in view of (1.7) the electrostatic potential), and the current densities.

3.2.1 . The electrostatic field equation

Treatment of Poisson's equation is based upon the well known result from the theory of differential equations¹ that for any second order equation of the type

$$y'' = F(y, y') \quad (3.7)$$

(i.e. the independent variable does not appear on the right hand side) the first integral can always be found analytically. In Poisson's equation the independent variable does not appear on the right hand side if an appropriate average value $\bar{N}$ is introduced for the doping profile. This indicates that by employing $\bar{N}$ the first integral of (1.5) can be obtained analytically. To show that this is indeed the case Poisson's equation requires rearrangement.

Multiplication of (1.5) by E , after local charge density is expressed by (1.6), gives

$$E \frac{dE}{dx} = \frac{q}{\epsilon} (pE - nE + NE). \quad (3.8)$$

The diffusion-drift equations, (1.1) and (1.2), can be used to express the products pE and nE as functions of the mobile charge carrier density gradients and the current densities, i.e.

$$pE = \left(\frac{J_p}{qD_p} + \frac{dp}{dx} \right) V_T, \quad (3.9)$$

$$nE = \left(\frac{J_n}{qD_n} - \frac{dn}{dx} \right) V_T. \quad (3.10)$$

Combining (3.8)-(3.10) results in the expression

$$EdE = \frac{qV_T}{\epsilon} \left(dp + dn + \frac{J_p}{qD_p} - \frac{J_n}{qD_n} dx + N \frac{E}{V_T} dx \right), \quad (3.11)$$

which, provided the term containing the electrostatic field on the right hand side can be eliminated, is integrated once to obtain the electrostatic field as a function of the charge carrier densities, current

densities and distance.

In an interval $x_0, x_0 + \delta x$ the integral of (3.11) is

$$E(x) = \pm \left[E(x_0)^2 + \frac{2qV_T}{\epsilon} (p(x) - p(x_0) + n(x) - n(x_0)) + \int_{x_0}^x \frac{J_p}{qD_p} dx - \int_{x_0}^x \frac{J_n}{qD_n} dx + \right. \\ \left. + \bar{N} \int_{x_0}^x \frac{E}{V_T} dx \right]^{\frac{1}{2}}, \quad (3.12)$$

where $\bar{N}$ stands for the mean value of doping in the interval of integration and $E(x_0)$ is the arbitrary constant of integration. The sign before the square root is determined by the general behaviour of the electrostatic potential function. The equation (3.12) is exact for uniform distributions of impurities only. Otherwise it is approximate and its use is confined to small intervals δx .

The right hand sides of the expressions derived so far, (3.5), (3.6) and (3.12), all contain the term $\int \frac{E}{V_T} dx$. This suggests that, instead of trying to eliminate it from (3.12), it may be profitable to treat this term as an auxiliary variable. Of course, the interrelation between this and the original variable, distance, must be known. It turns out that in this case that relation is not analytic. However, with the help of a suitable algorithm for evaluating the ratio of the two variables numerically, the above idea could still be followed.

So far the original equations have been reduced to an equivalent set of three, eqns. (3.5), (3.6), and (3.12), in which the mobile charge carriers and the electrostatic field are expressed in terms of diffusivities, the electrostatic potential, and the current densities.

With the aid of the two continuity equations, (1.3) and (1.4), the current densities may be expressed through appropriate boundary conditions for the charge carriers, the generation-recombination law, and the electrostatic potential. This is shown in Chapter 5. The remaining part of this chapter is devoted to the problem of defining a convenient auxiliary variable and its introduction into the reduced set of equations in form which is suitable for machine calculations. The current densities are assumed to be solenoidal.

3.3 Auxiliary variable

Consider the equations (3.5), (3.6), and (3.12) in a semi-open interval $[x_0, x)$. Following the discussion of the previous section, define the quantity $e(x)$

$$e(x) = \exp\left(\int_{x_0}^x \frac{E}{V_T} dt\right). \quad (3.13)$$

As indicated previously, the choice of the reference potential level determines the integration constants in (3.5) and (3.6). Denote by x_0 the point at which the potential is set to zero. Then,

$$A = p(x_0),$$

$$B = n(x_0).$$

Using the definition (3.13), the reduced equations become

$$p(x) = p(x_0)e(x) - e(x) \int_{x_0}^x \frac{J_p}{e(t)qD_p(t)} dt, \quad (3.14)$$

$$n(x) = n(x_0) \frac{1}{e(x)} + \frac{1}{e(x)} \int_{x_0}^x e(t) \frac{J_n}{qD_n(t)} dt, \quad (3.15)$$

$$E(x) = \pm \left[E(x_0)^2 + \frac{2qV_T}{\epsilon} (p(x) - p(x_0) + n(x) - n(x_0)) + \int_{x_0}^x \left(\frac{J_p}{qD_p(t)} - \frac{J_n}{qD_n(t)} \right) dt + \bar{N} \ln e(x) \right]^{\frac{1}{2}}. \quad (3.16)$$

Having chosen a point x_0 as the reference, the equations (3.13)-(3.16) define the quantities p , n , and E at an arbitrary point in space. However, the integrations indicated in these equations can only be carried out numerically.

From (3.13) it follows that

$$\delta x = \frac{V_T \ln e_0}{\bar{E}(x_0)}, \quad (3.17)$$

where $\bar{E}(x_0)$ is the mean value of $E(x)$ in δx , and $e_0 = e(x_0 + \delta x)$. Finding the relation between the auxiliary variable e and the distance thus depends upon finding the mean value of the electrostatic field in δx . Since δx is a small increment in the space coordinate, e_0 is always close to unity. This permits some simplifications to be introduced while deriving the relations between e_0 and p, n and E at $x_0 + \delta x$.

Because of the small variation of e in δx , for all practical purposes it can be replaced by its mean in δx . Consequently, $e(x)$ and $1/e(x)$ in the integrands of (3.14) and (3.15) are replaced by their respective average values (the average value of a quantity will simply

imply taking its arithmetic mean in a given space interval, unless specified otherwise). If, in addition, the variations of the diffusivities are calculated stepwise (i.e. they are treated as constants within each interval δx) the equations (3.14) and (3.16) become

$$p(x_0 + \delta x) = p(x_0) e_0 - \frac{J_p (1+e_0) \delta x}{2qD_p(N(x_0), E(x_0))} \quad , \quad (3.18)$$

$$n(x_0 + \delta x) = n(x_0) / e_0 + \frac{J_n (1+e_0) \delta x}{2qe_0 D_n(N(x_0), E(x_0))} \quad , \quad (3.19)$$

$$E(x_0 + \delta x) = \pm \left[E(x_0)^2 + \frac{2qV_T}{\epsilon} (p(x_0)(e_0 - 1) + n(x_0)(1 - e_0)/e_0 + A_{p1} w_1 \delta x + A_{n2} w_2 \delta x + \bar{N} \ln e_0) \right]^{\frac{1}{2}} \quad , \quad (3.20)$$

where the following abbreviations have been introduced

$$w_1 = \frac{1-e_0}{2} \quad , \quad w_2 = \frac{1-e_0}{2e_0} \quad , \quad A_{p,n} = \frac{J_{p,n}}{qD_{p,n}(N(x_0), E(x_0))} \quad .$$

Once the value of e_0 is selected, the set of equations (3.17)-(3.20) determines the values of the dependent variables p, n , and E at $x_0 + \delta x$, given the values of these quantities at the point x_0 . At each step e_0 can be adjusted, thus giving a continual control over the step-length δx .

3.4 Local iteration loop

To calculate the charge carrier densities and the electrostatic field using the equations of the previous section, the mean value of the electrostatic field in (3.17) must be known. This introduces some additional computations, since at every step $\bar{E}$ will have to be

evaluated.

The algorithm which defines an iterative procedure for evaluating $\bar{E}$, called the local iteration loop, can be formulated as follows: assume certain value $\bar{E} = E_1$. From (3.17) the first estimate of δx , δx_1 , is readily obtainable. With this δx_1 from (3.18)-(3.20) the corresponding estimates of p , n , and E at $x_0 + \delta x$ are determined. The value $E(x_0 + \delta x_1)$ is now used to define a better approximation for $\bar{E}$ by forming a simple arithmetic mean, i.e.

$$E_{i+1} = \frac{1}{2}(E(x_0) + E(x_0 + \delta x_i)), \quad (3.21)$$

where $i=1$ at the end of the first local iteration cycle. Using this improved approximation for $\bar{E}$ the computation of p , n , and E is repeated and the new values compared with those computed in the previous loop. The whole process is repeated until this comparison shows that the differences between the values of p , n , and E computed in two successive loops indicate the required accuracy. The last estimates are then taken to be the values of the dependent variables at $x_0 + \delta x$ and the calculations for the next step can follow.

It is immediately clear that the required number of local iterations depends upon the initial guess E_1 . The computations are normally initiated by taking for the first guess of $\bar{E}$ the value of the electrostatic field $E(x_0)$. Of course, if the computations start from a zero-field point, or cross through a zero-field point, the precautions must be taken to ensure that the denominator of (3.17) never becomes zero.

The flow-chart of the above algorithm is shown in Fig. 3.1.

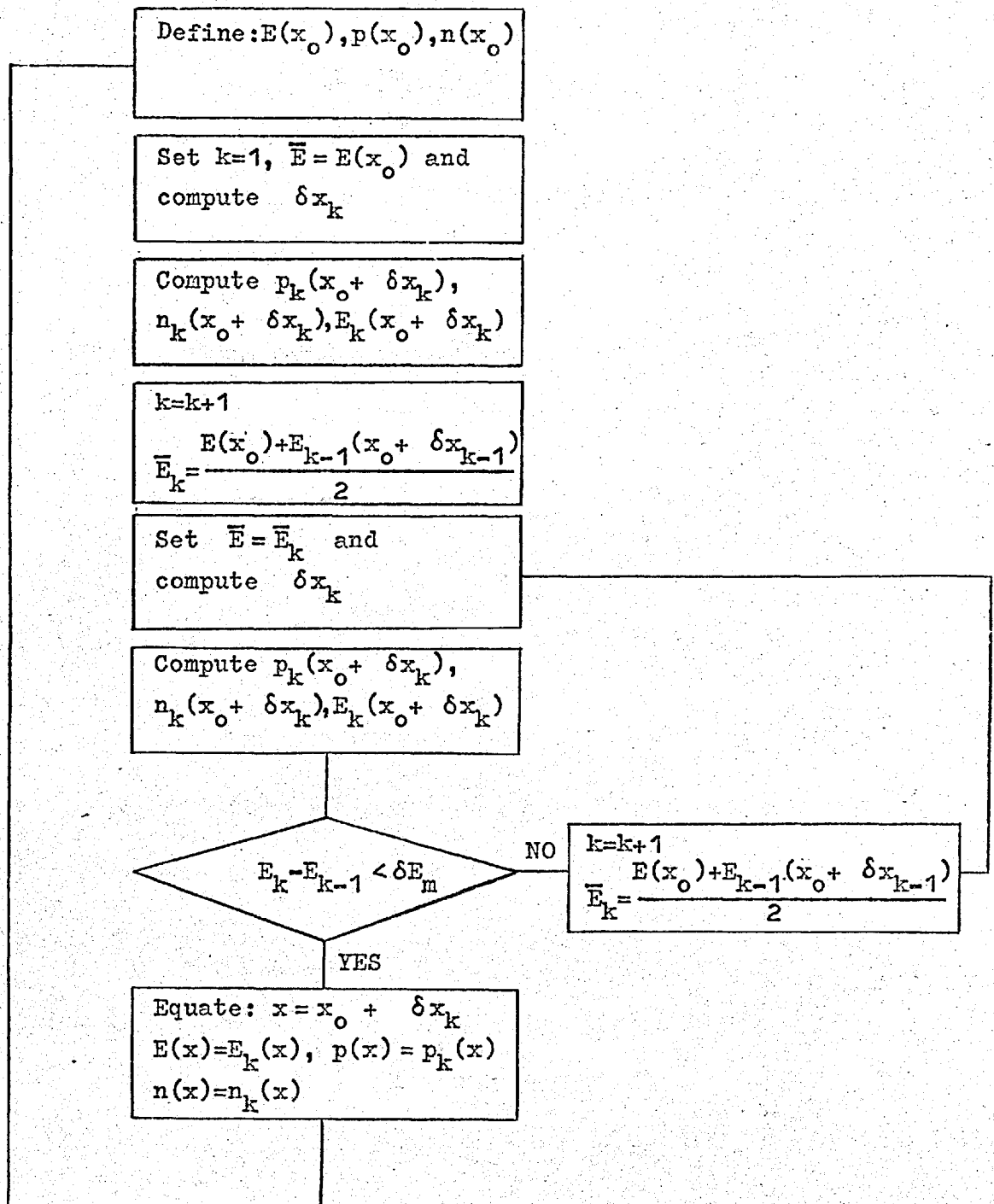


Fig.3.1

A complete procedure for practical calculations would always involve a more complicated flow-chart, but the one shown in Fig. 3.1 describes the main loop which is always present in all computations that involve the local iteration loop.

3.5 The over-all iteration loop

Two major difficulties arise in solving the p-n junction problem. The first one, as pointed out at the beginning of this chapter and illustrated in Appendix 2, is the stiffness of the solutions. The iterative procedure of the previous section allows computing the convergent solutions with the precision fixed by the preassigned accuracy of the local iteration loop. The second difficulty is establishing a self-consistent set of initial values. An over-all iterative scheme for solving this problem is suggested in this section. (The alternative approach, whereby the boundary values rather than initial values are specified for the p-n junction problem, is described in Chapter 5.)

The outline of the iterative scheme is given here considering the general form of Poisson's equation. In terms of the electrostatic potential, Poisson's equation is

$$\frac{d^2 u}{dx^2} = F(x, u), \quad (3.22)$$

where $F(x, u)$ stands for the negative local space charge. (This form is

obtainable through the use of (3.5) and (3.6).) In a given structure the potentials at the structural end points, $x=a$ and $x=b$, could be specified as $u(a)=u_a$ and $u(b)=u_b$, say. This defines a nonlinear two-point boundary value problem.

However, it is theoretically always possible to reduce the solution of a boundary value problem to the solution of a sequence of initial value problems. Let $u(x, -E_a)$ denote the solution of the initial value problem resulting from the above problem by replacing the condition for $u(b)$ by the condition $u'(a)=-E_a$, where E_a is a parameter. The discussed boundary value problem is then equivalent to solving the (in general nonlinear) equation $u(b, -E_a)=u_b$ for E_a . Each evaluation of $u(x, -E_a)$ requires the solution of an initial value problem. This is a so called "shooting" technique²⁴. The problem of computing the solutions for a junction structure involves the system of equations, but the concept of generation of the sequence of initial value problems formulated for Poisson's equation applies to this system, since the relations (3.5) and (3.6) express the relationships between u , and p and n .

A physically meaningful solution of this problem can be taken for granted on the ground that no matter how the fixed charge density $N(x)$ varies with position, the mobile charge carriers should be able to distribute themselves so that a steady-state equilibrium is produced. Formally, the unique solution of the problem is guaranteed by the Cauchy-Lipschitz theorem (e.g. ref. 24, p.15) provided F is continuous and $\partial F/\partial u$ is bounded in the strip (a,b) . Details as regards $\partial F/\partial u$ are

elaborated in Chapter 5. For the present purposes it will suffice to assume that the above conditions are satisfied in the physical systems studied in this work.

It was shown by Morgan and Smits³⁰ that due to the stiffness of the original equations, the errors made in specifying a set of initial values grow monotonically as the integration progresses, until one or all of the dependent variables violate the criteria which define the self-consistent behaviour of the solutions. This property of the basic equations ensures that, when solving the p-n junction problem by generating a sequence of initial value problems, it is not always necessary to perform the integration over the full length of an investigated structure. It will suffice to stop at the point at which at least one of the consistency-defining criteria is violated. The initial guesses are then corrected in conjunction with the type of divergence.

In a p-n junction structure it is usually possible to sketch the behaviour of at least one of the physical variables determining its state. For example, in an abrupt junction it can be specified that the absolute value of the electrostatic field has a maximum at the metallurgical junction, and reduces monotonically towards the bulk of both sides of the junction. In very simple structures it may be possible to sketch the behaviour of all of the variables involved. In more complicated cases these general assumptions may not be obvious, and obtaining some of them may only be possible after careful physical considerations. A practical implementation of this technique of specifying the over-all

behaviour of the solutions and relating it to the corresponding set of initial values is described in the following chapter.

CHAPTER 4

NUMERICAL ANALYSIS OF UNIFORM-BASE

TRANSISTOR STRUCTURES

4.1 Introduction

The iterative scheme described at the end of the previous chapter is applied here to the structure at a uniform-base pnp transistor. The solutions are calculated for the charge carrier densities and the electrostatic field over a range of operating conditions.

The developed numerical procedure solves the 'reverse' problem: a current density through the structure is specified first and then the applied voltages together with the relevant distributions are determined. From consideration of the structure as a two-port, it is evident that the solution at this problem is not unique. A set of solutions is thus obtained for each assumed current density. These are then related to the different biasing voltages which could give rise to the assumed current.

4.2 Strategy of the method

It was found expedient to treat separately the regions of the structure which have different impurity contents. Further

divisions of these uniform regions into sections have also been carried out in order to assist the computations. The complete solutions are obtained by matching the sectional solutions at the corresponding boundaries.

A sketch of the investigated structure is shown in Fig. 4.1. The sections are separated by the dotted lines and numbered. The lengths of the uniformly doped regions, and consequently those of the sections, are not fixed at the outset of the computations. Instead, for a selected doping pattern, they are calculated as functions of the applied biases. A complete transistor structure is synthesized by fixing the lengths of these 'building blocks' through matching the solutions at their boundaries. The numbering sequence in Fig. 4.1 coincides with the order in which the sections are calculated.

4.3 Self-consistent behaviour of the solutions in a p^+ collector

The assumptions concerning the self-consistent behaviour of the solutions in a uniformly doped p^+ collector are relatively straightforward. They are formulated below, assuming that the metal-semiconductor contacts of the device are characterized by an infinite recombination rate:

- (a) The state of a heavily doped collector region, in so far as the majority carriers are concerned, cannot be significantly perturbed by the usual collector-base biases. Change of the equilibrium state is concentrated to the vicinity of the impurity transition. Out in the bulk, however, the distribution remains practically unchanged.

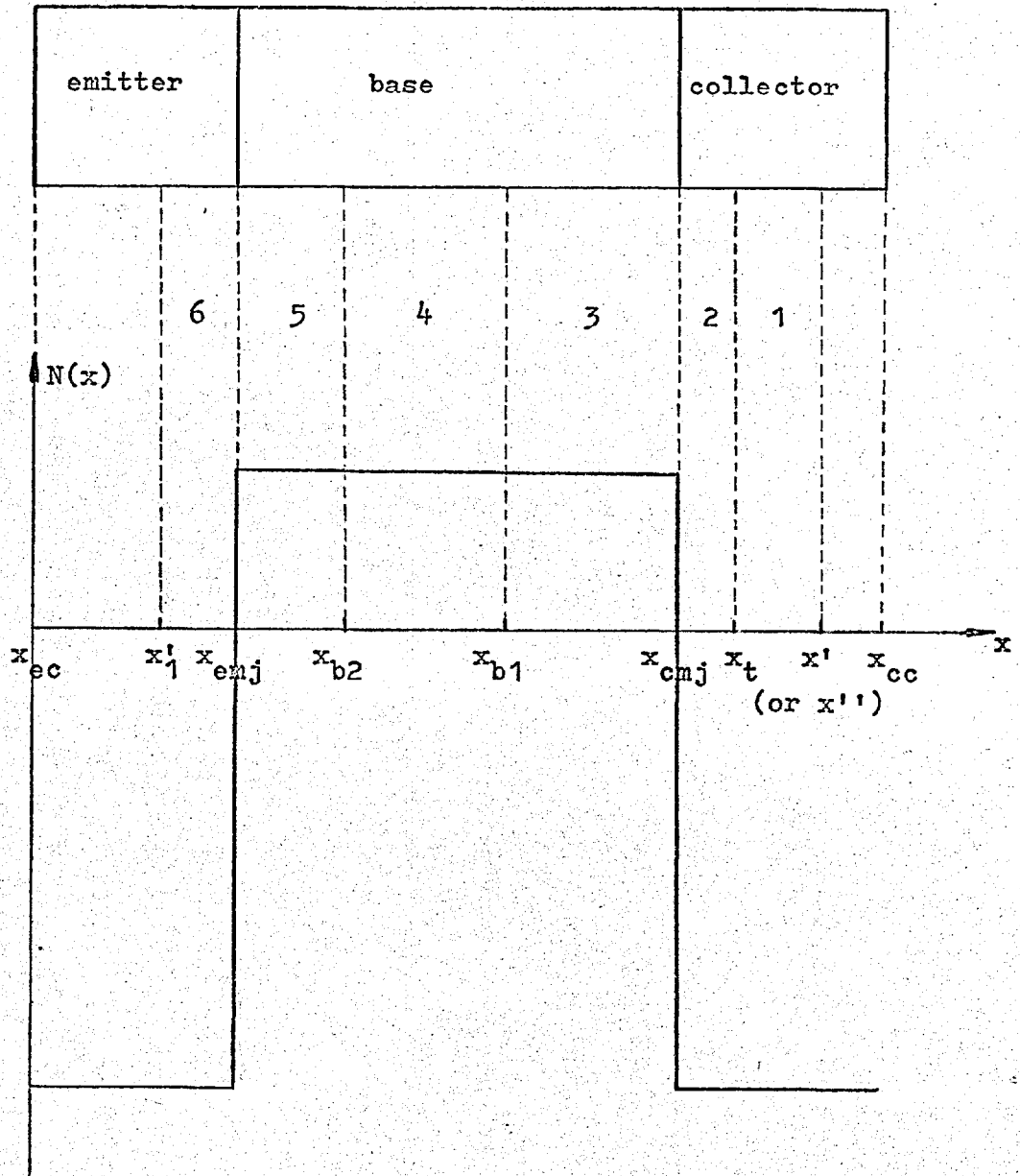


Fig.4.1

Consequently, the majority carrier distribution increases monotonically from the metallurgical junction converging towards its thermal equilibrium value at the collector external contact;

(b) variation of the electrostatic field, governed by the local space charge, is closely related to the behaviour of the more abundant charge carriers. Since they approach the original equilibrium state progressing away from the metallurgical junction, the electrostatic field distribution reduces monotonically from large value in the vicinity of the metallurgical junction to a limiting value E_{drift} in the bulk;

(c) the third junction variable, the electron density, is considerably suppressed compared to the equilibrium state. It eventually reaches the equilibrium state at the external contact, but its contribution to the properties of the collector region is generally quite negligible. Therefore, to a very good approximation the minority carrier density and its gradient can be completely neglected* ;

(d) the minority carrier current density is negligibly small.

This follows from (c).

The assumption (a) is conveniently expressed in terms of the

* It should be noted that, owing to a finite precision available on a digital computer, the minority carrier density is automatically neglected in all expressions involving *sums and differences of* both the majority and minority carriers.

following inequalities:

$$p \leq p_{po} , \quad (4.1a)$$

$$\frac{dp}{dx} \geq 0 , \quad (4.1b)$$

$$\frac{d^2 p}{dx^2} \leq 0 , \quad (4.1c)$$

for all $x_{cmj} \leq x \leq x_{cc}$. Here p_{po} stands for the hole density in the p^+ bulk, eqn.(2.1b).

The corresponding mathematical representation of the assumption (b) is

$$E \geq E_{drift} , \quad (4.2a)$$

$$\frac{dE}{dx} \leq 0 , \quad (4.2b)$$

$$\frac{d^2 E}{dx^2} \geq 0 . \quad (4.2c)$$

The limit E_{drift} denotes the electrostatic field that would exist in the bulk when (4.1) and (4.2) are reduced to the limiting equalities, $E_{drift} = J_p / (q\mu_p p_{po})$.

The assumptions (c) and (d) eliminate the eqn.(3.19) and simplify (3.20). The set of equations of the p^+ collector region thus reduces to

$$\delta x = \frac{V_T \ln e_o}{\bar{E}} , \quad (4.3)$$

$$p(x_o + \delta x) = p(x_o) e_o - \frac{J_p (1 + e_o) \delta x}{2qD_p (N(x_o), E(x_o))} , \quad (4.4)$$

$$E(x_0 + \delta x) = \pm (E(x_0)^2 + \frac{2qV_T}{\epsilon} (p(x_0)(e_0 - 1) + A_{p1} + N_a \ln e_0))^{\frac{1}{2}}. \quad (4.5)$$

The inequalities (4.1) and (4.2) supply the necessary criteria for governing the sequence of initial value problems discussed in section 3.5.

4.3.1 Iterative calculation of solutions

If at some point of a p^+ collector a hole density p_t is assumed to exist, then with the help of (4.3)-(4.5) the solutions for p and E between this point and the collector contact can be computed by iterating for the corresponding initial value E_t .

It can easily be shown from the differential equations that an integral curve $p(x)$ which once crosses the quasi-neutral solution p_{po} can never recross, since it has positive second derivative thenceforth, while by assumption it has non-positive second derivative. Similarly, an integral curve $E(x)$ which crosses the limiting value E_{drift} going downward has negative second derivative thenceforth, and can never recross.

Typical integral curves $p(x)$ and $E(x)$ are shown in Fig. 4.2. By improving the guess for E_t systematically, it is possible to arrive at the solutions which satisfy (4.1) and (4.2) and approach the limits p_{po} and E_{drift} to a preassigned accuracy.

The iterative procedure for improving E_t is contained in Fig. 4.2. The choice of p_t is straightforward since $p(x)$ is practically

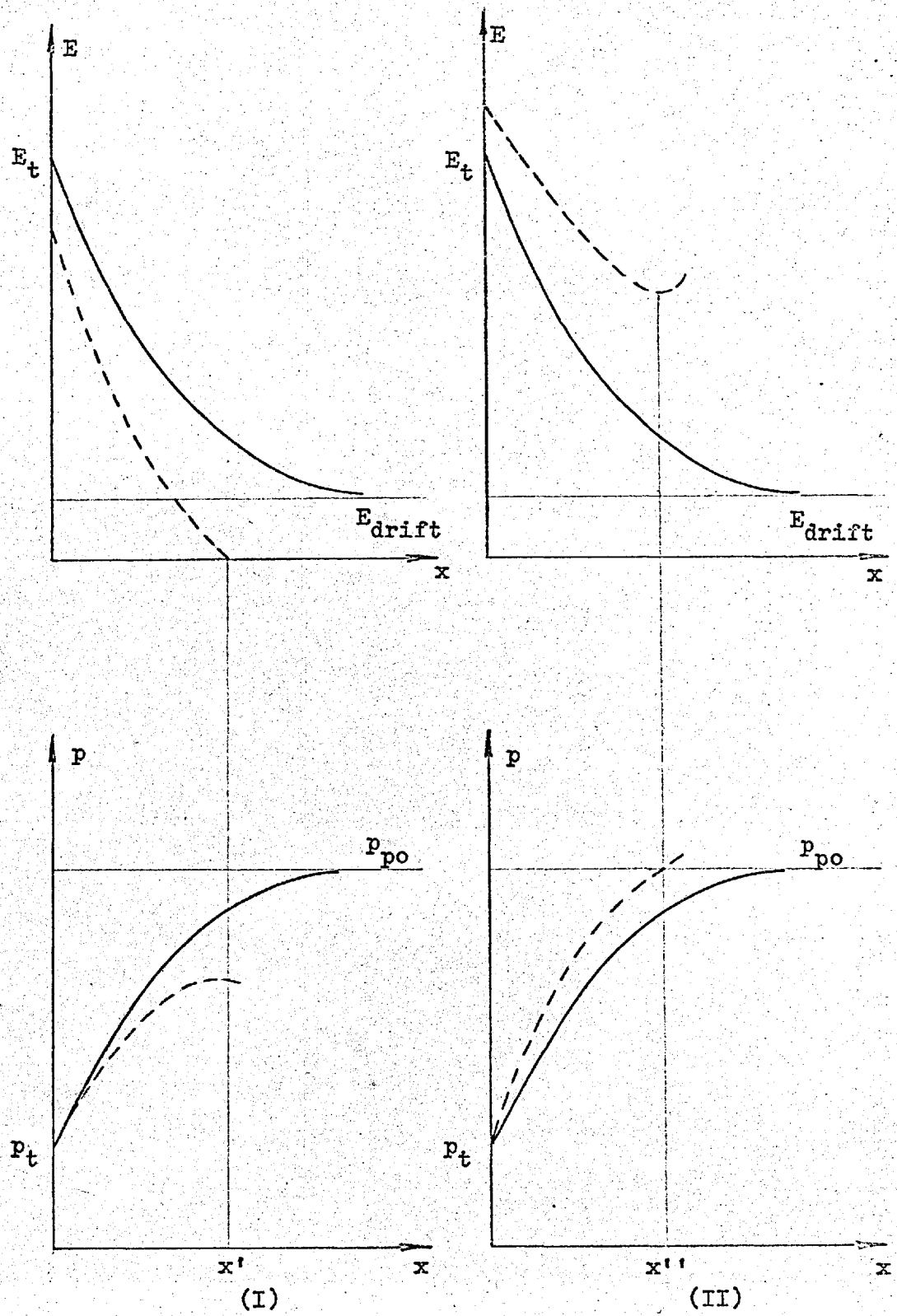


Fig.4.2

confined to the thermal equilibrium values. Moreover, its position in space does not have to be specified at this stage*.

Conceptually, the assumptions (a) and (b) define the upper bound for the hole density distribution and the lower bound for the electrostatic field, respectively. In the region situated between p_t and the collector contact each iteration for E_t gives either an improved lower bound $E_L(x)$ for the field (case I in Fig. 4.2) or an improved upper bound $p_U(x)$, for the hole density (case II in Fig. 4.2). When E_t eventually becomes known to an accuracy which is compatible with the accuracy at the local iteration loop, the solutions over this region are

$$E(x) = \begin{cases} E_L(x) & , \quad x \leq x' \\ E_{\text{drift}} & , \quad x' < x \leq x_{cc} \end{cases} \quad (4.6)$$

$$p(x) = \begin{cases} p_U(x) & , \quad x \leq x'' \\ p_{po} & , \quad x'' < x \leq x_{cc} \end{cases} \quad (4.7)$$

where $E_L(x)$ and $p_U(x)$ are the last estimates of the respective bounds.

The computations are easily mechanized by examining for the zero slope of $p(x)$ (case I) or of $E(x)$ (case II). Flow-chart of the program which iterates for E_t using this technique is shown in Fig. 4.3. As the iterations approach the correct E_t , the distances x' and x'' of Fig. 4.2 show sharp maxima. This is illustrated in Fig. 4.4 (the numerical values of N_a , p_t and J_p are also shown; the material constants

* For the calculations of this section the position of p_t may be taken as the reference, $x_t = 0$.

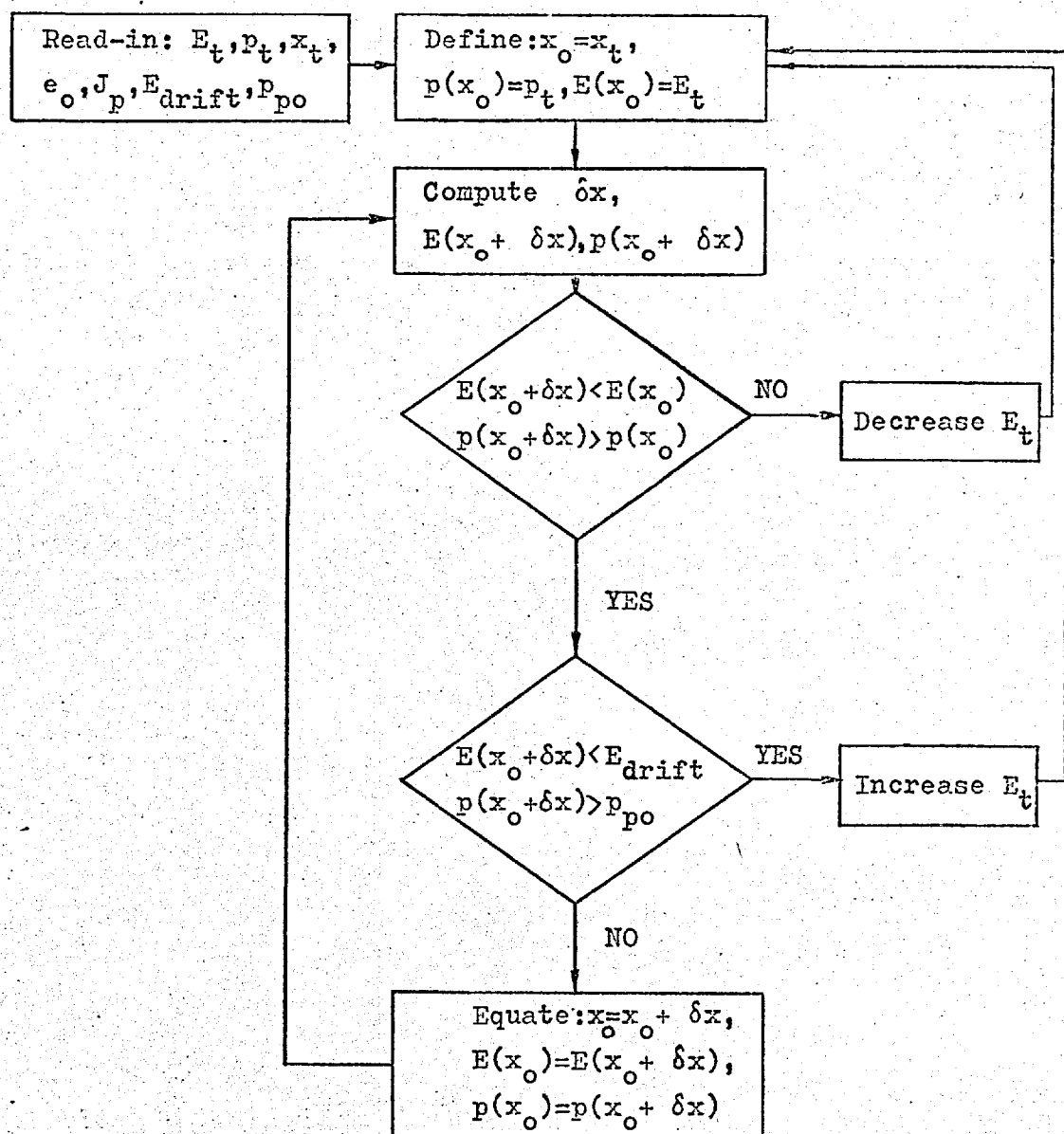


Fig. 4.3

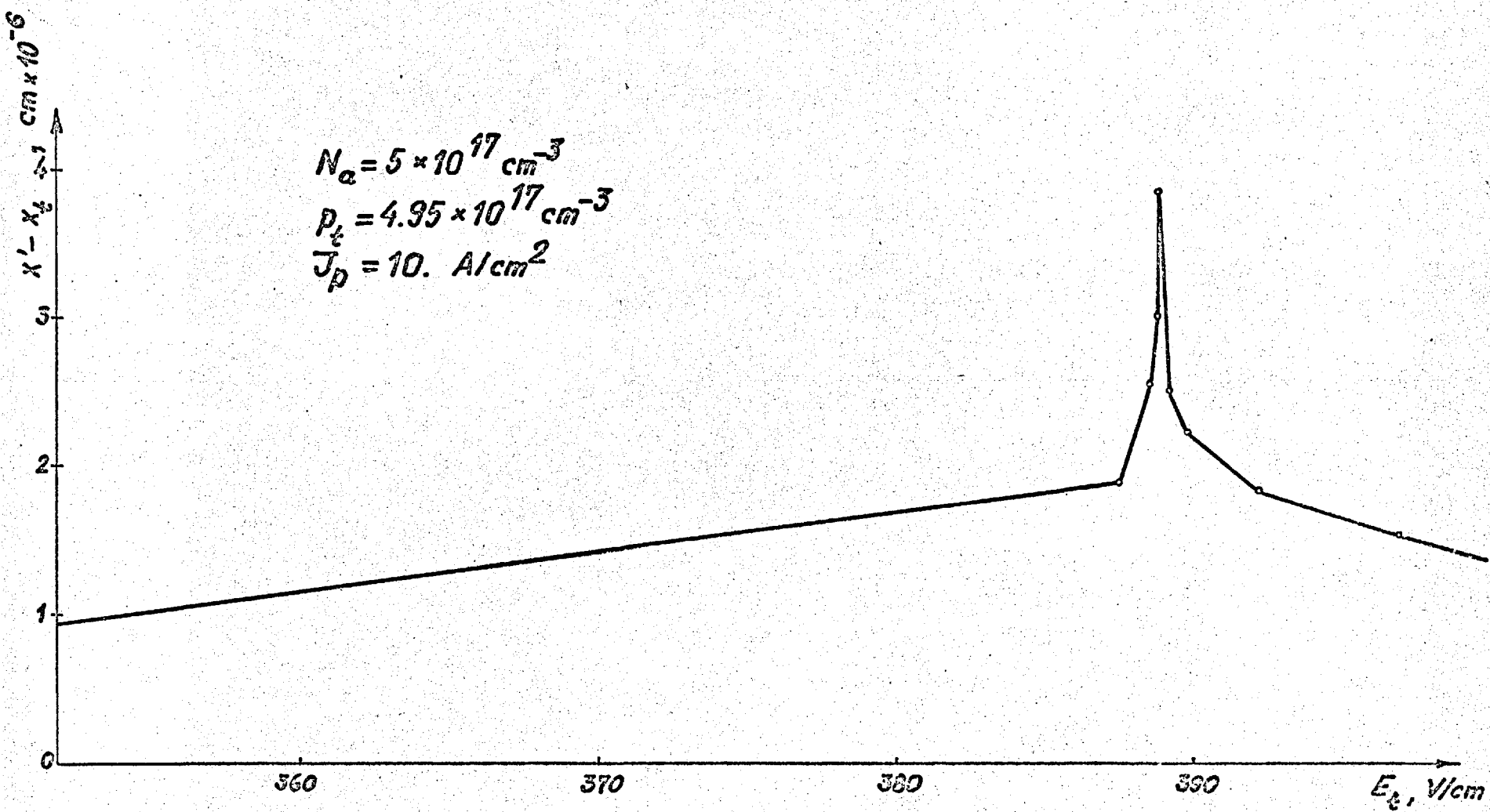


Fig. 4.4

ϵ and n_i correspond to germanium at room temperature).

The parameters x' and x'' are limited by the accuracy of the calculations. The total length of this section ($x_{cc} - x_t$), however, can be made arbitrarily long simply by adjusting the neutral parts of the section, $x_{cc} - x'$ and $x_{cc} - x''$.

4.3.2 The near-base section of the collector

The completion of integration of the p^+ collector is now quite simple since the initial values at x_t are known. A single round of calculations using p_t , E_t and equations (4.3)-(4.5) yields the solutions for this section, ending eventually with the collector-base metallurgical junction*.

Length of this section is a function of the applied collector-base voltage. All of the computed pairs (p, E) which satisfy the inequalities $p < p_{jc}$ and $E > E_{jc}$, but before avalanche multiplication, could mark the end of the section. The selection of the pair which does denote the metallurgical junction (and consequently the length of the section) is carried out in the process of synthesizing a particular transistor structure.

* Now $e_0 < 1$, thus the integration progresses from x_t towards the metallurgical junction.

4.4 The numerical analysis of the base

The total basewidth is divided into three sections. Descriptions of the self-consistent behaviour of the relevant physical variables are different in each section. There are, however, two assumptions common to all of them. These are:

(i) The electrostatic field in the base is a monotonically decreasing function from the collector towards the emitter (this is obvious from the geometry shown in Fig. 4.1);

(ii) The electron current density throughout the base is negligible. This is an approximation of the physical case, considered to be consistent with the one-dimensional character of the analysis. Treatment of very high currents, when the electron current density contributes significantly to the base region solutions, is thus excluded from the present analysis. Hence, throughout the base

$$\frac{dE}{dx} \geq 0, \quad (4.8)$$

$$J_n = 0. \quad (4.9)$$

4.4.1 The electron-depleted base section, next to the collector

The state of this section, dominated by the collector reverse bias, is essentially controlled by the large electrostatic fields.

The assumptions, additional to (i) and (ii), are:

(iii) the electron density is still negligible owing to the collector reverse bias. This is a reasonable assumption, since by (ii) the analysis of extremely high currents is excluded;

(iv) the hole density is monotonically decreasing from the collector into the base, not falling below

$$p_{\min} = \frac{J_p V_T}{q D_p (N_d)(E_{c1} - E_{c2})^{\frac{1}{2}}} \quad (4.10)$$

The limit (4.10) is derived in Appendix 3. It follows from (1.15) and applies as long as $E > E_{c2}$. The other boundary of the section thus coincides with the point $E = E_{c2}$.

The governing equations are still (4.3)-(4.5), except that in (4.5) N_a is replaced by $-N_d$. Since a range of initial values at the collector metallurgical junction is available from the calculations of section 2, the integration is straightforward. The parameter is again the width of the section as function of the collector-base voltage. This is illustrated in Fig. 4.5. for the doping densities $N_a = 5 \times 10^{17} \text{ cm}^{-3}$, $N_d = 5 \times 10^{14} \text{ cm}^{-3}$ and the indicated currents through the structure.

4.4.2 The low-field mid-base section

At the boundary where $E = E_{c2}$ and $p = p_{\min}$ the total current is entirely drift-controlled. The position is basically different at $E = 0$ where the mechanism of diffusion is entirely responsible for the total current. This mid-base section is the strip of the base between these two extremes.

The assumptions as regards the self-consistent behaviour of

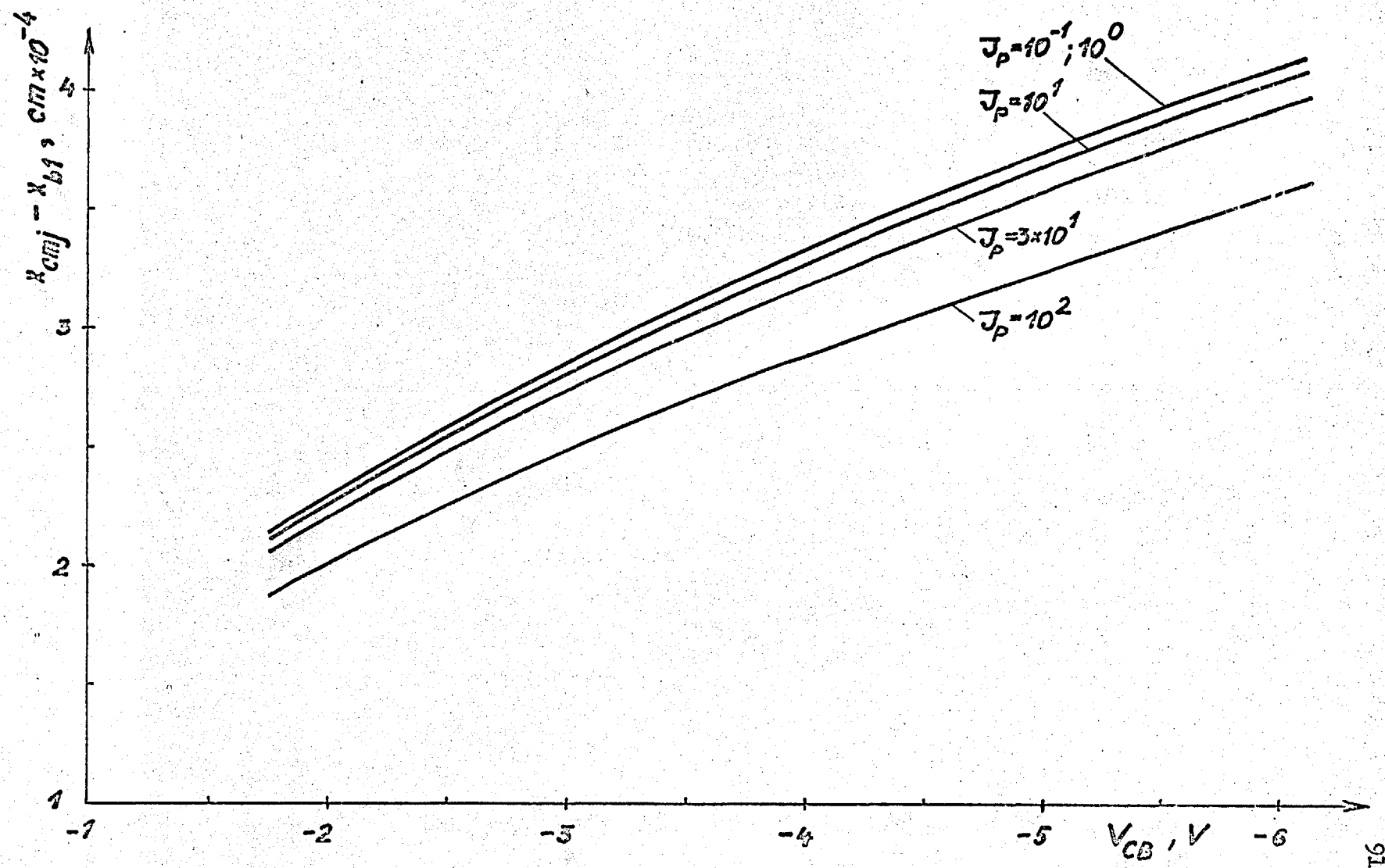


Fig. 4.5

the solutions, apart from (i) and (ii), are:

(iiia) the electron density is no longer negligible, hence the reduced form of (3.19) and a non-zero electron density term in (4.5) are included in the set of governing equations;

(iva) except at $E = E_{c2}$ the slope of the hole density distribution is negative,

$$\frac{dp}{dx} < 0 ; \quad (4.11)$$

(v) At the boundary $E = 0$ there is a range of values that the hole density can take at a given current level, depending upon the ratio of the biasing voltages. This is illustrated schematically in Fig. 4.6. The approximate limits for p at this boundary are:

$$p_{\text{high}} = p_{\text{min}} + \frac{J_p}{q D_p (N_d)} (x_{b1} - x_{b2}) , \quad (4.12)$$

which follows if $E(x) = 0$ throughout the section, and

$$p_{\text{low}} = p_{\text{min}} , \quad (4.13)$$

which denotes the limiting case that arises at the punch-through conditions in the base.

The objective of the analysis of this section is to establish the initial values for the electron density at $E = 0$, such that the distributions $p(x)$ and $E(x)$ fit their respective values at the other boundary, p_{min} and E_{c2} , for every $p = p_{b2}$, $p_{\text{low}} < p_{b2} < p_{\text{high}}$. A sequence of initial value problems is generated to compute these initial values n_{b2} and the corresponding solutions for $n(x)$, $p(x)$ and $E(x)$.

It is easy to see from the differential equations that for

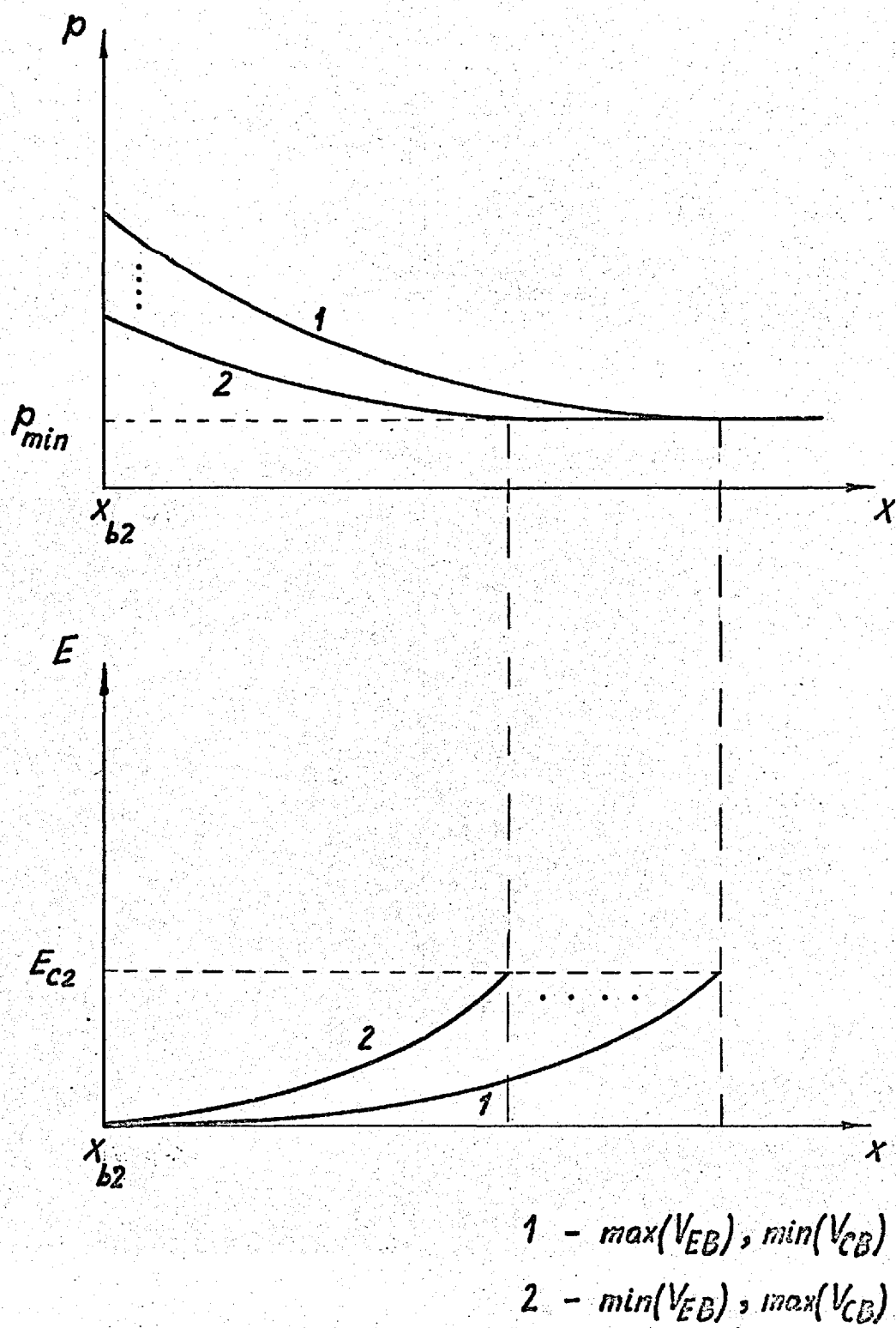


Fig. 4.6

every p_{b2} the integration over the section yields at the other boundary $E > E_{c2}$ if n_{b2} is smaller, and $E < E_{c2}$ if n_{b2} is greater than the corresponding correct initial value. From (4.8) it also follows that $n_{b2} < p_{b2} + N_d$. The flow-chart of the program which computes iteratively n_{b2} and the solutions for this section is shown in Fig. 4.7.

For $N_d = 5 \times 10^{14} \text{ cm}^{-3}$ the width of this section is plotted as function of p_{b2} at several current levels (p_{b2} conveniently represents the joint effect at both biasing voltages). The results are shown in Fig. 4.8 (full lines). The values n_{b2} , plotted in Fig. 4.9, show that the equilibrium majority carrier density is substantially increased at the current densities in excess of 100 A/cm^2 .

4.4.3 The negative-field base section, next to the emitter

This last section of the base is integrated in a straightforward manner since all initial values at x_{b2} are available. The position of the emitter metallurgical junction cannot be fixed at this stage and the width of the section remains unknown. It is obvious, however, that in the vicinity of the emitter metallurgical junction the solutions $p(x)$ and $E(x)$ satisfy the respective inequalities

$$p(x) > p_{je} , \quad (4.14)$$

$$E(x) < E_{je} . \quad (4.15)$$

This defines a narrow strip Δx , shown schematically in Fig. 4.10, where the emitter metallurgical junction must be situated. Its precise

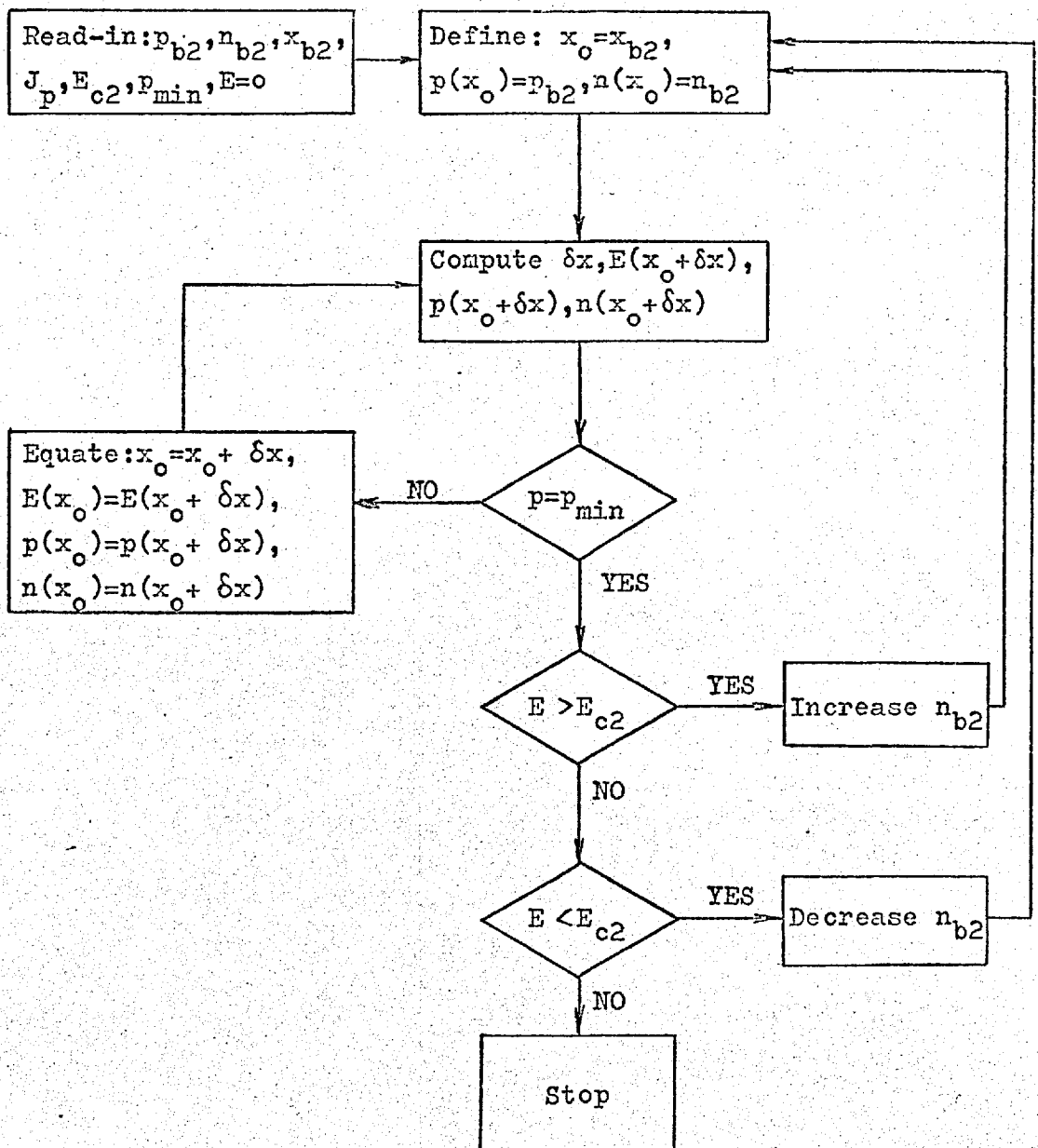


Fig. 4.7

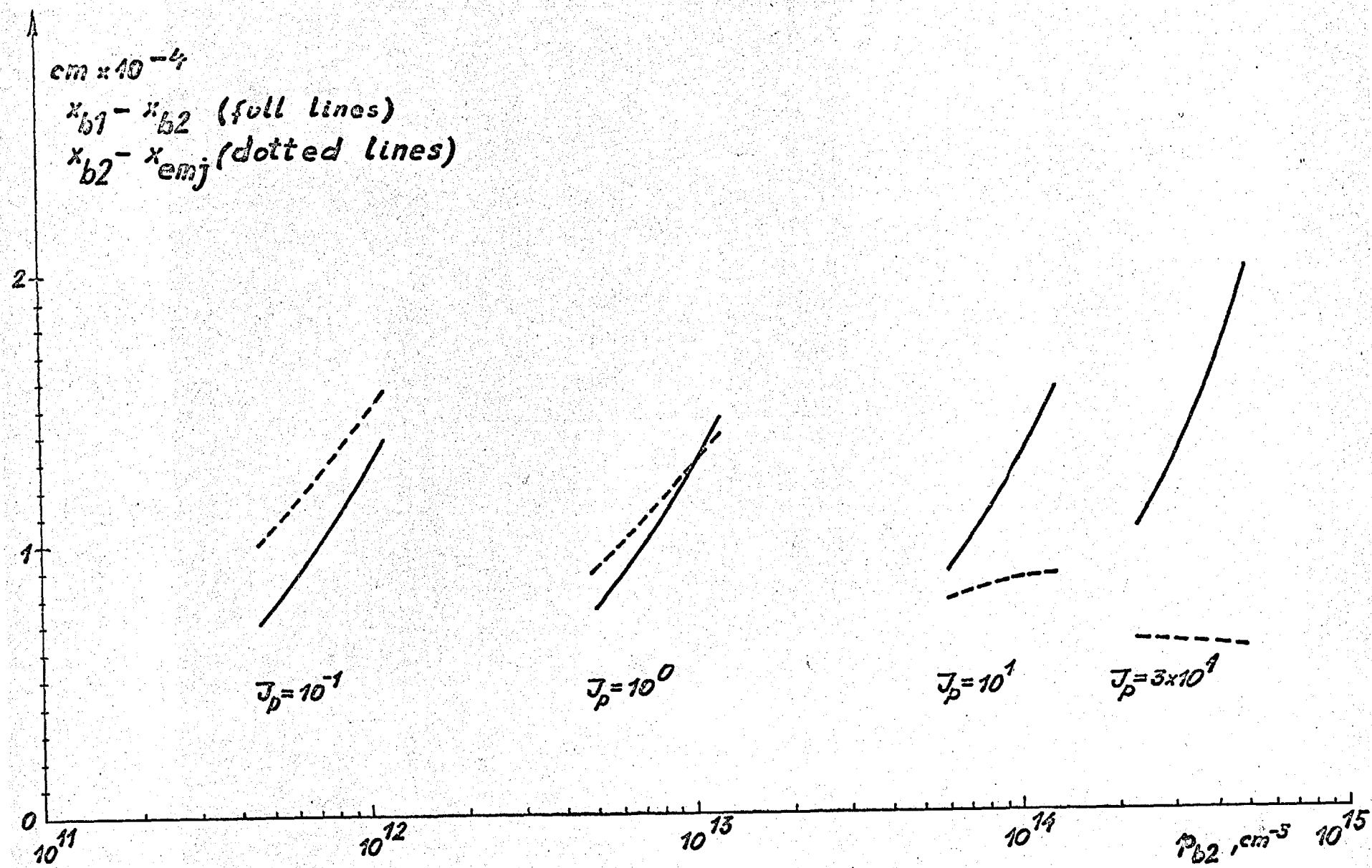


Fig. 4.8

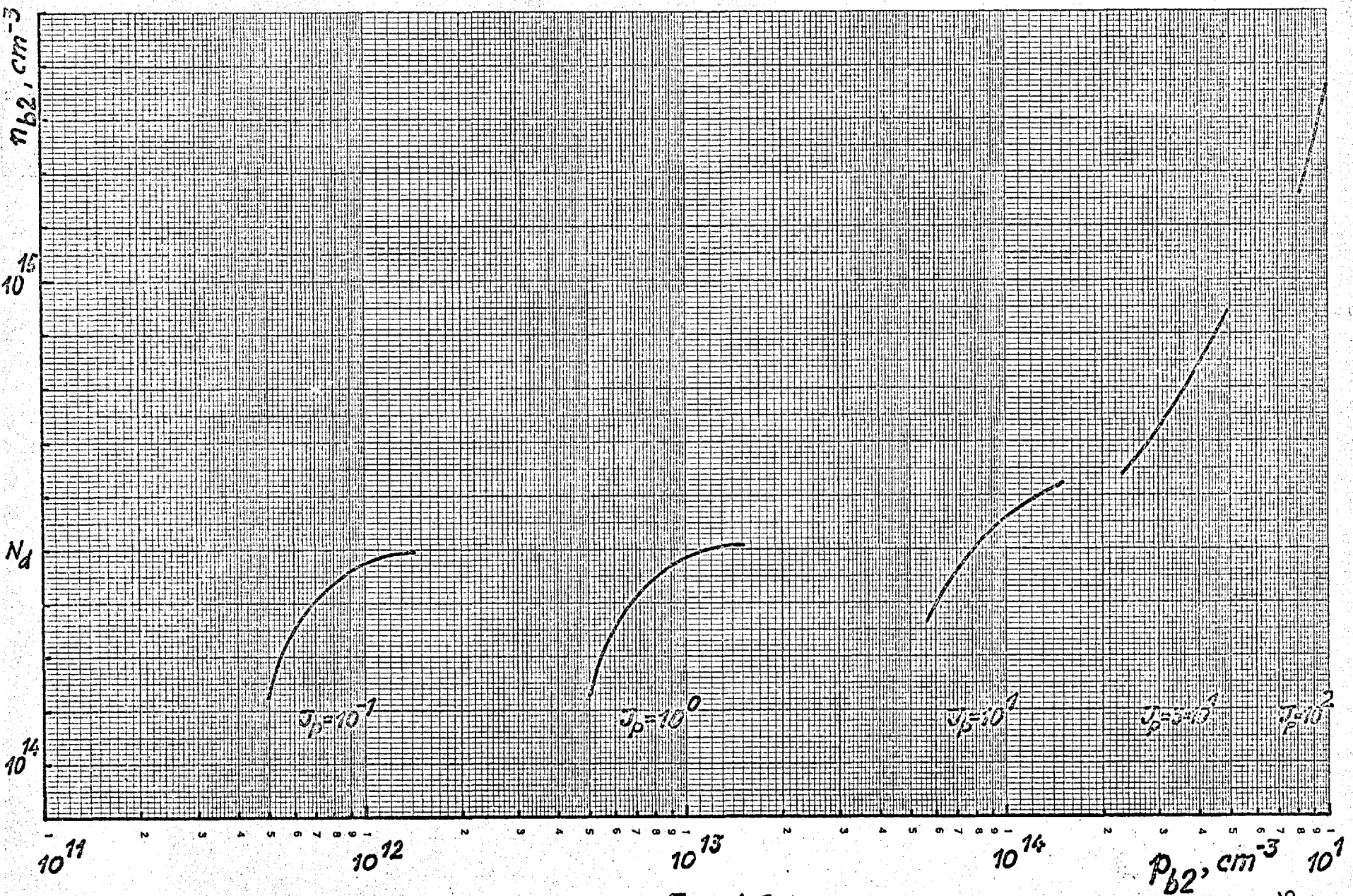


Fig. 4.9

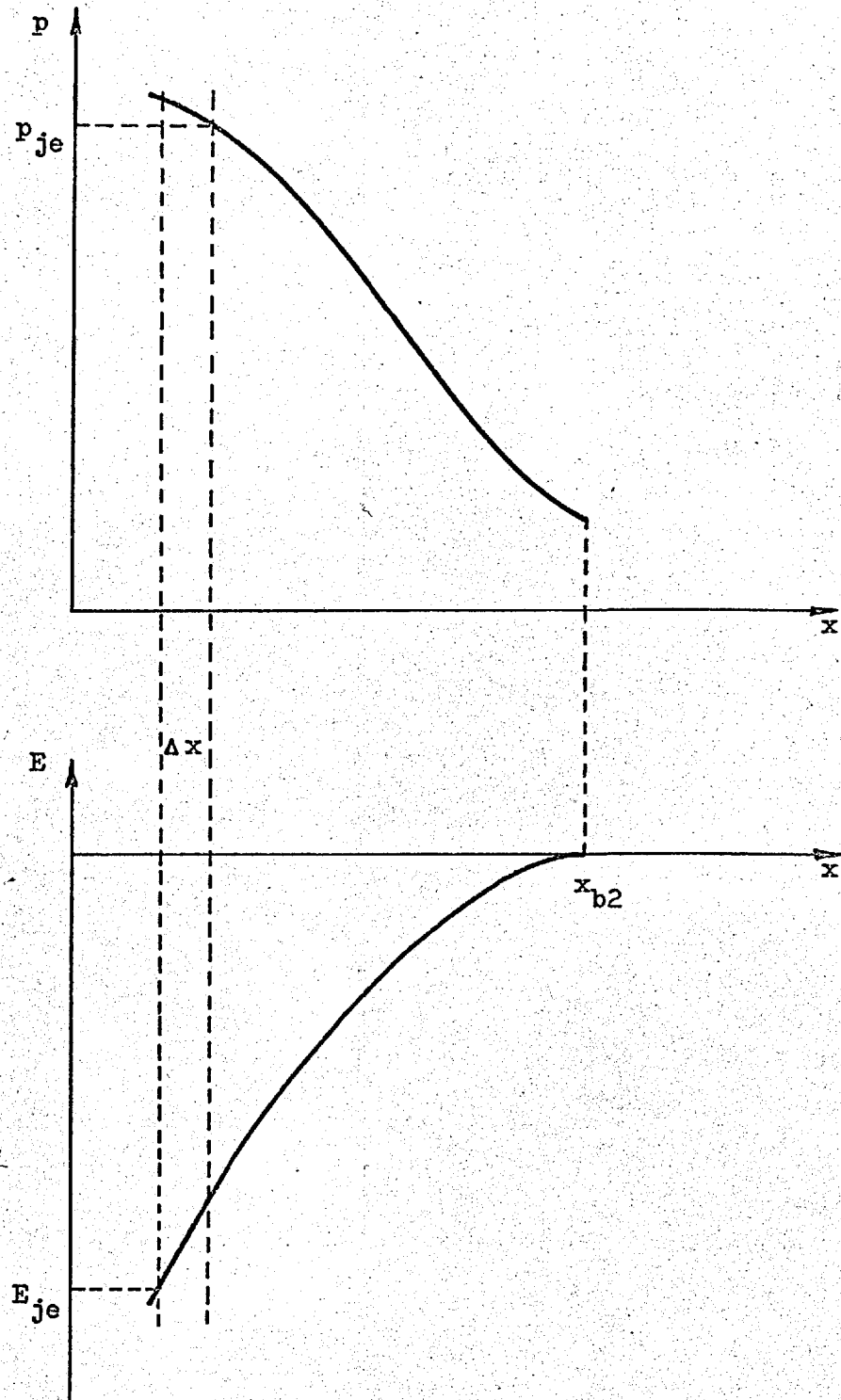


Fig.4.10

position within this strip is fixed by relating the solutions of this section to those of the p^+ emitter region.

4.5 The p^+ emitter region

The assumptions (a) and (b) of section 4.3, describing the self-consistent behaviour of the hole density and the electrostatic field, also apply to the p^+ emitter region. For geometrical reasons the inequalities (4.1) and (4.2) now read

$$p \leq p_{po}, \quad (4.16a)$$

$$\frac{dp}{dx} \leq 0, \quad (4.16b)$$

$$\frac{d^2p}{dx^2} \leq 0, \quad (4.16c)$$

and

$$E \leq E_{\text{drift}}, \quad (4.17a)$$

$$\frac{dE}{dx} \leq 0, \quad (4.17b)$$

$$\frac{d^2E}{dx^2} \geq 0. \quad (4.17c)$$

On the other hand, the electron density and the electron current density cannot be neglected as in section 4.3. The calculations are, however, performed assuming $J_n = 0$. Then, from the slope of the electron density distribution in the neutral part of the emitter a finite value for the electron current density is obtained. (It is assumed that this emitter electron current escapes 'laterally' through the base).

The set of discrete values for p , n and E in Δx , Fig. 4.10, is scanned pointwise to determine the initial values for this section by performing the integrations of the section for each set* (p, n, E) from Δx . The width of the domain where $p(x)$ and $E(x)$ satisfy (4.16) and (4.17) respectively, $(x_{emj} - x_1')$, shows a sharp maximum for the best fit of the initial values. This is illustrated in Fig. 4.11 for the indicated acceptor doping and the hole current density.

The solutions for the emitter can now be written in the form

$$p(x) = \begin{cases} p_{U1}(x) & , \quad x_{emj} \geq x \geq x_1' \\ p_{po} & , \quad x_1' > x \geq x_{ec} \end{cases} \quad (4.18)$$

$$n(x) = \begin{cases} n_p(x) & , \quad x_{emj} \geq x \geq x_1' \\ n_p(x_1') - \frac{n_p(x_1') - n_{po}}{x_1' - x_{ec}}(x - x_{ec}), & x_1' > x \geq x_{ec} \end{cases} \quad (4.19)$$

$$E(x) = \begin{cases} E_{L1}(x) & , \quad x_{emj} \geq x \geq x_1' \\ E_{drift} & , \quad x_1' > x \geq x_{ec} \end{cases} \quad (4.20)$$

where $p_{U1}(x)$, $n_p(x)$ and $E_{L1}(x)$ are the solutions for $\max(x_{emj} - x_1')$. In (4.19) the low-level approximation for the electron density distribution in the p^+ -neutral emitter, $x < x_1'$, is employed. The corresponding electron current density is

$$J_n \cong q D_n (N_a) \frac{n_p(x_1') - n_{po}}{x_1' - x_{ec}} \quad (4.21)$$

*In fact, scanning continues only until x_1' increases. Once it starts decreasing, the best fit for the initial values has been found.

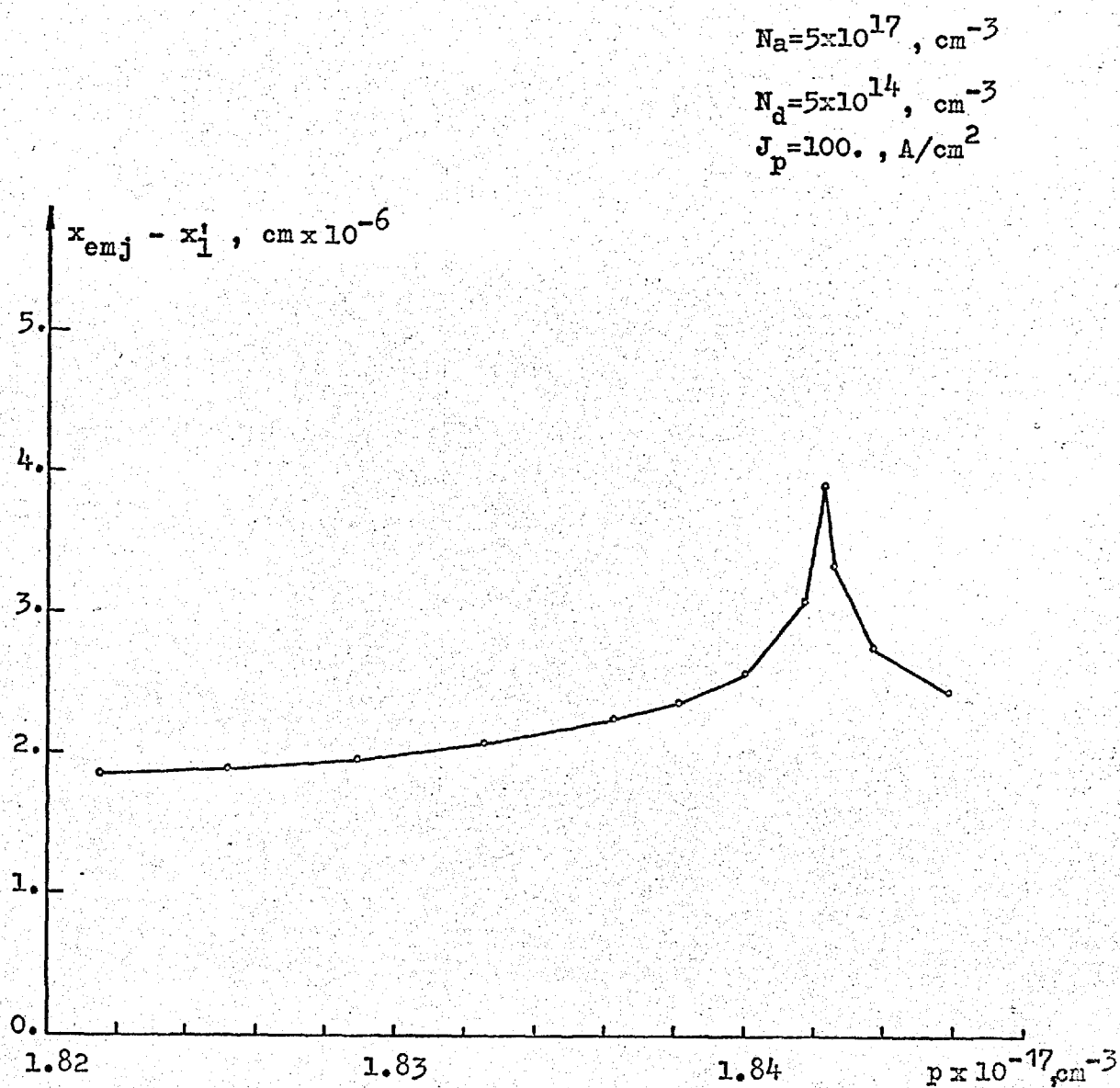


Fig. 4.11

The iterative calculations of this section fix the position of the emitter metallurgical junction and, consequently, conclude the calculations of section 5. The resulting width of section 5 is plotted dashed in Fig. 4.8.

A summary of all sectional calculations is given in Appendix 4.

4.6 The complete solutions for a particular pnp structure

The numerical examples of the sectional solutions presented in this chapter are now combined in the set of solutions for a particular uniform-base pnp transistor.

The doping densities at the emitter, base and collector have been chosen during the computations of the sectional solutions. The choice that remains to be made concerns the physical dimensions of a transistor: the metallurgical basewidth and the widths of the emitter and collector bodies.

The procedure for combining the sectional solutions involves the following steps:

- choose a set of desired w_b , L_e and L_c ;
- Figs. 4.8 and 4.5 determine all combinations of $(x_{b1} - x_{b2}) + (x_{b2} - x_{emj})$ and $(x_{cmj} - x_{b1})$ which add up to w_b , at selected discrete current levels;
- each choice of $(x_{cmj} - x_{b1})$ defines a set of values at the collector metallurgical junction, i.e. defines the width $(x_t - x_{cmj})$.

Since $(x'_t - x_t)$ is constant at a selected current level, the width of the remaining neutral part of the collector is adjusted to fit the chosen L_c ;

- similarly, the width $(x_{emj} - x'_1)$ follows automatically from a selected $(x_{b1} - x_{b2}) + (x_{b2} - x_{emj})$. Again, the width of the neutral part of the emitter is set to complement L_e ;

- the integrals of $E(x)$, with respect to a selected reference point in the base, define the applied voltages.

The above procedure is applied to obtain the solutions for the transistor structure which is defined by the following set of data: the emitter and collector doping densities $N_a = 5 \times 10^{17} \text{ cm}^{-3}$, the base doping density $N_d = 5 \times 10^{14} \text{ cm}^{-3}$, $w_b = 4.86 \text{ } \mu\text{m}$, $L_e = L_c = 1 \text{ } \mu\text{m}$.

Fig. 4.12 shows the distributions of the mobile charge carrier densities, electrons and holes, throughout the structure at $V_{CB} = -2\text{V}$ and the respective current densities of 0.1, 1.0, 10., and $30. \text{ A/cm}^2$. The corresponding electrostatic field distributions are plotted in Fig. 4.13 (to avoid overlapping of curves only the two extreme cases are shown).

The space charge distributions in the base at 0.1 A/cm^2 and $30. \text{ A/cm}^2$, and $V_{CB} = -2\text{V}$ and -3V respectively are plotted in Fig. 4.14. Widening of the 'neutral' base region at higher currents is observable from these distributions. This phenomenon is further demonstrated in Fig. 4.15 where the collector transition region width is plotted as a function of the collector current density, with V_{CB} as a parameter. (The transition region boundary has been defined as the point at which

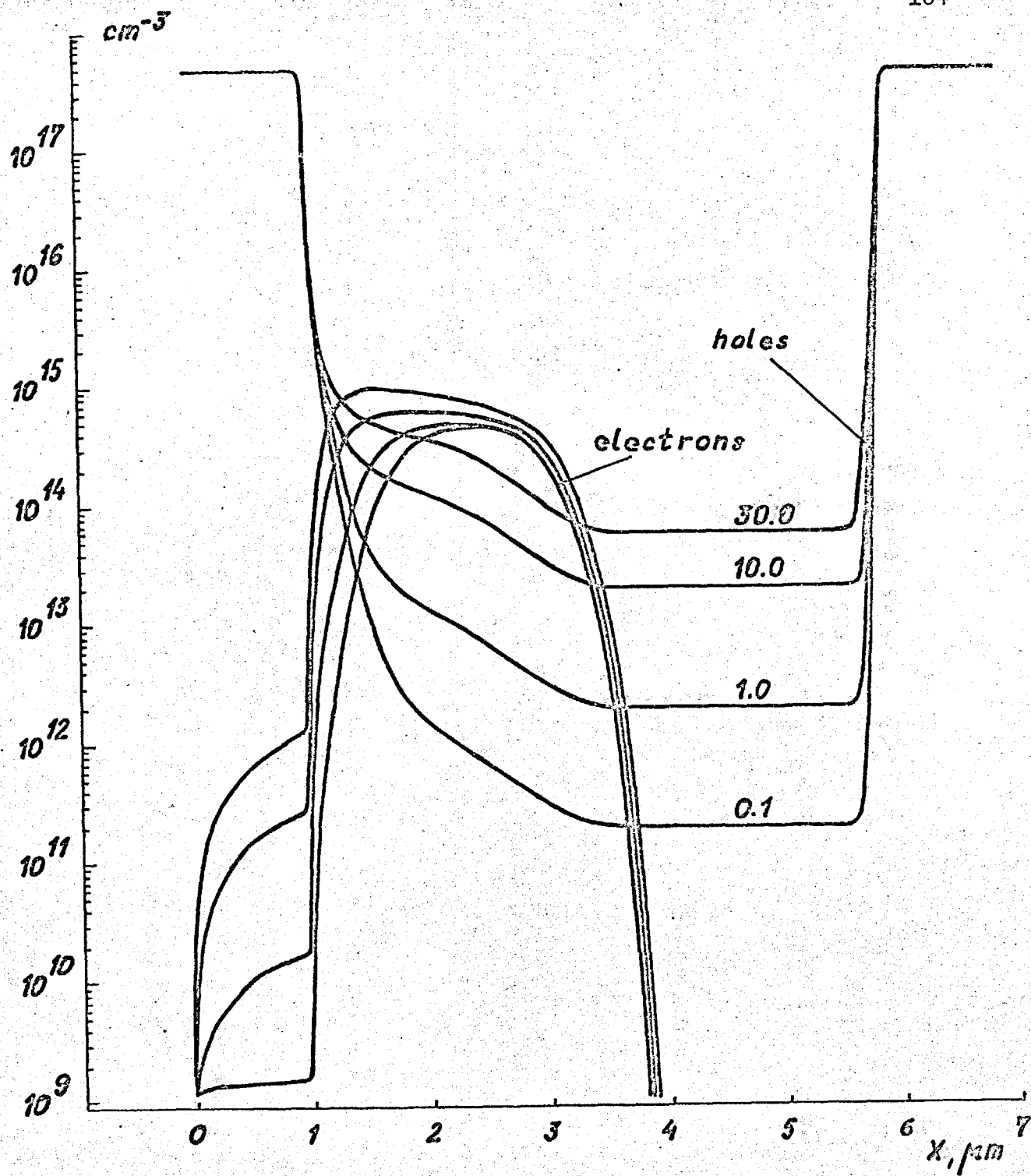


Fig. 4.12

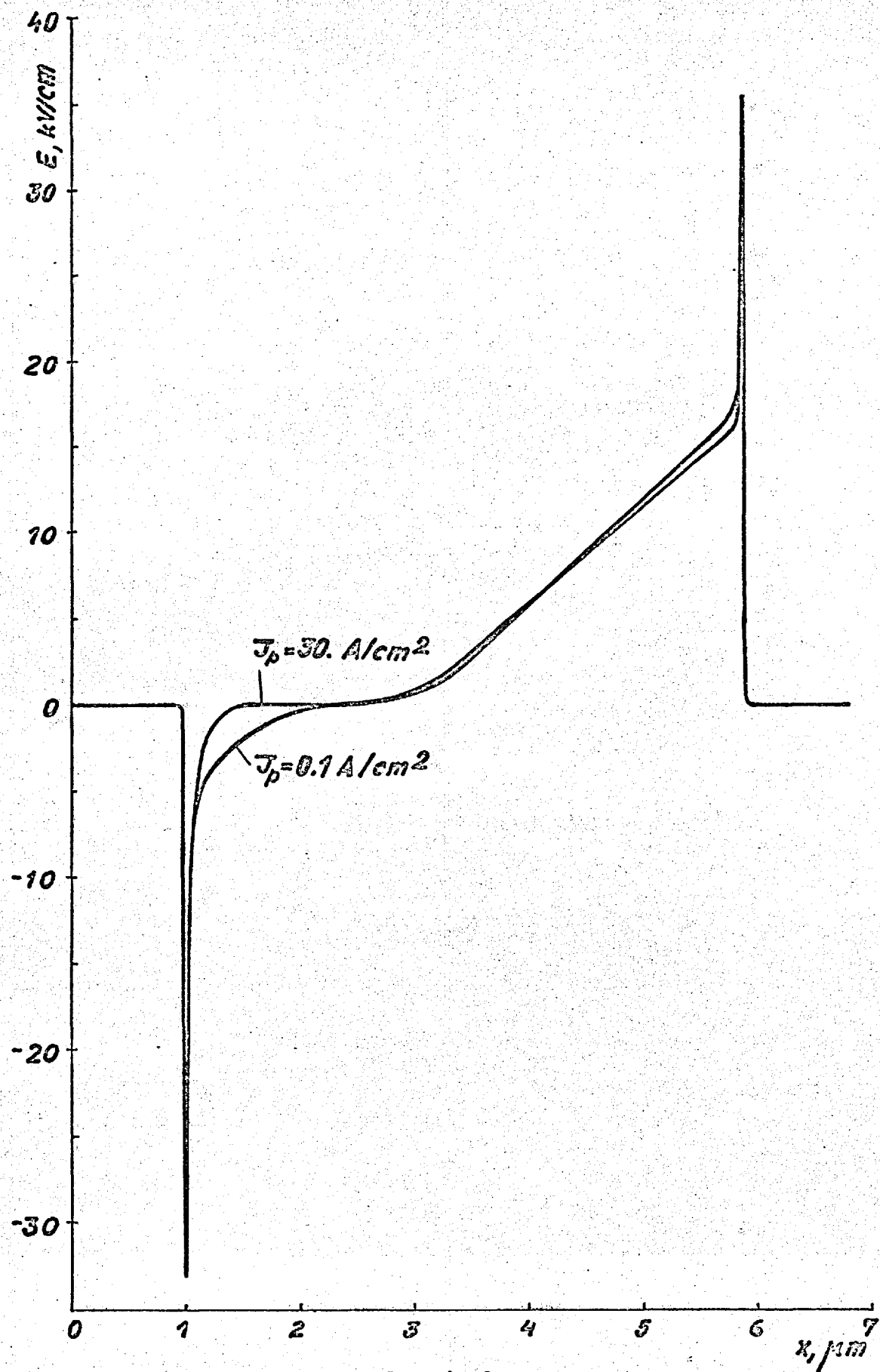


Fig. 4.13

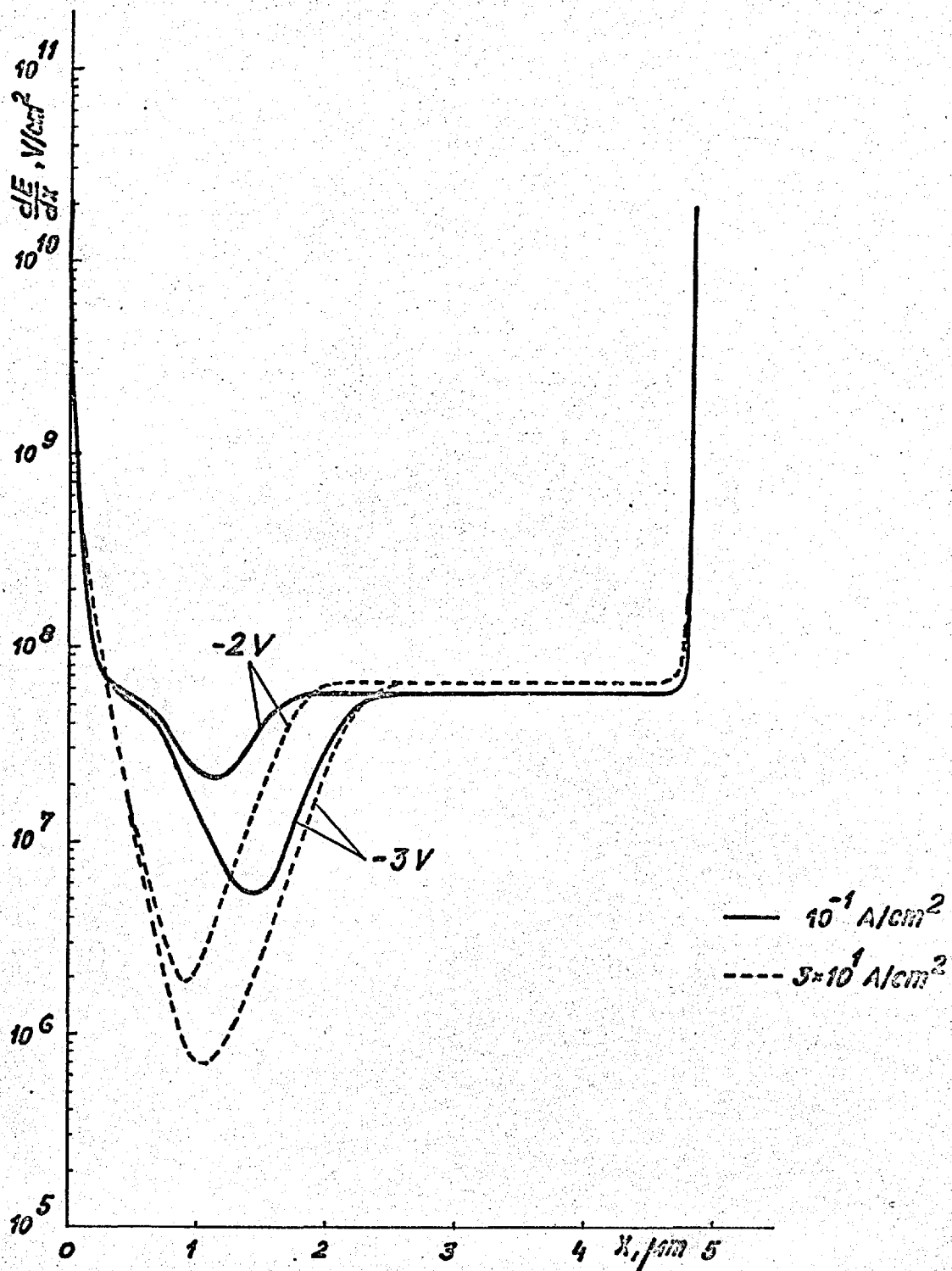


Fig. 4.14

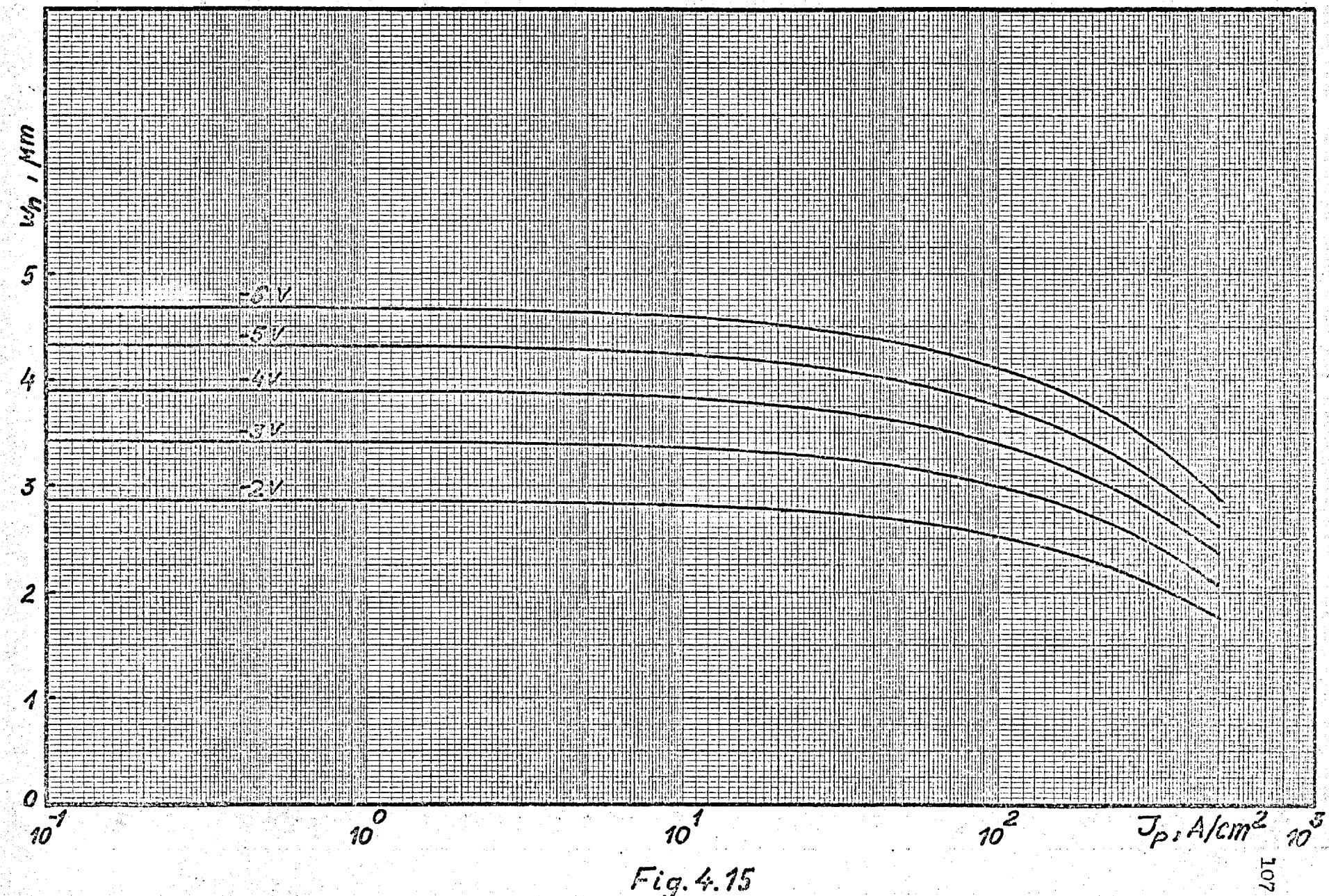


Fig. 4.15

dE/dx has fallen to half its midregion value).

4.7 Conclusions

The numerical analysis of the steady-state properties of uniform-base transistor structures by reducing the two-point boundary value problem to a sequence of initial value problems offers what is essentially the one-current solution of the problem.

A successful implementation of this technique is subject to an expedient separation of the interior of a device into several characteristic sections where the governing equations can be suitably simplified.

The results obtained by this technique apply to a particular doping pattern and thus to any device which fits this pattern. Generalization to arbitrary doping, however, is not possible since the sections identifiable in a uniformly doped device do not necessarily appear in devices possessing different doping patterns.

Despite the claims of Fulkerson and Nussbaum¹¹³ and more recently of Sanchez¹³⁷, this approach is insufficiently powerful for tackling cases of an arbitrary complexity.

CHAPTER 5

GENERAL ITERATIVE SCHEME FOR NUMERICAL TREATMENT
OF SEMICONDUCTOR JUNCTION STRUCTURES

5.1 Introduction

The mathematical instability exhibited by the initial value problems which are associated with equations (1.1)-(1.5) (hence partitioning of a structure to suppress its influence in chapter 4) prevents the technique based upon generating a sequence of initial value problems of acquiring the desired generality. Development of the procedures which attack the given two-point boundary value problem more directly is obviously desirable.

The iterative procedure proposed by Gummel¹⁰⁵ is of a general character. Two sets of boundary conditions for the electrostatic potential and the quasi-Fermi potentials are applied at the points representing the external contacts of a device, and the problem is treated as a classical two-point boundary value problem. The analytical formulation of the numerical algorithm for computing this set of equivalent variables involves the introduction of the suitably constructed functions. The set of variables defined by eqns.(1.1)-(1.7), on the other hand, allows a derivation of the relevant equations directly from the basic equations. This permits a formulation of an efficient numerical algorithm for computing the original variables, which has the advantage of offering a direct insight into the physical processes taking

place in the interior of a device. Moreover, it can be derived in the form which makes it applicable at arbitrary bias conditions. The general considerations are presented in this chapter discussing a single junction structure (Fig. 5.2).

The approach requires specifying the set of boundary conditions that completes the mathematical formulation of the problem presented by eqns.(1.1)-(1.5) and the subsidiary equations (1.6)-(1.7). These fix the mobile charge carrier densities and the electrostatic potential at the end points (the external contacts) of a device. In general, the carrier boundary values are related to the current densities and the impurity densities, while the boundary values of the electrostatic potential are directly related to the externally applied voltage V_a and the built-in potential V_o . Taking either of the potential boundary values as a reference, the general form of the boundary conditions can be written as

$$p(o) = p(N(o), J_p(o), J_n(o)), \quad (5.1a)$$

$$n(o) = n(N(o), J_p(o), J_n(o)), \quad (5.1b)$$

$$p(L) = p(N(L), J_p(L), J_n(L)), \quad (5.1c)$$

$$n(L) = n(N(L), J_p(L), J_n(L)), \quad (5.1d)$$

$$u(o) - u(L) = V_o - V_a. \quad (5.1e)$$

5.2 Outline of the method

The derivation of the expressions (3.5) and (3.6) in Chapter 3 has laid down the basis for establishing the relations which are

alternative to those obtained by Gummel*. With the help of (1.7), the equations (3.5) and (3.6) can be rewritten to read

$$p(x) = \exp\left(-\frac{u(x)}{V_T}\right) \left(A - \int \frac{\exp(u(t)/V_T)}{qD_p(t)} J_p(t) dt\right), \quad (5.2)$$

$$n(x) = \exp\left(\frac{u(x)}{V_T}\right) \left(B + \int \frac{\exp(-u(t)/V_T)}{qD_n(t)} J_n(t) dt\right). \quad (5.3)$$

5.2.1 The treatment of the charge carrier densities and the current densities

Definite forms of (5.2) and (5.3) are obtained if 0 and x are taken as the limits of integration and the constants A and B are expressed in terms of the boundary conditions at x=0, i.e.

$$p(x) = \exp\left(-\frac{u(x)}{V_T}\right) \left(p(0) \exp\left(\frac{u(0)}{V_T}\right) - \int_0^x \frac{\exp(u(t)/V_T)}{qD_p(t)} J_p(t) dt\right), \quad (5.4)$$

* It should be pointed out that a similar treatment of (1.1) and (1.2) has been proposed earlier in efforts to analyse the junction properties analytically^{55,122}. It is only recently that this approach in handling (1.1) and (1.2) has been shown to be feasible for pursuing a numerical analysis of the junction transport equations^{108,138,139,140}. An almost identical procedure to the one described in this chapter has been recently reported by Demari^{108,140}, who analysed a special case of a uniformly doped junction, assuming the absence of recombination and constant mobilities.

$$n(x) = \exp\left(\frac{u(x)}{V_T}\right) \left(n(0) \exp\left(-\frac{u_0}{V_T}\right) + \int_0^x \frac{\exp(-u(t)/V_T)}{qD_n(t)} J_n(t) dt \right). \quad (5.5)$$

From the continuity equations, (1.3) and (1.4), the current densities are

$$J_p(x) = \int_0^x q U(t) dt + J_{po}, \quad (5.6)$$

$$J_n(x) = - \int_0^x q U(t) dt + J_{no}, \quad (5.7)$$

where the constants of integration J_{po} and J_{no} , evaluated with the help of (5.4) and (5.5) at $x=L$, are

$$J_{po} = \frac{p(0) \exp(u_0/V_T) - p(L) \exp(u_L/V_T) - \int_0^L \frac{\exp(u(t)/V_T)}{qD_p(t)} \left(\int_0^t q U(t') dt' \right) dt}{\int_0^L \frac{\exp(u(t)/V_T)}{qD_p(t)} dt}, \quad (5.8)$$

$$J_{no} = \frac{n(L) \exp(-u_L/V_T) - n(0) \exp(-u_0/V_T) + \int_0^L \frac{\exp(-u(t)/V_T)}{qD_n(t)} \left(\int_0^t q U(t') dt' \right) dt}{\int_0^L \frac{\exp(-u(t)/V_T)}{qD_n(t)} dt}. \quad (5.9)$$

If the electrostatic potential were known as a function of distance, the charge carrier densities and the current densities could be readily computed from (5.4)-(5.9). This, however requires solving Poisson's equation, i.e. the second order nonlinear differential equation. In principle it is possible to obtain a valid solution of Poisson's equation through quadratures by proceeding from equation (3.12).

Unfortunately, the process of integrating (3.12) numerically can be very seriously affected by the sensitivity of the square-root operator to the sign of the function on the right hand side of (3.12). Unless a function representing the potential is very close to the exact potential distribution, the algorithm breaks down since, in general, the quantity under the square root becomes negative*. It is therefore necessary to develop a different treatment of Poisson's equation in which this sign-problem is not present.

The generalized Newton-Raphson method (e.g. ref. 24, p.355) provides a basis for formulating an iterative procedure for numerical computation of the potential distribution, provided an initial guess of the potential function reasonably close to the exact distribution is available.

5.2.2 Treatment of Poisson's equation

Assume that there exists a potential function $u^{(0)}(x)$ which is close to the exact solution of Poisson's equation

$$u'' = F(x,u), \quad (5.10)$$

given a set of boundary conditions $u(0)=u_0$, $u(L)=u_L$.

* The quantities on the right hand side of (3.12), p , n , J_p , and J_n are computed first from the starting potential distribution, employing eqns.(5.4)-(5.9) respectively.

The exact potential distribution can now be written as

$$u(x) = u^{(0)}(x) + \delta u(x), \quad (5.11)$$

where $\delta u(x)$ is a small difference between the initial guess and the exact potential distribution. The function $F(x, u)$ can be expanded in a Taylor series in terms of $\delta u(x)$, in the vicinity of $u^{(0)}(x)$.

Then,

$$F(x, u) = F(x, u^{(0)}) + \left(\frac{\partial F}{\partial u} \right)_{u^{(0)}} \delta u(x) + \left(\frac{\partial^2 F}{\partial u^2} \right)_{u^{(0)}} \frac{\delta u(x)^2}{2} + \dots \quad (5.12)$$

From (5.10)-(5.12), neglecting the square and other high order terms in (5.12), the second order linear differential equation for $\delta u(x)$ follows

$$\delta u'' - \frac{\partial F}{\partial u} \delta u = -u^{(0)''} + F(x, u^{(0)}). \quad (5.13)$$

Introducing in $F(x, u^{(0)})$ the expressions for the mobile charge carrier densities, (5.4) and (5.5), the equation (5.13) becomes (see Appendix 5)

$$\delta u'' - \delta u \frac{q}{V_T \epsilon} (p(x) + n(x)) = -u^{(0)''} + \frac{q}{\epsilon} (p - n + N)_{u^{(0)}}. \quad (5.14)$$

The equation (5.14) constitutes the linear boundary value problem of the general class

$$\delta u'' = f(x, \delta u), \quad (5.15a)$$

i.e. $\delta u'$ does not appear on the right hand side of (5.15a) which is, in addition, linear in δu . Since by (5.1e) the boundary values $u(0)$ and $u(L)$ are specified at the outset, the boundary conditions for the problem described by (5.14) are

$$\delta u(0) = 0; \quad \delta u(L) = 0. \quad (5.15b)$$

Since f in (5.15a), in addition to satisfying the condition of continuity and a Lipschitz condition, is such that $\partial f / \partial u$ is continuous and non-negative in $(0, L)$, the boundary value problem (5.15) has a unique solution.²⁴

By considering $\delta u(x)$ at a sufficiently dense set of points in $0 \leq x \leq L$, the differential equation (5.15) can be converted into a system of difference equations. Provided a three-point finite difference formula is employed, the left-hand side of this system forms a "tridiagonal" matrix T , say. Now, $\delta u(x)$ and $K(x) = -u^{(0)''} + \frac{q}{\epsilon}(p-n+N)u^{(0)}$ are represented as two column vectors, and the system of difference equations, in the matrix notation, is

$$T \delta u(x) = -R_e(x). \quad (5.16)$$

The new column vector $u^{(1)}$ which corresponds to the first improved solution for the potential function is

$$u^{(1)} = u^{(0)} - T^{-1}R_e, \quad (5.17)$$

provided the inverse of T exists. Finding the inverse of the matrix T is greatly facilitated by its property that the nonzero elements are situated in the main diagonal and the nearest adjacents only. The technique for forming T and R_e is outlined in the following section. An efficient method for inverting T is given in Appendix 6.

5.2.2.1 Formation of the matrix T

For the direct numerical solution of the boundary value problem defined by (5.15), the interval of integration $0 \leq x \leq L$ is divided into M small sections defined by the points $x_n = nh, (n=0, 1, \dots, M)$, where $h=L/M$. The setting up of a finite difference scheme permits determination of numbers δu_n which approximate the values of $\delta u(x_n)$ of the true solution at the points x_n . In general such a scheme is obtained by demanding that δu_n satisfy at interior mesh point x_n a difference equation

$$a_k \delta u_{n+k} + a_{k-1} \delta u_{n+k-1} + \dots + a_0 \delta u_n - h^2 (\beta_k f_{n+k} + \dots + \beta_0 f_n) = 0. \quad (5.18)$$

The problem of solving the differential equation (5.15) is thus reduced to solving a system of $M-1$ algebraic equations since δu_0 and δu_M are fixed by the boundary conditions. If $k > 2$, new unknown values such as δu_{-1} or δu_{M+1} are introduced for which (5.18) does not provide the required equations. This problem can be circumvented by suitably modifying the difference equations near the boundary points, but the case $k=2$ which defines a scheme suitable for direct implementation on a computer is particularly attractive in view of the fact that the matrix T in (5.16) assumes a very simple form. In general, the difference equations for $k=2$ can be written as

$$-\delta u_{n-1} + 2 \delta u_n - \delta u_{n+1} + h^2 (\beta_0 f_{n-1} + \beta_1 f_n + \beta_2 f_{n+1}) = 0. \quad (5.19)$$

In the further discussion the following vector and matrix

notation is used:

$$\delta u = \begin{bmatrix} \delta u_1 \\ \vdots \\ \delta u_{M-1} \end{bmatrix}, \quad f(\delta u) = \begin{bmatrix} f(x_1, \delta u_1) \\ \vdots \\ f(x_{M-1}, \delta u_{M-1}) \end{bmatrix}, \quad a = \begin{bmatrix} u(0) - \beta_0 h^2 f(x_0, \delta u_0) \\ \vdots \\ u(L) - \beta_2 h^2 f(x_M, \delta u_M) \end{bmatrix}$$

and

$$J = \begin{bmatrix} 2 & -1 & & 0 \\ -1 & 2 & -1 & \\ & \ddots & \ddots & \\ & -1 & 2 & -1 \\ 0 & & -1 & 2 \end{bmatrix}, \quad B = \begin{bmatrix} \beta_1 & \beta_2 & & 0 \\ \beta_0 & \beta_1 & \beta_2 & \\ & \ddots & \ddots & \\ & & \beta_0 & \beta_1 & \beta_2 \\ 0 & & & \beta_0 & \beta_1 \end{bmatrix}.$$

In the matrices J and B all elements not on the main diagonal or on the nearest adjacents are zero.

The system of equations arising from the demand that (5.19) hold for $n=1, 2, \dots, M-1$ can be compactly written in the form

$$J \delta u + h^2 B f(\delta u) = a. \quad (5.20)$$

The given differential equation, (5.15a), is linear, i.e. is of the form

$$f(x, \delta u) = g(x) \delta u + k(x), \quad (5.21)$$

where

$$g(x) = \frac{q}{V_T \epsilon} (p(x) + n(x)), \quad (5.22)$$

$$k(x) = -u^{(0)''} + \frac{q}{\epsilon} (p - n + N) u^{(0)} \quad (5.23)$$

are known functions, once the initial potential guess is chosen. Having

defined the diagonal matrix

$$G = \begin{bmatrix} g(x_1) & & & 0 \\ & g(x_2) & & \\ & & \ddots & \\ 0 & & & g(x_{M-1}) \end{bmatrix}$$

and the vector

$$K = \begin{bmatrix} k(x_1) \\ \vdots \\ k(x_{M-1}) \end{bmatrix},$$

it may be written

$$f(\delta u) = G \delta u + K. \quad (5.24)$$

The system (5.20) now reduces to the system of linear equations

$$T \delta u = R_e \quad (5.25)$$

where

$$T = J + h^2 B G \quad (5.26a)$$

$$R_e = a - h^2 B K. \quad (5.26b)$$

It is obvious that the matrix T shares with the matrices J and B the property of being tridiagonal, i.e. if $T = (t_{nm})$

$$t_{n,n} = 2 + h^2 \beta_1 g_n$$

$$t_{n,n-1} = -1 + h^2 \beta_0 g_{n-1}$$

$$t_{n,n+1} = -1 + h^2 \beta_2 g_{n+1}, \quad n=1,2,\dots,M-1$$

and $t_{nm} = 0$ for $|n-m| > 1$.

5.2.2.2 The discretization formula

The particular difference equation which is applied in the calculations presented in the subsequent chapters is

$$-\delta u_{n-1} + 2\delta u_n - \delta u_{n+1} + \frac{h^2}{12}(f_{n-1} + 10f_n + f_{n+1}) = 0. \quad (5.27)$$

Despite the simplicity, which is characteristic for all difference equations corresponding to $k=2$, the formula (5.27) possess a fairly high order of accuracy. An approximate measure of this accuracy is obtained if (5.27) is represented by its equivalent Taylor series in terms of h . The first non-zero term in this series, which indicates the order of error induced by approximating $\delta u(x_n)$ by δu_n , is associated with h^6 (e.g. ref. 24, p.298). This, in practice, eliminates the need for introducing any of the correcting terms in the formula (5.27).

5.2.3 The iterative procedure

It is now possible to formulate the iterative scheme for computing the solutions of the junction variables in an arbitrary single junction structure.

The equations (5.1)-(5.17) describe how an improved potential distribution can be found if a reasonable potential guess was made. With this improved approximation it is possible to enter the equations (5.4)-(5.7) and compute the corresponding improved solutions for the mobile charge carrier densities and the current densities. These, in turn, specify the next improved potential distribution as described in the section 5.2.2. If the original potential guess is sufficiently

close to the exact potential distribution a rapid convergence of this sequence of iterations can be expected*.

A flow-chart representation of this iterative scheme is given in Fig. 5.1.

5.2.4 Convergence of the iterative procedure

The three point discretization formula (5.27) yields $M-1$ independent equations which can be solved for δu_n provided T is non-singular. In a general case the elements $t_{n,n-1}$ and $t_{n,n+1}$ are non-zero, i.e.

$$t_{n,n-1} \neq 0, \quad (5.28a)$$

$$t_{n,n+1} \neq 0, \quad (5.28b)$$

and T is irreducible. (If either $t_{n,n-1}$ or $t_{n,n+1}$ were zero for some n , a part of the system (5.25), contrary to the physical case, could be solved without paying attention to the remaining equations.) If the conditions (5.28) are further reinforced by demanding that

$$t_{n,n-1} \leq 0, \quad (5.29a)$$

$$t_{n,n+1} \leq 0, \quad (5.29b)$$

* If the recombination processes are significant, the problem of computing the recombination currents in the first iteration loop arises since at that stage the charge carrier distributions are not available. The computation of $p(x)$ and $n(x)$ in the first loop must be carried out assuming the absence of recombination. The distributions $p(x)$ and $n(x)$ obtained in this way are then used to estimate the recombination terms for the subsequent loop.

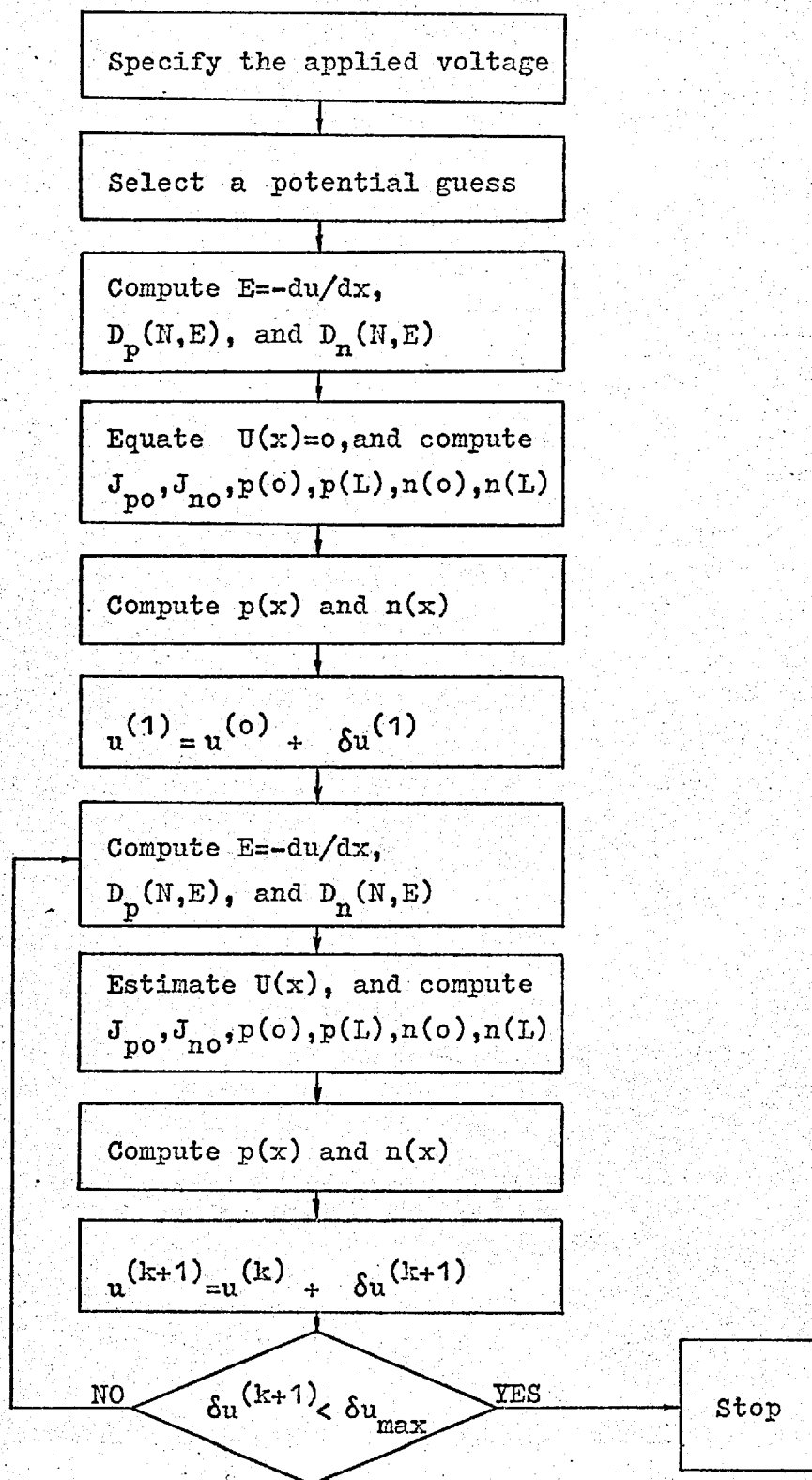


Fig.5.1

and

$$\sum_{j=1}^{M-1} t_{ij} \begin{cases} \geq 0 & i=1,2,\dots, M-1 \\ > 0 & \text{for at least one } i, \end{cases} \quad (5.30)$$

T is monotone and therefore nonsingular*. In view of the definitions of t_{ij} the conditions (5.29) are satisfied if

$$h^2 < 12 / \left(\frac{q}{V_T \epsilon} (p+n) \right)_{\max}, \quad (5.31)$$

i.e. for sufficiently small values of h . With an h chosen to meet (5.31) the convergence of the iterative scheme of section 5.2.3 takes place if the following two requirements are fulfilled:

a) h is sufficiently small that the solutions of the finite difference equations (5.25), δu_n , converge to the true solutions $\delta u(x_n)$ at the points $x_n = nh$ ($n=1,2,\dots,M-1$);

b) the initial guess $u^{(0)}$ is sufficiently close to the true solution of the system (5.25).

Denote by $u^{(0)}(x)$ a guessed potential function differentiable at least six times (the discretization formula (5.27) is under consideration). The following constants can be introduced:

$$Y_m = \max \left| \frac{d^6 u}{dx^6} \right|, \quad (5.32a)$$

* A matrix T is called monotone if $Tz \geq 0$ implies $z \geq 0$. If T is monotone, and $Tz \leq 0$, then, since $-Tz = T(-z) \geq 0$, it follows that $-z \geq 0$ or $z \leq 0$. Thus if $Tz = 0$, z must satisfy both $z \leq 0$ and $z \geq 0$, hence $z = 0$. Consequently $\det(T) \neq 0$ and T is nonsingular.

$$R_m = \max |u^{(0)} - F(x, u^{(0)})|, \quad (5.32b)$$

$$L_m = \max \left| \frac{\partial^2 F}{\partial u^2} \right|. \quad (5.32c)$$

Quantitatively, the main condition which guarantees convergence of the scheme of section 5.2.3 turns out to be (see Appendix 7)

$$\frac{L_m^4 (R_m + h^4 Y_m G_6)}{64} \leq \frac{1}{2}, \quad (5.33)$$

where $G_6 = 1/240$ is the constant associated with the first nonzero term of the Taylor series of (5.27). The limiting cases of (5.33), when either R_m or Y_m are negligible are of particular interest.

If the initial guess for the potential function $u^{(0)}$ is represented by a polynomial of a degree less than 6, $Y_m = 0$ and (5.33) specifies the maximum tolerable error by which the equations (5.20) fail to hold

$$R_m \leq \frac{32}{L^4 L_m}, \quad (5.34)$$

or after differentiating $F(x, u)$ twice with respect to u (see Appendix 5)

$$R_m \leq \frac{32 V_T^2 \epsilon}{L^4 q |n(x) - p(x)|_{\max}}. \quad (5.35)$$

Before completing the first iteration of the scheme, the inequality (5.35) offers a test for assessing the validity of an initial potential guess, provided of course, it consists of a polynomial of an order less than 6. Moreover, by considering the signs of the residual terms of (5.20) improving of the guess is possible, until eventually a valid guess is acquired.

If the computations now proceed by modifying slightly the exact solution $u(x)$ to match the modified boundary conditions, $R_m = 0$ and the method converges if

$$h^4 \leq \frac{32}{L^4 L_m G_6 Y_m} . \quad (5.36)$$

Fortunately, it turns out that the first order theory provides valid starting potential guesses, at least at small current levels. (Cubic distributions are obtained by approximating a diffused profile by an equivalent linear impurity function.) Approaching an arbitrary current level is then straightforward by adjusting gradually the boundary potentials $u(0)$ and $u(L)$.

5.3 Modifications of the analytical formulation

When using (5.4) and (5.5) for calculating $p(x)$ and $n(x)$ respectively, certain numerical difficulties may arise. The type of these difficulties is shown in this section on the example of a single junction structure, schematically shown in Fig. 5.2. A method for surmounting them is proposed.

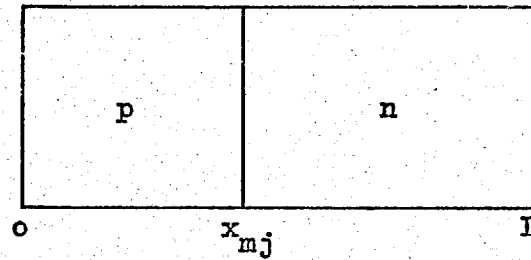


Fig. 5.2

5.3.1 Choice of a suitable reference point

Computation of $p(x)$ may lose a great deal of accuracy if the terms on the right hand side of (5.4) are nearly equal. Evaluation of the difference between two nearly equal numbers which are known with a certain finite precision could introduce a serious hindrance in achieving a required accuracy. A rearrangement of (5.4) to avoid this problem can be done as follows.

Denote by $I(x)$ the integral

$$I(x) = \int_0^x \frac{\exp(u(t)/V_T)}{qD_p(t)} J_p(t) dt, \quad (5.37)$$

and by $I_c(x)$ the integral over the rest of the domain $(0, L)$, i.e.

$$I_c(x) = \int_x^L \frac{\exp(u(t)/V_T)}{qD_p(t)} J_p(t) dt. \quad (5.38)$$

Obviously, for all x between 0 and L

$$I(L) = I(x) + I_c(x), \quad (5.39)$$

or

$$I(x) = I(L) - I_c(x). \quad (5.40)$$

The integral $I(L)$ can be expressed in terms of the boundary values, i.e. from (5.4)

$$I(L) = p(0)\exp(u_0/V_T) - p(L)\exp(u_L/V_T), \quad (5.41)$$

and the rearranged expression for $p(x)$ is now

$$p(x) = \exp(-u(x)/V_T) \left(p(L)\exp(u_L/V_T) + \int_x^L \frac{\exp(u(t)/V_T)}{q_p^D(t)} J_p(t) dt \right). \quad (5.42)$$

This rearrangement, in fact, redefines the reference point in the original equation so that $p(x)$ is now computed in the direction of increasing $p(x)$.

For the structure of Fig. 5.2 the integral on the right hand side of (5.5) is a non-negative quantity and redefinition of the reference point is not needed. Physically, it is easy to visualize that the electron density is increasing from the p-region contact, $x=0$, towards the n-region contact, $x=L$, so that $x=0$ is a good reference point. (Obviously, in an np structure these directions are reversed, thus requiring the modification of (5.5) while (5.4) remains unchanged).

In general, the considerations of this type govern the choice of the reference points in an arbitrary junction structure.

5.3.2 Shifting of the potential origin

The presence of the exponentially dependent terms in the equations (5.4), (5.5), (5.8) and (5.9) is a source of another type of numerical difficulty associated with these equations. When the applied bias exceeds several volts in the reverse direction, the exponential terms in these equations exceed in magnitude the permissible range of most of the currently available computers. A further modification of the basic formulation of the numerical procedure is needed to overcome this problem.

If $u_{r,n}$ and $u_{r,n+1}$ denote two potential levels separated by the maximum allowed potential variation, then in the interval $u_{r,n} \leq u \leq u_{r,n+1}$ the equations (5.5) and (5.42) can be written as

$$n(x) = \exp((u(x) - u_{r,n})/V_T) \left(n_{r,n} + \int_{x_{r,n}}^x \frac{\exp((u_{r,n} - u(t))/V_T)}{qD_n(t)} J_n(t) dt \right), \quad (5.43)$$

$$p(x) = \exp((u_{r,n+1} - u(x))/V_T) \left(p_{r,n+1} + \int_x^{x_{r,n+1}} \frac{\exp((u(t) - u_{r,n+1})/V_T)}{qD_p(t)} J_p(t) dt \right), \quad (5.44)$$

where the values $u_{r,n}$ and $u_{r,n+1}$ are treated as a given set of boundary conditions for the electrostatic potential. The total variation of the electrostatic potential between u_0 and u_L can be divided into m sections, e.g.: $u_0 = u_1, u_1 - u_2, \dots, u_{m-1} - u_L$, subject to the condition $|(u_k - u_{k+1})/V_T| \leq K_m$, where K_m is a positive number such that

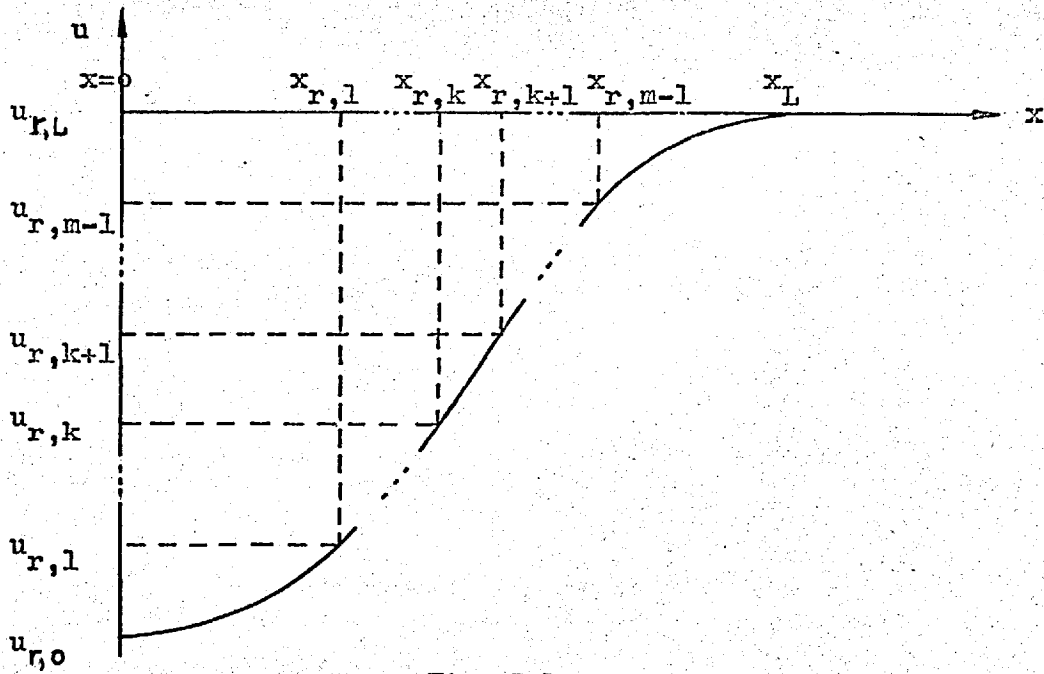


Fig. 5.3

$\exp(+K_m)$ still falls within the permissible range. Schematically this is shown in Fig. 5.3. The potential values, together with the values p_k and n_k in the equations (5.43) and (5.44) are redefined as the integration progresses. This corresponds to a shifting of the potential origin along the trajectory of integration in order to avoid the overflows or underflows in the registers of the computer arithmetic unit.

The problem is somewhat different when the definite integrals in (5.8) and (5.9) are evaluated. Shifting of the potential origin is not possible here and a different approach is required. The exponential variation of the integrand functions restricts the significant contribution to the integrals in (5.8) and (5.9) to a relatively narrow part of the total region of integration (reverse bias conditions are under discussion). The technique of neglecting the insignificant terms is discussed for the integrals in (5.8) only. The analogy of the approach

for computing the integrals in (5.9) is complete.

The overwhelming contribution to the integrals in (5.8) comes from the region where $u(x)$ is large, i.e. from the last section (u_{m-1}, u_L) of the total potential variation. In addition, for a u_0 which approaches or exceeds the limit $V_{Tm} K_m p(0) \exp(u_0/V_T) \ll p(L) \exp(u_L/V_T)$ and the first term on the right hand side of (5.8) can be omitted. Therefore for any $|V_a| > V_{Tm} K_m p(0) \exp(u_0/V_T)$ in (5.8) is ignored and the corresponding integrals are calculated only over the last section of the potential distributions. Applying this rule, the constant current density J_{po} can be calculated under arbitrary bias conditions.

Similarly, in equation (5.9) the term $n(L) \exp((u_0 - u_L)/V_T)$ is negligible under reverse bias conditions and the integrals in (5.9) are calculated only over the first section of the potential distribution.

CHAPTER 6

APPLICATION OF THE GENERAL ITERATIVE SCHEME FOR NUMERICAL ANALYSIS OF SINGLE JUNCTION STRUCTURES

6.1 Introduction

The iterative scheme considered in chapter 5 is applied here to the specific junction structures. In the first part of the chapter the steady-state electrical properties of a diffused junction diode are calculated. A number of authors have tackled successfully the problem of solving numerically the transport equations for forward biased junctions. Gummel¹²⁹ and Demari¹⁰⁸ considered uniformly doped abrupt systems; Kennedy and O'Brien¹²¹ treated linearly graded structures; Caughey¹⁴⁵ computed the solutions for a forward biased diffused junction diode. The difficulties caused by large potential variations which are present in reverse biased junctions prevented most of these analyses from obtaining the solutions for reverse biased junctions. Demari's treatment¹⁰⁸ overcomes this problem, but he does not consider the recombination processes and assumes constant mobilities. The set of solutions for the diffused structure which is presented in this chapter includes these effects, thus closing this gap in the literature on the subject.

The second part of the chapter is devoted to the application of the developed numerical technique for calculating the properties of

field-induced junctions. It is shown that the cut-off frequency for transconductance of idealized MOS structures can be improved by 'tailoring' expediently the substrate doping in the direction perpendicular to the oxide-semiconductor interface. This result is obtained assuming that the drain voltage is sufficiently small.

6.2 The numerical solutions for a diffused junction diode

The specific impurity profile analyzed in this section is assumed to result from a two-step diffusion process* (a brief summary of the simple diffusion theory is included in Appendix 8). The profile

$$N(x) = 8 \cdot 10^{15} - 10^{18} \exp(-x^2 / 1.864 \cdot 10^{-10}) \quad (6.1)$$

(N is in cm^{-3} , x in cm) is depicted in Fig. 6.1.

The external contacts, situated at $x = 0$ and $x = 2 \mu\text{m}$ respectively, are assumed to be characterized by an infinite recombination rate. In the interior at the device the recombination processes are simulated by a single Shockley-Read-Hall recombination level positioned half-way across the forbidden energy gap, i.e. $p_1 = n_1 = n_i = 1.45 \cdot 10^{10} \text{ cm}^{-3}$. The limiting lifetimes are taken to be $\tau_{p0} = 1 \text{ nsec}$ and $\tau_{n0} = 2 \text{ nsec}$.

* A sheet of acceptor impurity of $1.21 \cdot 10^{13} \text{ cm}^{-2}$ is deposited on a $8 \cdot 10^{15} \text{ cm}^{-3}$ donor-doped silicon wafer and then driven-in for 2 min 17 sec at the temperature 1100°C (the diffusivity taken to be $D = 3.4 \cdot 10^{-13} \text{ cm}^2 \text{ sec}$).

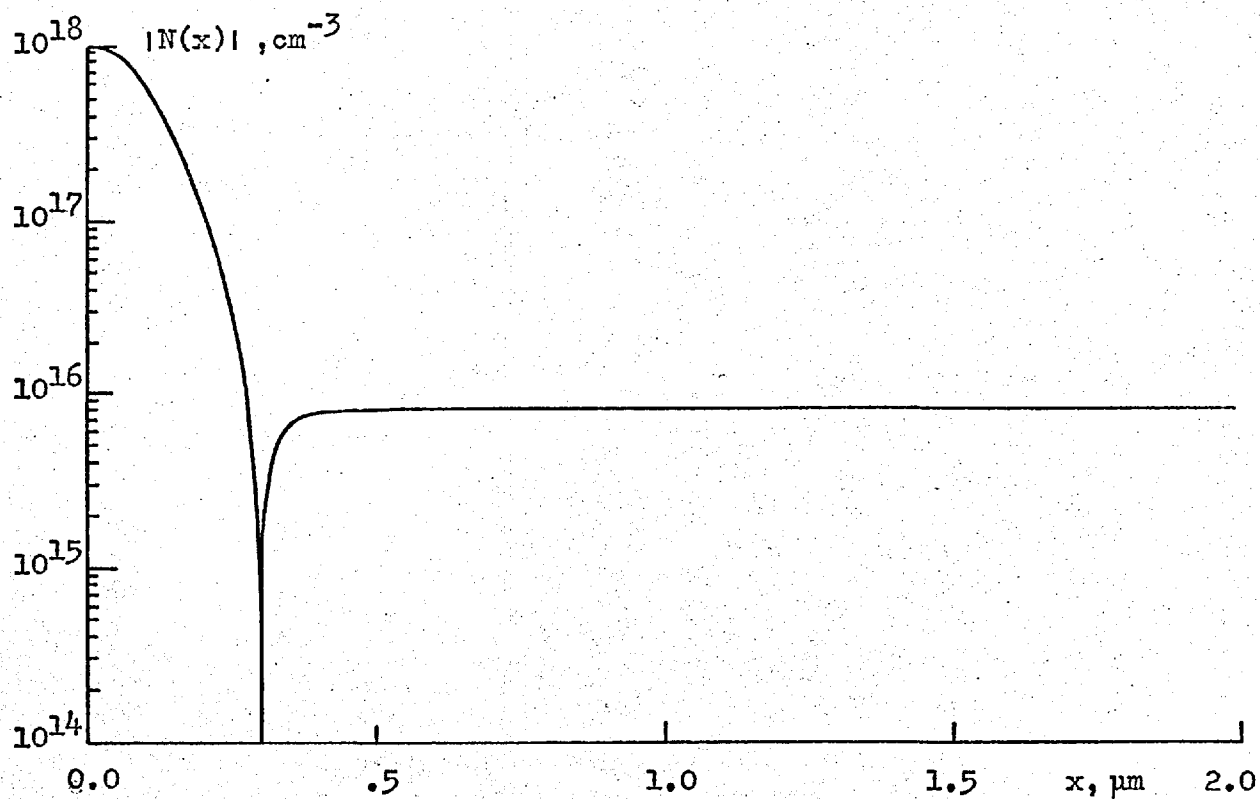


Fig. 6.1

6.2.1 The internal distributions

For various applied voltages the electrostatic potential as function of position is shown in Fig. 6.2. The coincident mobile charge carrier distributions are shown in Figs. 6.3 (holes) and 6.4 (electrons). The net space charge is plotted in Fig. 6.5.

The noteworthy feature of the carrier distributions at reverse biases is the relatively small variation of the minority carrier densities at the edges of the transition region. The classical Boltzmann relation is in error by many orders of magnitude.

At forward biases the positions of the transition layer

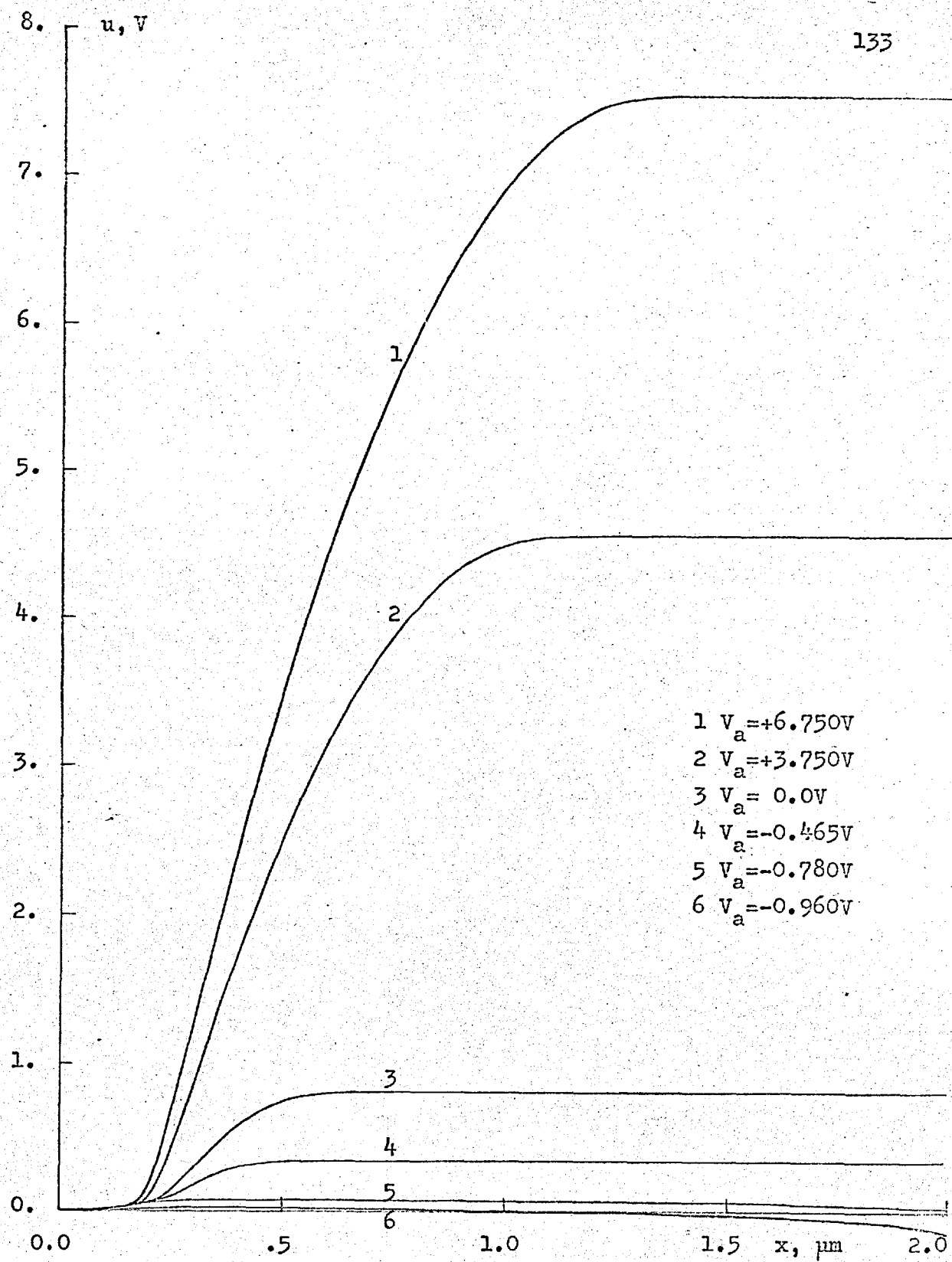


Fig.6.2

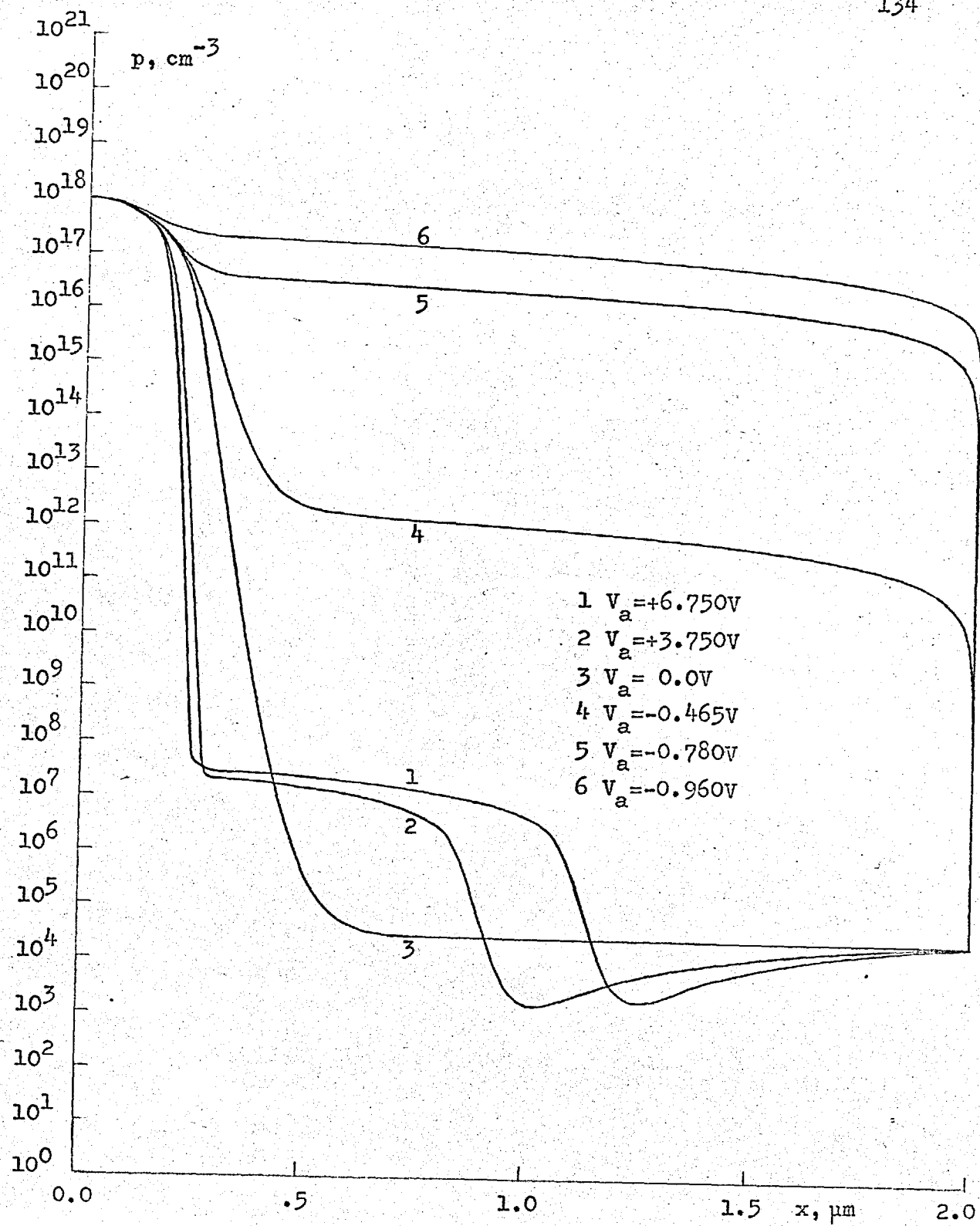


Fig.6.3

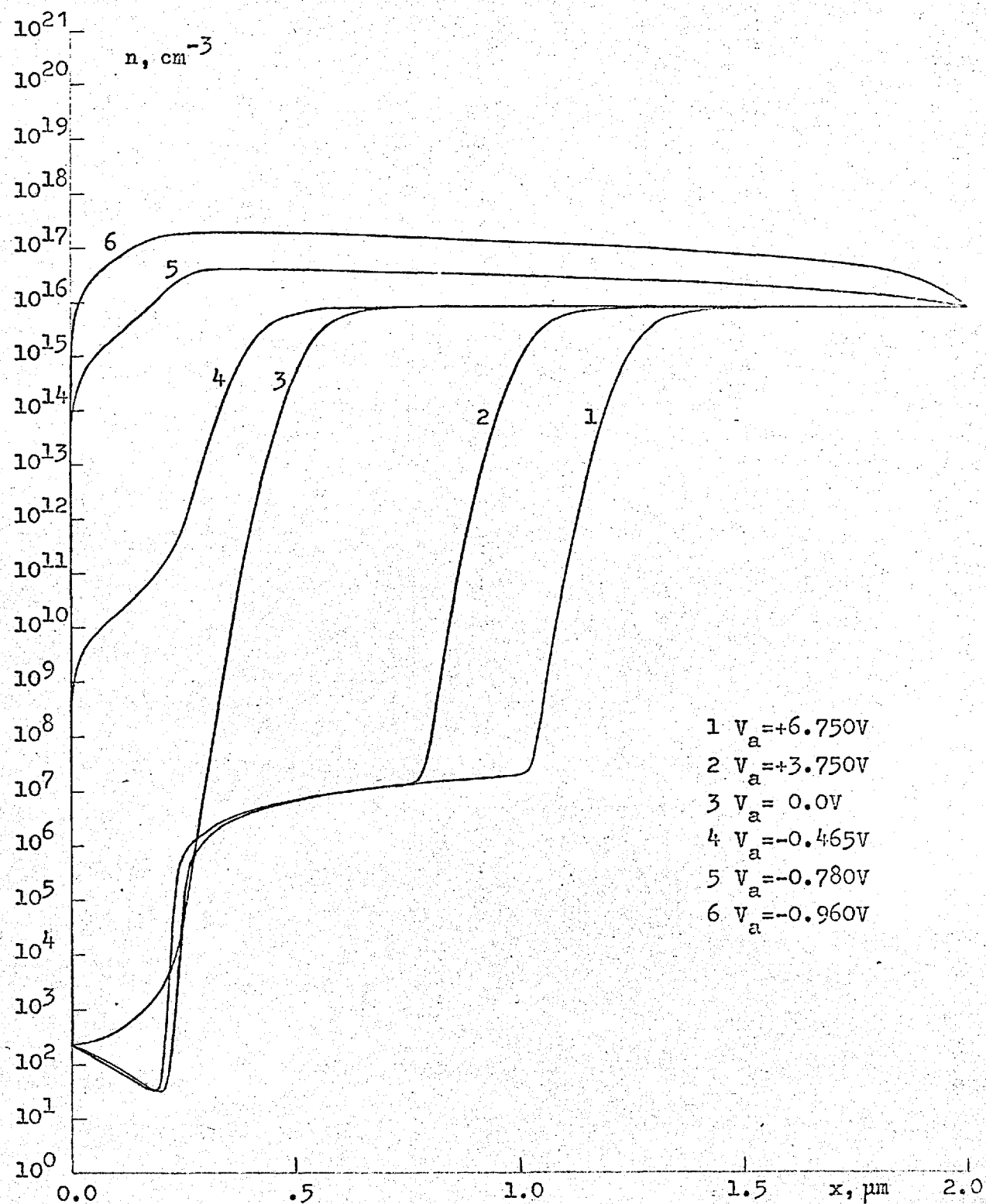


Fig.6.4

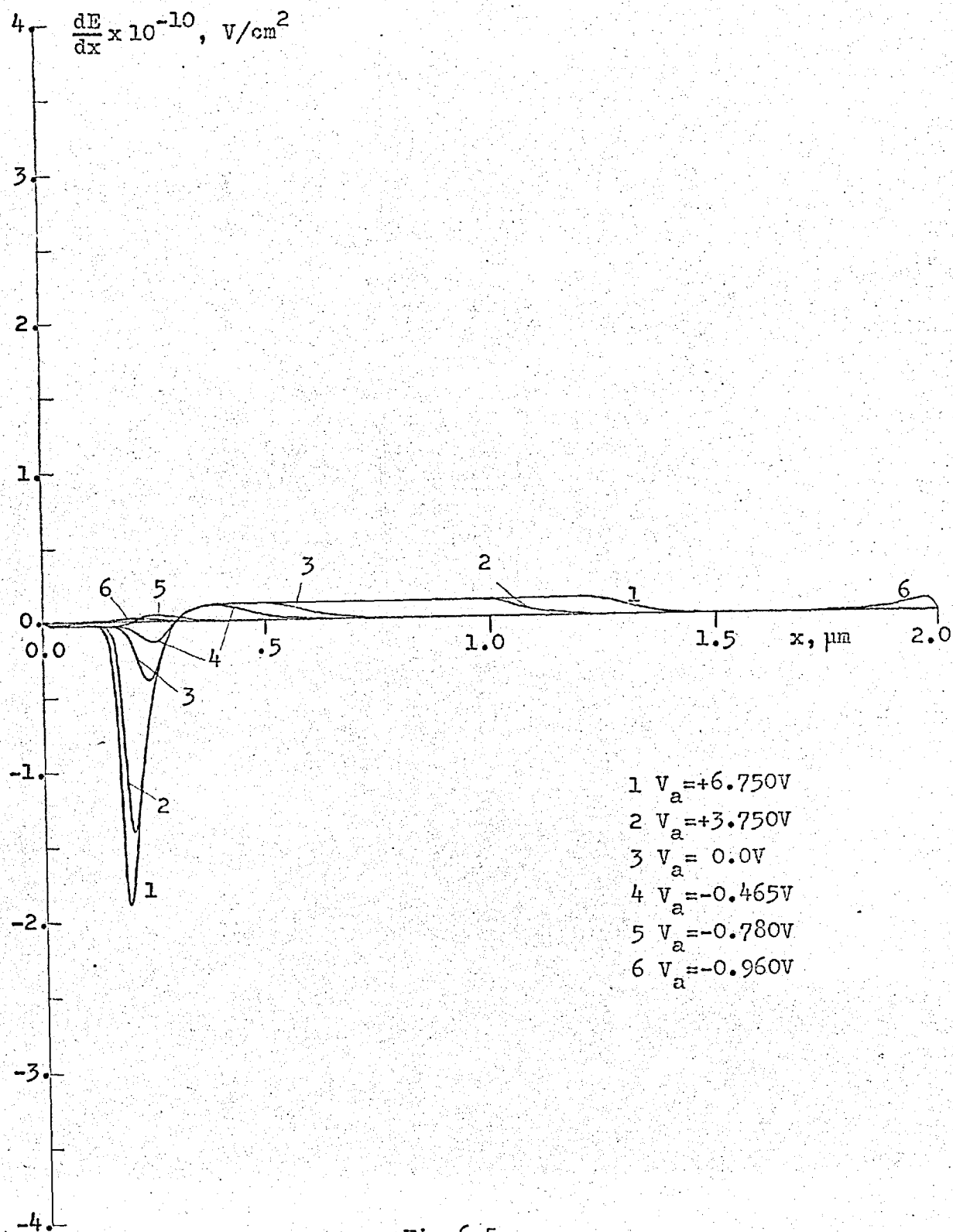


Fig.6.5

boundaries become uncertain. The eventual collapse of the space charge layer at high currents is accompanied by the charge build up in the vicinity of the contact of the low conductivity side. This follows as a consequence of the 'ohmic' contact assumption which prevents the conductivity modulation of this near-contact region. Considerable electric fields must rise to carry the current.

6.2.2 The terminal characteristics

The forward V-I characteristic of the device is depicted in Fig. 6.6 (full line). It exhibits the expected slopes at the low- and medium injections, and at very high currents the novel feature of the electron contribution to the total current (the ----- line) exceeding its hole counterpart (the dashed line). This can be interpreted through the higher electron mobility and the presence of considerable electric fields in the diode base.

The non-saturating reverse V-I characteristic is shown in Fig. 6.7 (note the difference in the ordinate scales for J_p and J_n).

The incremental capacitance, viewed at the external terminals of the device, is obtained with the aid of two successive solutions corresponding to two slightly different voltages applied at the terminals*. If Q is the total charge of one polarity (per-unit-area)

* The time constants associated with changing of the relevant quantities are neglected, thus a sufficiently low frequency is implied. A representation of the capacitive effects associated with a junction valid at high frequencies requires the knowledge of the time-dependent solutions of the junction transport equations.

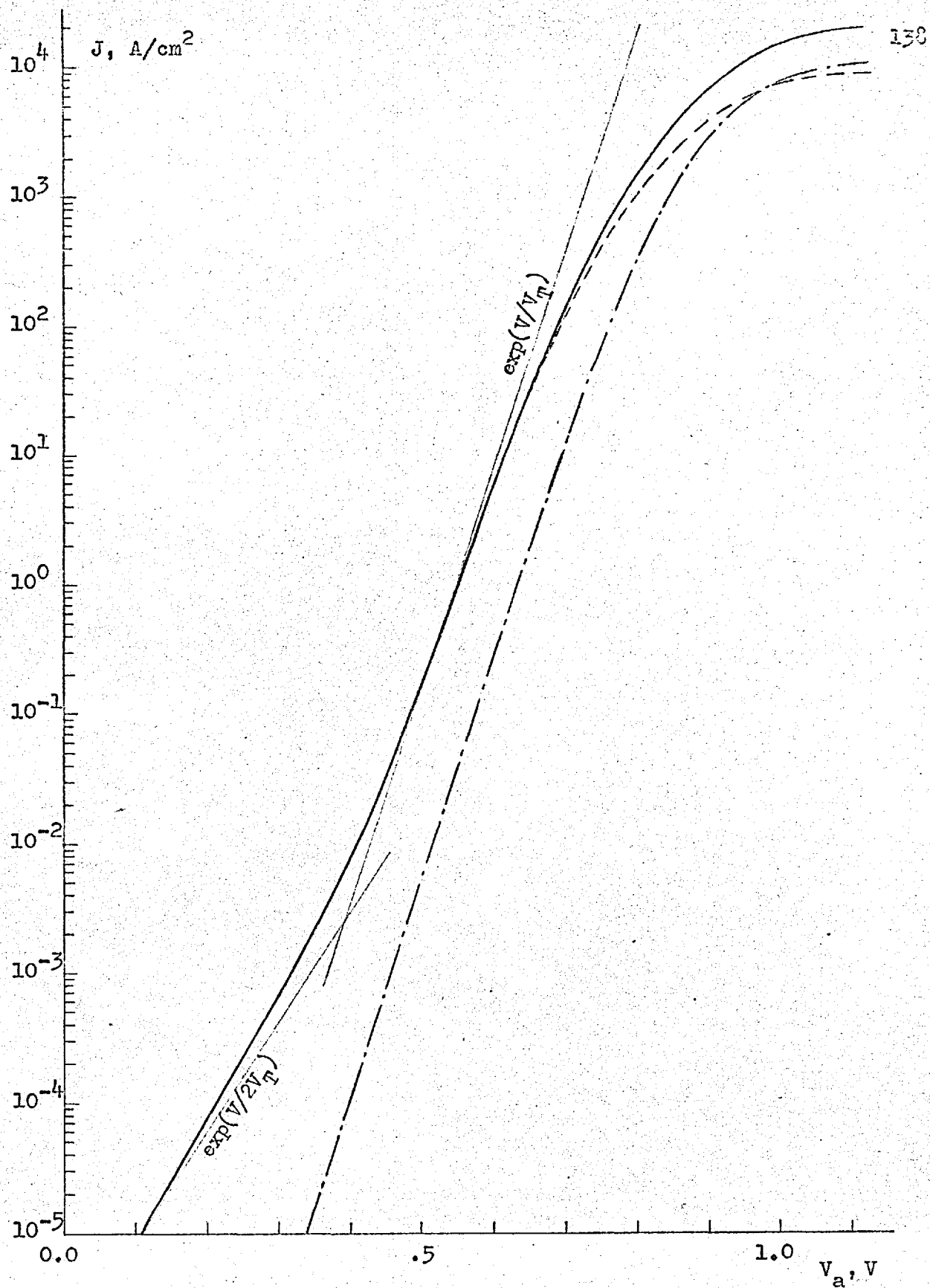


Fig.6.6

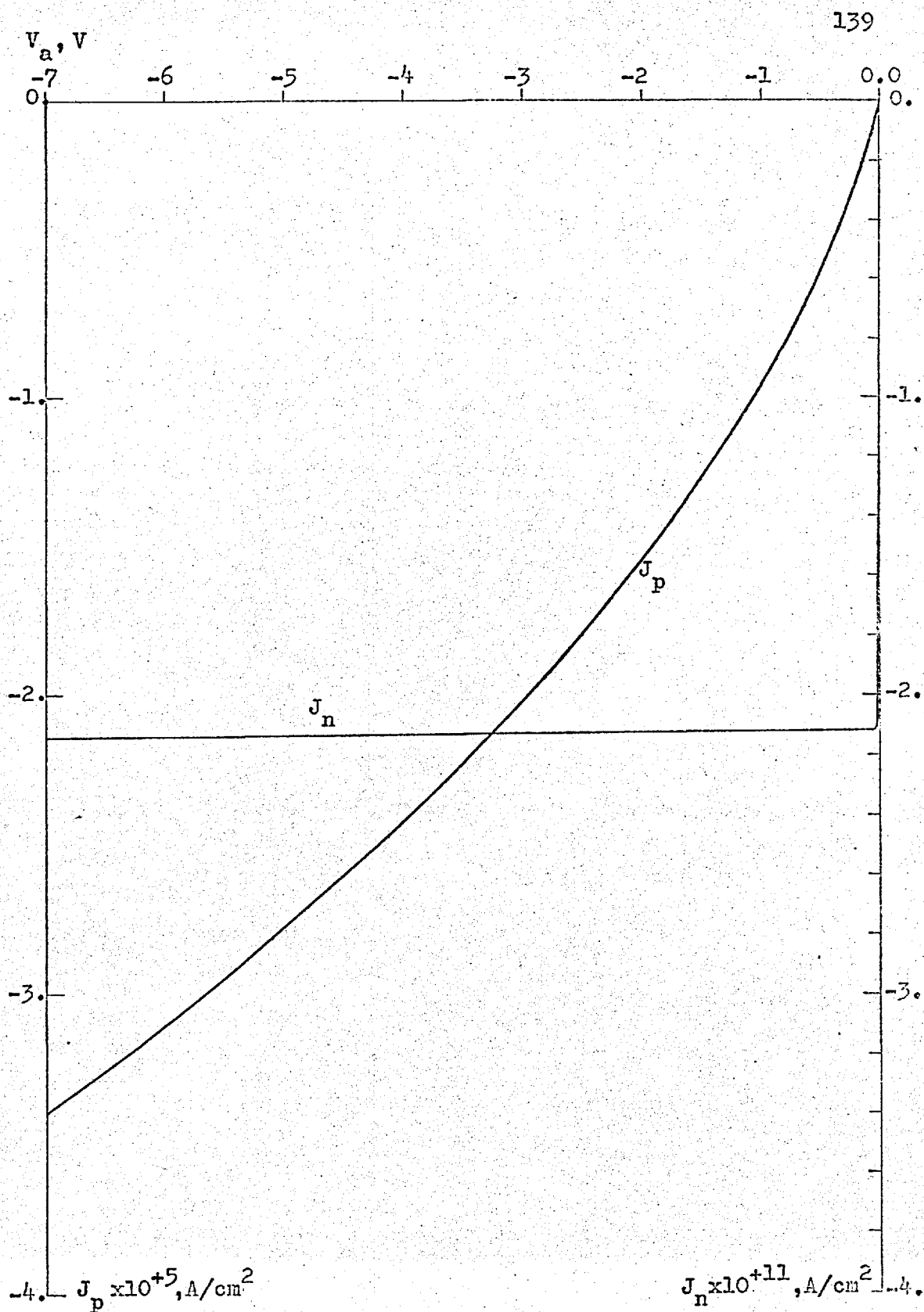


Fig.6.7

in the device, the incremental, per-unit-area capacitance, at a specified applied voltage V_a , is defined as

$$C(V_a) = \left| \frac{dQ}{dV} \right|_{V=V_a} \quad (6.2)$$

The total charge of one polarity is deducible from Poisson's equation by integrating it between the external contacts, $x = 0$ and $x = L$, i.e.

$$\int_0^L (p - n + N) dx = \frac{\epsilon}{q} (E(L) - E(0)). \quad (6.3)$$

Differentiation of (6.3) with respect to the applied voltage yields

$$\frac{d}{dV} \left(\int_0^L p dx \right)_{V=V_a} = \frac{d}{dV} \left[\int_0^L n dx + \frac{\epsilon}{q} (E(L) - E(0)) \right]_{V=V_a} \quad (6.4)$$

In terms of two successive solutions for p or n , the junction capacitance is

$$C(V_a) = \int_0^L \frac{|p - p_1|}{|V_a - V_{a1}|} dx = \left| \int_0^L \frac{n - n_1}{V_a - V_{a1}} dx + \frac{\epsilon}{q} \frac{E(L) - E_1(L) + E_1(0) - E(0)}{V_a - V_{a1}} \right|, \quad (6.5)$$

where $V_{a1} = V_a + \delta V$ and the subscript 1 denotes the solutions obtained at V_{a1} .

The per-unit-area junction capacitance given by (6.5) is plotted in Fig. 6.8 for the indicated range of reverse voltages. Also shown are the curves $1/C^2$ and $1/C^3$. The dashed line corresponds to $1/C^2$ curve for the uniformly doped $p + n$ junction of the same base doping. Although the $1/C^2$ curve obtained from (6.5) is almost linear, it differs from the

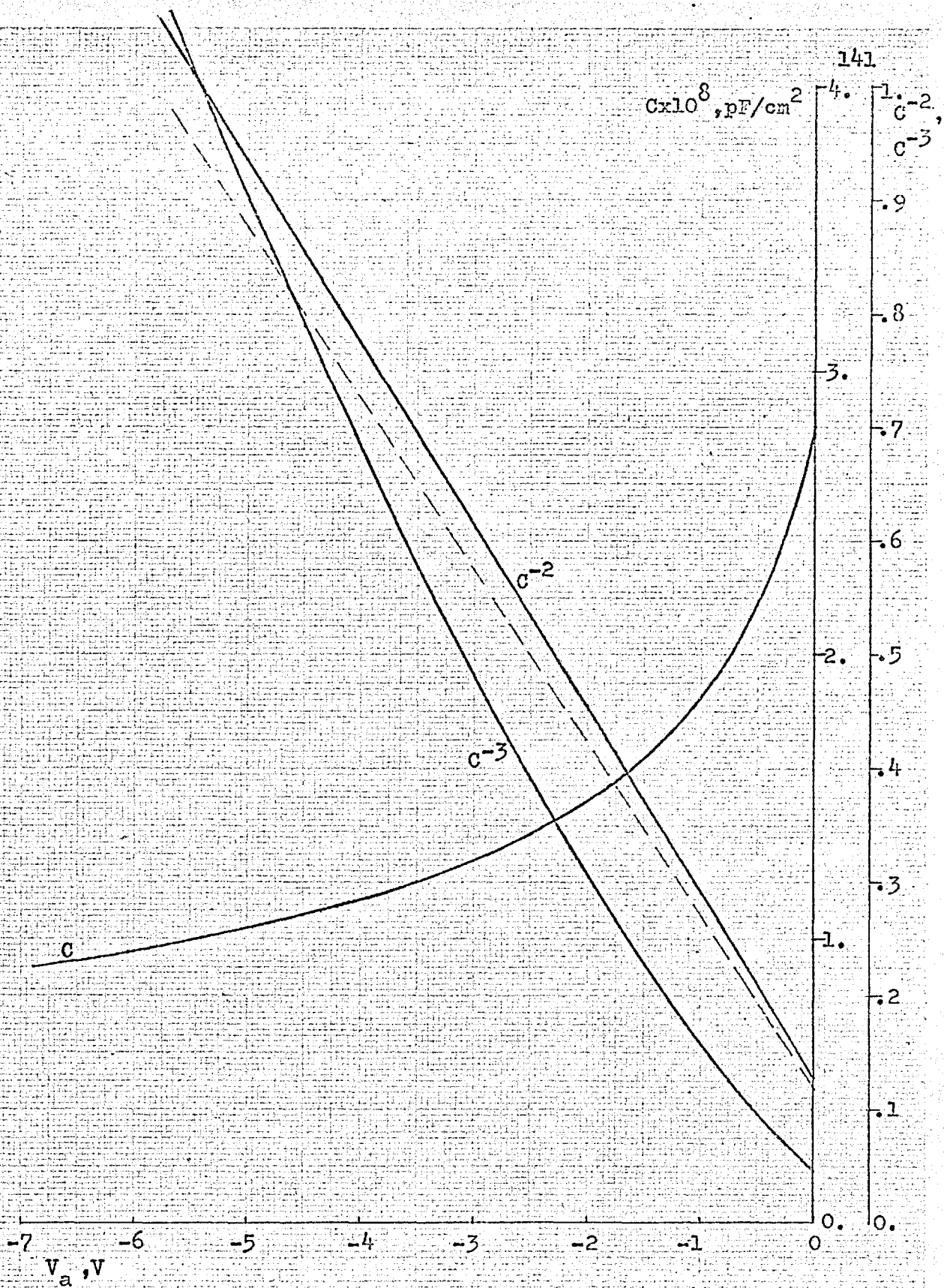


Fig.6.8

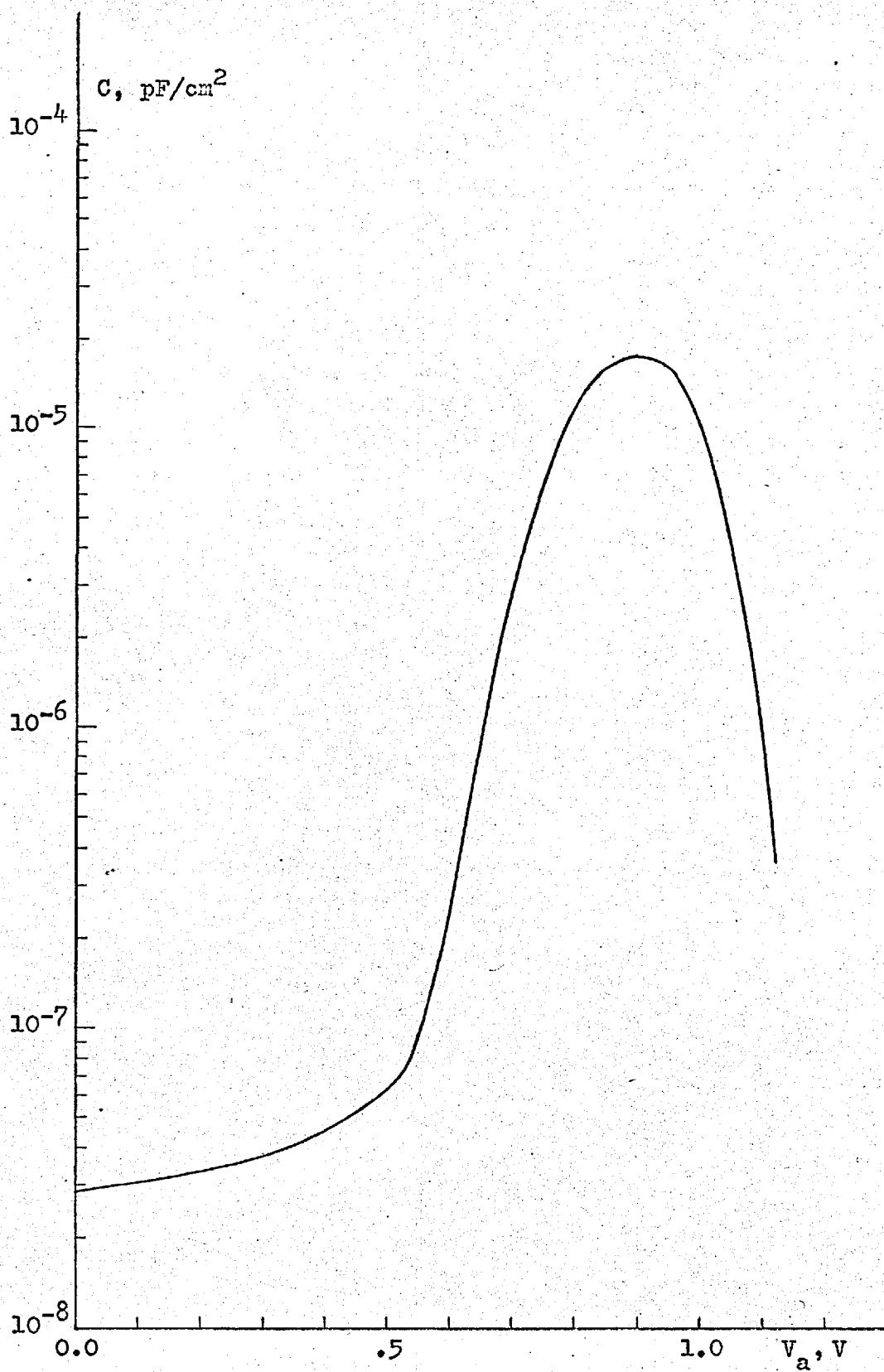


Fig.6.9

abrupt junction approximation in both the slope and the intercept at $V = 0$. The nonlinear $1/C^3$ curve shows that the linearly graded junction approximation of the profile of Fig. 6.1 also does not provide a good approximation for the capacitance computed by (6.5). The capacitance fall-off at very high currents displayed in Fig. 6.9 *accentuates* the tendency towards inductive behaviour of the device at large forward biases.

6.3 Selected one-dimensional calculations of MOS structures

The one-dimensional technique developed so far is inadequate for undertaking a systematic analysis of MOS devices which present themselves as at least two-dimensional systems. However, under suitable bias conditions some aspects of the behaviour of an MOS system can be described through convenient one-dimensional representations.

In the remaining part of this chapter an analysis of the channel conductance and gate capacitance of MOS transistors in the linear region is presented.

6.3.1 Input capacitance and transconductance of MOST's

The structure of an MOS n-channel transistor is shown schematically in Fig. 6.10.

Under conditions when V_D is small and $V_g \gg V_D$ the properties of the p-region between the two n^+ contacts could be considered

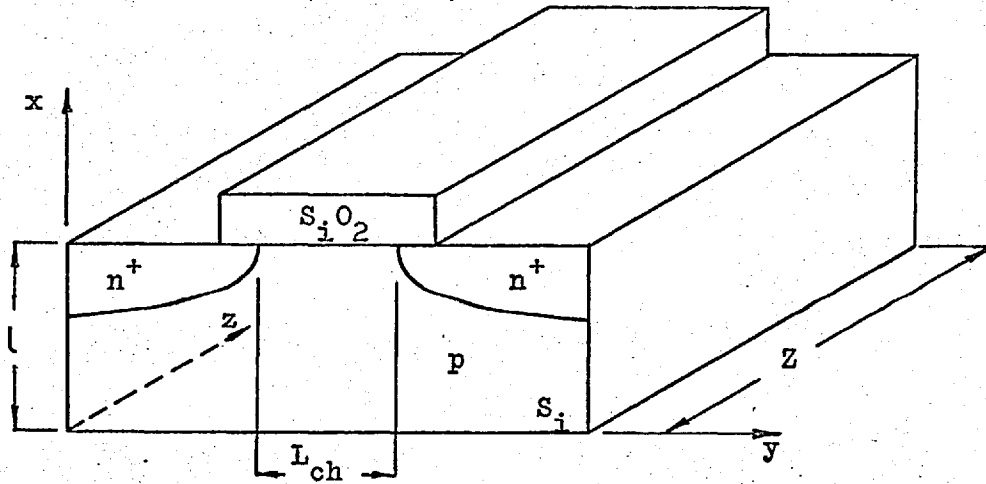


Fig. 6.10.

uniform along the z - and y -axes (see Fig. 6.10).

The conductance of the channel along L_{ch} is

$$g_{ch} = \frac{Z}{L_{ch}} \int_{x_i}^l q \mu_n n(x) dx, \quad (6.6)$$

where x_i is a suitably defined distance below the surface indicating the depth of penetration of the gate voltage (dominant contribution to the integral (6.6) comes from a narrow region just under the surface and the definition of x_i is not crucial. For the present purposes, it is convenient to assume $x_i = 0$). In terms of the electron per-unit-area charge induced by the gate voltage, Q_n , (6.6) can be written as

$$g_{ch} = \frac{Z}{L_{ch}} \mu_n Q_n \quad (6.7)$$

and the drain current is

$$I_D = \frac{Z}{L_{ch}} \mu_n Q_n V_D . \quad (6.8)$$

The transconductance is defined by

$$\epsilon_m = \frac{\partial I_D}{\partial V_g} = \frac{Z}{L_{ch}} \mu_n V_D \left(\frac{\partial Q_n}{\partial V_g} \right) . \quad (6.9)$$

The total gate capacitance at a voltage V_g is

$$C_g = \left| \frac{\partial Q_g}{\partial V_g} \right| , \quad (6.10)$$

where Q_g denotes the total charge at the gate. Define by Q_s the total charge per-unit-area in the silicon and by C_o the capacitance per-unit-area of the oxide layer. Then, starting from

$$V_g = V_s + \frac{|Q_s|}{C_o} , \quad (6.11)$$

the input capacitance is

$$C_g = \left| \frac{\partial Q_g}{\partial V_g} \right| = \left| \frac{\partial Q_s}{\partial V_g} \right| , \quad (6.12)$$

or using (6.11)

$$C_g = \frac{C_o C_s}{C_o + C_s} , \quad (6.13)$$

where $C_s = \left| \frac{\partial Q_s}{\partial V_s} \right|$ is the capacitance per-unit-area of the surface space charge region in the semiconductor and V_s is the semiconductor

surface potential*.

The maximum frequency of operation of an MOST is

$$f_T = \frac{g_m}{2\pi C_g}, \quad (6.14)$$

or in terms of the quantities defined so far

$$f_T = \frac{\mu_n V_D}{L_{ch}^2} \left| \frac{\partial Q_n}{\partial V_g} \right| \left(1/C_o + 1/\left| \frac{\partial Q_s}{\partial V_s} \right| \right). \quad (6.15)$$

By calculating Q_n and Q_s as

$$Q_n = \int_0^l q n(x) dx \quad (6.16)$$

and

$$Q_s = \int_0^l q(p-n+N) dx \quad (6.17)$$

the quantities $\frac{\partial Q_n}{\partial V_g}$ and $\frac{\partial Q_s}{\partial V_s}$ are obtained, similarly to (6.5), from the solutions which correspond to two slightly different gate voltages.

6.3.2 Graded channel MOST structures

If the substrate doping in the vicinity of the oxide-semiconductor interface is heavier than in the bulk of the semiconductor material, a built-in field results, aiding the flow of minority carriers away from the surface. Consequently, the number of minority carriers attracted to the surface by the gate voltage is slightly larger compared to the one which would have resulted if the substrate was uniformly

* Absence of any contact potential or work function difference between metal and semiconductor is assumed.

doped. This, in turn, produces a larger increase in the conductivity of the channel, i.e. a larger transconductance. Since the total gate capacitance beyond the turn-on voltage saturates very quickly at C_o , an increase of f_T should follow.

On the basis of this argument the technique of chapter 5 is applied to calculate the quantities defined in the previous section for a series of MOS structures*. The impurity profiles of the structures in the direction perpendicular to the oxide-semiconductor interface are shown in Fig. 6.11.

The transconductance and gate capacitance, defined respectively by (6.9) and (6.10), are computed as functions of the gate voltage. The results are shown in Fig. 6.12.

The cut-off frequencies for each of the calculated profiles are displayed in Fig. 6.13. Notable increases in f_T confirm the validity of the original qualitative argument.

Calculation of these parameters at arbitrary bias conditions requires the development of more powerful schemes, capable of solving two-dimensional problems. Such a scheme is proposed in chapter 8. It can only be concluded here that an improvement of the frequency response of MOS transistors in the linear region can be achieved by doping the substrate more heavily near the silicon-silicon-oxide

*In these calculations both current densities are zero thus greatly increasing the efficiency of the calculations.

$$1- N(x)=-10^{16}$$

$$2- N(x)=-10^{16} \operatorname{erfc}\left(\frac{1.5 \cdot 10^{-4}-x}{1.28965 \cdot 10^{-4}}\right)$$

$$3- N(x)=-\left(9 \cdot 10^{15} \operatorname{erfc}\left(\frac{1.5 \cdot 10^{-4}-x}{4 \cdot 10^{-5}}\right)+10^{15}\right)$$

$$4- N(x)=-\left(9 \cdot 10^{15} \operatorname{erfc}\left(\frac{1.5 \cdot 10^{-4}-x}{1.6 \cdot 10^{-5}}\right)+10^{15}\right)$$

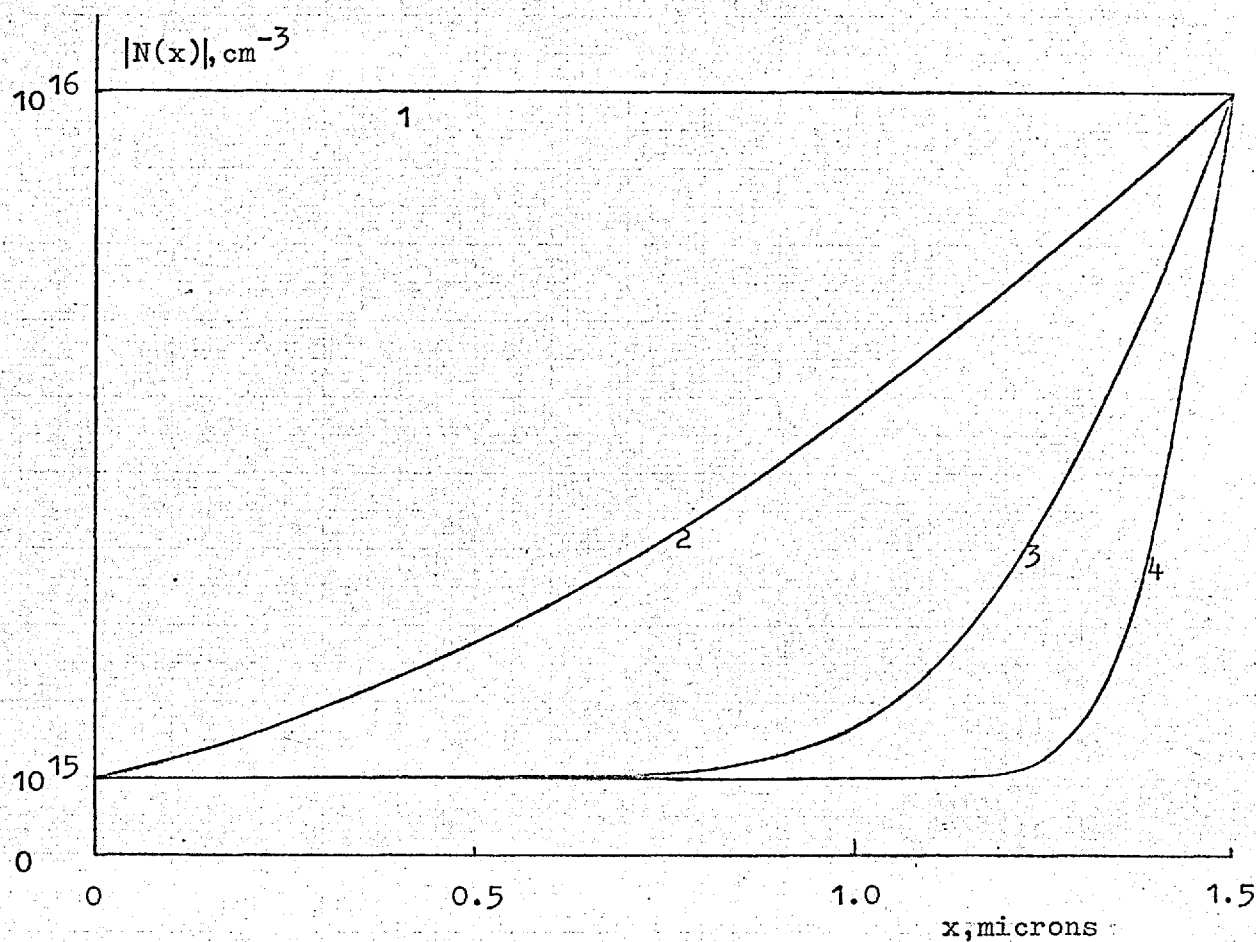


Fig.6.11

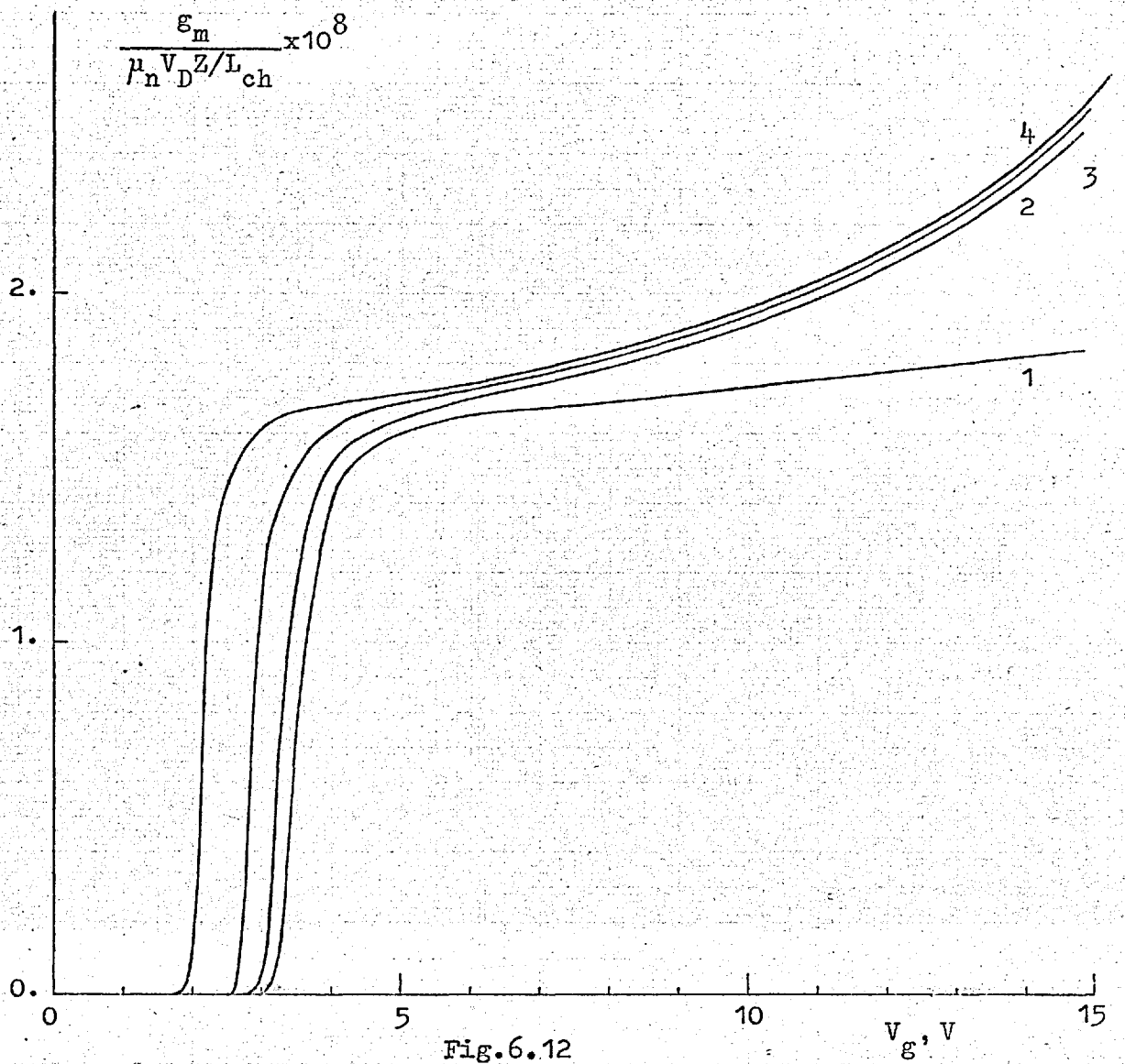
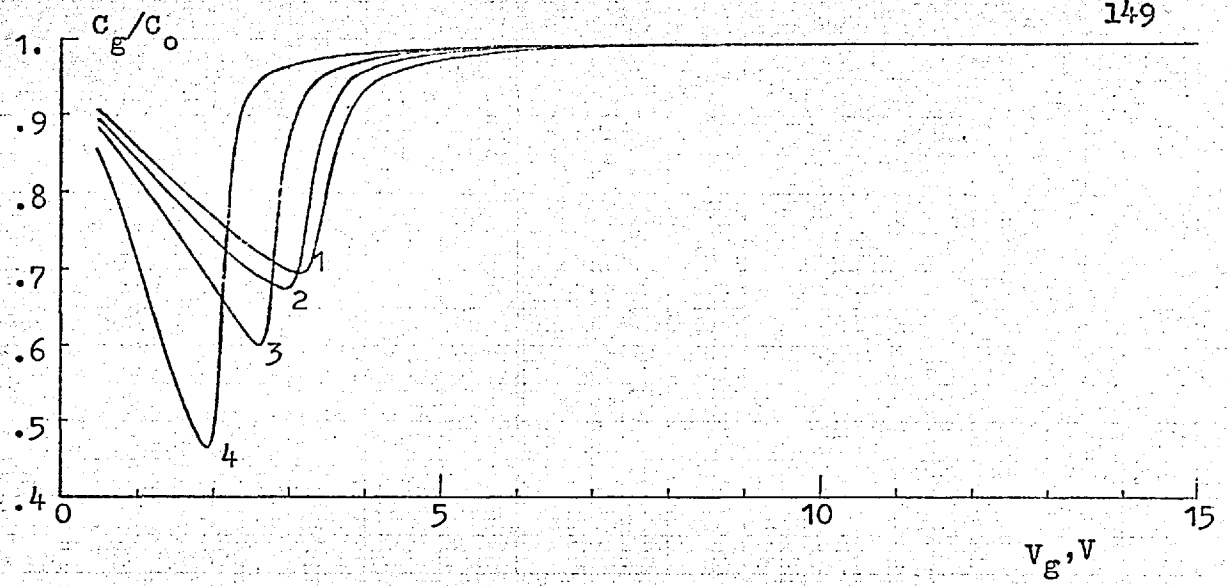


Fig. 6.12

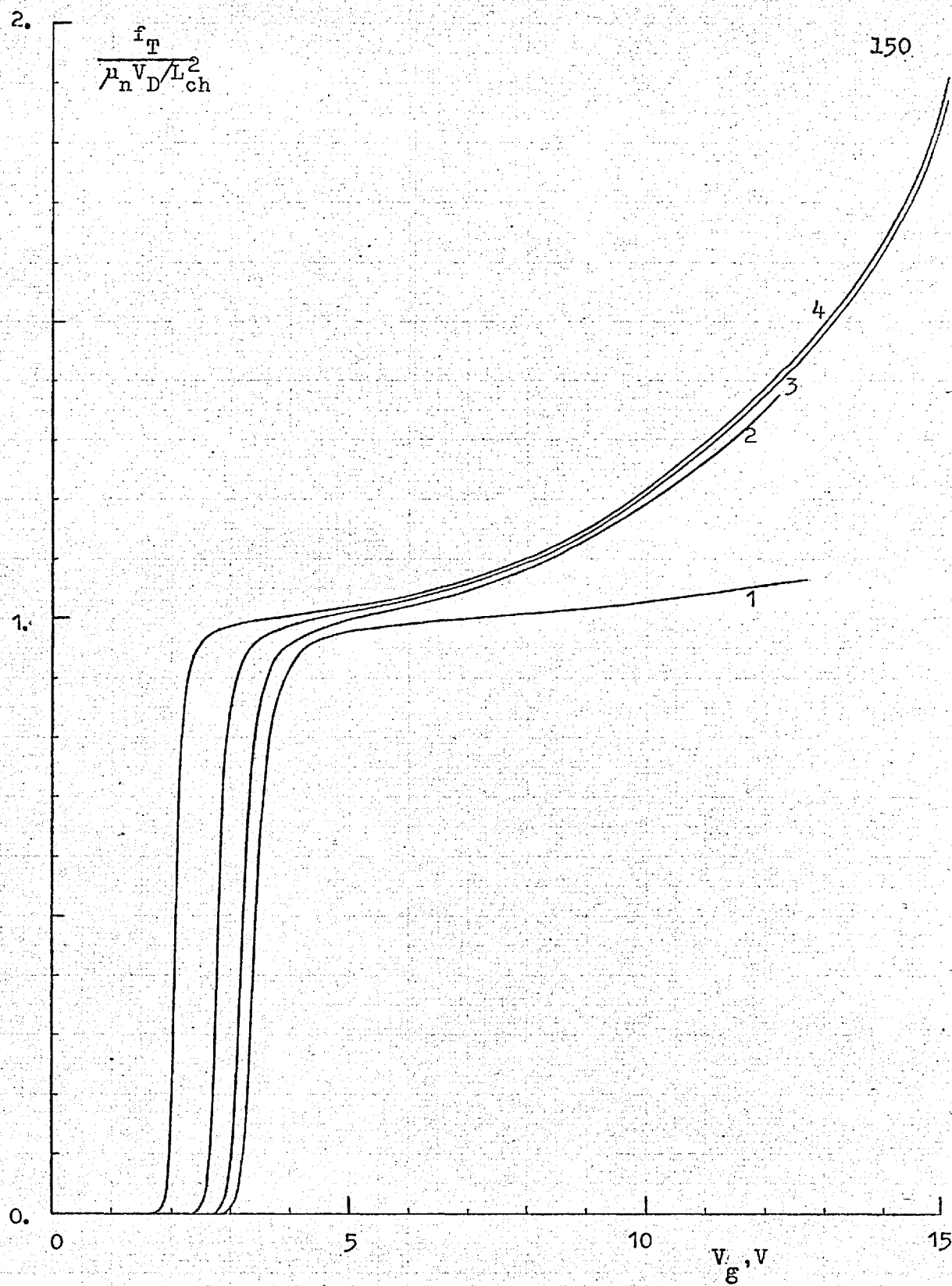


Fig.6.13

interface than in the bulk of the semiconductor material.

6.4 Accuracy of the results

Relatively complicated relations between the variables involved in these calculations could make unrealistic an estimation of the accuracy of the results through the error bounds derived in Appendix 7. Alternatively, the achieved accuracy may be judged by testing the consistency of the computed results with a set of relations derived from the fundamental system (1.1)-(1.5). Examples of such relations are $pn = n_i^2$ at zero bias conditions, the double equality (6.5), etc. Comparing the electrostatic field obtained from (1.7) to the one that follows from integrating the net space charge (equation 1.6)) is another possibility for estimating the accuracy of the final results. The distributions of the relevant quantities presented in this chapter are obtained with a relative error smaller than 10^{-5} .

CHAPTER 7

THE NUMERICAL ANALYSIS OF DOUBLE-DIFFUSEDTRANSISTOR STRUCTURES7.1 Introduction

Following Gummel's original paper¹⁰⁵ there have been several attempts to use the same approach in computing the numerical solutions for the bipolar transistor structures. However, having selected the same set of variables as Gummel, neither Caughey¹⁴⁶ nor Ghosh et al.¹⁴⁷ could calculate the solutions which correspond to the usual collector-base biases.

In this chapter the technique developed in chapter 5 for dealing with reverse biased junctions is applied to the collector-base junction of bipolar transistors. As a result, a sound numerical algorithm is developed, capable of solving arbitrary transistor structures under arbitrary bias conditions. The algorithm is demonstrated by computing the solutions for a double-diffused high frequency transistor assuming more realistic bias conditions at the collector.

7.2 The elements of the analysis

The expressions (5.4)-(5.9) for the mobile charge carriers and the algorithm of section 5.2.3 for correcting the potential distribution do not depend upon the impurity profile of a device. The set of boundary conditions, however, must be modified to complement the mathematical description of each particular problem.

For a transistor structure, the boundary conditions for the mobile charge carriers are, similarly to those described by (5.1), specified at the external contacts of a device. The potential boundary conditions are more complicated than (5.1e) and the choice of the potential reference is now subject to some preliminary considerations.

Input data for the calculations are:

- doping profile of the transistor;
- mobility variation with doping and electric field;
- generation-recombination law;
- applied emitter and collector biases;
- a potential guess.

Doping profile of the double-diffused transistor which is calculated in this chapter is defined first and then the specification of the boundary conditions and their incorporation in the general description of the transistor problem are resolved.

7.3 Doping profile of the analysed transistor

Successive diffusions of e.g. p- and n-type impurities into an n-type silicon wafer produce the n-p-n configuration, with junctions occurring where complete compensation of impurities takes place. Ideally, the impurity profile of a double-diffused device is composed of two error functions or of two Gaussian functions (or of these two combined in a way determined by the order of execution of the diffusions employed). Practical diffusions inevitably encounter the deviations from the ideal theory outlined in Appendix 8. High sensitivity of the diffused profiles to the physical conditions that exist during a particular process invariably leads to the structures sufficiently peculiar to that process.

The modifications of the base diffusion owing to the out-diffusion and redistribution of impurities during thermal oxidation are further complicated by the "emitter-dip" effect which has no mathematical representation as yet¹⁴³. Very high densities of the diffusants involved in emitter diffusions cause the departures from the ideal theory, additional to those attributable to the field-aided diffusion¹²⁵. Detailed study of the modifications pertaining to the practical double-diffused profiles is beyond the scope of this work. The profile of the double-diffused high frequency transistor which is analysed in this chapter is based partly on the empirical data taken to be a reasonable approximation of the practical transistors¹⁴⁴.

The n-p-n profile considered hereafter is described analytically

by the following equations:

$$N(x) = \begin{cases} 10^{21} \operatorname{erfc}(x/1.33 \cdot 10^{-5}) - 5.9157698 \cdot 10^{18} + 8.0 \cdot 10^{15}, & x \leq x_a \\ 10^{21} \operatorname{erfc}(x/1.33 \cdot 10^{-5}) - 10^{20} \operatorname{erfc}(x/1.625 \cdot 10^{-5}) + 8 \cdot 10^{15}, & x > x_a \end{cases} \quad (7.1)$$

where N is in cm^{-3} , x in cm and $x_a = 2.5 \cdot 10^{-5} \text{ cm}$. The complete profile is shown in Fig. 7.1.

7.4 The boundary conditions

The emitter and collector contacts are normally situated well outside the active region of a device. This is conveniently expressed by demanding that at these contacts, $x = 0$ and $x = L$, the carrier equilibrium and space charge neutrality prevail. Then, recalling (2.1), the boundary values for the mobile charge carrier densities are

$$n(0) = \frac{N(0)}{2} \left[1 + \left(1 + \frac{4n_i^2}{N(0)^2} \right)^{\frac{1}{2}} \right], \quad p(0) = \frac{n_i^2}{n(0)}; \quad (7.2a)$$

$$n(L) = \frac{N(L)}{2} \left[1 + \left(1 + \frac{4n_i^2}{N(L)^2} \right)^{\frac{1}{2}} \right], \quad p(L) = \frac{n_i^2}{n(L)}. \quad (7.2b)$$

The approach in choosing the reference for the boundary potentials resides upon the fact that the equilibrium majority carrier distribution within a part of the transistor base is very little affected

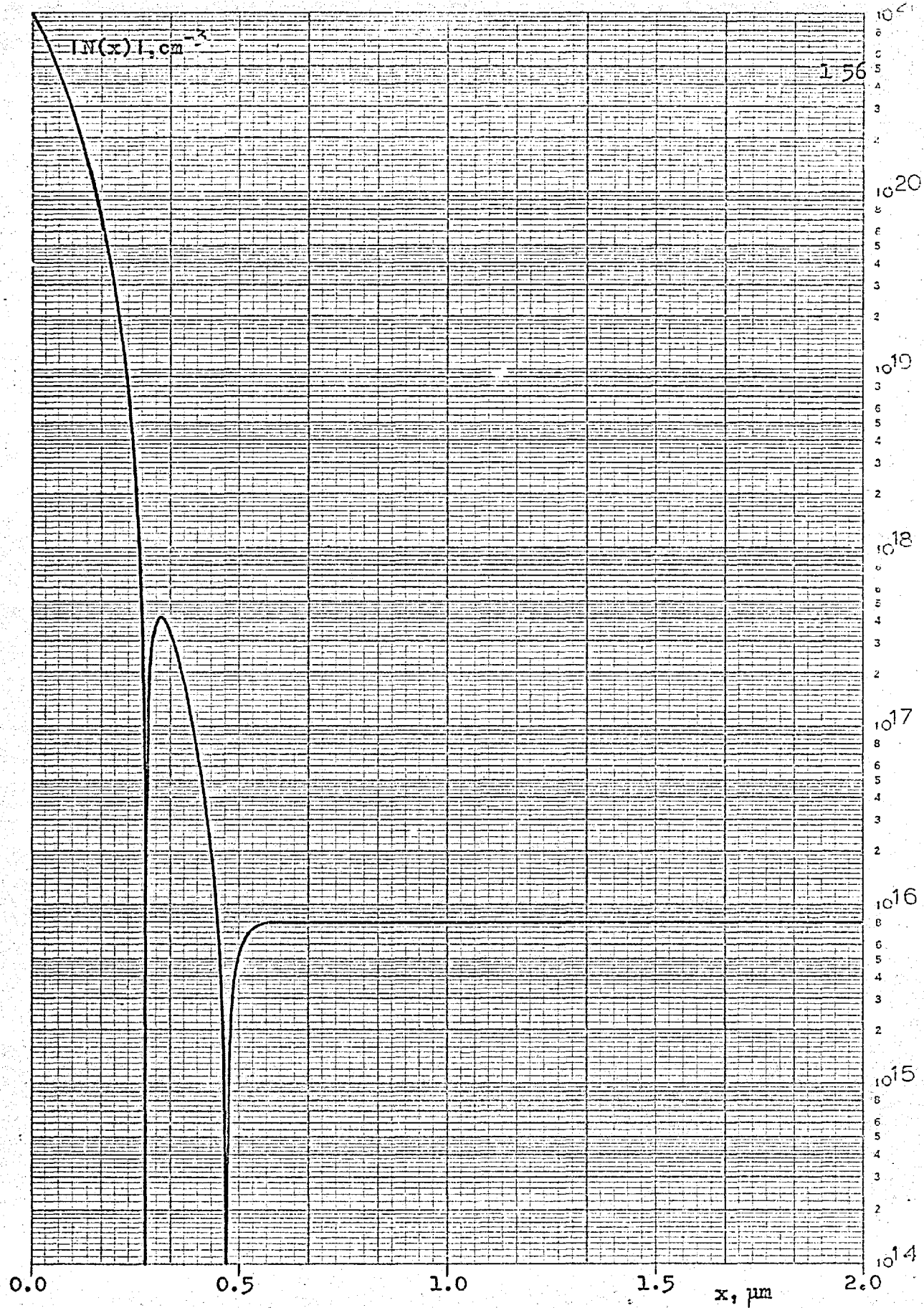


Fig.7.1

by the applied biases. This permits defining the applied voltages as the total potential steps minus built-in voltages with respect to a point in this part of the base.

If the base resistivity is sufficiently lower from the one of the collector body, the "penetration depth" of the collector reverse bias into the base is very small. Furthermore, in the region after the base potential minimum (an n-p-n configuration is under consideration) transport of the charge carriers is substantially drift-controlled. The base majority carrier density in this part is essentially unchanged up to very high current levels. The position of this region can be easily localized from the thermal equilibrium solutions which can be computed assuming an arbitrary potential reference. Selecting the reference point within this domain is not critical. (At extremely high current densities when this choice may become significant, the lateral base current also becomes significant and the whole of this one-dimensional analysis is inadequate).

Let $x=x_m$ be the position of the reference point. Then

$$u(x_m) = 0. \quad (7.3)$$

The boundary potentials at the contacts are

$$u(0) - u(x_m) = V_{oe} + V_{EB} \quad (7.4)$$

$$u(L) - u(x_m) = V_{oc} + V_{CB} \quad (7.5)$$

The "built-in" voltages V_{oe} and V_{oc} are calculated with respect to x_m using the thermal equilibrium value of $p(x_m)$ and the $p(0)$ and $p(L)$ given by (7.2).

The conditions (7.3)-(7.5) are formulated for computing the transistor common-base characteristics. By shifting the zero potential level to $x=0$ or $x=L$, similar conditions follow for the common-emitter or common-collector calculations respectively.

7.5 The expressions for the charge carrier densities and constant current densities

Under active bias conditions the electron current density in an n-p-n structure is a negative quantity (the geometry of Fig. 7.1 is under consideration). A rearrangement of (5.5) is needed in order to avoid the accuracy problem discussed in section 5.3.1. Applying the same method as in 5.3.1, the modified expression for $n(x)$ is

$$n(x) = \exp\left(\frac{u(x)}{V_T}\right) \left(n(L) \exp\left(-\frac{u_L}{V_T}\right) - \int_x^L \frac{\exp(-u(t)/V_T)}{qD_n(t)} J_n(t) dt \right). \quad (7.6)$$

Analogously to (5.9) the constant electron current density is

$$J_{no} = \frac{n(L) \exp(-u_L/V_T) - n(0) \exp(-u_0/V_T) + \int_0^L \frac{\exp(-u(t)/V_T)}{qD_n(t)} \left(\int_0^t qU(t') dt' \right) dt}{\int_0^L \frac{\exp(-u(t)/V_T)}{qD_n(t)} dt}, \quad (7.7)$$

except that now u_0 and u_L have the meanings different from those in (5.9).

The expressions for the hole density and the constant hole current density follow directly from (5.4) and (5.8) respectively. However, since the presence of a zone (strictly speaking a single point x_m)

of undisturbed hole density distribution in the base has been postulated, two separate domains, the emitter domain $0 \leq x \leq x_m$, and the collector domain $x_m \leq x \leq L$, must be considered.

7.5.1 Emitter domain, $0 \leq x \leq x_m$

From (5.4) and (5.8) the hole density and the emitter-controlled constant hole current density are

$$p(x) = \exp\left(-\frac{u(x)}{V_T}\right) \left(p(0) \exp\left(\frac{u_0}{V_T}\right) - \int_0^x \frac{\exp(u(t)/V_T)}{qD_p(t)} J_p(t) dt \right), \quad (7.8)$$

and

$$J_{pe} = \frac{p(0) \exp(u_0/V_T) - p(x_m) - \int_0^{x_m} \frac{\exp(u(t)/V_T)}{qD_p(t)} \left(\int_0^t qU(t') dt' \right) dt}{\int_0^{x_m} \frac{\exp(u(t)/V_T)}{qD_p(t)} dt}. \quad (7.9)$$

The hole current density in this domain is

$$J_p(x) = J_{pe} + q \int_0^x U(t) dt. \quad (7.10)$$

7.5.2 Collector domain, $x_m \leq x \leq L$

Starting from the same basic equations as in the section above, the hole density and the collector-controlled constant hole

current density are

$$p(x) = \exp\left(-\frac{u(x)}{V_T}\right) \left(p(x_m) - \int_{x_m}^x \frac{\exp(u(t)/V_T)}{qD_p(t)} J_p(t) dt \right), \quad (7.11)$$

and

$$J_{pc} = \frac{p(x_m) - p(L) \exp(u_L/V_T) - \int_{x_m}^L \frac{\exp(u(t)/V_T)}{qD_p(t)} \left(\int_0^t qU(t') dt' \right) dt}{\int_{x_m}^L \frac{\exp(u(t)/V_T)}{qD_p(t)} dt} \quad (7.12)$$

The hole current density in this domain is

$$J_p(x) = J_{pc} + q \int_0^x U(t) dt. \quad (7.13)$$

7.5.3 Terminal current densities

The emitter and collector currents are made up of electron and hole contributions which combine, at the boundaries $x=0$ and $x=L$, in the currents that appear in the external circuits. The emitter current density is

$$J_E = J_n(0) + J_p(0) = J_{no} + J_{pe}. \quad (7.14)$$

The collector current density is

$$J_C = J_n(L) + J_p(L) = J_{no} + J_{pc}. \quad (7.15)$$

The base current density is

$$J_B = J_E - J_C = J_{pe} - J_{pc} \quad (7.16)$$

7.6 The electrostatic potential and iteration loop

Since the electrostatic potential is specified at three points, namely at $x = 0$, $x = x_m$ and $x = L$, the algorithm of section 5.2.3 is applied to the emitter domain and the collector domain separately. The corresponding boundary values for the potential correction δu are now: $\delta u(0) = \delta u(x_m) = \delta u(L) = 0$.

The complete procedure involves the following steps:

- a guess for the potential distribution is made;
- the charge carrier distributions and the current densities within the respective regions are calculated employing (7.6)-(7.13);
- The algorithm of section 5.2.3 is applied to the emitter and collector domains separately to obtain an improved potential distribution.

The last two steps are alternately performed until the solutions are obtained to a required accuracy.

The convergence of this iterative process is subject to the conditions derived in section 5.2.4. From (5.31) and (5.36) it is evident that the more heavily doped emitter domain must be processed using smaller discretization steps compared to the ones that may be employed in the collector domain.

7.7 Modifications pertaining to reverse collector biases

The equations derived for the collector domain must be modified in order to avoid the numerical difficulties of the type discussed in section 5.3.2. For that purpose the potential variation across the collector domain is divided in the sections: $u(x_m) - u_{r1}, u_{r1} - u_{r2}, \dots, u_{r,m-1} - u_L$, not necessarily of the same size but such that $|u_{r,k} - u_{r,k+1}| \leq K_m V_T$, where K_m is a constant restricted by the condition that $\exp(\pm K_m)$ does not exceed the permissible range (K_m , of course, depends upon the machine which is employed for the calculations). Schematically this is shown in Fig. 7.2. With the number and the sizes of the potential sections selected, the technique of shifting the reference values $u_{r,k}$, $p_{r,k}$ and $n_{r,k}$ during the process of computing $p(x)$ and $n(x)$ is analogous to the one described in section 5.3.2. Hence the equations (7.6) and (7.11) in the k -th potential section of the collector domain become

$$n(x) = \exp((u(x) - u_{r,k+1})/V_T) (n_{r,k+1} - \int_x^{x_{r,k+1}} \frac{\exp((u_{r,k+1} - u(t))/V_T)}{qD_n(t)} J_n(t) dt), \quad (7.17)$$

$$p(x) = \exp((u_{r,k} - u(x))/V_T) (p_{r,k} - \int_{x_{r,k}}^x \frac{\exp((u(t) - u_{r,k})/V_T)}{qD_p(t)} J_p(t) dt). \quad (7.18)$$

Calculating the constant current densities J_{no} and J_{pc} , although in principle follows the technique discussed in 5.3.2, involves some additional features because of the different form of potential distribution in this case.

The definite integrals in (7.7) are evaluated only between $x=0$

losing the accuracy of integration due to the saturating effect*.

This gives the following expression for J_{no}

$$J_{no} = \frac{-n(o)\exp(-u_o/V_T) + \int_0^{x_m} \frac{\exp(-u(t)/V_T)}{qD_n(t)} J_{rg}(t) dt - \int_{x_{r1}}^{x_m} \frac{\exp(-u(t)/V_T)}{qD_n(t)} J_{rg}(t) dt}{\int_0^{x_m} \frac{\exp(-u(t)/V_T)}{qD_n(t)} dt - \int_{x_{r1}}^{x_m} \frac{\exp(-u(t)/V_T)}{qD_n(t)} dt}, \quad (7.19)$$

where $J_{rg}(x) = \int_0^x qU(t)dt.$

The expression (7.12) for calculating J_{pc} is first normalized with respect to $\exp(u_L/V_T)$. It is obvious that the required integrations are carried out only over the part $x_{r1} - L$, which is indicated in full

* The saturating effect is best exposed if numerical integration of a constant function $f(x)=f_o$, using a constant integration step length Δx , is considered. It is easy to visualize that after certain distance x_s in the interval of integration (a,b) , say, the ratio $f_o \Delta x / (f_o(x_s - a))$ may fall out of the permissible range. As a result the total contribution to the integral from $(b - x_s)$ is lost. The integral thus saturates at $f_o(x_s - a)$. The problem can be resolved by splitting (a,b) into several parts and summing up the results of their individual integrations.

lines in Fig. 7.2. The collector-controlled constant hole current density is *

$$J_{pc} = \frac{-p(L) - \int_{x_{ri}}^L \frac{\exp((u(t)-u_L)/V_T)}{qD_p(t)} J_{rg}(t) dt}{\int_{x_{ri}}^L \frac{\exp((u(t)-u_L)/V_T)}{qD_p(t)} dt} \quad (7.20)$$

7.8 Limitations in the collector domain analysis

At very high current densities, or at moderately high current densities and very short limiting lifetimes of the charge carriers, the recombination current density in the collector domain becomes quite significant. The overwhelming contributions to this current density must come from the emitter and base, thus in $x_{ri} - L$ the current density J_{rg} is essentially constant, equal to $J_{rg}(L)$. The second term on the right hand side of (7.20) becomes considerably larger than $p(L)$, giving the limiting value for the collector-controlled constant hole current density

$$J_{pc} \approx - \int_0^L qU(t) dt = -J_{rg}(L). \quad (7.21)$$

* V_{CB} is assumed sufficiently large that $p(x_m)\exp(-u(L)/V_T)$ is negligibly small. Otherwise (7.12) applies.

Under conditions when this limit is approached, the influence of the local round-off error in calculating $J_p(x)$ becomes noticeable. A direct consequence is the loss of accuracy in computing $p(x)$ over the part of the collector next to the external contact. Increasing the precision in calculating the relevant quantities is necessary to avoid this problem. Fortunately, in reasonably extrinsic collectors the contribution of this "tail" of the hole density distribution to the terminal properties of a device is negligible. Considering the increases in the complexity of the program, storage requirements, and running times, the introduction of these double-precision calculations cannot be justified. (In the calculations presented in this chapter no attempt is made to increase the precision of the collector domain calculations. FORTRAN IV version of the computer program for calculating the structure of Fig. 7.1 is given in Appendix 9).

7.9 The numerical results for the structure of Fig. 7.1

The steady-state calculations discussed so far yield directly the transistor d.c. characteristics. Since the internal distributions are also known, the results contain information pertinent to a.c. transistor operation, such as low-frequency capacitances, stored charge, signal delay time, etc. The results which are presented in this division are classified into two groups: the internal distributions and the terminal characteristics of the device.

The calculations are performed assuming two different collector-base voltages and two different sets of limiting lifetimes τ_{no} and τ_{po} . The graphs denoted by I correspond to $V_{CB} = 1V$, $\tau_{no} = 400$ ns, and $\tau_{po} = 200$ ns; the graphs denoted by II are obtained for $V_{CB} = 3V$, $\tau_{no} = 4$ ns, and $\tau_{po} = 2$ ns. The internal distributions have been computed with a relative error less than 10^{-5} .

7.9.1 The internal distributions

The distributions of electrons for the indicated values of the emitter and collector biases are shown in Figs. 7.3 and 7.4. These results demonstrate the internal consequences of forward biasing of the emitter: the electron flooding of the emitter junction region, their injection into the base and transition across the collector space charge region. The coinciding hole density distributions are depicted in Figs. 7.5 and 7.6. Considerable injection of holes into the emitter at high forward biases is well displayed by these distributions. The unexpected feature is the behaviour of the hole density distribution in the collector transition region. The initial reduction of $p(x)$ is attributed to the increased contribution of the recombination term in (7.20). The subsequent raising of the hole distribution results from the changes in the potential distribution which are caused by large electron current densities. Unfortunately, owing to the limitations of the single-precision calculations discussed in division 7.8, the

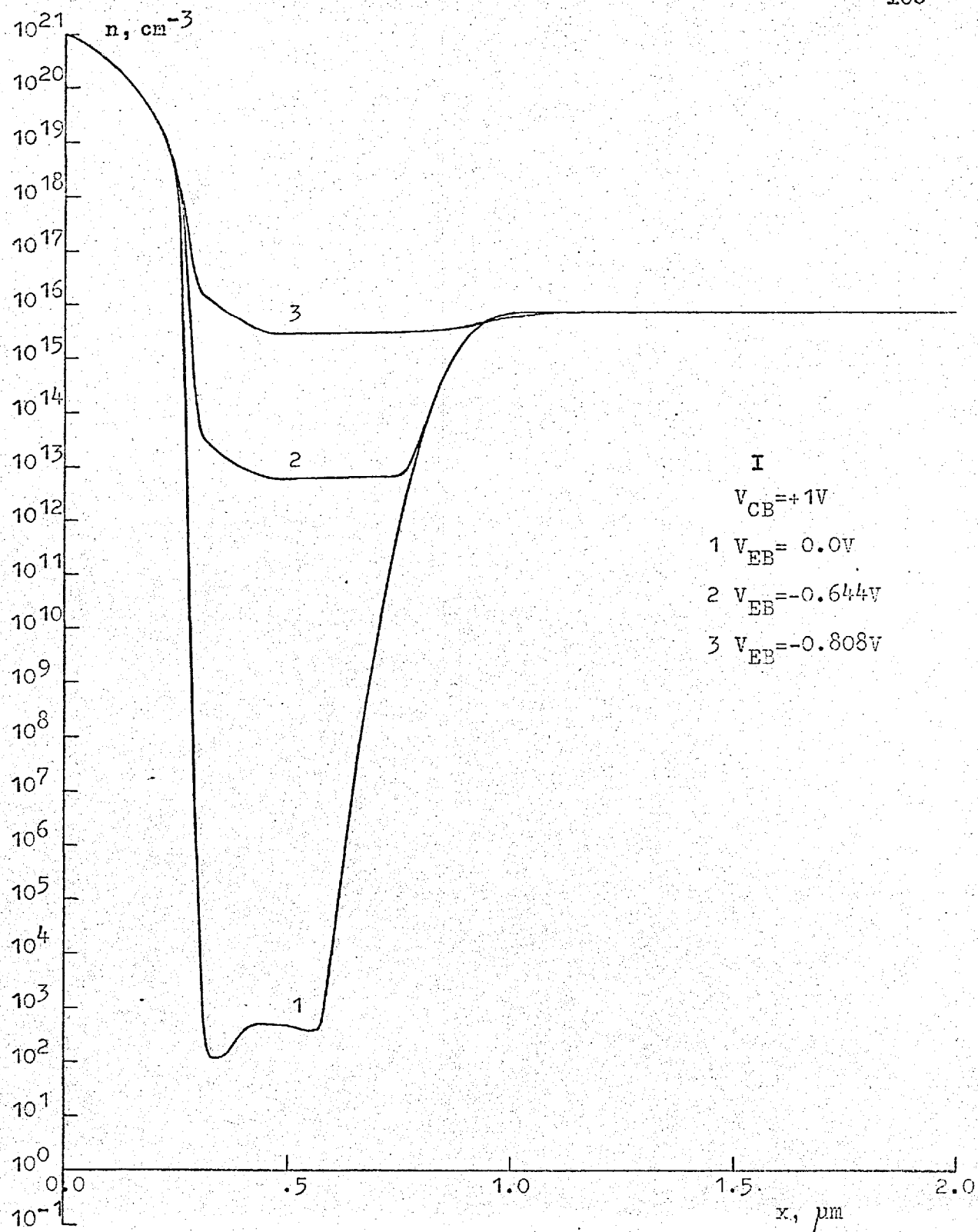


Fig.7.3

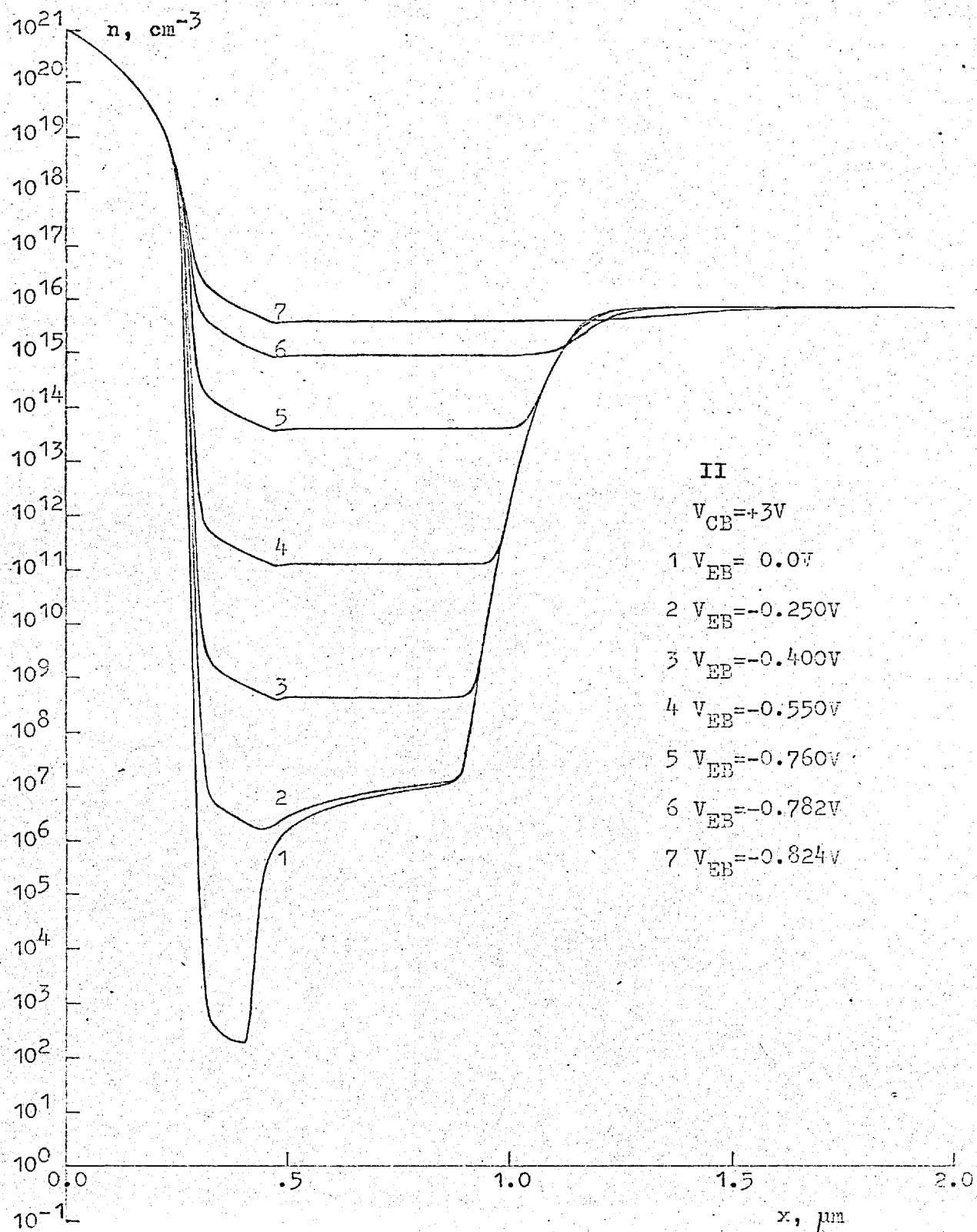


Fig.7.4

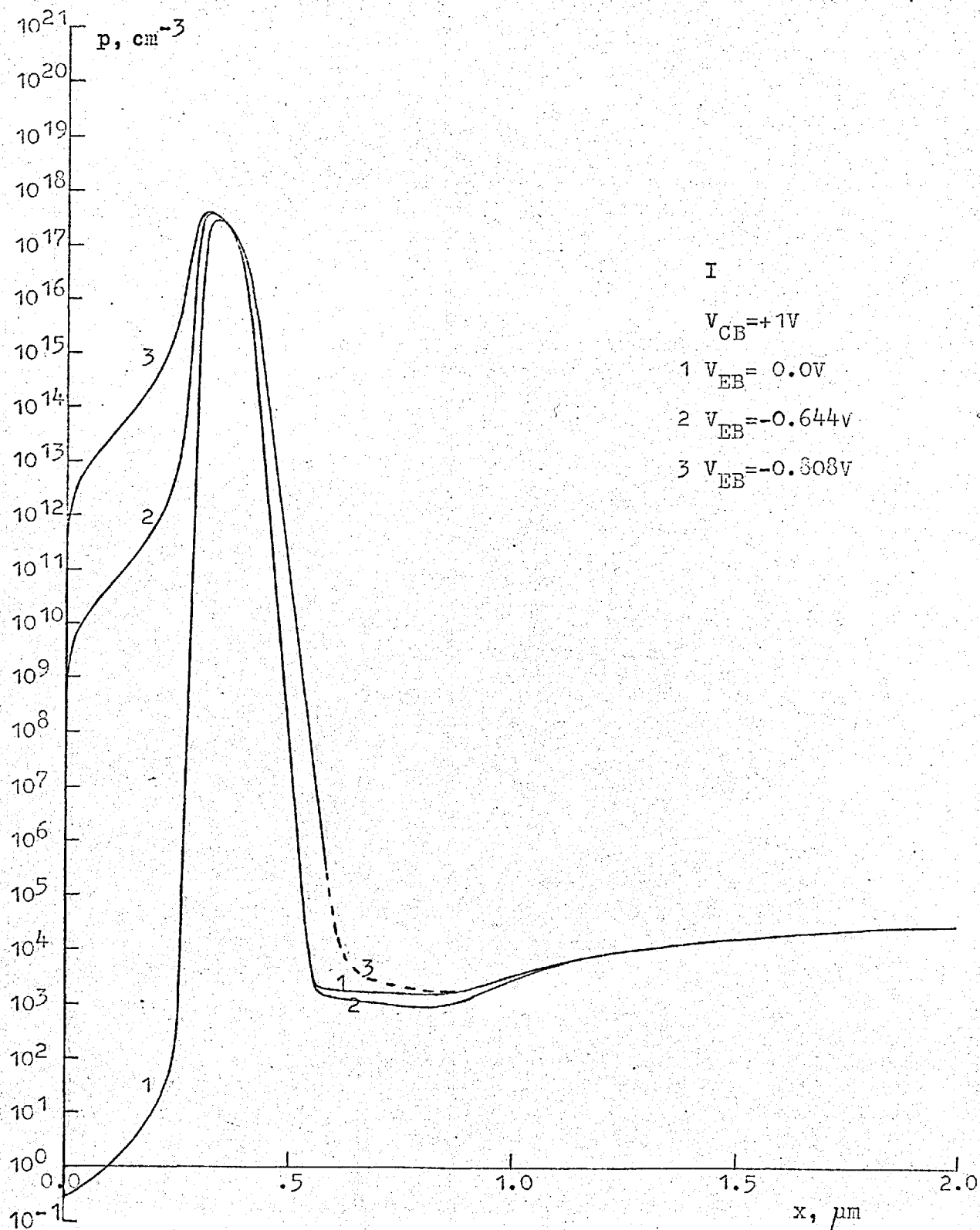


Fig.7.5

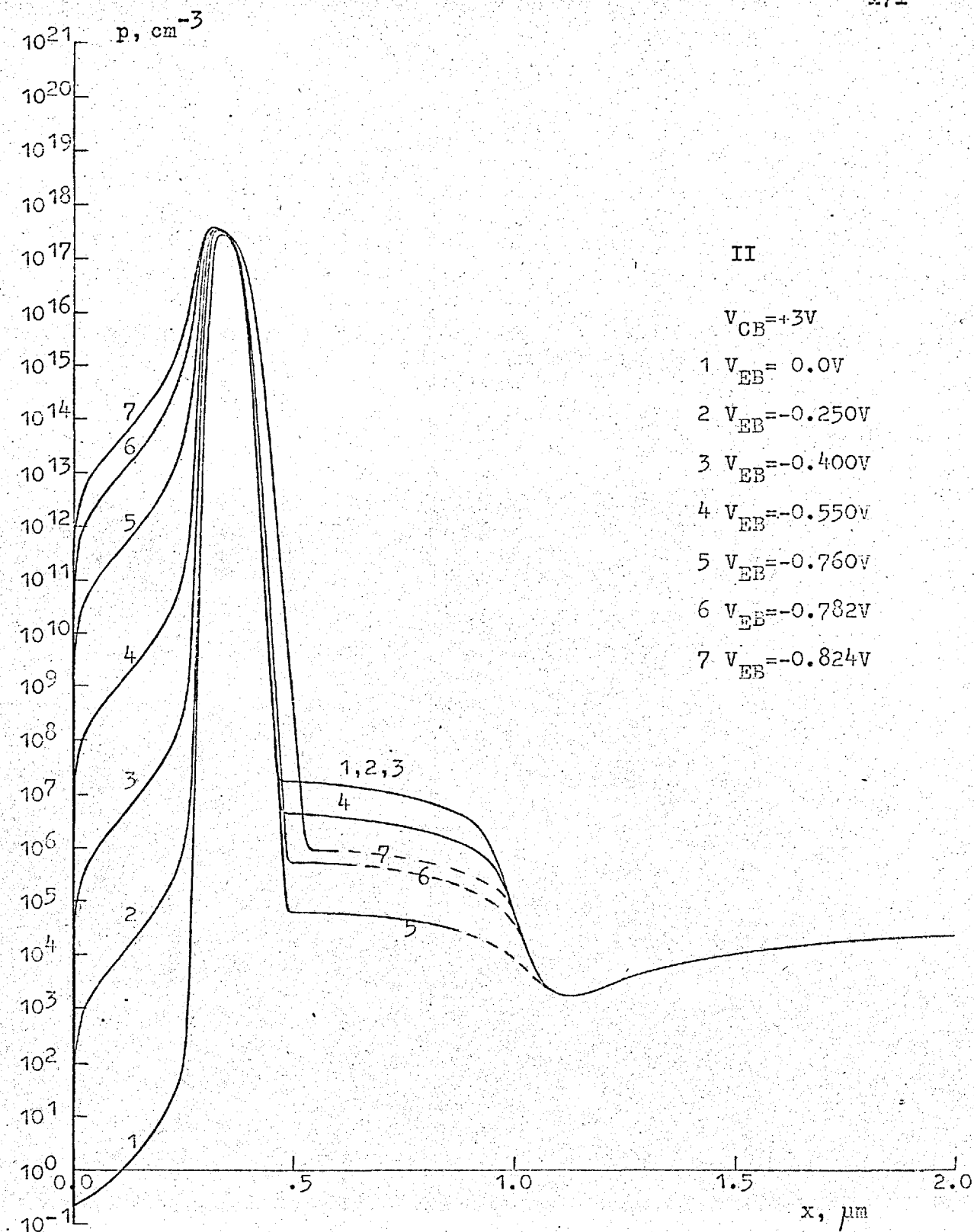


Fig. 7.6

control over this part of the hole density distribution is lost at high current levels. The dotted lines in Figs. 7.5 and 7.6 indicate the extrapolated hole density distributions at high levels.

The potential distributions which correspond to these carrier density distributions are shown in Figs. 7.7 and 7.8. Shifting of the distribution into the collector at high current levels demonstrates the so-called "base push-out" effect (Kirk effect). It is accompanied by a noticeable flattening of the emitter junction barrier.

Both of these two effects are further illustrated by the space charge distributions depicted in Figs. 7.9 and 7.10. Details of the movement of the collector dipole layer into the collector are shown in Figs. 7.11 and 7.12.

7.9.2 Terminal characteristics of the device

The V-I characteristics of the emitter-base diode for the two sets of collector-base voltages and recombination parameters are shown in Fig. 7.13. The expected slopes $\exp(V/V_T)$ and $\exp(V/2V_T)$ exhibited by the curve which corresponds to the shorter limiting lifetimes indicate that the practical lifetimes of injected carriers should be expected to be in the region of several nano seconds.

The two cases of different recombination parameters are further compared in Fig. 7.14. Here the incremental common-emitter current gains for the two cases are plotted as functions of the collector current

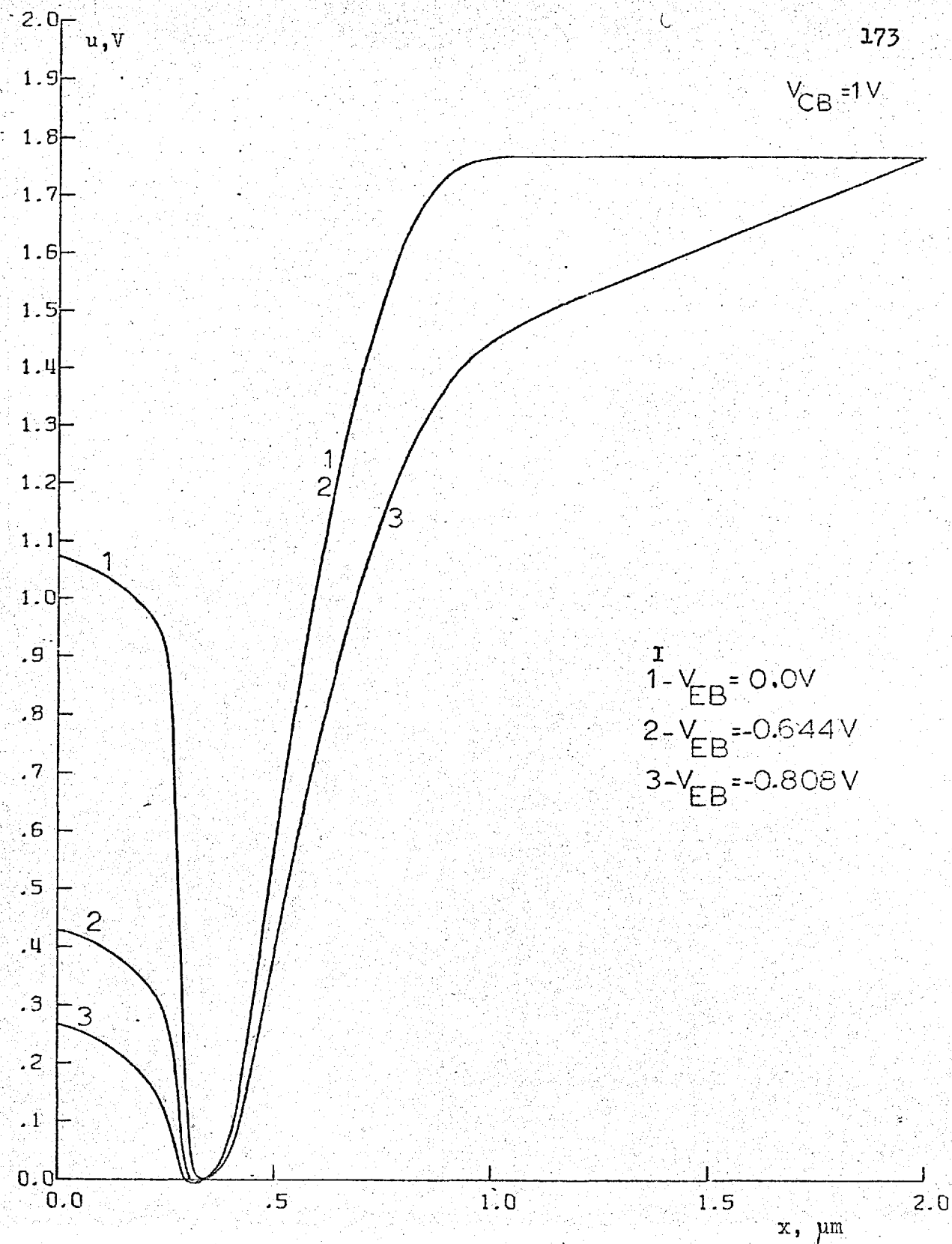


Fig.7.7

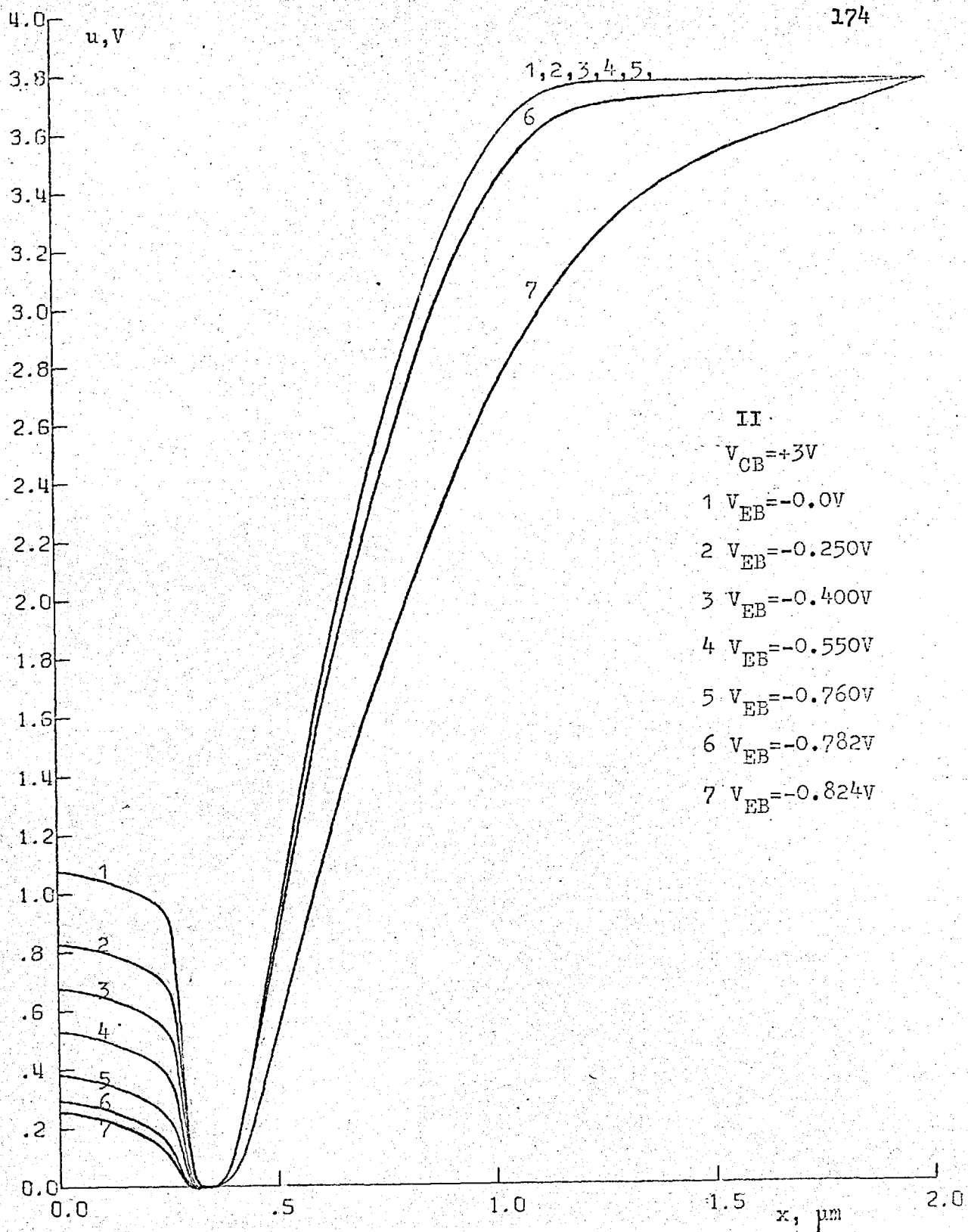


Fig. 7.8

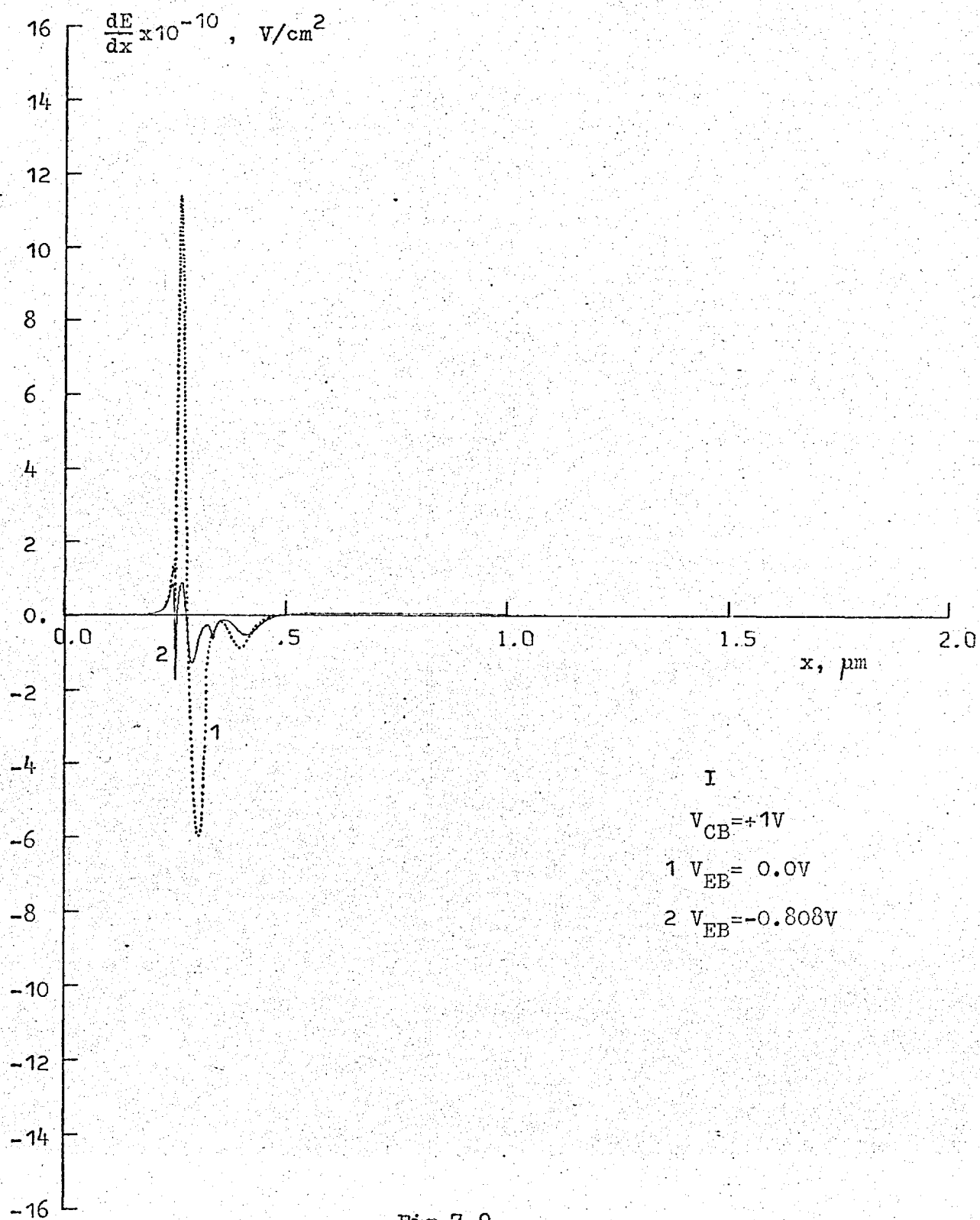
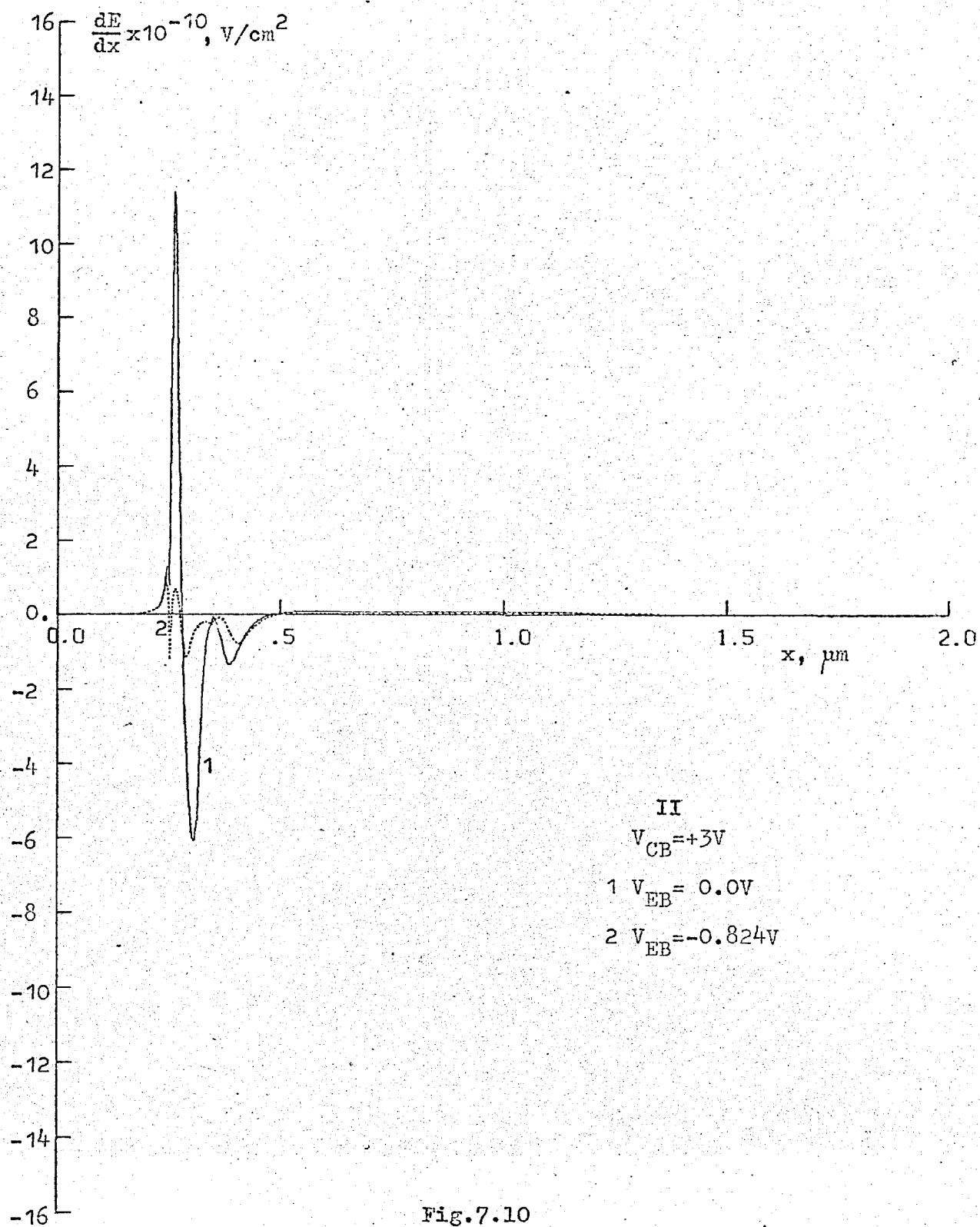


Fig.7.9



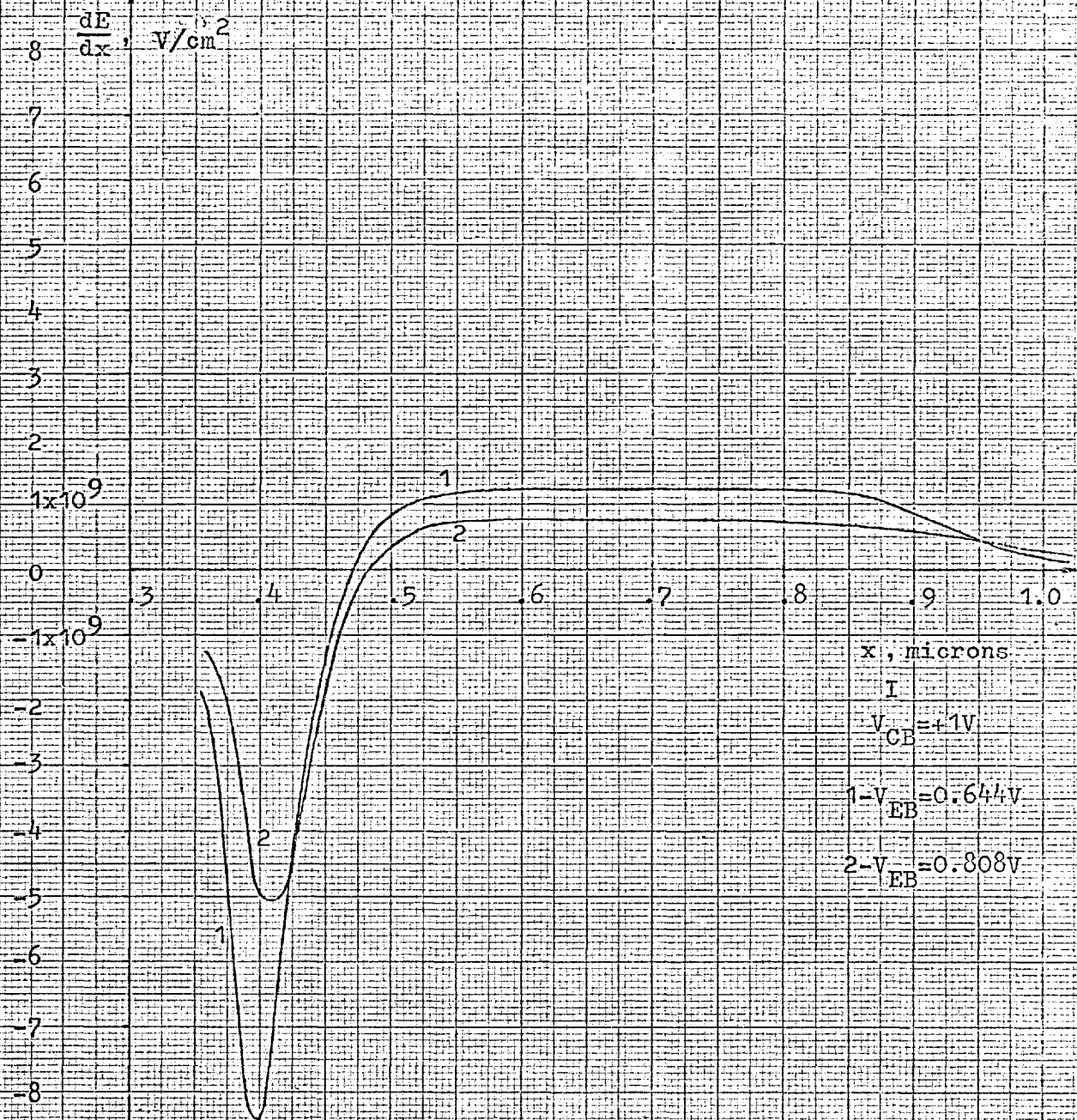


Fig. 7.11

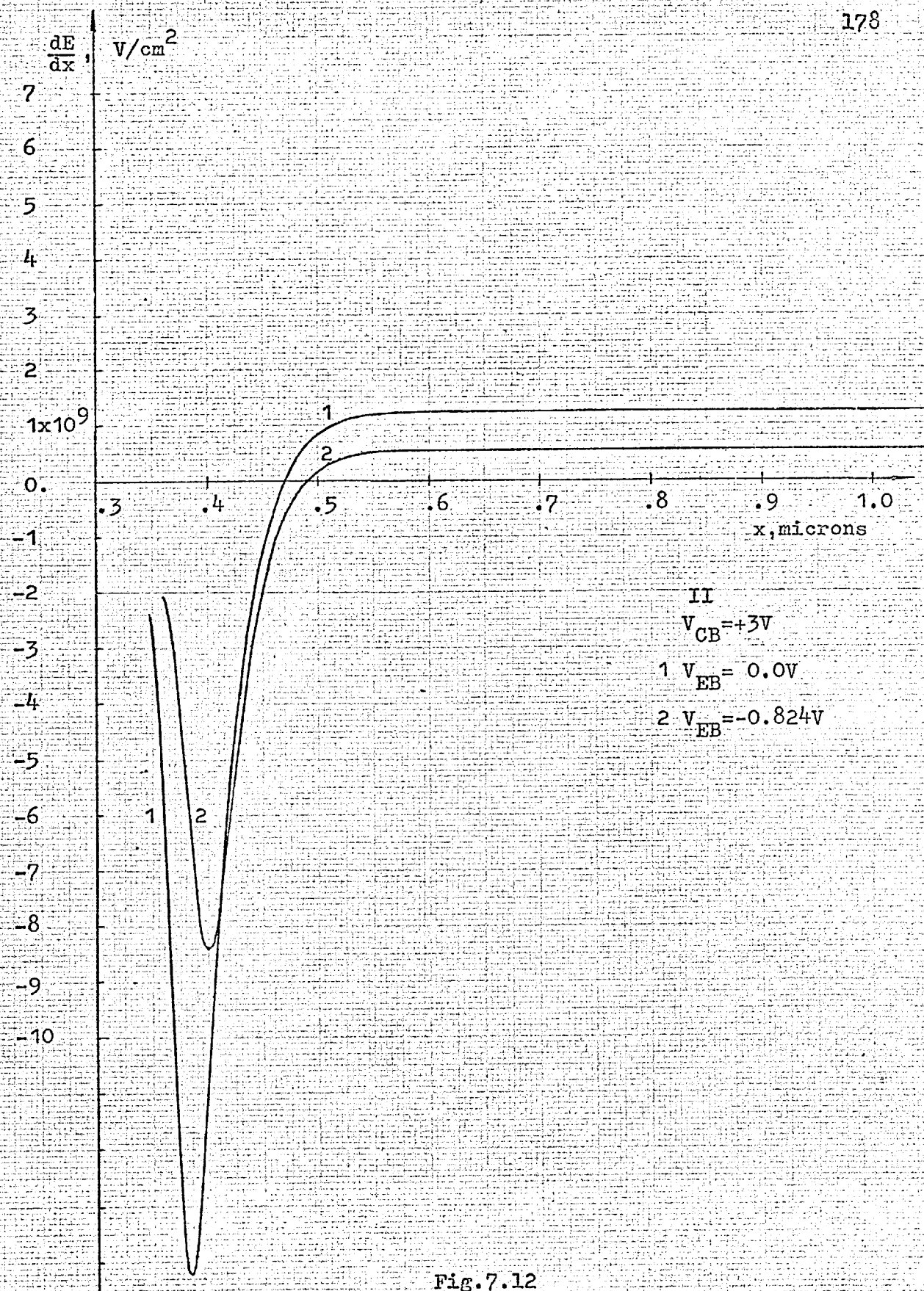


Fig. 7.12

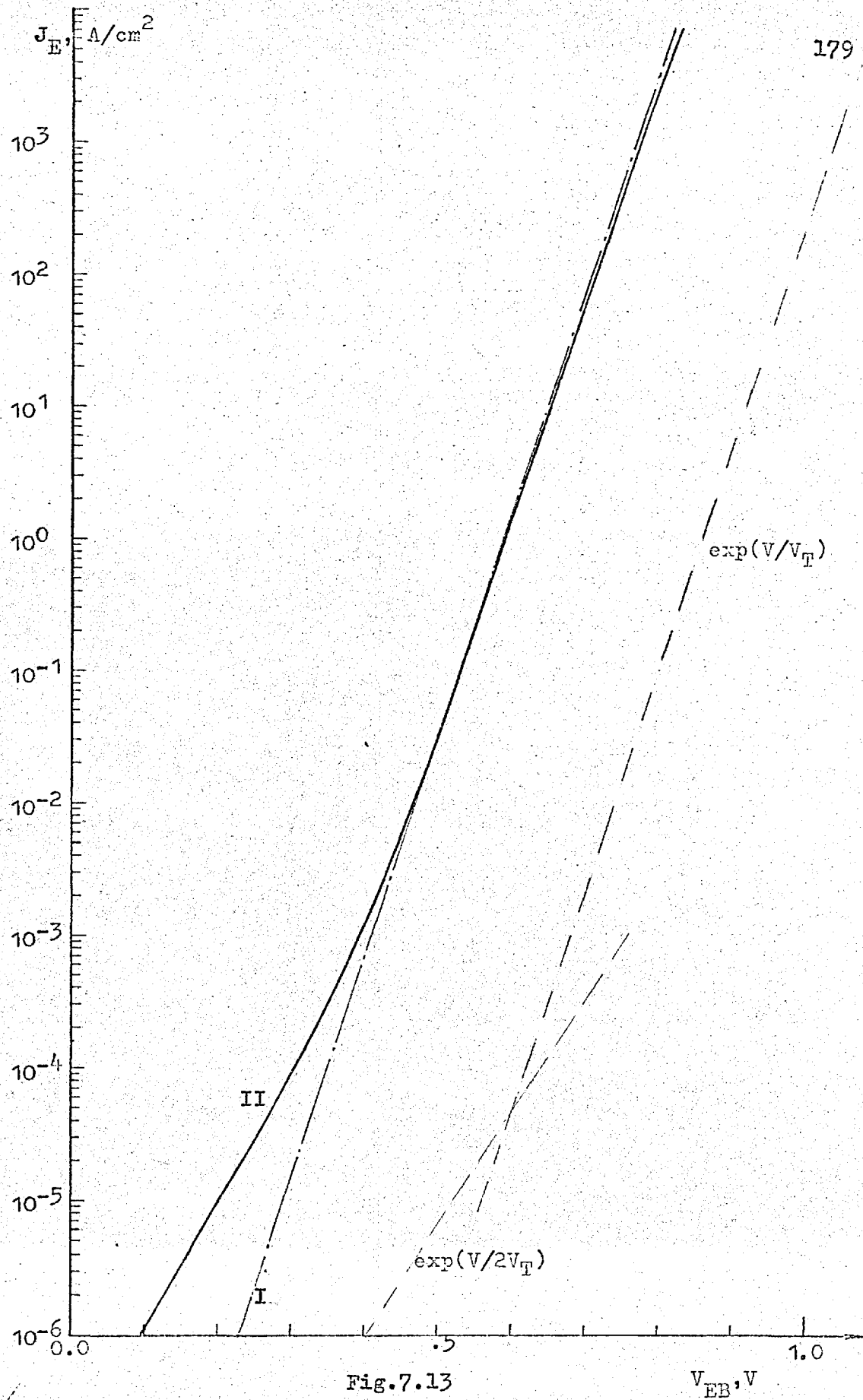


Fig.7.13

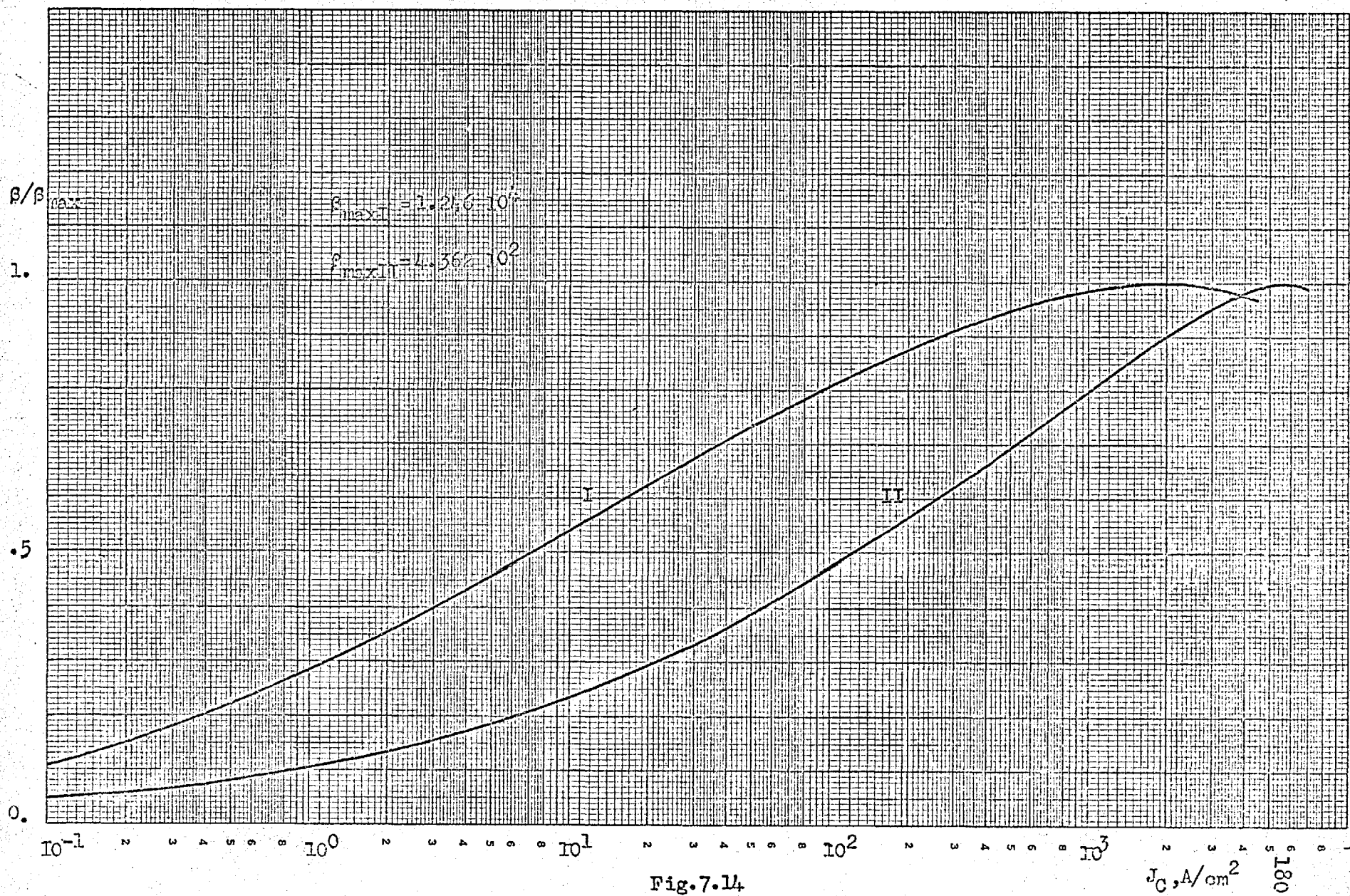


Fig.7.14

$J_C, \text{A/cm}^2$ 180

density. The substantial difference in the two normalizing factors $\beta_{\max}$ reflects the well known sensitivity of the current gain of transistors to the recombination which takes place in the interior of a device.

The dependences of the input per-unit-area parameters, capacitance and transconductance, upon the collector current density are shown in Figs. 7.15 and 7.16 respectively. The derived parameter, the gain-bandwidth product, is plotted in Fig. 7.17. The effect of widening of the transistor base at high current levels appears here as the high-current fall-off of the maximum useful frequency of the device.

Finally the output per-unit-area parameters, incremental conductance and junction capacitance, are shown in Figs. 7.18 and 7.19 as functions of the collector-base voltage, with $V_{EB} = 0$. The curves C_{CB}^{-2} and C_{CB}^{-3} shown in Fig. 7.19 suggest, as in chapter 6, that the capacitance of a diffused junction cannot be approximated by either abrupt or linearly graded junction approximation.

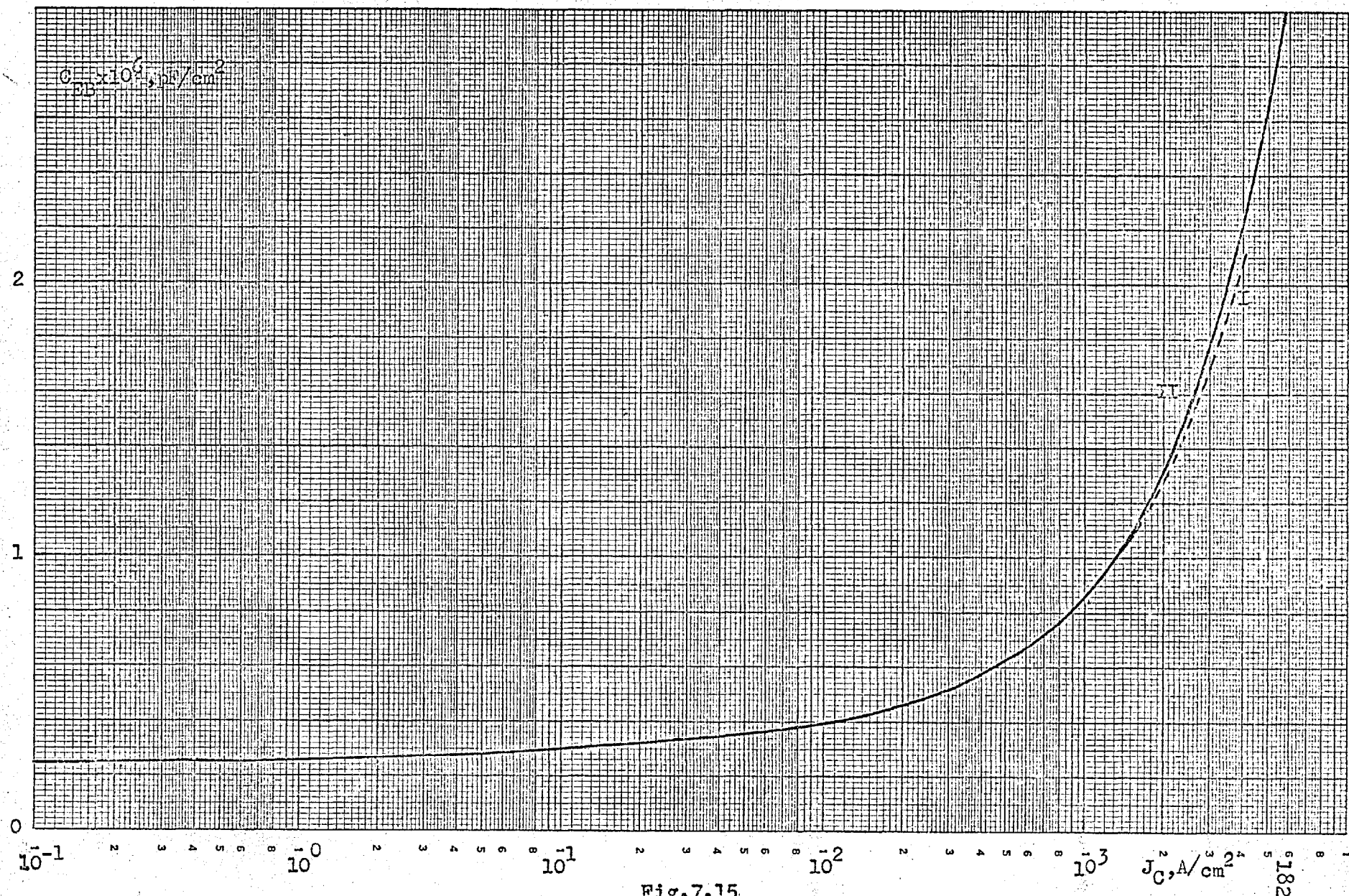


Fig. 7.15

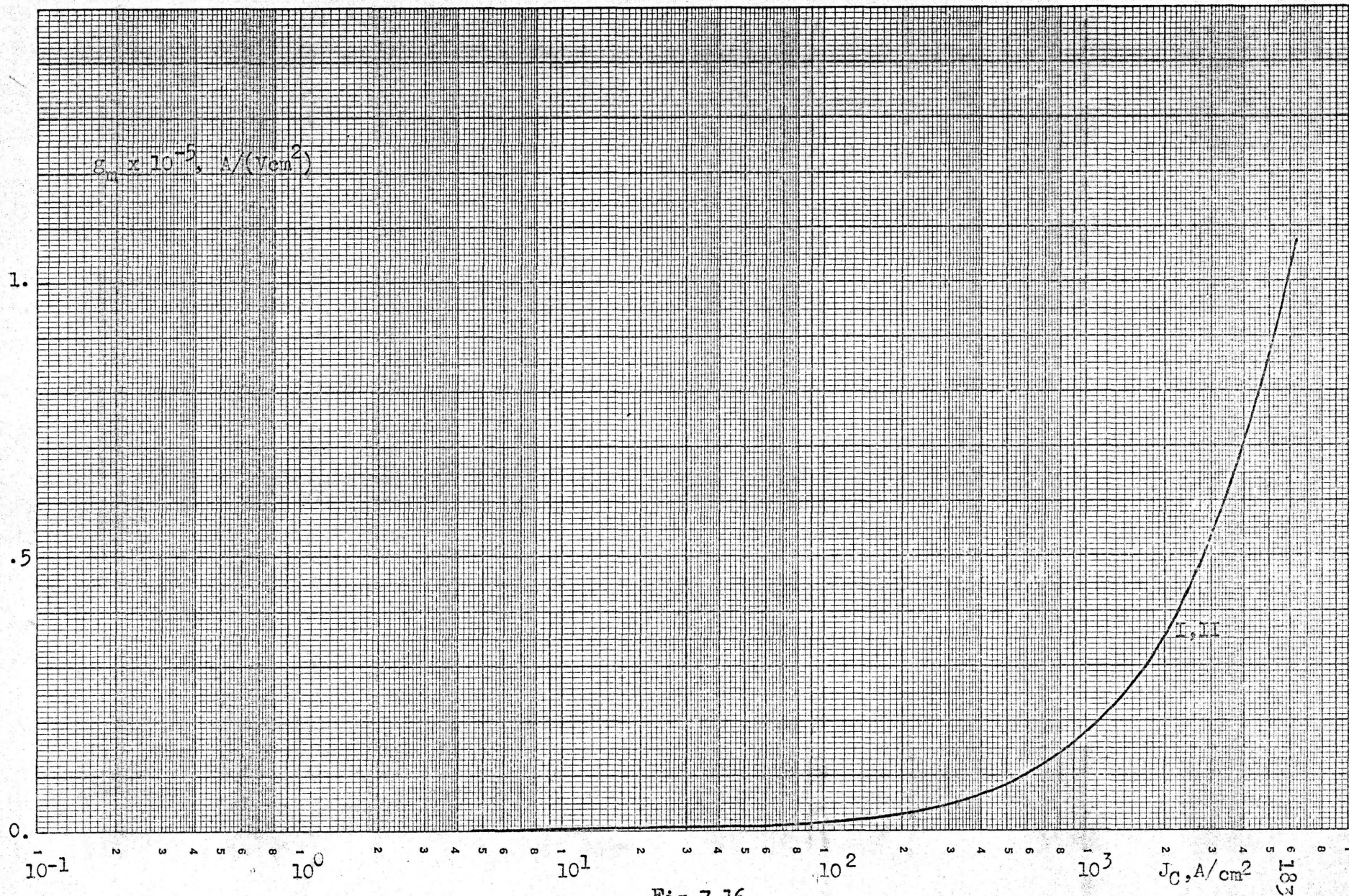


Fig. 7.16

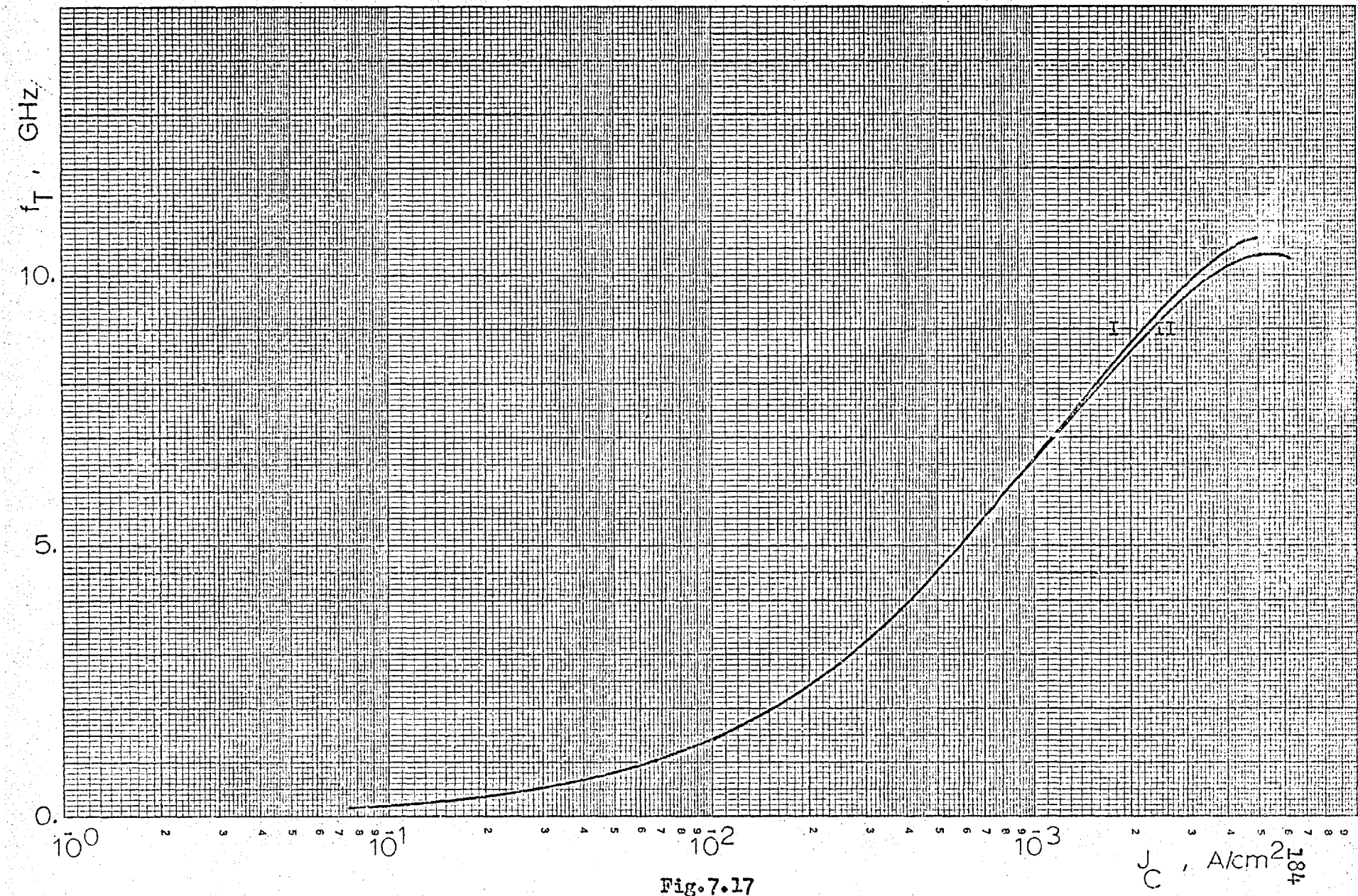


Fig.7.17

J_C , A/cm^2 184

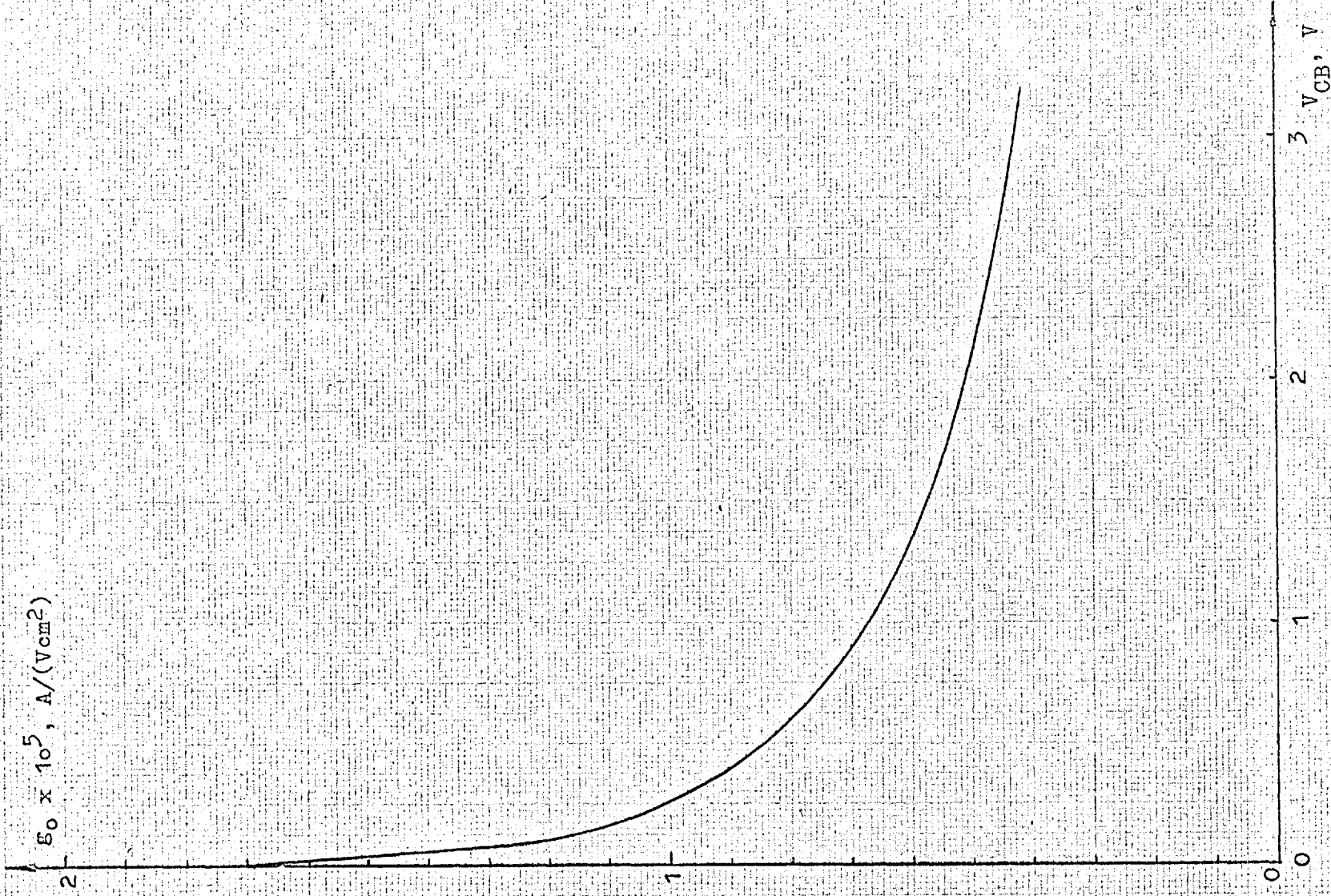


Fig. 7.18

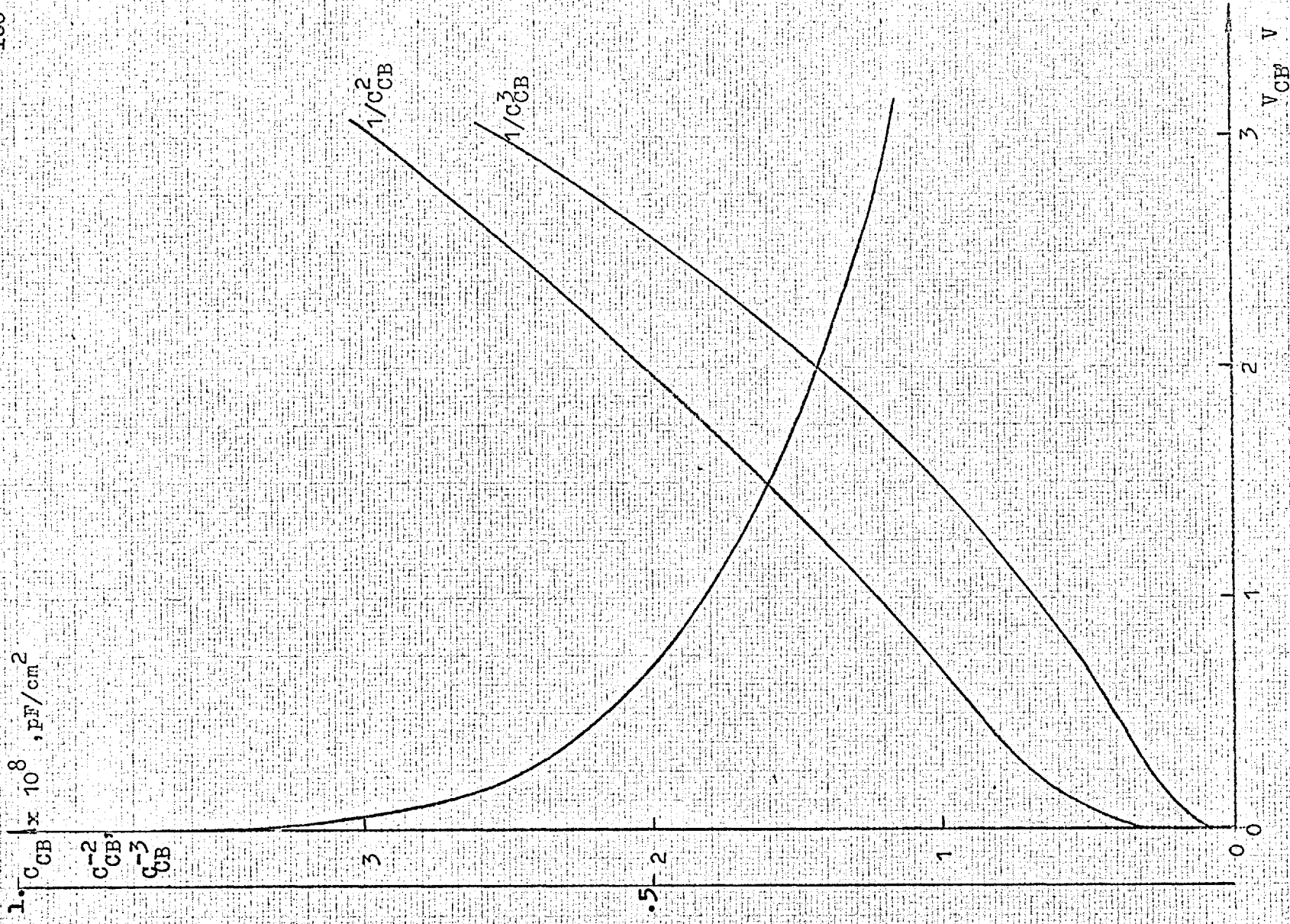


Fig. 7.19

CHAPTER 8

CONCLUSIONS8.1 General conclusions

An investigation of the methods for solving the problem of steady-state current flow in semiconductor junction devices is performed. The general case of doping- and field-dependent transport coefficients has been treated.

The analytical methods for solving the problem have been examined by considering the structures of mathematical models pertaining to various analytical approaches. It was possible to carry out a systematic classification of these methods. It was concluded that a comprehensive treatment of the problem could not be obtained by analytical means.

An initial investigation of the possibilities for applying numerical methods to the problem has shown that general integrating routines, like Runge-Kutta or predictor-corrector, could not be used profitably because of the stiffness of the original system of equations. To overcome this difficulty suitable integral representations are introduced in the diffusion-drift equations and Poisson's equation. By defining an auxiliary variable, related to the potential increment per integration step, an iterative, variable step size integration method

was formulated. The junction transport equations are solved by generating a suitable sequence of initial value problems. The feasibility of this method is tested by applying it to a uniform-base transistor structure. The method involves dividing up a device into several regions in order to prevent an excessive accumulation error. This, in turn, reduces the efficiency of the calculations, except for some special cases, such as a uniformly doped junction in thermal equilibrium. It was not possible to obtain the generalizations which are required for numerical analysis of arbitrary doping profiles under arbitrary bias conditions.

By resorting to the methods for direct solution of two-point boundary value problems it was possible to obtain a general iterative algorithm for solving the steady-state junction transport equations. The aforementioned integral representations for diffusion-drift equations are crucial for formulating this generalized method. The convergency criteria for both, the discretization error and the quality of an initial potential guess have been obtained. The choice of the junction variables in the fundamental system permits formulating efficient numerical algorithms for treating arbitrary bias conditions in arbitrary junction profiles.

By computing the solutions for a diffused junction diode the capability of the method to handle efficiently high reverse biases is demonstrated. A notion concerning the improvement of the gain-bandwidth product of MOS devices was put forward and then substantiated by the

quantitative results which have been obtained applying a version of the developed algorithm.

The method is extended to include the analysis of the steady-state transport phenomena in junction transistors. A detailed numerical study of the steady-state d.c. and a.c. properties of a double-diffused transistor structure under active bias conditions was performed.

8.2 Further research

The numerical technique founded in chapter 5 and extended in chapter 7 lays down a guideline for tackling profitably several interesting research problems. Two different lines of development could be suggested. They are discussed below.

8.2.1 Further applications of the developed numerical technique

Two problems of different types are mentioned here:

(a) temperature sensitivity of the electrical characteristics of junction devices can be analysed by introducing in the present numerical scheme the temperature dependences of the relevant parameters, such as intrinsic carrier density, lifetimes of charge carriers, etc. Predicting temperature behaviour of the characteristics like: collector saturation voltage, current gain, collector reverse saturation current, etc. is of interest to circuit designers. It may also result in

improved designs of junction devices;

(b) recent assertion by Wei¹⁴⁸ that the ions in a nerve axon follow the same physical principles and have similar physical environment as the electrons and holes in a p-n-p transistor makes this numerical technique suitable for the applications in medicine and biology. If it was possible to specify the required input data, the present numerical technique may supply the solutions which could lead towards better understanding of nervous conduction.

8.2.2 Generalizations of the present numerical technique

The specific proposals can be made as regards generalizing the present numerical technique to include the time-dependent one-dimensional and steady-state two-dimensional calculations.

The one-dimensional time dependent calculations can be outlined as follows:

(a) under transient conditions the time derivatives do not vanish from the continuity equations which become parabolic partials (boundary-value type in space and initial-value in time). Poisson's equation remains an ordinary boundary-value type. The spacial boundary conditions are fixed, as in the steady-state case, by the applied voltages. The initial conditions in time are the steady-state solutions immediately before a disturbance of bias.

The distinction between the time-dependent and the steady-

state analysis is made in the treatment of the time partials. Under steady-state conditions these are set to zero. In transient analysis they must be represented at each instant of time. Finite difference approximation, e.g. of the Crank-Nicholson type

$$\frac{p(t_0 + \Delta t) - p(t_0)}{\Delta t} = \frac{\frac{\partial p}{\partial t}(t_0) + \frac{\partial p}{\partial t}(t_0 + \Delta t)}{2} \quad (8.1)$$

offers a simple and relatively accurate formula for estimating the contributions of the time partials. The solutions at each instant of time are obtained as in the steady-state case, except that now the current densities J_p and J_n have additional, time-dependent terms.

The estimates of $\frac{\partial p}{\partial t}$ and $\frac{\partial n}{\partial t}$ are not available in the first iteration loop after the disturbance of a steady-state. If suitable guesses for these terms cannot be made, they are set to zero during the first iteration. At each subsequent instant of time the current densities are calculated from

$$J_p(x, t_i) = J_{p0} + q \int_0^x U(\lambda, t_i) d\lambda - q \int_0^x \frac{\partial p}{\partial t}(\lambda, t_i) d\lambda, \quad (8.2)$$

$$J_n(x, t_i) = J_{n0} - q \int_0^x U(\lambda, t_i) d\lambda + q \int_0^x \frac{\partial n}{\partial t}(\lambda, t_i) d\lambda, \quad (8.3)$$

where the formula (8.1) is used to calculate the time partials;

(b) in small-signal analysis the time partials are

$$\frac{\partial p}{\partial t} = j\omega \tilde{p}, \quad \frac{\partial n}{\partial t} = j\omega \tilde{n}, \quad (8.4)$$

where $j = (-1)^{\frac{1}{2}}$, ω - angular frequency, and $\tilde{p}$ and $\tilde{n}$ are the amplitudes of the corresponding sinusoidal perturbations of $p(x)$ and $n(x)$.

Since the small-signal behaviour is linear, the expansion

$$F(x,u) = F(x,u^{(0)}) + \frac{\partial F}{\partial u}(x,u^{(0)})\delta u \quad (8.5)$$

is exact and only one execution of the algorithm of section 5.2.2 gives the correct potential increments $\delta u(x)$. The corresponding new distributions $p(x)$ and $n(x)$ and the old steady-state values $p(x)^{(0)}$ and $n(x)^{(0)}$ determine the amplitudes $\tilde{p}(x)$ and $\tilde{n}(x)$. The current densities are obtained by inserting (8.4) into (8.2) and (8.3) where J_{po} , J_{no} and U retain their old steady-state values.

Two-dimensional steady-state calculations are outlined considering an MOS transistor structure.

The hole and electron current densities, the electrostatic field and the carrier density gradients are treated as two-dimensional vectors. The boundary conditions are specified at the external contacts. (Assume that a suitable two-dimensional mesh of $(n \times m)$ points (x_j, y_k) is laid down. The x-axis is parallel to the oxide-semiconductor interface and the y-axis is perpendicular to it). The calculations in the semiconductor substrate may proceed as follows:

- supply a guess for the potential distribution;
- along each of the m lines in the x-direction the expressions like (5.4) and (5.9) are employed to calculate the line carrier density distributions and current densities;

- the linearized Poisson's equation in the x-direction, in terms of $\delta u_p(x)$,

$$\delta u_p'' - \frac{\partial F}{\partial u}(x, y, u^{(0)}) \delta u_p = - u_{xx}^{(0)} - \frac{q}{\epsilon} (p - n + N)_u^{(0)}, \quad (8.6)$$

gives the potential corrections along each of the m lines;

- the last two steps are then performed for each of the n lines in the y -direction giving the potential corrections $\delta u_t(y)$ for each line;

This alternating direction technique is performed until a required accuracy is achieved.

The oxide region presents the classical Dirichlet problem. The solutions for the oxide and the substrate are matched at the interface by demanding that the potential and displacement are continuous functions.

Appendix 1

Two different approximations have been employed in calculating the functions $Si(t)$ and $Ci(t)$ in equation (1.11). If $t \leq 1$, the following series representations apply²²

$$Si(t) = t - \frac{t^3}{6} + \frac{t^5}{600} - \frac{t^7}{35080},$$

$$Ci(t) = 0.5772156 + \ln(t) - \frac{t^2}{4} + \frac{t^4}{96} - \frac{t^6}{4320} + \frac{t^8}{322560}.$$

If $t > 1$, the complete expression for the mobility (1.11) is²³

$$\mu = \mu_L \left(1 + \frac{t^8 + a_1 t^6 + a_2 t^4 + a_3 t^2 + a_4}{t^8 + b_1 t^6 + b_2 t^4 + b_3 t^2 + b_4} \right),$$

where

$$a_1 = 42.242855$$

$$b_1 = 48.196927$$

$$a_2 = 302.757865$$

$$b_2 = 482.485984$$

$$a_3 = 352.018498$$

$$b_3 = 1114.978885$$

$$a_4 = 21.821899$$

$$b_4 = 449.690326.$$

The relative errors of both of these approximations are less than 3.110^{-7} .

Appendix 2

Several direct integration routines have been applied to compute the solutions for a uniformly doped p^+n junction in thermal equilibrium. (This case is chosen since a set of exact initial values can be determined at the metallurgical junction). The set of basic equations is reduced to

$$\frac{dE}{dx} = \frac{q}{\epsilon}(p - n + N), \quad (A2.1a)$$

$$\frac{dp}{dx} = pE \frac{1}{V_T}, \quad (A2.1b)$$

$$\frac{dn}{dx} = -nE \frac{1}{V_T}. \quad (A2.1c)$$

Brief outlines of the applied methods and a sample result of the calculations are reported here.

- Runge-Kutta Methods - For a system of differential equations

$$y' = f(x, y) \quad (A2.2)$$

(y and f are vectors) the methods of Runge-Kutta type are represented by the formula

$$y_{n+1} = y_n + hf(x_n, y_n; h), \quad (A2.3)$$

where $\bar{f}$ is a weighted average of the evaluations of the function f , with the arguments in each evaluation depending upon the preceding one.

In a fourth order method $\bar{f}$ is

$$\bar{f} = a_1 k_1 + a_2 k_2 + a_3 k_3 + a_4 k_4, \quad (A2.4)$$

where for the classical Runge-Kutta fourth order method

$$\begin{aligned} k_1 &= f(x, y), \\ k_2 &= f\left(x + \frac{1}{2}h, y + \frac{1}{2}hk_1\right), \\ k_3 &= f\left(x + \frac{1}{2}h, y + \frac{1}{2}hk_2\right), \\ k_4 &= f(x + h, y + hk_3), \end{aligned} \quad (A2.5)$$

and $a_1 = a_4 = 1/6$, $a_2 = a_3 = 1/3$. For the Runge-Kutta-Gill method the above coefficients are

$$\begin{aligned} k_1 &= f(x, y), \\ k_2 &= f\left(x + \frac{1}{2}h, y + \frac{1}{2}hk_1\right), \\ k_3 &= f\left(x + \frac{1}{2}h, y + \left(-\frac{1}{2} + \frac{1}{\sqrt{2}}\right)hk_1 + \left(1 - \frac{1}{\sqrt{2}}\right)hk_2\right), \\ k_4 &= f\left(x + h, y + \left(\frac{1}{\sqrt{2}}\right)hk_2 + \left(1 + \frac{1}{\sqrt{2}}\right)hk_3\right), \end{aligned} \quad (A2.6)$$

$$\text{and } a_1 = a_4 = 1/6, \quad a_2 = \frac{1}{3}\left(1 - \frac{1}{\sqrt{2}}\right), \quad a_3 = \frac{1}{3}\left(1 + \frac{1}{\sqrt{2}}\right).$$

- Taylor series method - Introduce the power series representation of the variables E, p and n in (A2.1),

$$E(x) = \sum_{k=0}^{\infty} a_k x^k, \quad (A2.7)$$

$$p(x) = \sum_{k=0}^{\infty} b_k x^k, \quad (A2.8)$$

$$n(x) = \sum_{k=0}^{\infty} c_k x^k. \quad (A2.9)$$

By substituting (A2.7)-(A2.9) into (A2.1) and applying the method of undetermined coefficients, the following recurrent formulae for the

coefficients a_i , b_i , and c_i are obtained:

$$a_n = \frac{c}{\epsilon} \frac{1}{n} (b_{n-1} - c_{n-1}), \quad (A2.10)$$

$$b_n = \frac{1}{V_T} \frac{1}{n} \sum_{k=0}^{n-1} b_k a_{n-k-1}, \quad (A2.11)$$

$$c_n = -\frac{1}{V_T} \frac{1}{n} \sum_{k=0}^{n-1} c_k a_{n-k-1}. \quad (A2.12)$$

An m -th order integration routine follows if the series (A2.7)-(A2.9) are truncated after first m terms. (In the present calculations $m=7$).

- Predictor-corrector method - The sixth order finite difference method described by Ralston and Wilf³¹ can be summarized as follows.

For the system of differential equations (A2.2) the forward difference equation for predicting y_{n+1} , with the values $y_{n-5} - y_n$ known, is

$$y_{n+1} = y_{n-5} + \frac{3}{10}h(11y'_n - 14y'_{n-1} + 26y'_{n-2} - 14y'_{n-3} + 11y'_{n-4}). \quad (A2.13)$$

A corrected value of y_{n+1} is obtained from

$$y_{n+1} = y_{n-3} + \frac{2}{45}h(7y'_{n+1} + 32y'_n + 12y'_{n-1} + 32y'_{n-2} + 7y'_{n-3}), \quad (A2.14)$$

where the y_{n+1} from (A2.13) is employed to calculate y'_{n+1} .

The described Taylor series method has been used to start the computations.

None of the described methods has produced the convergent solutions. Applying the method proposed by Sparkes²⁹ the convergent

solutions for (A2.1) have been obtained. These are compared to those calculated by the methods described here. Fig. A2.1 shows the relative difference between the electrostatic field computed by these methods and the one that follows from Sparkes' algorithm (the point $x = 0$ corresponds to the metallurgical junction).

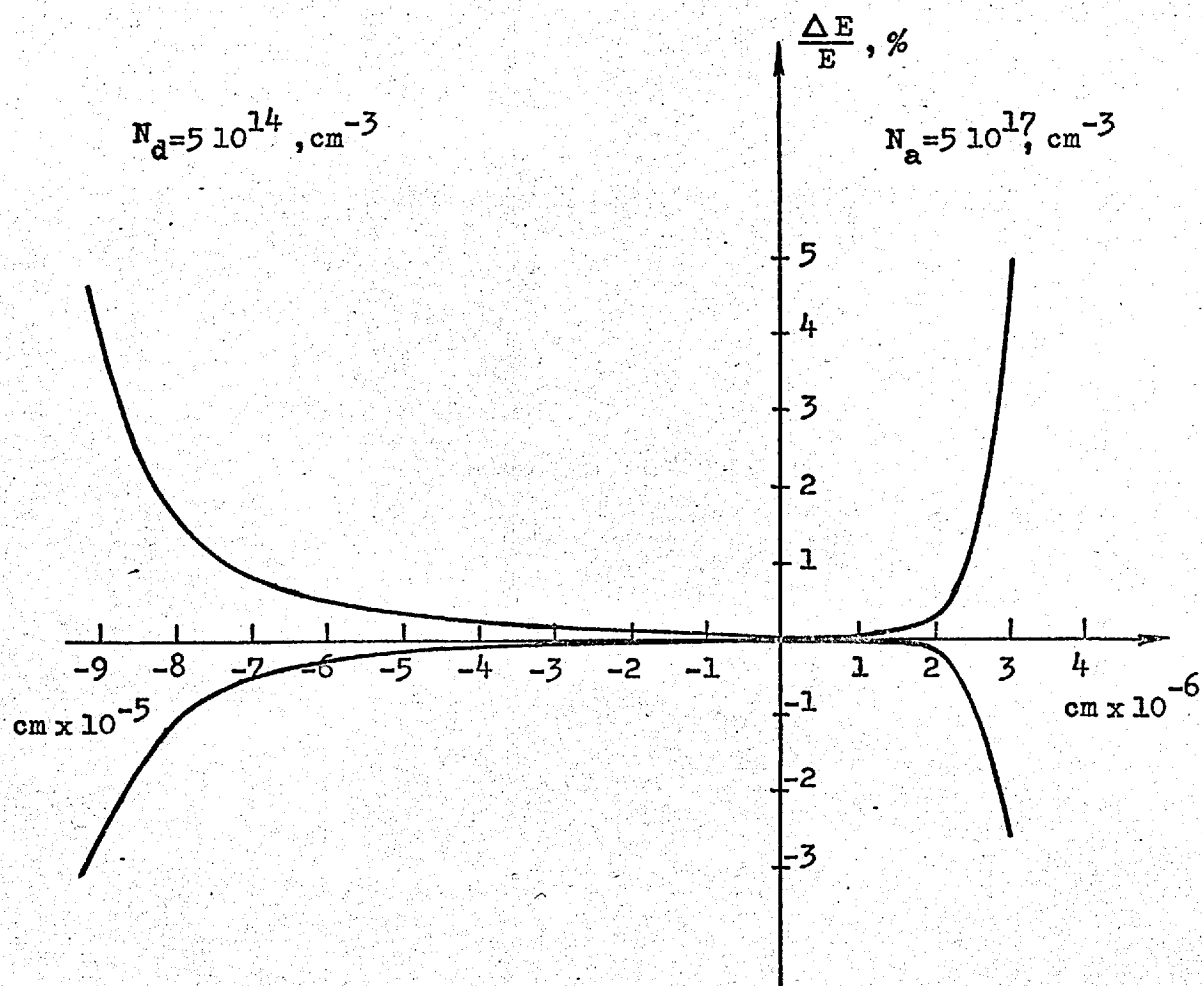


Fig.A2.1

Appendix 3

The equation governing the hole density distribution is

$$\frac{dp}{dx} = \frac{pE}{V_T} - \frac{J_p}{qD_p} \quad (A3.1)$$

By (1.14) and (1.15)

$$D_p = \frac{D(N_d) (E_{c1} E_{c2})^{\frac{1}{2}}}{E} \quad (A3.2)$$

for all $E \geq E_{c2}$. It follows that (A3.1) may be written as

$$\frac{dp}{dx} = \frac{E}{V_T} \left(p - \frac{J_p V_T}{qD_p (N_d) (E_{c1} E_{c2})^{\frac{1}{2}}} \right) \quad (A3.3)$$

The second term on the right hand side of (A3.3) defines the lower limit $p_{\min}$ for the hole density in the electron depleted base section, next to the collector.

It is obvious from (A3.3) that all higher derivatives of p can be recurrently expressed as products of $(p - p_{\min})$ and the corresponding functions involving the derivatives of E . Consequently, at $p = p_{\min}$ all derivatives of p reduce to zero and p does not change as long as (A3.3) applies.

Appendix 4

Summary of the calculations in chapter 4

The purpose of this appendix is to summarize the procedure described in chapter 4. The sections are indicated following the notation of Fig. 4.1.

Section 1 - The electron density and electron current density are negligible; for a chosen p_t , such that $p_{jc} < p_t < p_{po}$, vary E_t to obtain $\max(x' - x_t)$ or $\max(x'' - x_t)$ (the flow chart of Fig. 4.3).

Section 2 - The electron density and electron current density are negligible; using the pair p_t, E_t obtained in section 1 perform a single computation of $p(x)$ and $E(x)$ towards the collector junction.

Section 3 - The electron density and electron current density are negligible; using various pairs (p, E) obtained by the integration of section 2, such that $E > E_{jc}$ and $p \leq p_{jc}$, perform the integrations of the "electron depleted" base section. (Each integration gives a set of solutions which corresponds to a different V_{CB} voltage).

Section 4 - The electron current density is negligible; for a chosen p , such that $p_{low} < p < p_{high}$, and $E = 0$ vary n to obtain the solutions which end at the point (p_{min}, E_{o2}) (the flow chart of Fig. 4.7).

Section 5 - The electron current density is negligible; using various pairs (p_{b2}, n_{b2}) , obtained from the calculations of section 4 at a given current level, and $E = 0$, perform the integrations of the negative-field base section. (Each integration gives a set of solutions which corresponds to a different V_{EB} voltage).

Section 6 - The electron current density is negligible; the

sets (p_k, n_k, E_k) obtained from the calculations of section 5, such that $p_k > p_{je}$ and $|E_k| < |E_{je}|$, are varied to obtain $\max(x_{emj} - x_1)$; the electron current density is estimated by (4.21).

Appendix 5

The local charge density, denoted by $F(x,u)$ in the section 5.2.2, can be expressed symbolically in terms of x and u as

$$F(x,u) = -\frac{q}{\epsilon} (p(x,u) - n(x,u) + N(x)), \quad (A5.1)$$

where the terms $p(x,u)$ and $n(x,u)$ are given by eqns.(5.4) and (5.5) of the section 5.2.1 respectively. The partial derivative of F with respect to u is now

$$\frac{\partial F}{\partial u} = -\frac{q}{\epsilon} \left(\frac{\partial p}{\partial u} - \frac{\partial n}{\partial u} \right). \quad (A5.2)$$

($N(x)$ is potential independent). Using (5.4) and (5.5)

$$\frac{\partial p}{\partial u} = \frac{-1}{V_T} \exp(-u(x)/V_T) (p(o) \exp(u_o/V_T) - \int_0^x \frac{\exp(u(t)/V_T) J_p(t)}{q D_p(t)} dt), \quad (A5.3)$$

$$\frac{\partial n}{\partial u} = \frac{1}{V_T} \exp(+u(x)/V_T) (n(o) \exp(-u_o/V_T) + \int_0^x \frac{\exp(-u(t)/V_T) J_n(t)}{q D_n(t)} dt), \quad (A5.4)$$

i.e.

$$\frac{\partial p}{\partial u} = -\frac{p(x)}{V_T}, \quad (A5.5)$$

$$\frac{\partial n}{\partial u} = \frac{n(x)}{V_T},$$

and

$$\frac{\partial F}{\partial u} = \frac{q}{\epsilon V_T} (p + n). \quad (A5.6)$$

The second partial derivative of F with respect to u is obviously

$$\frac{\partial^2 F}{\partial u^2} = \frac{q}{\epsilon V_T^2} (n - p). \quad (A5.7)$$

Appendix 6The method for inverting the matrix T

The algorithm for solving the linear system (5.25) can be formulated by an adaptation of the Gaussian algorithm as follows.

Assume that it is possible to find two nonsingular matrices $Q = (q_{nm})$ and $S = (s_{nm})$ of the special form

$$Q = \begin{bmatrix} 1 & & & & \\ q_{21} & 1 & & & \\ & q_{32} & 1 & & \\ & & & \ddots & \\ & & & & 1 \end{bmatrix}, \quad q_{nm} = 1, \quad n > m$$

$$, \quad q_{nm} = 0 \text{ if } \begin{cases} n > m \\ n < m-1 \end{cases}$$

$$S = \begin{bmatrix} s_{11} & s_{12} & & & \\ & s_{22} & s_{23} & & \\ & & & \ddots & \\ & & s_{M-2,M-2} & s_{M-2,M-1} & \\ & & & & s_{M-1,M-1} \end{bmatrix}, \quad s_{nm} = 0 \text{ if } \begin{cases} n < m \\ n > m+1 \end{cases}$$

having the property

$$QS = T. \quad (A6.1)$$

In order to solve (A6.1) determine the vector z such that

$$Qz = R_e \quad (A6.2)$$

and then

$$S \delta u = z. \quad (A6.3)$$

Since $\delta u = S^{-1} Q^{-1} R_e = T^{-1} R_e$, the vector δu thus determined satisfies (5.25).

To carry out this program (A6.1) is written as

$$s_{11} + s_{12} = t_{11} + t_{12}$$

$$(s_{11} q_{21}) + (s_{12} q_{21} + s_{22}) + (s_{23}) = t_{21} + t_{22} + t_{23}$$

$$(s_{22} q_{23}) + (s_{23} q_{32} + s_{33}) + (s_{34}) = t_{32} + t_{33} + t_{34} \quad (A6.4)$$

...

$$(s_{M-2, M-2} q_{M-1, M-2}) + (s_{M-2, M-1} q_{M-1, M-2} + s_{M-1, M-1}) = t_{M-1, M-2} + t_{M-1, M-1}$$

Equating the corresponding coefficients yields

$$s_{11} = t_{11}, \quad (A6.5a)$$

$$s_{n-1, n-1} q_{n, n-1} = t_{n, n-1}, \quad (A6.5b)$$

$$s_{n-1, n} q_{n, n-1} + s_{n, n} = t_{n, n} \quad (A6.5c)$$

$$s_{n, n+1} = t_{n, n+1}. \quad (A6.5d)$$

The relation (A6.5d) directly yields $s_{n, n+1}$; the relations (A6.5b) and (A6.5c) may be rearranged to give $q_{n, n-1}$ and $s_{n, n}$ recursively as follows

$$s_{11} = t_{11}, \quad (A6.6)$$

$$q_{n, n-1} = t_{n, n-1} / s_{n-1, n-1}, \quad (A6.7a)$$

$$s_{n, n} = t_{n, n} - q_{n, n-1} t_{n-1, n}. \quad (A6.7b)$$

The vector z can be determined simultaneously with Q . From (A6.2) is

$$\begin{aligned} z_1 &= r_1 \\ z_1 q_{21} + z_2 &= r_2 \\ z_2 q_{32} + z_3 &= r_3 \\ &\dots \\ z_{M-2} q_{M-1, M-2} + z_{M-1} &= r_{M-1} \end{aligned} \quad (A6.8)$$

or

$$\begin{aligned} z_1 &= r_1 \\ z_n &= r_n - q_{n,n-1} z_{n-1}. \end{aligned} \quad (\text{A6.10})$$

Writing out (A6.3) in components yields

$$\begin{aligned} s_{11} \delta u_1 + s_{12} \delta u_2 &= z_1 \\ s_{22} \delta u_2 + s_{23} \delta u_3 &= z_2 \\ &\dots \\ s_{M-1,M-1} \delta u_{M-1} &= z_{M-1}. \end{aligned} \quad (\text{A6.11})$$

The components of δu , starting from the last, are now

$$\delta u_{M-1} = z_{M-1} / s_{M-1,M-1} \quad (\text{A6.12})$$

$$\delta u_n = (z_n - t_{n,n-1}) / s_{n,n}. \quad (\text{A6.13})$$

The complete procedure can now be summarized as follows:

1) Compute $s_{n,n}$ and z_n , starting with $n=1$ from the relations

$$s_{11} = t_{11}$$

$$z_1 = r_1$$

$$q_{n,n-1} = t_{n,n-1} / s_{n-1,n-1}$$

$$s_{n,n} = t_{n,n} - q_{n,n-1} t_{n-1,n}$$

$$z_n = r_n - q_{n,n-1} z_{n-1};$$

2) Calculate δu_n , starting with $n=M-1$, from the relations

$$\delta u_{M-1} = z_{M-1} / s_{M-1,M-1}$$

$$\delta u_n = (z_n - s_{n,n+1} \delta u_{n+1}) / s_{n,n}.$$

This algorithm breaks down when $s_{n-1,n-1} = 0$. (If this is the case, then,

denoting by $\det(T)$ the determinant of the matrix T , $\det(T) = \det(S)\det(Q) =$

$s_{11}s_{22}\dots s_{M-1,M-1} = 0$, and T is singular).

Appendix 7

Convergency criterion and the discretization error of the iterative scheme of section 5.2.3

The conditions which ensure the convergence of the iterative scheme of section 5.2.3 are contained in the theorem originally proved by Kantorovich¹⁴² which is quoted here in a form suitable for the problem at hand (reference 24 p.367).

Assume that the following conditions are satisfied:

(i) For $u=u^{(0)}$, the initial approximation, the matrix $T(u^{(0)})$ has an inverse $I_T = T^{-1}$, and an estimate of its norm is known:

$$|I_T| \leq B_0; \quad (A7.1)$$

(ii) The vector $u^{(0)}$ approximately satisfies the system of equations (5.25) in the sense that

$$|I_T R_e(u^{(0)})| \leq \eta_0; \quad (A7.2)$$

(iii) In the region defined by inequality (A7.5), the components of the vector $R_e(u^{(0)})$ are twice continuously differentiable with respect to u and satisfy

$$h^2 \left| \frac{\partial^2 F}{\partial u^2} \right| \leq F_0; \quad (A7.3)$$

(iv) The constants B_0 , η_0 , and F_0 introduced above satisfy the inequality

$$h_0 = B_0 \eta_0 F_0 \leq \frac{1}{2}; \quad (A7.4)$$

Then the system of equations (5.25) has a solution u which is located in

$$|u - u^{(0)}| \leq \frac{1 - \sqrt{1 - 2h_0}}{h_0} \eta_0. \quad (A7.5)$$

Moreover, the successive approximations $u^{(k)}$ defined by (5.17) exist and converge to u , and the speed of convergence may be estimated by the inequality

$$|u^{(k)} - u| \leq \frac{1}{2^{k-1}} (2h_0)^{2^{k-1}} \eta_0. \quad (A7.6)$$

By definitions (5.26) $T > J$, $B > 0$, and $G > 0$. Under conditions established by (5.31)

$$T^{-1} \leq J^{-1}. \quad (A7.7)$$

As J is a special matrix, (see definitions in 5.2.2.1) its norm can be written explicitly as

$$|J^{-1}| \leq \frac{M^2}{8}, \quad (A7.8)$$

where $M=L/h$. In view of (A7.7) the condition (A7.1) is observed for

$$B_0 = \frac{L^2}{8h^2}. \quad (A7.9)$$

In relation to the initial approximation $u^{(0)}$ the following constants are useful

$$Y_m = \max \left| \frac{d^6 u^{(0)}}{dx^6} \right|, \quad (A7.10)$$

$$R_m = \max |u^{(0)''} - F(x, u^{(0)})|, \quad (A7.11)$$

$$L_m = \max \left| \frac{\partial^2 F}{\partial u^2} \right|, \quad (A7.12)$$

for all $0 \leq x \leq L$.

By applying (5.27) to $u(x)$ and introducing Taylor series

representation for $u(x \pm h)$, it follows that

$$| -u(x-h) + 2u(x) - u(x+h) + \frac{h^2}{12}(u(x-h)'' + 10u(x)'' + u(x+h)') | \leq \frac{h^6}{240} Y_m. \quad (A7.13)$$

Considering also (A7.11), for a selected $u^{(0)}$

$$| -u_{n-1} + 2u_n - u_{n+1} + \frac{h^2}{12}(F_{n-1}'' + 10F_n'' + F_{n+1}') | \leq h^2 R_m + \frac{h^6}{240} Y_m. \quad (A7.14)$$

The conditions (A7.2) of the above theorem is satisfied for

$$\eta_0 = \frac{L^2}{8} (R_m + h^4 Y_m / 240). \quad (A7.15)$$

Thus the condition which guarantees the convergence of the iterative process, (A7.4), becomes

$$\frac{L^4 L_m (R_m + h^2 Y_m / 240)}{64} \leq \frac{1}{2}. \quad (A7.16)$$

A bound for the discretization error

As a corollary of the convergency theorem, a bound for the discretization error can be obtained. If the iterative process is started with a $u^{(0)}$ very close to the exact solution u , denote by e_r the vector with components e_{rn} ,

$$| u^{(0)} - u | = | e_r |. \quad (A7.17)$$

Assuming that (A7.16) holds (i.e. h is sufficiently small), it follows from (A7.5), using (A7.15),

$$| e_r | \leq \frac{1 - \sqrt{1 - 2h_0}}{h_0} \frac{L^2 h^4 Y_m / 240}{8} \quad (A7.18)$$

where h_0 is defined by (A7.4). Since $h_0 \leq \frac{1}{2}$,

$$1 < \frac{1 - \sqrt{1 - 2h_0}}{h_0} < 2 \quad (\text{A7.19})$$

and a simpler error bound is

$$|e_r| \leq \frac{L^2 h^4 y_m / 240}{4} \quad (\text{A7.20})$$

Appendix 8

The most effective way of controlling the type and concentration of impurities within specific regions of a semiconductor crystal is through solid-state diffusion. Consequently, the diffusion of various impurities in semiconductors has become the principal method in the fabrication of junction devices. A successful control over the process of junction formation by solid-state diffusion has become possible only after the process was understood sufficiently well to develop an adequate model. A brief outline of the results relevant to specification of the impurity profiles of diffused junction devices is given in this appendix.

- Basic equations - Diffusion processes generally are described in terms of the so-called Fick's laws¹³². The flow density of diffusing atoms, crossing an arbitrary plane, is related to the concentration gradient at this plane through first Fick's law

$$F = -D \text{ grad } N. \quad (\text{A8.1})$$

The scalar proportionality factor D , diffusivity, is highly temperature dependent. This is reflected quantitatively by $D = D_0 \exp(-W_a/kT)$, where W_a is the activation energy for the particular type of impurity and D_0 is a constant.

Application of continuity equation to (A8.1) yields Fick's second law

$$\frac{\partial N}{\partial t} = D \nabla^2 N. \quad (\text{A8.2})$$

The electric field associated with this process is assumed to be

sufficiently small that the field-aided diffusion does not occur.

However, if the density of diffusing atoms approaches the density of intrinsic carriers at the temperature of diffusion, doubling of the diffusion coefficient has been suggested¹³² to account for the phenomena associated with the field-aided diffusion.

Equation (A8.2) is of fundamental importance in solid-state diffusion. When it is solved and appropriate boundary conditions are applied, the result is an expression for impurity distribution in a semiconductor crystal.

- Diffusion from vapour of constant impurity concentration - Passing a vapour of constant impurity concentration over a semiconductor wafer which has been raised to a temperature near melting point results in diffusion of impurity atoms from the vapour into the wafer. Provided the period of adjustment at the semiconductor surface is much shorter than the time of exposure*, the impurity distribution in the wafer is obtained by solving (A8.2) subject to the boundary conditions

$$N(0,t) = N_s \quad (\text{A8.3a})$$

$$N(\infty,t) = 0, \quad (\text{A8.3b})$$

* The surface concentration cannot jump instantaneously from zero to its final constant value, and the boundary condition (A8.3a) need be replaced by the condition relating the flux to the surface via mass transfer to the flux away from the surface via solid-state diffusion. However, if the times involved exceed several minutes, the solutions which account for this external limitation to the rate of transport of the impurities merge into the complementary error function¹²⁵.

and the initial condition

$$N(x,0)=0. \quad (\text{A8.4})$$

The result is the complementary error function

$$N(x,t)=N_s \operatorname{erfc}(x/2\sqrt{Dt}). \quad (\text{A8.5})$$

- Diffusion from a planar source - This is a two-step process. A fixed amount of impurity N_0 is predeposited on the surface of a wafer, and then subjected to a high temperature treatment, usually carried out in an oxidizing ambient. The oxide layer which is formed at the surface tends to seal the diffusant inside the wafer. Approximating the predeposited profile by a delta function*, the boundary conditions for the second step are

$$N(0,0)=N_0 \quad (\text{A8.6a})$$

$$N(\infty,t)=0. \quad (\text{A8.6b})$$

The impurity distribution, subject to the above approximation is given by a Gaussian profile

$$N(x,t) = \frac{N_0}{\sqrt{\pi Dt}} \exp(-x^2/4Dt). \quad (\text{A8.7})$$

* This approximation applies if the penetration of the predeposited profile is negligibly small in comparison to that of the final profile after the drive-in step. Otherwise, the problem is much more complicated and its solution requires application of numerical methods¹²³.

C APPENDIX 9

C LIST OF DATA WHICH ARE READ-IN FOR EFFECTING THE CALCULATI-
C ONS OF THE STRUCTURE OF FIG.7.1

C Q - ELECTRONIC CHARGE , IN COULOMBS
C VT - THERMAL VOLTAGE (KT/Q) , IN VOLTS
C EPS - DIELECTRIC CONSTANT OF THE SEMICONDUCTOR, IN PF/CM
C DOPE - SURFACE DONOR DENSITY OF THE EMITTER DIFFUSION, IN CM-3
C DOPB1 - CONCENTRATION OF THE FLAT SECTION OF THE ACCEPTOR
C DISTRIBUTION IN THE EMITTER, IN CM-3
C DOPB2 - 'EQUIVALENT' SURFACE ACCEPTOR DENSITY OF THE BASE
C DIFFUSION, IN CM-3
C DOPC - COLLECTOR BACKGROUND DOPING, IN CM-3
C ED1,ED2 - DENOMINATORS IN THE ARGUMENTS OF THE COMPLEMENTARY
C ERROR FUNCTIONS ASSOCIATED WITH THE EMITTER AND BASE DIFFUSI-
C ONS RESPECTIVELY, IN CM
C E1MAX,E2MAX - LIMITS FOR THE ARGUMENTS OF THE COMPLEMENTARY
C ERROR FUNCTIONS AFTER WHICH THESE FUNCTIONS BECOME NEGLIGIBLE
C E1SMAX,E2SMAX - LIMITS OF THE ARGUMENTS OF THE EXPONENTIAL
C FUNCTIONS AFTER WHICH THESE FUNCTIONS BECOME NEGLIGIBLE
C XEJ - POSITION OF THE EMITTER-BASE METALLUR. JUNCTION, IN CM
C XCJ - POSITION OF THE COLLECTOR-BASE METALLUR. JUNCTION, IN CM
C XMAX - POSITION OF THE COLLECTOR CONTACT, IN CM
C XK1 - POSITION OF THE POTENTIAL REFERENCE POINT, IN CM
C DX - DISCRETIZATION STEP IN THE COLLECTOR DOMAIN, IN CM
C ECH,ECE - THE CHARACTERISTIC FIELDS FOR THE HOLE AND ELECTRON
C MOBILITIES, RESPECTIVELY, DEFINED BY EQUATION(1.15A) AND GIVEN
C IN TABLE 2B
C DELU - REQUIRED RELATIVE ACCURACY OF CALCULATING THE NORMALI-
C ZED ELECTROSTATIC POTENTIAL(NORMALIZING FACTOR IS VT)
C USMALL - LOWER LIMIT FOR THE NORMALIZED POTENTIAL AFTER WHICH
C THE ACCURACY OF CALCULATIONS IS NOT TESTED, IN VT
C VAPE0 - EMITTER BIAS VOLTAGE, IN VOLTS
C VAPC0 - COLLECTOR BIAS VOLTAGE, IN VOLTS
C VAPES,VAPEB - SMALL AND LARGE INCREMENTS RESPECTIVELY IN THE
C EMITTER BIAS, IN VOLTS
C VAPCS,VAPCB - SMALL AND LARGE INCREMENTS RESPECTIVELY IN THE
C COLLECTOR BIAS, IN VOLTS
C ANI - INTRINSIC CARRIER DENSITY, IN CM-3
C B0,B1,B2 - COEFFICIENTS IN THE DISCRETIZATION FORMULA (5.27)
C HAVING VALUES 1/12,10/12 AND 1/12, RESPECTIVELY
C TPO,TNO - HOLE AND ELECTRON LIMITING LIFETIMES, IN SECONDS
C HDR,EDR - HOLE AND ELECTRON CONCENTRATIONS RELATED TO THE
C ENERGY LEVEL OF TRAPS, IN CM-3
C XAP - LENGTH OF THE FLAT PART OF ACCEPTOR DISTRIBUTION IN
C EQUATION (7.1), IN CM
C USF0 - MAGNITUDES OF THE FIRST (N-1) POTENTIAL SECTIONS IN

C THE COLLECTOR DOMAIN, IN VT
C HDK1 - THERMAL EQUILIBRIUM HOLE DENSITY AT THE POTENTIAL
C REFERENCE POINT, IN CM-3
C DX1 - DISCRETIZATION STEP IN THE EMITTER DOMAIN, IN CM
C VCCOR - ABSOLUTE VALUE OF THE REDUCTION OF POTENTIAL DISTRI-
C BUTION IN THE COLLECTOR TRANSITION REGION PER 1 MILLIVOLT OF
C EMITTER BIAS(NONZERO AT VERY LARGE CURRENTS ONLY), IN VOLTS
C KMAX - TOTAL NUMBER OF DISCRETE POINTS IN A STRUCTURE
C K1 - NUMBER OF DISCRETE POINTS IN THE EMITTER DOMAIN
C IG - NUMBER OF INCREMENTS OF EMITTER BIAS PER RUN OF THE
C PROGRAM
C ITERM - MAXIMUM NUMBER OF ITERATION TOLERATED BEFORE THE
C RELATIVE ACCURACY DELU IS ACHIEVED
C KWRITE - THE RESULTS FOR EACH KWRITE-TH POINT IN THE EMITTER
C DOMAIN ARE WRITTEN OUT, STARTING WITH K=1
C LIME, LIMC - NUMBERS OF DISCRETE STEPS IN THE EMITTER AND
C COLLECTOR DOMAINS RESPECTIVELY
C NC - NUMBER OF INCREMENTS OF COLLECTOR BIAS PER RUN OF THE
C PROGRAM
C MAN - INDEX DETERMINING WHICH BOUNDARY POTENTIAL IS CHANGED,
C MAN=0 REFERS TO THE EMITTER, OTHERWISE TO THE COLLECTOR
C IO - EACH IO-TH SET OF COMPUTED INTERNAL DISTRIBUTIONS IS
C WRITTEN OUT
C KW1 - INTEGER MULTIPLE OF KWRITE DETERMINING THE LAST POINT
C IN THE EMITTER DOMAIN FOR WHICH THE RESULTS CAN BE OUTPUTED
C KW2 - INTEGER MULTIPLE OF KWRITE DETERMINING THE LAST POINT
C IN THE COLLECTOR DOMAIN FOR WHICH THE RESULTS CAN BE OUTPUTED
C KWRITE1 - THE RESULTS FOR EACH KWRITE1-TH POINT IN THE COLLEC-
C TOR DOMAIN ARE WRITTEN OUT, STARTING WITH K=K1
C KREC - ALWAYS GREATER THAN K1, USUALLY CORRESPONDS TO A POINT
C NEAR COLLECTOR-BASE TRANSITION REGION BOUNDARY
C QN0, QP0 - TOTAL ELECTRON AND HOLE CHARGES, RESPECTIVELY, IN A
C DEVICE AT THERMAL EQUILIBRIUM

```

C      THE FORTRAN IV VERSION OF THE COMPUTER PROGRAM FOR CALCULA-
C      TING THE TRANSISTOR STRUCTURE OF FIG.7.1

C      PRELIMINARIES, INTRODUCTION OF DATA AND SPECIFICATION OF CON-
C      STANTS AND ARRAYS
      DIMENSION U(1674),HD(1673),ED(1673),DELTA(1673),USF(10),KR(10)
      COMMON/AR/GR(1673),CHCI(1673),CECI(1673),HCI(1673),ECI(1673),
      *GRI(1673)
      COMMON/POCO/DX,TM,B0,B1,B2,DXSQB0,DXSQB1,DXSQB2,TOVT,KM,KMA,
      *K1,K1M1,K1M2,K1P1,K1P2,L0,DX1,DX1SB0,DX1SB1,DX1SB2,TM1,XK1
      COMMON/DFUN/XAP,DOPE,DOPB1,DOPB2,DOPC,ED1,ED2,E1MAX,E2MAX,
      *E1SMAX,E2SMAX
      COMMON/DIFFS/VT,ECH,ECE
      READ(5,55) Q,VT,EPS,DOPE,DOPB1,DOPB2,DOPC,ED1,ED2,E1MAX,E2MAX,
      1E1SMAX,E2SMAX,XEJ,XCJ,XMAX,XK1,DX,ECH,ECE,DELU,USMALL,VAPE0,
      2VAPC0,VAPES,VAPEB,VAPCS,VAPCB,ANI,B0,B1,B2,TP0,TN0,HDR,EDR,
      3XAP,USF0,HDK1,DX1,VCCOR
55  FORMAT(E14.7)
      READ(5,58) KMAX,K1,IG,ITERM,KWRITE,LIME,LIMC,NC,MAN,10,KW1,
      1KW2,KWRIT1,KREC
58  FORMAT(I5)
      READ(5,155) QN0,QP0
155  FORMAT(E14.7)
      WRITE(6,66)
66  FORMAT(1H1,4X,10HINPUT DATA)
      WRITE(6,60) Q,VT,EPS,DOPE,DOPB1,DOPB2,DOPC,ED1,ED2,E1MAX,E2MAX,
      1E1SMAX,E2SMAX,XEJ,XCJ,XMAX,XK1,DX,ECH,ECE,DELU,USMALL,VAPE0,
      2VAPC0,VAPES,VAPEB,VAPCS,VAPCB,ANI,B0,B1,B2,TP0,TN0,HDR,EDR,
      3XAP,USF0,HDK1,DX1,VCCOR
60  FORMAT(5X,1PE14.7)
      WRITE(6,64)
64  FORMAT(1H0,4X,12HINTEGER DATA)
      WRITE(6,65) KMAX,K1,IG,ITERM,KWRITE,LIME,LIMC,NC,MAN,10,KW1,
      1KW2,KWRIT1,KREC
65  FORMAT(5X,15)
      WRITE(6,596)
596  FORMAT(1H0,4X,23HTHE EQUILIBRIUM CHARGES)
      WRITE(6,597) QN0,QP0
597  FORMAT(5X,1PE14.7)
      T=Q/EPS
      ANIS=ANI*ANI
      KMAX1=KMAX + 1
      KMA=KMAX - 1
      KM=KMAX - 2
      K1M1=K1 - 1
      K1M2=K1 - 2
      K1P1=K1 + 1
      K1P2=K1 + 2
      LO=KM - K1

```

```

KREC1=KREC + 1
N=0
IVP=0
IE=0
IC=0
I=0
FLIME=FLOAT(LIME)
FLIMC=FLOAT(LIMC)
DINC=FLOAT(KWRITE)
DXW=DX*DINC
DINC1=FLOAT(KWRIT1)
DX1W=DX1*DINC1
VAPPLE=VAPE0
VAPPLC=VAPC0
TOVT=T/VT
TM=-T*DX*DX/VT
DXSQB0=DX*DX*B0
DXSQB1=DX*DX*B1
DXSQB2=DX*DX*B2
TM1=-T*DX1*DX1/VT
DX1SB0=DX1*DX1*B0
DX1SB1=DX1*DX1*B1
DX1SB2=DX1*DX1*B2
CON=TP0*EDR + TN0*HDR
DX2=DX/2.
DX12=DX1/2.

```

```

C POTENTIAL GUESS, FIRST ORDER THEORY
X=0.
DON0=DOP(X)
S=ANI/DON0
ED(1)=DON0*(1. + SQRT(1. + 4.*S*S))/2.
HD(1)=ANIS/ED(1)
X=XMAX
DONL=DOP(X)
S=ANI/DONL
ED(KMAX)=DONL*(1. + SQRT(1. + 4.*S*S))/2.
HD(KMAX)=ANIS/ED(KMAX)
HD(K1)=HDK1
X=XEJ
AEJ=DERDOP(X)
X=XCJ
ACJ=DERDOP(X)
VEQ1=+VT*ALOG(HD(K1)/HD(1))
VEQ2=-VT*ALOG(HD(KMAX)/HD(K1))
VEMI=VEQ1 + VAPE0
VCOL=VEQ2 + VAPC0
AEJA=ABS(AEJ)
ACJA=ABS(ACJ)
VEA=ABS(VEMI)
VCA=ABS(VCOL)
VEMIN=VEMI/VT

```

```

VCOLN=VCOL/VT
AEL=(3.*EPS/(2.*Q*AEJA)*VEA)**(1./3.)
XEP=XEJ - AEL
XEN=XEJ + AEL
EEJ=Q*AEJ*AEL*AEL/(2.*EPS)
ACL=(3.*EPS/(2.*Q*ACJA)*VCA)**(1./3.)
XCN=XCJ - ACL
XCP=XCJ + ACL
ECJ=Q*ACJ*ACL*ACL/(2.*EPS)
U(1)=VEMIN
U(K1)=0.
U(KMAX)=VCOLN
A1=-Q*AEJ/(6.*EPS*VT)
A2=Q*AEJ*XEJ/(2.*EPS*VT)
A3=-Q*AEJ*XEP*(2.*XEJ - XEP)/(2.*EPS*VT)
A4=U(1)+Q*AEJ*XEP*XEP*(XEJ/2. - XEP/3.)/(EPS*VT)
B11=-Q*ACJ/(6.*EPS*VT)
B22=Q*ACJ*XCJ/(2.*EPS*VT)
B33=-Q*ACJ*XCN*(2.*XCJ - XCN)/(2.*EPS*VT)
B44=U(K1)+Q*ACJ*XCN*XCN*(XCJ/2. - XCN/3.)/(EPS*VT)
X=0.
DO 901 K=2,K1M1
X=X + DX1
IF(X.GT.XEP) GO TO 902
U(K)=U(1)
GO TO 901
902 IF(X.GT.XEN) GO TO 903
U(K)=A1*X*X*X + A2*X*X + A3*X + A4
GO TO 901
903 U(K)=U(K1)
901 CONTINUE
DO 905 K=K1P1,KMA
X=X + DX
IF(X.GT.XCN) GO TO 906
U(K)=U(K1)
GO TO 905
906 IF(X.GT.XCP) GO TO 907
U(K)=B11*X*X*X + B22*X*X + B33*X + B44
GO TO 905
907 U(K)=U(KMAX)
905 CONTINUE
U(KMAX1)=2.*U(KMAX) - U(KMA)

```

```

C   WRITING OUT THE POTENTIAL GUESS
    WRITE(6,61)
61  FORMAT(1H0,4X,15HPOTENTIAL GUESS)
    X=0.
    DO 162 K=1,KW1,KWRIT1
    UR=U(K)*VT
    WRITE(6,62) X,UR
162 X=X + DX1W
62  FORMAT(5X,1PE14.7,3X,E14.7)
    X=XK1 + FLOAT(KW2 - K1)*DX

```

```

DO 163 K=KW2,KMAX,KWRITE
UR=U(K)*VT
WRITE(6,62) X,UR
163 X=X + DXW
VEB1=VAPPLE
VCB1=VAPPLC
WRITE(6,71)
71 FORMAT(1H1,30X,26HDOUBLE DIFFUSED TRANSISTOR)
LA=0
ITER=1
GO TO 35
300 ITER=ITER + 1
IF(VAPPLE.EQ.0...AND.VAPPLC.EQ.0.) GO TO 35

C RECOMBINATION RATE
GR(1)=0.
GR(KMAX)=0.
DO 110 K=2,KMA
110 GR(K)=- (HD(K)*ED(K) - ANIS)/(TP0*ED(K) + TN0*HD(K) + CON)

C RECOMBINATION CURRENT DENSITY
GRI(1)=0.
DO 111 K=2,K1
111 GRI(K)=GRI(K-1) + (GR(K-1) + GR(K))*DX12
GRIR=GRI(K1)
GRI(K1)=0.
DO 211 K=K1P1,KREC
211 GRI(K)=GRI(K-1) + (GR(K-1) + GR(K))*DX2
DO 1211 K=K1,KREC
1211 GRI(K)=GRIR + GRI(K)
GRIR1=GRI(KREC)
GRI(KREC)=0.
DO 2211 K=KREC1,KMAX
2211 GRI(K)=GRI(K-1) + (GR(K-1) + GR(K))*DX2
DO 3211 K=KREC,KMAX
3211 GRI(K)=GRIR1 + GRI(K)

C COUNTING THE NUMBER OF COLLECTOR DOMAIN POTENTIAL SECTIONS
302 X=0.
ANOS=ABS(U(KMAX) - U(K1))/USF0
NOS=INT(ANOS) + 1
NOS1=NOS + 1
USF(1)=0.
IF(NOS.GT.1) GO TO 621
USF(NOS1)=U(KMAX)
GO TO 1302

C NUMBER OF SECTIONS AND THE INTERMEDIATE POTENTIAL REFERENCES
621 DO 125 M=2,NOS
125 USF(M)=USF(M-1) + USF0
USF(NOS1)=U(KMAX)
1302 X=0.

```

```

C      EMITTER DOMAIN INTEGRANDS FOR THE CURRENT INTEGRALS
DO 1288 K=1,K1M1
E=ABS((U(K+1) - U(K))/DX1)*VT
DOP1=ABS(DOP(X))/1.0E+16
DP=DH(X,E,DOP1)
DN=DE(X,E,DOP1)
HCI(K)=EXP(U(K))/DP
ECI(K)=1./(EXP(U(K))*DN)
1288 X=X + DX1

C      NORMALIZED FUNCTIONS FOR THE COLLECTOR DOMAIN INTEGRALS
M=1
KR(M)=K1
X=XK1
UREF=U(K1)
DO 2288 K=K1,KMAX
E=ABS((U(K+1) - U(K))/DX)*VT
DOP1=ABS(DOP(X))/1.0E+16
DP=DH(X,E,DOP1)
DN=DE(X,E,DOP1)
IF(K.EQ.KMAX) GO TO 8282
IF(ABS(U(K)).GT.ABS(USF(M+1))) GO TO 288
8282 HCI(K)=EXP(U(K) - UREF)/DP
ECI(K)=EXP(UREF - U(K))/DN
GO TO 2288

C      SHIFTING THE POTENTIAL REFERENCE POINT
288 MT=M + 1
IF(MT.EQ.NOS1) GO TO 8282
M=MT
UREF=U(K-1)
KR(M)=K-1
HCI(K)=EXP(U(K) - UREF)/DP
ECI(K)=EXP(UREF - U(K))/DN
2288 X=X + DX
KR(NOS1)=KMAX
IF(VAPPLE.EQ.0..AND.VAPPLC.EQ.0.) GO TO 631

C      CONSTANT HOLE CURRENT DENSITY, EMITTER DOMAIN
HCINDE=0.
HCINNE=0.
DO 2506 L=2,K1
K=K1 - L + 2
HCINDE=HCINDE + (HCI(K-1) + HCI(K))
2506 HCINNE=HCINNE + (GRI(K-1)*HCI(K-1)+GRI(K)*HCI(K))
HCINNE=HCINNE*DX12
HCINDE=HCINDE*DX12
AHC0E=(HD(1)*EXP(U(1))-HD(K1)*EXP(U(K1))-HCINNE)/HCINDE
IF(NOS.GT.1) GO TO 2302

C      CONSTANT HOLE CURRENT DENSITY, COLLECTOR DOMAIN
C      SINGLE SECTION CASE
HCINDC=0.

```

```

HCINNC=0.
DO 118 K=K1P1,KMAX
  HCINDC=HCINDC + (HCI(K-1) + HCI(K))
118 HCINNC=HCINNC + (GRI(K-1)*HCI(K-1)+GRI(K)*HCI(K))
  HCINDC=HCINDC*DX2
  HCINNC=HCINNC*DX2
  CH=HD(K1)*EXP(U(K1)) - HD(KMAX)*EXP(U(KMAX))
  AHCOC=(CH - HCINNC)/HCINDC

```

```

C   CONSTANT ELECTRON CURRENT DENSITY, SINGLE SECTION
ECIND=0.
ECINN=0.
DO 313 K=2,K1
  ECINN=ECINN + (GRI(K-1)*ECI(K-1) + GRI(K)*ECI(K))
313 ECIND=ECIND + (ECI(K-1) + ECI(K))
  ECINN1=0.
  ECIND1=0.
DO 113 L=K1P1,KMAX
  K=KMAX - L + K1P1
  ECINN1=ECINN1 + (GRI(K-1)*ECI(K-1)+GRI(K)*ECI(K))
113 ECIND1=ECIND1+(ECI(K-1) + ECI(K))
  ECINN=ECINN*DX12 + ECINN1*DX2
  ECIND=ECIND*DX12 + ECIND1*DX2
  CE=ED(KMAX)/EXP(U(KMAX)) - ED(1)/EXP(U(1))
  AECO=(CE + ECINN)/ECIND
  GO TO 631

```

```

C   CONSTANT HOLE CURRENT DENSITY, COLLECTOR DOMAIN
2302 K=KMA
880 UC=U(K) - U(KMAX)
  IF(ABS(UC).GT.USF0) GO TO 881
  K=K - 1
  GO TO 880
881 KI=2*(K/2) + 1
  K=KI
  X=XK1 + FLOAT(KI - K1)*DX
  UREF=U(KMAX)
  HCINDC=0.
  HCINNC=0.
  E1=ABS((U(K+1) - U(K))/DX)*VT
  DOP1=ABS(DOP(X))/1.E+16
  T22=EXP(U(K) - UREF)/DH(X,E1,DOP1)
  DO 2507 K=KI,KMA
    X1=X + DX
    T11=T22
    E2=ABS((U(K+2) - U(K+1))/DX)*VT
    DOP2=ABS(DOP(X1))/1.E+16
    T22=EXP(U(K+1) - UREF)/DH(X1,E2,DOP2)
    HCINDC=HCINDC + (T11 + T22)
    HCINNC=HCINNC + (GRI(K)*T11 + GRI(K+1)*T22)
2507 X=X + DX
  HCINDC=HCINDC*DX2
  HCINNC=HCINNC*DX2

```

AHCOC=(-HD(KMAX) - HCINNC)/HCINDC

C CONSTANT ELECTRON CURRENT DENSITY

KAUX1=2*(KR(2)/2) - 1

ECIND=0.

ECINN=0.

DO 3505 K=2,K1

ECINN=ECINN + (GRI(K-1)*ECI(K-1) + GRI(K)*ECI(K))

3505 ECIND=ECIND + (ECI(K-1) + ECI(K))

ECINN1=0.

ECIND1=0.

DO 2505 L=K1P1,KAUX1

K=KAUX1 - L + K1P1

ECINN1=ECINN1 + (GRI(K-1)*ECI(K-1)+GRI(K)*ECI(K))

2505 ECIND1=ECIND1+(ECI(K-1) + ECI(K))

ECINN=ECINN*DX12 + ECINN1*DX2

ECIND=ECIND*DX12 + ECIND1*DX2

AEC0=-(ED(1)/EXP(U(1)) - ECINN)/ECIND

C HOLE DENSITY DISTRIBUTION, EMITTER DOMAIN

631 CHCI(1)=0.

HDEXP=HD(1)*EXP(U(1))

CHCI(2)=(HCI(1)*(AHC0E+GRI(1)) + HCI(2)*(AHC0E+GRI(2)))*DX12

HD(2)=(HDEXP - CHCI(2))/EXP(U(2))

K=2

5050 K=K + 1

DCHCI=(HCI(K-1)*(AHC0E+GRI(K-1))+HCI(K)*(AHC0E+GRI(K)))*DX12

IF(AHC0E.EQ.0.) GO TO 4015

QUOT=DCHCI/CHCI(K-1)

IF(ABS(QUOT).LT.DELU) GO TO 5051

4015 CHCI(K)=CHCI(K-1) + DCHCI

HD(K)=(HDEXP - CHCI(K))/EXP(U(K))

IF(K.LT.K1) GO TO 5050

GO TO 5151

5051 HDEXP=HD(K-1)*EXP(U(K-1))

CHCI(K-1)=0.

CHCI(K)=(HCI(K-1)*(AHC0E+GRI(K-1)) + HCI(K)*(AHC0E+GRI(K)))*DX12

HD(K)=(HDEXP - CHCI(K))/EXP(U(K))

IF(K.LT.K1) GO TO 5050

C HOLE DENSITY DISTRIBUTION, COLLECTOR DOMAIN

5151 CHCI(K1)=0.

M=1

NREF=KR(M)

UREF=U(NREF)

CHCI(K1P1)=(HCI(K1)*(AHCOC+GRI(K1))+HCI(K1P1)*(AHCOC+
*GRI(K1P1)))*DX2

HD(K1P1)=(HD(NREF) - CHCI(K1P1))*EXP(UREF - U(K1P1))

K=K1P1

2910 K=K + 1

CHCI(K)=CHCI(K-1) + (HCI(K-1)*(AHCOC+GRI(K-1))+HCI(K)*
*(AHCOC+GRI(K)))*DX2

HD(K)=(HD(NREF) - CHCI(K))*EXP(UREF - U(K))

```

IF(K.EQ.KMA) GO TO 3666
IF(K.EQ.KR(M+1)) GO TO 4040
GO TO 2910

```

C SHIFTING THE POTENTIAL REFERENCE POINT

```

4040 M=M + 1
NREF=KR(M)
UREF=U(NREF)
X=XK1 + FLOAT(NREF - K1)*DX
CHCI(NREF)=0.
E=ABS((U(NREF+1) - U(NREF))/DX)*VT
DOP1=ABS(DOP(X))/1.E+16
HCI(NREF)=1./DH(X,E,DOP1)
K=NREF + 1
CHCI(K)=(HCI(NREF)*(AHCOC+GRI(NREF))+HCI(K)*(AHCOC+GRI(K)))*DX2
HD(K)=(HD(NREF) - CHCI(K))*EXP(UREF - U(K))
IF(K.EQ.KMA) GO TO 3666
GO TO 2910

```

C ELECTRON DENSITY DISTRIBUTION, COLLECTOR DOMAIN

```

3666 CECI(KMAX)=0.
M=NOS1
NREF=KR(M)
NREF1=KR(M-1)
UREF=U(NREF)
UREF1=U(NREF1)
COR=EXP(UREF - UREF1)
DX22=COR*DX2
CECI(KMA)=(ECI(KMAX)*(AECO-GRI(KMAX))+ECI(KMA)*(AECO-GRI(KMA)))
1*DX22
ED(KMA)=(ED(NREF) - CECI(KMA))*EXP(U(KMA) - UREF)
K=KMA
4010 K=K - 1
IF(K.LT.K1) GO TO 4012
IF(K.EQ.K1) GO TO 4011
IF(K.EQ.KR(M-1)) GO TO 4020
4011 CECI(K)=CECI(K+1) + (ECI(K+1)*(AECO-GRI(K+1)) + ECI(K)*
*(AECO-GRI(K)))*DX22
ED(K)=(ED(NREF) - CECI(K))*EXP(U(K) - UREF)
GO TO 4010

```

C SHIFTING THE POTENTIAL REFERENCE POINT

```

4020 X=XK1 + FLOAT(K - K1)*DX
E=ABS((U(K+1)-U(K))/DX)*VT
DOP1=ABS(DOP(X))/1.E+16
DN=DE(X,E,DOP1)
CECI(K)=CECI(K+1) + (ECI(K+1)*(AECO-GRI(K+1)) + (AECO-GRI(K))
*/DN)*DX22
ED(K)=(ED(NREF) - CECI(K))*EXP(U(K) - UREF)
M=M - 1
NREF=KR(M)
NREF1=KR(M-1)
UREF=U(NREF)

```

```

    UREF1=U(NREF1)
    COR=EXP(UREF - UREF1)
    DX22=COR*DX2
    CECI(NREF)=0.
    K=NREF - 1
    CECI(K)=(ECI(NREF)*(AECO-GRI(NREF))+ECI(K)*(AECO-GRI(K)))*
1DX2*COR
    ED(K)=(ED(NREF) - CECI(K))*EXP(U(K) - UREF)
    GO TO 4010

C    ELECTRON DENSITY DISTRIBUTION, EMITTER DOMAIN
4012 K=K1M1
    CECI(K1)=0.
    EDREF=ED(K1)
    CECI(K)=(ECI(K1)*(AECO-GRI(K1)) + ECI(K1M1)*(AECO-GRI(K1M1))
**DX12
    ED(K)=(EDREF - CECI(K))*EXP(U(K))
4030 K=K - 1
    DCECI=(ECI(K+1)*(AECO-GRI(K+1))+ECI(K)*(AECO-GRI(K)))*DX12
    IF(AECO.EQ.0.) GO TO 5052
    RATIO=DCECI/CECI(K+1)
    IF(ABS(RATIO).LT.DELU) GO TO 4014
5052 CECI(K)=CECI(K+1) + DCECI
    ED(K)=(EDREF - CECI(K))*EXP(U(K))
    IF(K.GT.2) GO TO 4030
    GO TO 4666
4014 EDREF=ED(K+1)/EXP(U(K+1))
    CECI(K+1)=0.
    CECI(K)=(ECI(K)*(AECO-GRI(K)) + ECI(K+1)*(AECO-GRI(K+1)))*DX12
    ED(K)=(EDREF - CECI(K))*EXP(U(K))
    IF(K.GT.2) GO TO 4030

C    COUNTING THE NUMBER OF ITERATIONS
4666 X=0.
    IF(LA.EQ.1) GO TO 303
    IF(ITER.GT.ITERM) GO TO 3
    WRITE(6,102) ITER
102  FORMAT(4X,13HITERATION NO.,12)

C    CORRECTION TO THE POTENTIAL DISTRIBUTION
    CALL POTCOR(HD,ED,U,DELTA,X)

C    TESTING THE ACHIEVED ACCURACY
    DO 180 K=2,KMA
    UC=ABS(U(K))
    IF(UC.LE.USMALL) GO TO 180
    AD=ABS(DELTA(K))
    ABRD=AD/UC
    IF(ABRD.GT.DELU) GO TO 830
180  CONTINUE
    DO 800 K=2,KMA
800  U(K)=U(K) + DELTA(K)
    U(KMAX1)=2.*U(KMAX) - U(KMA)

```

LA=1
GO TO 300

C OUTPUTING

C APPLIED VOLTAGES

303 WRITE(6,77) VAPPLE,VAPPLC
77 FORMAT(1H0,4X,4HVEB=,1PE14.7,4X,4HVCB=,E14.7)

C STORING THE LAST ITERATION ON THE TAPE B5
WRITE(9) (U(K),HD(K),ED(K), K=1,KMAX)
REWIND 9

C CONSTANT CURRENT DENSITIES

ECDO=AECO*Q
HCDOE=AHCOE*Q
HCDOC=AHDOC*Q
WRITE(6,72) ECDO,HCDOE,HCDOC
72 FORMAT(1H0,4X,4HECD=,1PE14.7,3X,5HHCDE=,E14.7,3X,5HHCDC=,E14.7)

C STORED CHARGES OF DIFFERENT POLARITIES

HDI=0.
EDI=0.
DO 770 K=1,K1M1
L=K1 - K + 1
HDI=HDI + (HD(K) + HD(K+1))
770 EDI=EDI + (ED(L) + ED(L+1))
HDI1=0.
EDI1=0.
DO 769 K=K1,KMA
L=KMAX - K + K1
HDI1=HDI1 + (HD(L) + HD(L+1))
769 EDI1=EDI1 + (ED(K) + ED(K+1))
HDI=HDI*DX12 + HDI1*DX2
EDI=EDI*DX12 + EDI1*DX2
WRITE(6,777) HDI,EDI
777 FORMAT(1H0,4X,4HHDI=,1PE14.7,4X,4HEDI=,E14.7)
QN=Q*EDI
QP=Q*HDI

C CURRENT DENSITIES AT THE EXTERNAL CONTACTS

ECUR=ECDO + HCDOE
CCUR=ECDO + HCDOC
BCUR=HCDOE - HCDOC

C TEST FOR THE EMITTER VOLTAGE VARIATION

DVIN=VAPPLE - VEB1
IF(DVIN,EQ,0.) GO TO 3333

C COMMON-BASE A.C. CURRENT GAIN

ALFA=(CCUR - CCUR1)/(ECUR - ECUR1)

C A.C. INPUT CONDUCTANCE AND RESISTANCE

```

GIN=(ECUR - ECUR1)/DVIN
RIN=1./GIN

C    TRANSCONDUCTANCE
    TRANS=(CCUR-CCUR1)/DVIN

C    INPUT CAPACITANCE (THE ELECTRON CHARGE)
    CINN=(QN-QN1)/ABS(DVIN)

C    INPUT CAPACITANCE (THE HOLE CHARGE)
    CINP=(QP-QP1)/ABS(DVIN)

C    ELECTRON CHARGE TRANSIT TIME
    TIMETN=(QN-QN0)/ABS(CCUR)

C    HOLE CHARGE TRANSIT TIME
    TIMETP=(QP-QP0)/ABS(CCUR)

C    ELECTRON CHARGE CALCULATED LIMITING FREQUENCY
    OMTN=TRANS/CINN
    OMTN=OMTN/(2.*3.1415926)

C    HOLE CHARGE CALCULATED LIMITING FREQUENCY
    OMTP=TRANS/CINP
    OMTP=OMTP/(2.*3.1415926)

C    COMMON-EMITTER A.C. CURRENT GAIN
    BETA=ALFA/(1. - ALFA)

C    COMMON-BASE D.C. CURRENT GAIN
    ALFADC=CCUR/ECUR

C    COMMON-EMITTER D.C. CURRENT GAIN
    BETADC=ALFADC/(1. - ALFADC)

C    WRITING OUT THE DERIVED TERMINAL PARAMETERS
    WRITE(6,598) ALFA,GIN,RIN,TRANS,CINN,CINP,TIMETN,TIMETP,OMTN,
    *OMTP,ECUR,CCUR,BCUR,QN,QP,BETA,ALFADC,BETADC
598  FORMAT(5X,5HALFA=,1PE14.7//5X,4HGIN=,E14.7//5X,4HRIN=,E14.7//
    15X,6HTRANS=,E14.7//5X,5HCINN=,E14.7//5X,5HCINP=,E14.7//
    25X,7HTIMETN=,E14.7//5X,7HTIMETP=,E14.7//5X,5HOMTN=,E14.7//
    35X,5HOMTP=,E14.7//5X,5HECUR=,E14.7//5X,5HCCUR=,E14.7//
    *5X,5HBCUR=,E14.7//5X,3HQN=,E14.7//5X,3HQP=,E14.7//
    *5X,5HBETA=,E14.7//5X,7HALFADC=,E14.7//5X,7HBETADC=,E14.7)

C    TEST FOR THE COLLECTOR VOLTAGE VARIATION
3333 DVOUT=VAPPLC - VCB1
    IF(DVOUT.EQ.0.) GO TO 3334

C    SHORT-CIRCUIT OUTPUT ADMITTANCE
    YOUT=(CCUR - CCUR1)/DVOUT

C    SHORT-CIRCUIT REVERSE TRANSFER ADMITTANCE

```

```

      YRTA=(ECUR - ECUR1)/DVOUT
C      OUTPUT CAPACITANCE (HOLE CHARGE)
      COUTP=ABS((QP - QP1)/DVOUT)
C      OUTPUT CAPACITANCE (ELECTRON CHARGE)
      COUTN=ABS((QN - QN1)/DVOUT)
C      WRITING OUT THE DERIVED TERMINAL PARAMETERS
      WRITE(6,599) YOUT,YRTA,ECUR,CCUR,BCUR,QN,QP,COUTP,COUTN
599  FORMAT(5X,5HYOUT=,1PE14.7//5X,5HYTRA=,E14.7//
      15X,5HECUR=,E14.7//5X,5HCCUR=,E14.7//5X,5HBCUR=,
      2E14.7//5X,3HQN=,E14.7//5X,3HQP=,E14.7//
      35X,6HCOUTP=,E14.7//5X,6HCOUTN=,E14.7)
C      REDEFINING THE LAST ITERATION
3334 ECUR1=ECUR
      CCUR1=CCUR
      BCUR1=BCUR
      VEB1=VAPPLE
      VCB1=VAPPLC
      QN1=QN
      QP1=QP
C      RECORDING THE COMPUTED INTERNAL DISTRIBUTIONS
      I=I + 1
      IF(I.LE.10) GO TO 3002
3003 WRITE(6,78)
      78  FORMAT(1H0,5X,1HX,16X,1HU,16X,1HP,16X,1HN,16X,5HDE/DX,12X,
      *5HFIELD,12X,3HGRI)
      X=0.
      DO 602 K=1,KW1,KWRIT1
      RO=T*(DOP(X) - ED(K) + HD(K))
      UR=U(K)*VT
      FIELD=(U(K) - U(K+1))*VT/DX1
      WRITE(6,170)X,UR,HD(K),ED(K),RO,FIELD,GRI(K)
602  X=X + DX1W
170  FORMAT(1H ,4X,7(1PE14.7,3X))
      X=XK1 + FLOAT(KW2-K1)*DX
      DO 603 K=KW2,KMAX,KWRITE
      RO=T*(DOP(X) - ED(K) + HD(K))
      UR=U(K)*VT
      FIELD=(U(K) - U(K+1))*VT/DX
      WRITE(6,170)X,UR,HD(K),ED(K),RO,FIELD,GRI(K)
603  X=X + DXW
      I=1
3002 WRITE(6,688)
688  FORMAT(1H0,4X,27HTHE LAST ITERATION RECORDED)
C      NEW BOUNDARY POTENTIALS AND THE POTENTIAL GUESS
3001 IF(MAN.EQ.0) GO TO 31
      IF(N.GE.NC) GO TO 33

```

C SELECTING THE VARIATION IN THE COLLECTOR BOUNDARY VALUE

```

32 IC=IC + 1
   ICR=IC/2
   IC1=2*ICR
   IF(IC1.EQ.IC) GO TO 1717
   VAPC=VAPCS
   GO TO 1718
1717 VAPC=VAPCB
1718 VAPCN=VAPC/VT
   DVAPCN=VAPCN/FLIMC
   DO 2280 L=1,LIMC
   K=KMAX - L + 1
   KB=LIMC - L + 1
   FKB=FLOAT(KB)
2280 U(K)=U(K) + DVAPCN*FKB
   VAPPLC=VAPPLC + VAPC
   U(KMAX1)=2.*U(KMAX) - U(KMA)
   N=N + 1
   LA=0
   ITER=0
   GO TO 300

```

C SELECTING THE VARIATION IN THE EMITTER BOUNDARY VALUE

```

31 IF(IVP.GE.IG) GO TO 33
   IE=IE + 1
   IER=IE/2
   IE1=2*IER
   IF(IE1.EQ.IE) GO TO 1700
   VAPE=VAPES
   GO TO 1701
1700 VAPE=VAPEB
1701 VAPEN=VAPE/VT
   DVAPEN=VAPEN/FLIME
   DO 280 K=1,LIME
   KA=LIME - K + 1
   FKA=FLOAT(KA)
280 U(K)=U(K) + DVAPEN*FKA
   IVP=IVP + 1
   VAPPLE=VAPPLE + VAPE
   KC=(KMAX - K1)/2
   DVCORN=(VCCOR/VT)/FLOAT(KC)
   KCCOR=K1 + KC
   KCCOR1=KCCOR + 1
   DO 377 I1=K1P2,KCCOR
377 U(I1)=U(I1) - DVCORN*FLOAT(I1 - K1P1)
   DO 378 I1=KCCOR1,KMA
378 U(I1)=U(I1) - DVCORN*FLOAT(KMA - I1)
   U(KMAX1)=2.*U(KMAX) - U(KMA)
   LA=0
   ITER=0
   GO TO 300

```

C INTERMEDIATE STEP IN CORRECTING THE POTENTIAL DISTRIBUTION

```

830 IN=2
DO 181 K=IN,KMA
181 U(K)=U(K) + DELTA(K)
   U(KMAX1)=2.*U(KMAX) - U(KMA)
   GO TO 300

C   INTERMEDIATE STOP
3   WRITE(6,106)
106 FORMAT(1H0,4X,30HMAX NO. OF ITERATIONS EXCEEDED)
   REWIND 9
   WRITE(6,77) VAPPLE,VAPPLC
   ECDO=AECO*Q
   HCDOE=AHCOE*Q
   HCDOC=AHCOE*Q
   WRITE(6,72) ECDO,HCDOE,HCDOC

C   STORING THE INTERMEDIATE RESULTS ON TAPE B5
   WRITE(9) (U(K),HD(K),ED(K), K=1,KMAX)
   REWIND 9

C   DETAILS OF INTERMEDIATE INTERNAL DISTRIBUTIONS
   WRITE(6,178)
178 FORMAT(1H0,2X,1HX,10X,1HU,10X,1HP,10X,1HN,10X,3HHCI,8X,3HECI,
   *8X,5HDELTA,6X,2HGR,9X,3HGRI,8X,4HCHCI,7X,4HCECI)
   X=0.
   DO 601 K=1,KW1,KWRIT1
   WRITE(6,173)X,U(K),HD(K),ED(K),HCI(K),ECI(K),DELTA(K),
   *GR(K),GRI(K),CHCI(K),CECI(K)
601 X=X + DX1W
173 FORMAT(1H,1X,11(1PE11.4))
   X=XK1 + FLOAT(KW2-K1)*DX
   DO 604 K=KW2,KMAX,KWRITE
   WRITE(6,173)X,U(K),HD(K),ED(K),HCI(K),ECI(K),DELTA(K),
   *GR(K),GRI(K),CHCI(K),CECI(K)
604 X=X + DXW
   STOP

C   SETTING THE CURRENT DENSITIES AND RECOMBINATION TO ZERO
35 DO 135 K=1,KMAX
   GR(K)=0.
135 GRI(K)=0.
   AECO=0.
   AHCOE=0.
   AHCOE=0.
   GO TO 302
33 WRITE(6,79)
79 FORMAT(5X,/,5X,22HCOMPUTATIONS COMPLETED)
   STOP
   END

```

```

C      DOPING PROFILE OF A COMPUTED STRUCTURE
      FUNCTION DOP(X)
      COMMON/DFUN/XAP,DOPE,DOPB1,DOPB2,DOPC,ED1,ED2,E1MAX,E2MAX,
      *E1SMAX,E2SMAX
      IF(X.GT.XAP) GO TO 24
      E1=X/ED1
      DOP=DOPE*(1. - ERF(E1)) - DOPB1 + DOPC
      RETURN
24  E1=X/ED1
      E2=X/ED2
      IF(E2.GT.E2MAX) GO TO 25
      IF(E1.GT.E1MAX) GO TO 28
      DOP=DOPE*(1. - ERF(E1)) - DOPB2*(1. - ERF(E2)) + DOPC
      RETURN
28  DOP=-DOPB2*(1. - ERF(E2)) + DOPC
      RETURN
25  DOP=DOPC
      RETURN
      END

```

```

C      DERIVATIVE OF THE DOPING FUNCTION
      FUNCTION DERDOP(X)
      COMMON/DFUN/XAP,DOPE,DOPB1,DOPB2,DOPC,ED1,ED2,E1MAX,E2MAX,
      *E1SMAX,E2SMAX
      IF(X.GT.XAP) GO TO 24
      E1=X/ED1
      E1S=E1*E1
      DERDOP=-1.1283792*DOPE/(ED1*EXP(E1S))
      RETURN
24  E1=X/ED1
      E2=X/ED2
      E1S=E1*E1
      E2S=E2*E2
      IF(E2S.GT.E2SMAX) GO TO 25
      IF(E1S.GT.E1SMAX) GO TO 28
      DERDOP=-1.1283792*(DOPE/(ED1*(EXP(E1S))) - DOPB2/(ED2*
      1*(EXP(E2S))))
      RETURN
28  DERDOP=1.1283792*DOPB2/(ED2*EXP(E2S))
      RETURN
25  DERDOP=0.
      RETURN
      END

```

```

C      SUBROUTINE FOR CALCULATING CORRECTIONS TO POTENTIAL FUNCTION
      SUBROUTINE POTCOR(HD,ED,U,DELTA,X)
      DIMENSION U(1674),HD(1673),ED(1673),DELTA(1673)
      COMMON/AR/ANN(1673),ANNM1(1673),ANNP1(1673),UNN(1673),ZV(1673),
      *R(1673)
      COMMON/POCO/DX, TM, B0, B1, B2, DXSQB0, DXSQB1, DXSQB2, TOVT, KM, KMA,
      *K1, K1M1, K1M2, K1P1, K1P2, L0, DX1, DX1SB0, DX1SB1, DX1SB2, TM1, XK1
      COMMON/DFUN/XAP, DOPE, DOPB1, DOPB2, DOPC, ED1, ED2, E1MAX, E2MAX,
      *E1SMAX, E2SMAX

C      EMITTER DOMAIN CALCULATIONS
      DO 81 K=2, K1M1
      X=X + DX1
      X1=X - DX1
      X2=X + DX1
      81 R(K)=-U(K-1)+2.*U(K)-U(K+1)+TM1*(B0*(HD(K-1)+(DOP(X1)-ED(K-1)))
      1+B1*(HD(K)+(DOP(X)-ED(K)))+B2*(HD(K+1)+(DOP(X2)-ED(K+1))))
      DF1=TOVT*(HD(2) + ED(2))
      ANN(2)=2. + DX1SB1*DF1
      ANNM1(2)=-1. + DX1SB0*DF1
      DO 82 K=3, K1M2
      DF2=TOVT*(HD(K) + ED(K))
      ANNP1(K)=-1. + DX1SB2*DF2
      ANN(K)=2. + DX1SB1*DF2
      82 ANNM1(K)=-1. + DX1SB0*DF2
      DFM=TOVT*(HD(K1M1) + ED(K1M1))
      ANNP1(K1M1)=-1. + DX1SB2*DFM
      ANN(K1M1)=2. + DX1SB1*DFM
      UNN(2)=ANN(2)
      ZV(2)=-R(2)
      DO 84 K=3, K1M1
      ALNNM1=ANNM1(K-1)/UNN(K-1)
      UNN(K)=ANN(K) - ALNNM1*ANNP1(K)
      84 ZV(K)=-R(K) - ALNNM1*ZV(K-1)
      DELTA(K1M1)=ZV(K1M1)/UNN(K1M1)
      DO 85 L=2, K1M2
      K=K1M1 - L + 1
      85 DELTA(K)=(ZV(K) - ANNP1(K+1)*DELTA(K+1))/UNN(K)

C      COLLECTOR DOMAIN CALCULATIONS
      X=XK1
      DELTA(K1)=0.
      DO 810 K=K1P1, KMA
      X=X + DX
      X1=X - DX
      X2=X + DX
      810 R(K)=-U(K-1)+2.*U(K)-U(K+1)+TM*(B0*(HD(K-1)+(DOP(X1)-ED(K-1)))
      1+B1*(HD(K)+(DOP(X)-ED(K)))+B2*(HD(K+1)+(DOP(X2)-ED(K+1))))
      DF1=TOVT*(HD(K1P1) + ED(K1P1))
      ANN(K1P1)=2. + DXSQB1*DF1
      ANNM1(K1P1)=-1. + DXSQB0*DF1
      DO 820 K=K1P2, KM
      DF2=TOVT*(HD(K) + ED(K))

```

```

      ANNP1(K)=-1. + DXSQB2*DF2
      ANN(K)=2. + DXSQB1*DF2
820  ANNM1(K)=-1. + DXSQB0*DF2
      DFM=TOVT*(HD(KMA) + ED(KMA))
      ANNP1(KMA)=-1. + DXSQB2*DFM
      ANN(KMA)=2. + DXSQB1*DFM
      UNN(K1P1)=ANN(K1P1)
      ZV(K1P1)=-R(K1P1)
      DO 840 K=3,KMA
      ALNNM1=ANNM1(K-1)/UNN(K-1)
      UNN(K)=ANN(K) - ALNNM1*ANNP1(K)
840  ZV(K)=-R(K) - ALNNM1*ZV(K-1)
      DELTA(KMA)=ZV(KMA)/UNN(KMA)
      DO 850 L=1,L0
      K=KMA - L
850  DELTA(K)=(ZV(K) - ANNP1(K+1)*DELTA(K+1))/UNN(K)
      RETURN
      END

```

```

C      DIFFUSION COEFFICIENT OF HOLES
      FUNCTION DH(X,E,DOP1)
      COMMON/DIFFS/VT,ECH,ECE
      DH0=(47.7 + 447.3/(1. + (DOP1/6.3)**0.76))*VT
      EX=1. + E/ECH
      DH=DH0/EX
      RETURN
      END

```

```

C      DIFFUSION COEFFICIENT OF ELECTRONS
      FUNCTION DE(X,E,DOP1)
      COMMON/DIFFS/VT,ECH,ECE
      DE0=(65. + 1265./(1. + (DOP1/8.5)**0.72))*VT
      EY=E/ECE
      DE=DE0/SQRT(1.+EY*EY)
      RETURN
      END

```

C NOTE

C AFTER AN INTERMEDIATE STOP OF THE CALCULATIONS THE NECESSARY
C INTERNAL DISTRIBUTIONS FOR RESTARTING THE CALCULATIONS ARE
C AVAILABLE ON TAPE B5 AND THE FOLLOWING DECK SHOULD BE USED
C INSTEAD OF THE PART CALLED POTENTIAL GUESS, FIRST ORDER THEORY

C LAST ITERATION STORED ON TAPE B5

REWIND 9

READ(9) (U(K),HD(K),ED(K),K=1,KMAX)

REWIND 9

U(KMAX1)=2.*U(KMAX) - U(KMA)

VEB1=VAPPLE

VCB1=VAPPLC

WRITE(6,71)

71 FORMAT(1H1,30X,26HDOUBLE DIFFUSED TRANSISTOR)

LA=0

ITER=0

REFERENCES

1. Murphy G. M., "Ordinary Differential Equations and Their Solutions", D. Van Nostrand, Inc., 1960.
2. McKelvey P. J., Longini L. R., and Brody T. P., Physical Review, Vol. 123, No. 1, pp.51-57, July 1, 1961.
3. McKelvey P. J., J. Appl. Phys., Vol. 33, No. 3, pp.985-991, 1962.
4. Shockley W., Physical Review, Vol. 125, No.5, pp.1570-76, 1962.
5. Prior A. C., J. Phys. Chem. Solids, Vol. 12, p.175, 1960.
6. Ryder J. E., and Shockley W., Physical Review, Vol.81, p.139, 1951.
7. Sim C. A., IEE Proc., Vol. 106, part B, Suppl.15, pp.357-61, 1959.
8. Ryder J. E., Physical Review, Vol. 90, p.766, 1953.
9. Gunn J. B., J. Electronics, Vol.2, p.87, 1956.
10. Norris C. B., and Gibbons J. F., IEEE Trans. on Electron Devices, Vol. ED-14, pp.38-43, 1967.
11. Irvin J. C., B.S.T.J., Vol. 41, pp.387-410, 1962.
12. Okamoto K., and Nishizawa J., J. Appl. Physics, Vol.36, No.12, pp.3716-22, 1965.
13. Caughey D. M., and Thomas R. E., Proc. IEEE (Corr.), Vol. 55, pp.2192-3, 1967.
14. Prince M. B., Physical Review, Vol. 92, pp.681-87, 1953.
15. Prince M. B., Physical Review, Vol. 93, pp.1206-6, 1954.
16. Lindmayer J., and Wrigley G. Y., "Fundamentals of semiconductor devices", D. Van Nostrand, Princeton, N.J., 1965, p.127.
17. Conwell E., and Weisskopf V. F., Physical Review, Vol. 77, pp.388-90.
18. Van Roosbroeck W., B.S.T.J., Vol. 29, pp.560-608, 1950.
19. Debye, P. P., and Conwell E., Physical Review, Vol. 93, pp.693-706, 1954.
20. Conwell E., Proc. IRE, Vol.40, pp.1327-37, 1952.
21. Fletcher N. F., Proc. IRE, Vol. 45, pp.862-72, 1957.
22. Abramowitz M., and Stegun I. A., Eds., "Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables", Nat.Bur. of Standards, Applied Math. Series-55, 1964, p.232.

23. Hastings C., "Approximations for Digital Computers," Princeton Univ. Press, Princeton, N.J., 1955.
24. Henrici P., "Discrete Variable Methods in Ordinary Differential Equations", John Wiley & Sons, Inc., p.345, 1962.
25. Hall R. N., Physical Review, Vol.87, p.387, 1952.
26. Shockley W., and Read W. T., Physical Review, Vol.87, pp.835-43, 1952.
27. Adirovich E. J., Riabinkin Yu. S., and Temko K. V., Soviet Phys. - Techn. Phys., Vol. 3, 1958.
28. Passau H. P., and Van Styvendal M., Solid State Physics in Electronics and Telecommunications, Academic Press, New York, Vol. 1, pp.407-21, 1960.
29. Sparkes J. J., J. Electronics and Control, Vol.16, No.2, pp.152-68, 1964.
30. Morgan P. S., and Smits M. E., B.S.T.J., Vol.39, pp.1573-1602, 1960.
31. Ralston A., and Wilf S. H., "Mathematical Methods for Digital Computers", John Wiley & Sons, Inc., 1960, p.98.
32. Shockley W., B.S.T.J., Vol. 28, pp.435-89, 1949.
33. Middlebrook R. D., "An Introduction to the Junction Transistor Theory", John Wiley & Sons, Inc., 1957.
34. Reiss, H., J. Appl. Physics, Vol. 27, pp.530-37, 1956.
35. Rediker R. H., and Sawyer D. E., Proc. IRE, Vol. 45, pp.944-53, 1957.
36. Hall R. N., Proc. IRE, Vol. 40, pp.1512-18, 1952.
37. Shields J., Proc. IEEE, Vol. 106, Part B, Supplement No.15, pp.342-52, 1959.
38. Stafeev I. V., Soviet Phys. - Tech.Physics, Vol. 3, p.1502, 1958.
39. Aronov D. A., Izvestiya Acad. Sci. Uz.SSR, Ser.Math.-Phys.Sci., pp.68-77, 1960 (in Russian).
40. Moll, J. L., Proc. IRE, Vol. 46, pp.1076-82, 1958.
41. Rashba E. I., and Tolpygo K. B., Zh. Tekh. Phys., Vol.26, No. 7, p.1419, 1956 (in Russian).
42. Berkovskii M. F., Ryvkin M. S., and Strokan B. N., Soviet Phys.-Solid State, Vol.3, pp.1762-67, 1961.

43. Sokolov Yu. S., Radio Engineering and Electronic Physics, Vol.8, No.3, pp.425-23, 1963.
44. Stafeev I. V., Soviet Phys.-Solid State, Vol.3, pp.135-40, 1961.
45. Kinman T. A. et al., Proc.IEE, Vol.103, Part A, pp.89-111, 1956.
46. Ladany I., Proc. IRE (Corr.), Vol. 47, p.589, 1958.
47. Avakyants G. M., et al., Rad.Eng. and Elec.Phys., Vol.8, pp.1671-77, 1963.
48. Avakyants G. M., Rad.Eng. and Elec.Phys., Vol.10, pp.1281-86, 1965.
49. Avakyants G. M., et al., Rad.Eng. and Elec.Phys., Vol.8, pp.835-43, 1963.
50. Avakyants G. M., et al., Rad.Eng. and Elec.Phys., Vol.9, pp.707-13, 1964.
51. Avakyants G. M., and Leiderman A. Yu., Rad.Eng. and Elec.Phys., Vol.9, pp.544-48, 1964.
52. Leiderman A. Yu., and Karageorgiy-Alkalaev P. M., Rad.Eng. and Elec.Phys., Vol.9, pp.1550-55, 1964.
53. Aronov D. A., and Avakyants G. M., Izvestiya Acad.Sci.Uz.SSR, Ser. Phys.-Math.Sci., Vol. 6, p.27, 1959 (in Russian).
54. Leiderman A. Yu., and Karageorgiy-Alkalaev P. M., Rad.Eng. and Elec. Phys., Vol. 10, pp.611-17, 1965.
55. Kleinman D. A., B.S.T.J., Vol. 35, pp.685-706, 1956.
56. Jonscher A. K., J.Electronics and Control, Vol.5, pp.1-15, 1958.
57. Lampert M. A., and Rose A., Physical Review, Vol.121, p.26, 1961.
58. Gribnikov Z. S., Rad. Eng. and Elec.Phys., Vol.9, pp.127-35, 1964.
59. Gribnikov Z. S., Rad. Eng. and Elec.Phys., Vol.9, pp.692-700, 1964.
60. Jonscher A. K., J.Electronics and Control, Vol.5, pp.226-44, 1958.
61. Larrabee R. D., Physical Review, Vol.121, p.37, 1961.
62. Lieb D. P., et al., IRE Trans. on Electron Devices, Vol.ED-9, pp.143-53, 1962.
63. Nussbaum A., Physics of Semiconductors, Proceedings of the 7-th International Conference, Paris, 1964, pp.583-87.
64. Sah C. T. et al., Proc. IRE, Vol. 45, pp.1228-43, 1957.

65. Pell E. M., and Roe G. M., J.Appl.Physics, Vol.26, pp.658-65, 1955.
66. Bernard M. J., J.Electronics, Vol.2, pp.579-96, 1957 (in French).
67. Barber D. H., University of London Thesis, London, 1965.
68. Hauser R. J., Proc.IEEE (Corr.), Vol.53, p.743, 1965.
69. Chevychelov D. A., Soviet Phys.-Solid State, Vol.2, pp.1102-09, 1960.
70. Sah C. T., Proc. IRE, Vol. 49, pp.603-18, 1961.
71. Scarlett M. R., IRE Trans. on Electron Devices, Vol.ED-6, pp.405-08, 1959.
72. Lawrence H., and Warner M. R., B.S.T.J., Vol.39, pp.289-404, 1960.
73. Root D. C., IRE Trans. on Electron Devices, Vol.ED-7, pp.279-82, 1960.
74. Kennedy P. D., and O'Brien R. R., J. Electronics and Control, Vol.9, pp.303-15, 1961.
75. Kennedy P. D., and O'Brien R. R., IRE Trans. on Electron Devices, Vol.ED-9, pp.478-83, 1962.
76. Breitschwrdt G. K., IEEE Trans. on Electron Devices, Vol.ED-12, pp.13-19, 1965.
77. Kroemer H., RCA Rev., Vol. 17, pp.515-21, 1956.
78. Vul B. M., Doklady Akad. Sci. (Phys.), USSR, Vol.96, pp.257-59, 1954.
79. Giacoletto L. J., IRE Trans. on Electron Devices, Vol.ED-4, pp.207-16, 1957.
80. Vul M. B., Soviet Phys.-Solid State, Vol.3, pp.148-49, 1961.
81. Gribnikov S. Z., Soviet Phys.-Solid State, Vol.3, pp.1211-20, 1961.
82. Middlebrook R. D., Solid-State Electronics, Vol.6, pp.556-72, 1963.
83. Nosov Yu. R., Rad.Eng. and Elec.Phys., Vol.6, pp.194-206, 1961.
84. Nosov Yu. R., Rad.Eng. and Elec.Phys., Vol.9, pp.1763-69, 1964.
85. Nosov Yu. R., and Postnikova N. V., Rad.Eng. and Elec.Phys., Vol.9, pp.1769-72, 1964.
86. Shields J., J. Electronics and Control, Vol.4, pp.58-60, 1958.
87. Shields J., J. Electronics and Control, Vol.6, pp.130-48, 1959.
88. Ko H. W., Solid-State Electronics, Vol.3, pp.59-69, 1961.

89. Kano K., and Reich J. H., IEEE Trans. on Electron Devices, Vol.ED-11, pp.515-23, 1964.
90. Gossick R. B., Physical Review, Vol. 91, pp.1012-13, 1953.
91. Bray R., and Gossick R. B., Physical Review, Vol.91, pp.1011-12, 1953.
92. Shulman G. R., and McMahon E. M., J. Appl. Physics, Vol.24, pp.1267-72, 1953.
93. Steele E. L., J.Appl. Physics, Vol.25, pp.916-18, 1954.
94. Ko H. W., IRE Trans. on Electron Devices, Vol. ED-8, pp.123-31, 1961.
95. Lax B., and Neustadter F. S., J. Appl. Physics, Vol.25, pp.1148-54, 1954.
96. Kingston R. H., Proc. IRE, Vol.42, pp.829-34, 1954.
97. Henderson C. J., and Tillman J. R., Proc.IEE, Vol.104B, pp.318-33, 1957.
98. Byzkowski M., and Madigan R. R., J. Appl. Physics, Vol.28, pp.878-81, 1957.
99. Barsukov K. Yu., Soviet Phys.-Solid State, Vol.2, pp.1518-24, 1960.
100. Ilyenkov A. I., Rad.Eng. and Elec. Phys.,Vol.8, pp.843-47, 1963.
101. Kennedy P. D., IRE Trans. on Electron Devices, Vol.ED-9, pp.174-82, 1962.
102. Muto V. S., and Wang S., IRE Trans. on Electron Devices, Vol.ED-9, pp.183-87, 1962.
103. Goldberg C., Solid-State Electronics, Vol.7, pp.593-609, 1964.
104. Gold L., J. Electronics and Control, Vol.5, pp.427-31, 1958.
105. Gummel H., IEE Trans. on Electron Devices, Vol.ED-11, pp.455-65, 1964.
106. Penin N. A., Rad.Eng. and Elec.Phys., Vol.2, No.8, pp.147-58, 1957.
107. Bemski G., Proc.IRE,Vol.46, pp.990-1004, 1958.
108. Demari A., Electronics Letters, Vol.3, pp.142-44, 1967.
109. Trofimenkoff F. N., and Boothroyd A. R., International J. Electronics, Vol. 18, pp.165-76, 1965.
110. Agakhanyan T. M., Rad. Eng. and Elec.Phys., Vol.10,pp.1887-95, 1965.

111. Fletcher N. H., J. Electronics, Vol.2, pp.609-10, 1957.
112. Chang Y. F., J.Appl.Phys., Vol. 37, No.6, pp.2337-42, 1966.
113. Fulkerson D. E., and Nussbaum A., Solid-State Electronics, Vol. 9, pp.709-19, 1966.
114. Lade R. W., and Poncelet C. G., Proc.IEEE (Corr.), Vol.52, pp.629-30, 1964.
115. Loeb H. W., J. Electronics and Control, Vol. 12, pp.31-47, 1962.
116. Collard J. R., and Sterzer F., Appl.Phys.Letters, Vol.5, pp.165-67, 1964.
117. Nakahara O., Proc.IEEE (Corr.), Vol.51, p.1271, 1963.
118. Nicolet M. A., Proc.IEEE (Corr.), Vol.51, p.1789, 1963.
119. Gatland I. R., and Gold L., International J. Electronics, Vol.18, pp.219-21, 1965.
120. Kirk J. C., IRE Trans. on Electron Devices, Vol.ED-9, pp.164-74, 1962.
121. Kennedy D. P., and O'Brien R. R., IBM J. Res.Dev., Vol.11, pp.252-70, 1967.
122. Moll J. L., and Ross I. M., Proc.IRE, Vol.44, pp.72-78, 1956.
123. Kennedy D. P., and Murley P. C., Proc. IEEE (Corr.), Vol. 52, pp.620-21.
124. Greebe, C. A. A., and Maesen, Van der F., Philips Res. Reports, Vol. 18, pp.65-70, 1963.
125. Grove A. S., "Physics and technology of semiconductor devices", John Wiley & Sons, Inc., 1967, p.65.
126. Rose A., J.Appl.Phys., Vol.35, pp.2664-78, 1964.
127. Van Vliet K. M., Solid-State Electronics, Vol.9, pp.185-201, 1966.
128. Webster W. M., Proc.IRE, Vol.42, pp.914-920, 1954.
129. Gummel H., Solid-State Electronics, Vol.10, pp.209-212, 1967.
130. Lampert M., Proc.IRE, Vol.50, pp.1781-96, 1962.
131. Maesen, Van der F. et al., Philips Res. Reports, Vol.17, pp.479-512, 1962.
132. Smits F. M., Proc. IRE, Vol. 46, pp.1049-61, 1958.
133. Chang Y. F., Solid-State Electronics, Vol.10, pp.281-287, 1967.
134. Gummel H., and Scharfetter D. L., J.Appl.Phys., Vol.38, pp.2148-53, 1967.

135. Chang F. Y., J. Appl. Phys., Vol.34, pp.2056-60, 1963.
136. Muratov I. I., Rad.Eng. and Elec.Phys., Vol.10, pp.1895-98, 1965.
137. Sanchez M., Electronics Letters, Vol.3, No.4, pp.160-62, 1967.
138. Arandjelovic V., and Sparkes J. J., Electronics Letters, Vol.3, No.8, pp.357-9, 1967.
139. Arandjelovic V., and Sparkes J. J., "Numerical analysis of transistor properties in non-equilibrium conditions", paper presented at Conference on solid state devices, Manchester, England, 1967.
140. DeMari A., Solid-State Electronics, Vol.11, pp.33-58, 1968.
141. Fox L., "The numerical solutions of two-point boundary problems in ordinary differential equations", Oxford at the Clarendon Press, 1957, p.90.
142. Kantorovich L. V., Nat.Bur.Standards Rept. No.1509.
143. Nicholas K. N., Solid-State Electronics, Vol.9, pp.35-47, 1966.
144. Cave K. J. S., Allen Clark Res. Centre, The Plessey Company Ltd., England, Private communication.
145. Caughey D. M., Electronics Letters, Vol.3, No.12, 1967.
146. Caughey D. M., "The computer simulation of gigahertz transistors", the paper presented at IEEE International Electronics Conference, Toronto, Ont., Canada, September 1967.
147. Ghosh et al., Solid-State Electronics, Vol.10, pp.705-26, 1967 (also Proc. IEEE, Vol.55, No.11, pp.1897-912, 1967).
148. Wei L. Y., IEEE Spectrum, Vol. 3, pp.123-27, 1966.