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FISH1D 2.1 User's Manual

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FISH1D 2.1

User's Manual

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PREFACE

FISH1D is a computer program that solves the one-dimensional Poisson equation for electrostatic fields in semiconductor heterostructures. The program will print or plot the electrostatic potential, electric field, electron and hole densities, dopant density, ionized dopant density, and other quantities of interest versus position at an applied bias voltage (assuming zero current). A capacitance or sheet carrier concentration versus voltage analysis may also be performed. While FISH1D was originally written for the ternary $\text{Al}_x\text{Ga}_{1-x}\text{As}$, it has been modified to simulate $\text{Cd}_x\text{Hg}_{1-x}\text{Te}$, ZnSe, $\text{Ge}_x\text{Si}_{1-x}$, and Si as well, and the program can be readily modified to analyze other semiconductors through the addition of new material subroutines or using the most recent option, the MATDEF card. This card enables the user to enter new material definitions by layers in the input deck without having to recompile, an advantage of FISH1D 2.1 over FISH1D 2.0. The primary purpose of this document is explain how to use FISH1D; for a more thorough discussion of the numerical implementation of FISH1D, the user is directed to the references. A theoretical basis for FISH1D is provided in Appendix I of this manual.

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INPUT DECK STRUCTURE

The input deck for FISH1D is loosely based on the FORTRAN NAMELIST statement. An input card has the form:

```
NAME KEY1=VALUE1, KEY2=STRING2, ..., KEYn=VALUEn
+ ARRAY1=VA1/VA2/VA3/VA4, ARRAY2=WA1/WA2
+ ARRAY2=WA3/WA4
```

Each card begins in column 1 with its name; a card may be up to 5 lines long. Warning: do not use tabs in the input deck! If a card is longer than one line, the continuation symbol, +, must appear in column 1 for lines 2, 3, 4, etc. Commas or blanks are assumed to be separators; any number of separators may appear between assignments. An assignment cannot contain any blanks, i.e.

```
PARM = - 12.0
```

is not valid. The above assignment should read:

```
PARM=-12.0
```

Values are assigned to arrays by separating the values by /'s. In the example card shown above, values are defined for ARRAY1(1), ARRAY1(2), ARRAY1(3), ARRAY1(4), and for ARRAY2(1), ARRAY2(2), ARRAY2(3), and ARRAY2(4). Any parameter that does not appear in the card assumes its default value. Only those keys that are to be changed from their default value need to be specified. If the default values are to be used for all parameters of the card, the card need not appear.

Special care should be taken when continuing cards since array elements cannot be continued across lines. For example, the following card is NOT ALLOWED:

```
NAME KEY1=VALUE1, KEY2=STRING2, ..., KEYn=VALUEn
+ ARRAY1=VA1/VA2/VA3/VA4, ARRAY2=WA1/WA2/
+ WA3/WA4
```

The array should either be contained on one line or continued as shown above in the first example.

The input deck consists of a title followed by several other cards. The *TITLE card, which consists of up to 80 characters, is used to identify the simulation run; it must not be omitted. For the other cards, order is not significant. On the following pages, we briefly describe the allowed keys and their default values for of the cards.

GRID

The GRID card is used to specify the finite difference grid for the problem. Since the accuracy of the computed results is to a great extent determined by the quality of the grid, it should be carefully specified. When specifying the grid, several nodes should be placed in each of the material and doping layers defined. Nodes should also be concentrated where the electrostatic potential (or more precisely, the space-charge density) is expected to vary rapidly. It is also possible to direct the program to automatically choose a finite difference grid. The user should always assess the quality of the grid; it is easiest to do so by inspecting the plots of electrostatic potential or electric field versus position.

The GRID keys are:

AUTO

A logical variable that, if true, directs the program to automatically select a finite difference grid. Default value: AUTO=TRUE

NODES

The number of nodes to be used in the automatically generated grid. Allowed values are integers between 1 and 250. NODES refers to the number of interior nodes used in the finite difference grid. If NODES=250, for example, a node 0 is automatically placed at $x=0$, and a node 251 at $x=L$. Default value: NODES=250

XD(i)

The user-specified grid is defined by dividing the device length into a number of sections, then placing a specified number of nodes uniformly within each region. The XD(i) keys, where $1 \leq i \leq 20$, specify the right edge of each section in micrometers. Default value: XD(1)=10.

NXD(i)

The number of nodes to be placed within each of the sections. An NXD(i) value must be specified for each XD(i) specified. The sum of the NXD(i), the total number of nodes, must not exceed 251. Note that the $x = 0$ boundary node is not among these, but the boundary at $x = L$ is (the last node may be at most, node 251). Default value: NXD(1)=251

ND

The number of user-defined sections for the finite difference grid is an integer, ND, where $1 \leq ND \leq 20$. Default value: ND=1.

SOLVE

The SOLVE card is used to specify iteration and convergence criteria for the finite difference solution. For most applications, the default values of these parameters should be used. Note that changes to DVMAX can affect the accuracy of the results.

The SOLVE keys are:

DVMAX

Before iteration can be terminated, the maximum change in the electrostatic potential between iterations must be less than DVMAX. DVMAX is a dimensionless voltage measured in units of kT/q . Default value: DVMAX=1.0e-04

ITMAX

ITMAX is the maximum number of iterations allowed. The program aborts if convergence is not achieved in ITMAX or fewer iterations. Default value: ITMAX=50

DEVICE

The DEVICE card is used to specify certain device-related parameters for the simulation such as the device length, cross-sectional area, and operating temperature.

The DEVICE keys are:

TEMP

A real variable that specifies the operating temperature in degrees centigrade.
Default value: TEMP=27.0

LENGTH

The device length in micrometers. Default value: LENGTH=10.

AREA

The device cross-sectional area in square centimeters. Default value: AREA=1.0

XNSS

The position (in micrometers) at which a sheet of fixed charge is to be placed.
 $0.0 \leq \text{XNSS} \leq \text{LENGTH}$ Default value: XNSS=0.

NSS

The number of fixed charges per square centimeter (may be positive or negative).
Default value: NSS=0.0

DOPING

The DOPING card is used to specify the position-dependent donor and acceptor concentrations and related parameters.

The DOPING keys are:

XSTEP(i)

Doping profiles consisting of up to 20 piece-wise constant intervals may be specified. XSTEP(i), where $1 \leq i \leq 20$, specifies the right endpoint (in microns) of the ith section. Default value: XSTEP(1)=10.

NDSTEP(i)

The donor concentration per cubic centimeter in the ith section. NDSTEP(i) must be ≥ 0 . Default value: NDSTEP(1)=0.0

NASTEP(i)

The acceptor concentration per cubic centimeter in the ith section. NASTEP(i) must be ≥ 0 . Default value: NASTEP(1)=0.0

UDEFINE

A logical variable that, if true, tells the program that the user is supplying his/her own FORTRAN subroutine (UDOPE) to define the donor and acceptor concentrations versus position. Default value: UDEFINE=FALSE

IONIZE

A logical variable that, if true, causes the program to assume complete ionization of the donors and acceptors. Default value: IONIZE=TRUE

AUTOLEV

When IONIZE=FALSE and the material is $\text{Al}_x\text{Ga}_{1-x}\text{As}$, the donor energy level $E_C - E_D$ may be automatically computed as a function of the aluminum mole fraction. This is particularly useful if the alloying is graded. AUTOLEV is a logical variable that controls this feature. Default value: AUTOLEV=FALSE

EDSTEP(i)

When IONIZE=FALSE, the donor energy level $E_C - E_D$ in electron volts may be explicitly specified for each of the various sections. Default value: EDSTEP(1)=0.0

EASTEP(i)

When IONIZE=FALSE, the acceptor energy level $E_A - E_V$ in electron volts must be specified for each of the various sections. Default value: EASTEP(1)=0.0

GD

The donor degeneracy level (applies to donors in all of the sections). Default value: GD=2.0

GA

The acceptor degeneracy level (applies to acceptors in all of the sections). Default value: GA=4.0

MATTER

The MATTER card is used to specify the position-dependent material composition.

The MATTER keys are:

XHJ(i)

Material profiles consisting of up to 9 piece-wise constant intervals may be specified. XHJ(i), where $1 \leq i \leq 9$, specifies the right endpoint (in microns) of the ith section. Default value: XHJ(1)=10.

SEMI

A character variable specifying the semiconductor material. Allowed values are ALGAAS, CDHGTE, ZNSE, GESI, SILICON, or USERMAT for user-specified material definitions (see Appendix F for this option) . Different materials can be added in user-supplied subroutines (see Appendix E). Default value: SEMI='ALGAAS'

XMOLE(i)

The mole fraction in the ith section; $0 \leq \text{XMOLE}(i) \leq 1$. Note: XMOLE(i) must be given a value even if the material is not a ternary compound. Default value: XMOLE(i)=0.0

UDEFINE

A logical variable that, if true, indicates that the user is supplying a FORTRAN subroutine, UMAT, to define the mole fraction versus position. Default value: UDEFINE=FALSE

MODEL

The MODEL card is used to choose either Boltzmann or Fermi-Dirac statistics for electrons and holes. Be warned that the choice of Fermi-Dirac statistics significantly increases the execution time. The model card may also be used to specify the magnitude of the conduction band discontinuity.

The MODEL keys are:

FDIRAC

A logical variable that, if true, specifies the use of Fermi-Dirac statistics for carriers. Default value: FDIRAC=FALSE

DECFRC

A real variable that controls the magnitude of the conduction band discontinuity, ΔE_C . The program computes $\Delta E_C = \text{DECFRC} * \Delta E_G$, where ΔE_G is the bandgap difference between the two materials (the rule is applied to the Γ valley). Default value: DECFRC=0.65

CONTACT

The CONTACT card is used to specify the type of metal contact at $x = 0$ (at $x = L$, the contact is always ohmic).

The CONTACT keys are:

FRONT

A string that identifies the desired front contact. If FRONT=OHMIC, the front contact is ohmic (space-charge neutrality and equilibrium are assumed at $x=0$). If FRONT=MIS, the front contact is insulating, and the device is assumed to be in equilibrium for all applied biases. The applied bias in this case represents the surface potential in volts. If FRONT=SB, a Schottky-barrier front contact is assumed. Default value: FRONT=OHMIC

PHIB

If FRONT=SB, then the barrier energy, PHIB, in electron volts for the contact located at $x = 0$ must be specified. Default value: PHIB=0.0

BIAS

The BIAS card is used to specify the desired range of applied biases for the simulations. The back ($x = L$) contact is assumed to be grounded and the bias (in volts) is applied to the front ($x = 0$) contact. The total number of applied biases specified by this card must not exceed 250. The user should exercise some caution in interpreting the results obtained under bias. Since only Poisson's equation is solved, the program must guess the quasi-Fermi levels. Zero current is assumed and constant or piece-wise constant quasi-Fermi levels are used. The program generally treats Schottky barriers on a substrate with no pn junctions and single pn junctions with both contacts ohmic. For multiple junction or three terminal devices, only the equilibrium solution should be requested. The assumed quasi-Fermi levels are displayed on the energy band plot (the dashed line represents the electron quasi-Fermi level).

The BIAS keys are:

VSTART

The starting bias in volts. Default value: $VSTART=0.0$

VSTOP

The ending bias in volts. Default value: $VSTOP=0.0$

VDEL

The bias increment in volts. The total number of biases thus specified must not exceed 250. Default value: $VDEL=0.0$

COMPUTE

In addition to computing the solution to Poisson's equation, other computations may be specified on the COMPUTE card.

The COMPUTE keys are:

TYPE

An array of strings that specifies the desired computations.

TYPE=CV to compute the quasi-static capacitance at each bias.

If TYPE=CV is present, then TYPE=PROFILE will direct FISH1D to differentiate the C-V curve and extract an apparent carrier concentration profile.

TYPE=NSQUARE to compute the electron concentration per square centimeter for each of the material layers. Note that this option cannot be specified if UDEFINE=TRUE on the MATTER card.

PRINT

The PRINT card specifies the desired printed output.

The PRINT keys are:

INFO

An integer variable between 0 and 5 that controls the printing of diagnostic output. A value of INFO=2 is recommended. If the program aborts in an unusual manner, specifying INFO=5 may help to locate the source of the trouble. Default value: INFO=2

TABPRT

A logical variable that, if true, specifies that a table of position (x), adjacent nodes spacing (h), ionized doping density (dopi), band parameters (vp and vn), relative dielectric constant (krel), electrostatic potential (v), electron density (n), hole density (p), electric field (e), and space-charge density (rho) is to be printed. Default value: TABPRT=FALSE

JSTEP

The above-described table is printed at each JSTEPth node in the grid. Default value: JSTEP=1

VGPRT(i)

The table is to be printed at each of the VGPRT(i) biases. Note that each VGPRT(i) must be exactly one of the biases specified and that $1 \leq i \leq 9$. Default value: VGPRT(1)=0.0

PLOT

The PLOT card specifies the desired plotted output. The PLOT keys are:

TYPE

An array of strings to specify the desired plots. Allowed strings are:

DOPING to plot the net doping density $N_D - N_A$ and the net ionized doping density $N_D^+ - N_A^-$.

MOLE to plot the mole fraction versus position.

POTENT to plot the electrostatic potential versus position.

EFIELD to plot the electric field versus position.

ELECTRON to plot the electron density versus position.

HOLES to plot the hole density versus position.

EC to plot the conduction band edge and electron quasi-Fermi level versus position.

EV to plot the valence band edge and hole quasi-Fermi level versus position.

EBAND to plot an energy versus position diagram with the conduction band, valence band, electron quasi-Fermi level and the hole quasi-Fermi level.

NSQUARE to plot total electron concentration per cm^2 versus voltage, and electron concentration per cm^2 versus voltage in a user-specified layer.

CV to plot capacitance versus voltage and $\frac{1}{C^2}$ versus voltage.

VG PLOT

Plots are to be produced at the bias point given by VG PLOT. Note that VG PLOT must be exactly one of the biases specified. Default value: VG PLOT=0.0

XMIN

The left position boundary (in micrometers) for each of the plots. Default value:
XMIN=0.0

XMAX

The right position boundary (in micrometers) for each of the plots. Default value:
XMAX=10.0

LAYER

An integer variable that specifies the layer whose electron concentration per cm^2 is to be plotted. Default value: **LAYER=1**

SAVE

The SAVE card is used to store the computed results in data files.

The SAVE keys are:

VSAVE

The applied bias (in volts) for which the computed results are to be saved. The user is referred to Appendix D for the format of the stored results. If VSAVE=99., then no computed results will be saved. Default value: VSAVE=99.

TAG

TAG is a character variable which specifies the output filename tag, used to distinguish output files from different runs, and to prevent overwriting previous output files. Default value: TAG=XXX

REFERENCES

- [1] M.S. Lundstrom, S. Datta, R.J. Schuelke, S. Bandyopadhyay, and P. Sorlie, "Physics and Modeling of Heterostructure Semiconductor Devices," Annual Report for Semiconductor Research Corporation, Contract 83-01-001, August, 1984. (Also available as Technical Report TR-EE 84-35, School of Electrical Engineering, Purdue University, West Lafayette, Indiana, 47907.)
- [2] M.S. Lundstrom and R.J. Schuelke, "Numerical Simulation of Heterostructure Semiconductor Devices," *IEEE Trans. on Electron Devices*, Vol. ED-30, Sept. 1983.
- [3] M.S. Lundstrom and R.J. Schuelke, "Modeling Semiconductor Heterojunctions in Equilibrium," *Solid-State Electron*, Vol. 25, pp. 683-692, 1982.
- [4] M.S. Lundstrom, R.J. Schwartz and J.L. Gray, "Transport Equations for the Analysis of Heavily Doped Semiconductor Devices," *Solid-State Electronics*, Vol. 24, pp. 195-202, 1981.
- [5] J.L. Gray and M.S. Lundstrom, "Numerical Solution of Poisson's Equation with Application to C-V Analysis of III-V Heterostructure Capacitors," *IEEE Trans. Electron Dev.*, Vol. ED-32, pp. 2102-2109, 1985.

APPENDIX A: DEFAULT INPUT DECK

The default input deck is listed below.

```
*TITLE  DEFAULT INPUT DECK
GRID    AUTO=TRUE,NODES=250,ND=1,NXD=251,XD=10.0
SOLVE   DVMAX=1.0e-4,ITMAX=50
DEVICE  TEMP=27.0,LENGTH=10.0,AREA=1.0,XNSS=0.0,NSS=0.0
DOPING  XSTEP=10.0,NDSTEP=0.0,NASTEP=0.0,
+       UDEFINE=FALSE,IONIZE=TRUE,EDSTEP=0.0,
+       EASTEP=0.0,GD=2.0,GA=4.0,AUTOLEV=FALSE
MATTER  XHJ=10.0,SEMI=ALGAAS,XMOLE=0.0,UDEFINE=FALSE
MODEL   FDIRAC=FALSE,DECFRC=0.65
CONTACT FRONT=OHMIC,PHIB=0.0
BIAS    VSTART=0.0,VSTOP=0.0,VDEL=0.0
COMPUTE TYPE=NONE
PRINT   INFO=2,TABPRT=TRUE,JSTEP=1,VGPRT=0.0
PLOT    TYPE=NONE,XMIN=0.0,XMAX=10.0,VGPLOT=0.0
SAVE    VSAVE=99.,TAG=XXX
```

APPENDIX B: EXAMPLE INPUT DECKS

- 1) Compute the equilibrium solution for an n-n GaAs homojunction and print a table of results. Note that the cards with no keys present are not required but are shown merely to remind the user that default values are being assumed.

```
*title  example #1: n-n step junction
grid
solve
model
device  length=10.0,temp=27.0,area=1.0
matter
doping  xstep=0.5/10.0 ndstep=1.5e16/3.0e16
contact
bias
compute
print  tabprt=true, jstep=1, vgprt=0.0
plot
save
```

- 2) Repeat example 1 but for an n-n step AlGaAs/GaAs heterojunction. Plots of the results are also requested.

```
*title  example #2: n-n step heterojunction
grid
solve
model
device  length=10.0,temp=27.0,area=1.0
matter  xhj=0.50/10.0 xmole=0.0/0.30
doping  xstep=0.5/10.0 ndstep=1.5e16/3.0e16
contact
bias
compute
print  tabprt=true, jstep=1, vgprt=0.0
plot  type=doping/alum/potent/efield/electron/ec
+     xmin=0.0 xmax=1.0 vgplot=0.0
save
```

- 3) Repeat example 2 but with a Schottky barrier at $x=0$. A C-V curve is also requested. This example also illustrates the manual specification of a finite difference grid. For this example, impurity de-ionization in the AlGaAs is modeled. Complete ionization within the GaAs is forced by specifying a donor level of $E_c - E_d = -1.0$ eV.

```
*title example #3: cv of n-n step heterojunction
grid auto=false, nxd=25/75/25/50/25/25/26,
+ xd=0.25/0.48/0.52/0.75/1.2/2.5/10.0
solve
model
device length=10.0,temp=27.0,area=1.0
matter xhj=0.50/10.0 xmole=0.0/0.30
doping xstep=0.5/10.0 ndstep=1.5e16/3.0e16
+ edstep=-1.0/0.10 ionize=false
contact front=sb, phib=0.86
bias vstart=0.0,vstop=-5.50,vdel=-0.05
compute type=cv
print tabprt=true, jstep=1, vgprt=0.0
plot type=doping/alum/potent/efield/electron/cv
+ xmin=0.0 xmax=1.0 vgplot=-5.0
save
```

- 4) Repeat example 3, but with a graded, not abrupt, heterojunction (complete ionization of dopants is also assumed). The subroutine UMAT must be supplied to specify the desired compositional grading. A copy of the subroutine is also shown.

```
*title example #4: cv of n-n step GaAs/AlGaAs heterojunction
grid auto=true
solve
model
device length=10.0,temp=27.0,area=1.0
matter udefine=true,xhj=0.50/10.0 xmole=0.0/0.30
doping xstep=0.5/10.0 ndstep=1.5e16/3.0e16
contact front=sb, phib=0.86
bias vstart=0.0,vstop=-5.50,vdel=-0.05
compute type=cv
print tabprt=true, jstep=1, vgprt=0.0
plot type=doping/alum/potent/efield/electron/cv
+ xmin=0.0 xmax=1.0 vgplot=0.0
save
```



```
subroutine umat(x,xmole)
c
c specifies user-defined aluminum profiles....
c x is input in microns
c user returns aluminum fraction xal
c
c xj is the junction depth
c wg is the grading width
c
  xj = 0.5
  wg = 0.03
  cofx = 0.5*(1.-tanh((x-xj)/wg))
  xmole = 0.30*(1.0-cofx)
c
  return
end
```

- 5) Compute the electron concentration per cm^2 in an n-p HgCdTe heterojunction. Plot the total electron concentration per cm^2 , as well as the electron concentration per cm^2 in the second layer of the device. Save the computed equilibrium results in data files.

```
*title example #5: HgCdTe n-p heterojunction
grid
solve
model
device length=5.0,temp=27.0,area=1.0
matter xhj=0.2/5.0 semi=hgcdn
+ xmole=0.2/0.0
doping xstep=0.2/5.0 ndstep=1.0e18/0.0
+ nstep=0.0/1.0e18
contact
bias
compute type=nsquare
print tabprt=true, jstep=1, vgpert=0.0
plot type=nsquare/potent/electron layer=2
save vsave=0.0 tag=run1
```

- 6) Compute the equilibrium solution for a heterojunction bipolar transistor with abrupt grading. Use auto-leveling to set donor energy levels for incomplete ionization.

```
*title example #6: HBT with abrupt grading, auto-leveling ionization
grid
solve
device length=1.38
doping xstep=0.1/0.15/0.25/0.28/0.38/0.88/1.38 ndstep=5e18/5e18/5e17
+ ndstep=5e17/0.0/3e16/5e18 nastep=0.0/0.0/0.0/0.0/1e19/0.0/0.0
+ ionize=false autolev=true
matter xhj=0.1/0.15/0.25/0.28/0.38/0.88/1.38
+ xmole=0.0/0.0/0.3/0.3/0.0/0.0/0.0
model
contact
bias
compute
print tabprt=true info=2
plot type=doping/mole/eband/potent/efield/electron/holes
+ xmin=0.0 xmax=1.38
save
```

- 7) Compute the equilibrium solution of a MODFET, and do an electron concentration per cm^2 analysis of layer one of the device. Do not assume complete ionization of dopants and use Fermi-Dirac statistics.

```
*title example #7: MODFET in equilibrium
grid
solve
model fdirac=true, decfrc=0.60
device xlong=5.0,temp=27.0,area=1.0
matter xhj=0.2925/0.3000/5.0 xmole=0.30/0.30/0.0
doping xstep=0.2925/0.3/5.0
+ ndstep=3.0e17/0.0/0.0 nastep=0.0/0.0/5.0e14
+ ionize=false, edstep=0.060/-1.0
contact front=sb,phib=0.86
bias
compute type=nsquare
print info=5, tabprt=true, jstep=1, vgprt=0.0
plot type=nsquare/eband/doping/potent/electron layer=1
+ vgplot=0.0 xmin=0.0, xmax=0.5
save
```

APPENDIX C: EXAMPLE OUTPUT

Example #6 HBT in equilibrium

***** FISH1D - VERSION 2.1 *****

DATE: Thu Feb 9 14:33:26 1989

***** INPUT DECK *****

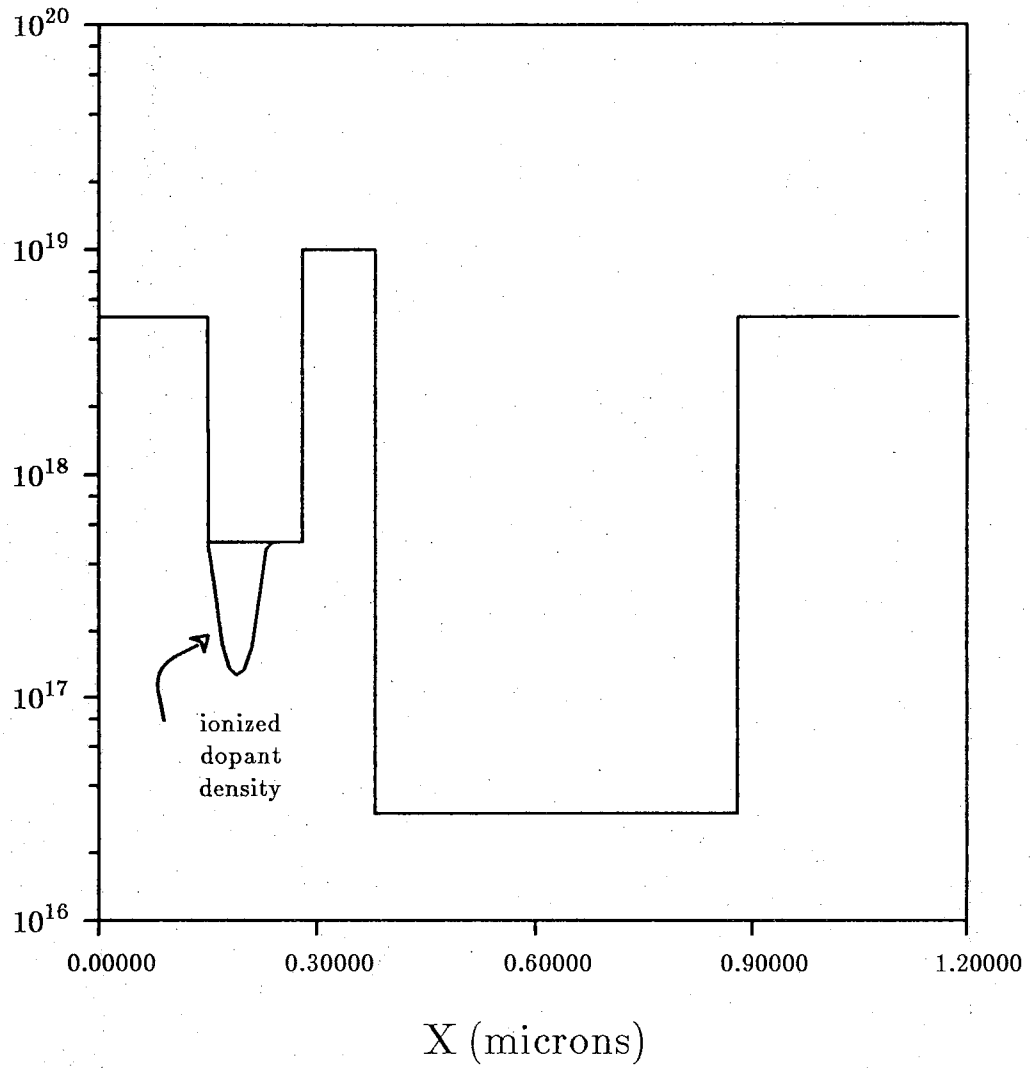
```
*title HBT with abrupt junction, auto-leveling de-ionization
grid
solve
device length=1.38
doping xstep=0.1/0.15/0.25/0.28/0.38/0.88/1.38 ndstep=5e18/5e18/5e17
+ ndstep=5e17/0.0/3e16/5e18 nastep=0.0/0.0/0.0/0.0/1e19/0.0/0.0
+ ionize=false autolev=true
matter xhj=0.1/0.15/0.25/0.28/0.38/0.88/1.38
+ xmole=0.0/0.0/0.3/0.3/0.0/0.0/0.0
model
contact
print tabprt=true jstep=5 info=2
plot type=doping/mole/cband/potent/efield/electron/holes
+ xmin=0.0 xmax=1.38
save vsave=0.0
```

*** results for $v_g = 0.000$ ***

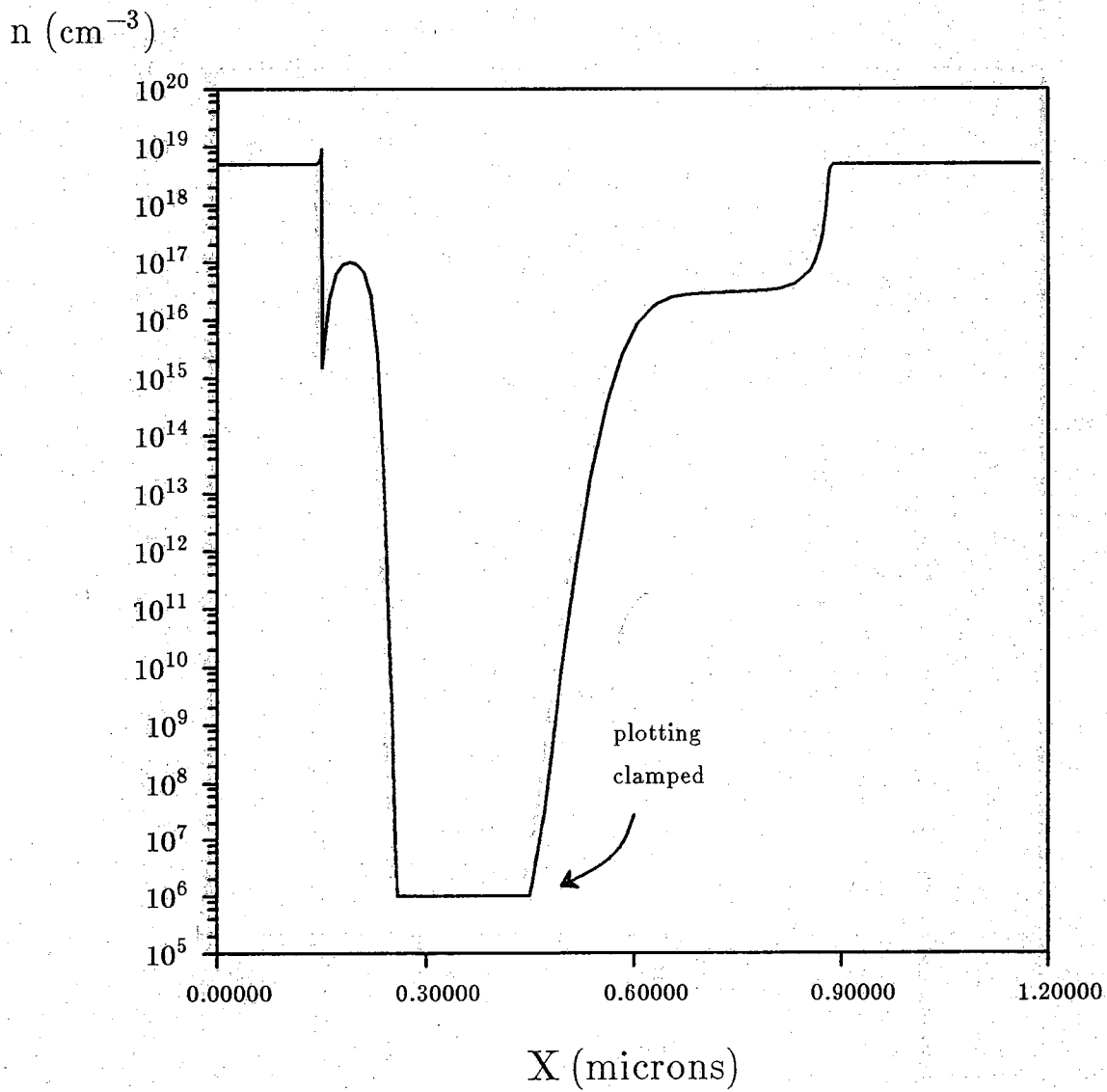
x(cm)	h(cm)	dopi(cm-3)	xal	ni	krel	v(volts)	n(cm-3)	p	e(v/cm)	rho/q	
0	0.000E+00	0.000E+00	0.500E+19	0.000	0.238E+07	12.847	0.734	0.500E+19	0.113E-05	-.253E-07	0.284E+07
1	0.808E-06	0.808E-06	0.500E+19	0.000	0.238E+07	12.847	0.734	0.500E+19	0.113E-05	-.902E-08	0.139E+06
2	0.162E-05	0.808E-06	0.500E+19	0.000	0.238E+07	12.847	0.734	0.500E+19	0.113E-05	-.434E-09	0.146E+05
7	0.566E-05	0.808E-06	0.500E+19	0.000	0.238E+07	12.847	0.734	0.500E+19	0.113E-05	0.217E-10	-.282E+04
12	0.843E-05	0.172E-06	0.500E+19	0.000	0.238E+07	12.847	0.734	0.500E+19	0.113E-05	0.000E+00	-.282E+04
17	0.929E-05	0.172E-06	0.500E+19	0.000	0.238E+07	12.847	0.734	0.500E+19	0.113E-05	-.198E-07	-.660E+06
22	0.984E-05	0.182E-07	0.500E+19	0.000	0.238E+07	12.847	0.734	0.500E+19	0.113E-05	-.323E-06	-.112E+08
27	0.994E-05	0.182E-07	0.500E+19	0.000	0.238E+07	12.847	0.734	0.500E+19	0.113E-05	-.508E-06	-.184E+08
32	0.100E-04	0.182E-07	0.500E+19	0.000	0.238E+07	12.847	0.734	0.500E+19	0.113E-05	-.817E-06	-.300E+08
37	0.101E-04	0.182E-07	0.500E+19	0.000	0.238E+07	12.847	0.734	0.500E+19	0.113E-05	-.131E-05	-.483E+08
42	0.104E-04	0.172E-06	0.500E+19	0.000	0.238E+07	12.847	0.734	0.500E+19	0.113E-05	-.475E-05	-.163E+09
47	0.112E-04	0.172E-06	0.500E+19	0.000	0.238E+07	12.847	0.734	0.500E+19	0.113E-05	-.375E-03	-.127E+11
52	0.120E-04	0.117E-06	0.500E+19	0.000	0.238E+07	12.847	0.734	0.500E+19	0.113E-05	-.220E-01	-.769E+12
57	0.126E-04	0.117E-06	0.500E+19	0.000	0.238E+07	12.847	0.734	0.500E+19	0.113E-05	-.439E+00	-.156E+14
62	0.133E-04	0.172E-06	0.500E+19	0.000	0.238E+07	12.847	0.734	0.500E+19	0.113E-05	-.118E+02	-.402E+15
67	0.141E-04	0.172E-06	0.500E+19	0.000	0.238E+07	12.847	0.734	0.503E+19	0.113E-05	-.930E+03	-.315E+17
72	0.148E-04	0.182E-07	0.500E+19	0.000	0.238E+07	12.847	0.740	0.633E+19	0.897E-06	-.361E+05	-.133E+19
77	0.149E-04	0.182E-07	0.500E+19	0.000	0.238E+07	12.847	0.744	0.745E+19	0.762E-06	-.595E+05	-.245E+19
82	0.150E-04	0.200E-07	0.478E+18	0.300	0.255E+04	11.900	0.752	0.152E+16	0.425E-08	-.101E+06	0.477E+18
87	0.200E-04	0.998E-06	0.134E+18	0.300	0.255E+04	11.900	0.858	0.918E+17	0.706E-10	0.507E+04	0.423E+17

Dopant Densities vs. Position

Nd - Na (cm^{-3})

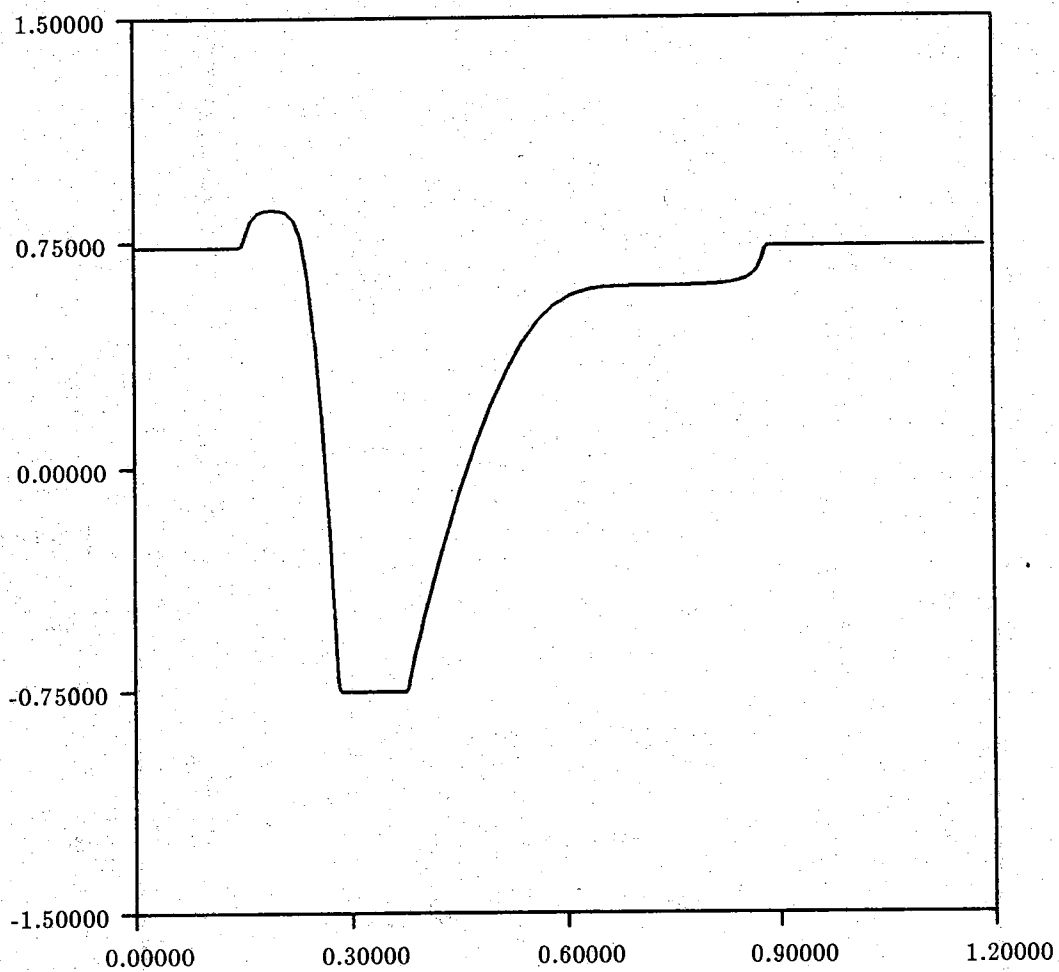


Electron Concentration vs. Position



Potential vs. Position

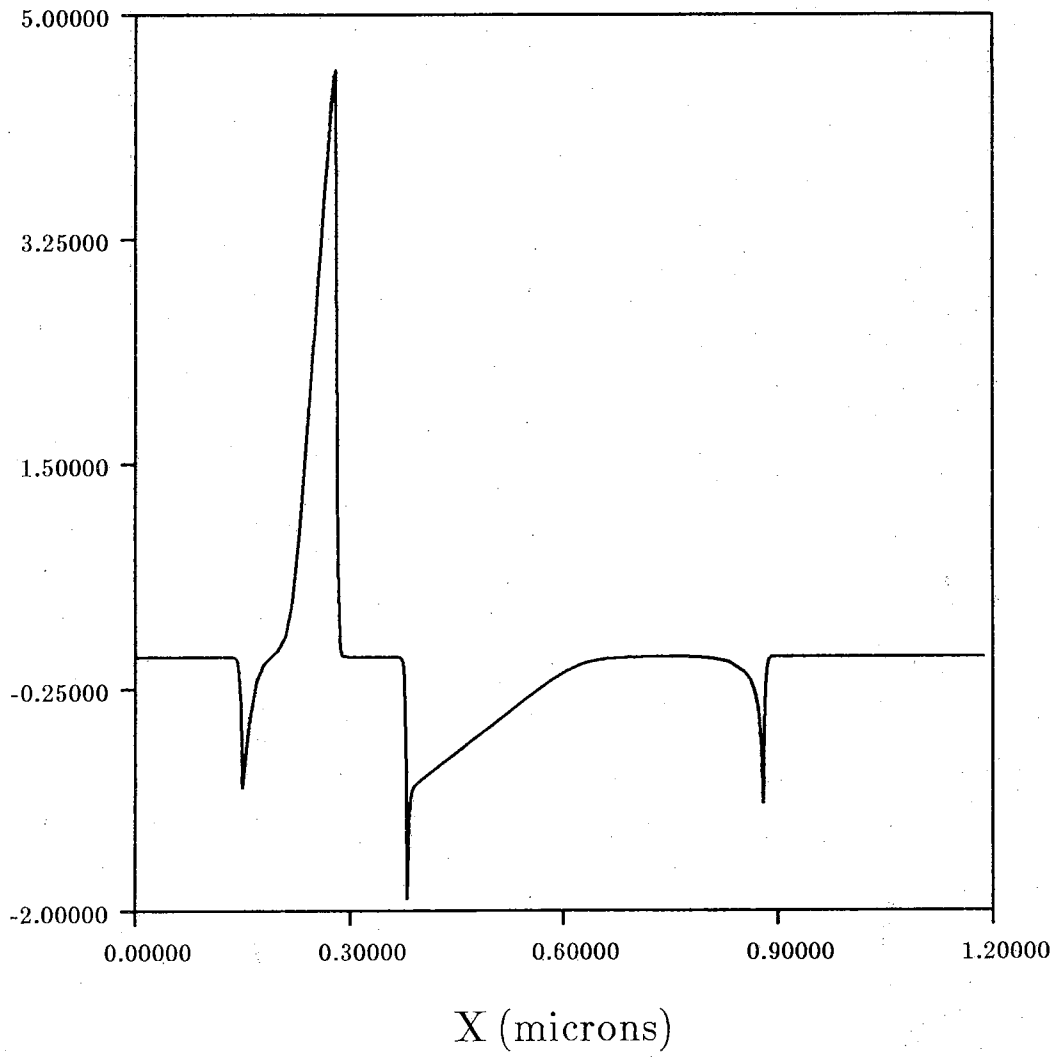
Potential (volts)



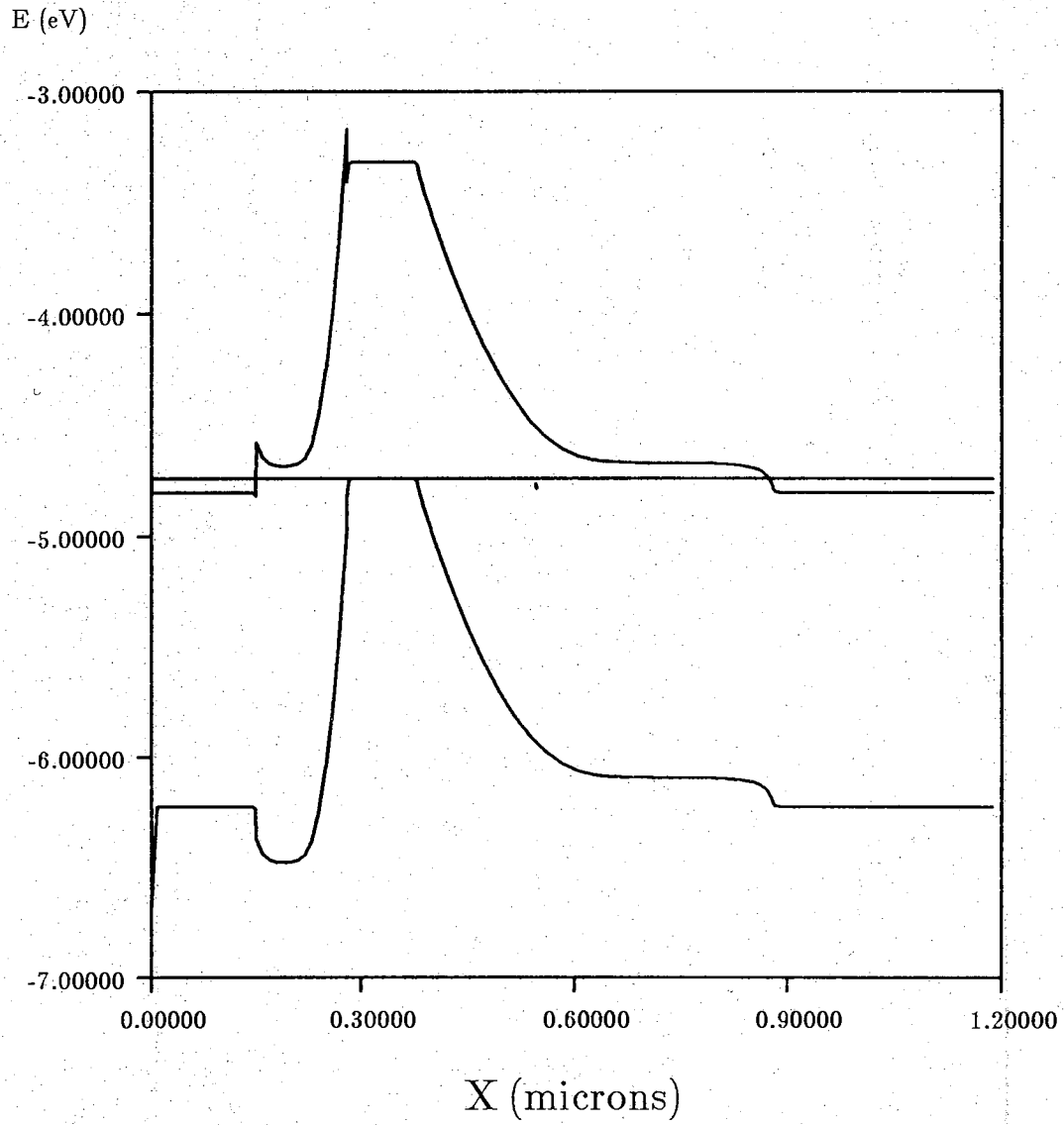
X (microns)

Electric Field vs. Position

e (v/cm) ($\times 10^5$)



Energy Bands vs. Position



APPENDIX D: DATA FILE OUTPUT

Use of the SAVE card directs FISH1D to store all calculated data at a specified bias. When this is done, FISH1D will create two files, f1d.mdat_xxx and f1d.fdat_xxx, where xxx is the data file tag as specified on the SAVE card. The structure of these files is as follows:

1) F1D.MDAT

F1D.MDAT is a file 9 columns wide by the number of nodes in the finite difference grid long. Data is ordered in the following manner:

- column #1: position (microns)
- column #2: N_D^+ (cm^{-3})
- column #3: N_A^- (cm^{-3})
- column #4: $N_D^+ - N_A^-$ (cm^{-3})
- column #5: $N_D - N_A$ (cm^{-3})
- column #6: mole fraction
- column #7: intrinsic carrier concentration (cm^{-3})
- column #8: relative dielectric constant
- column #9: electric field (volts per cm)

2) F1D.FDAT

F1D.FDAT is a file 9 columns wide by the number of nodes in the finite difference grid long. Data is ordered in the following manner:

- column #1: position (microns)
- column #2: electrostatic potential (volts)
- column #3: electron concentration (cm^{-3})
- column #4: hole concentration (cm^{-3})
- column #5: space-charge density (divided by electron charge)
- column #6: conduction band edge energy (eV)
- column #7: valence band edge energy (eV)
- column #8: electron quasi-Fermi level (eV)
- column #9: hole quasi-Fermi level (eV)

In addition if a C-V or electron concentration per cm^2 analysis is requested, FISH1D will store these results in the files f1d.cvdat_xxx and f1d.nsdatt_xxx. These files have a similar structure:

1) F1D.CVDAT

F1d.cvdat is a file 2 columns wide by the number of nodes in the finite difference grid long. Data is ordered in the following manner:

column #1: applied bias voltage (volts)
column #2: capacitance (farads)

2) F1D.NSDAT

F1d.nsdatt is a file of variable width and length. The number of columns is equal to the number of layers in the device plus two. The length is the number of nodes in the finite difference grid.

column #1: applied bias voltage (volts)
column #2: total electron concentration per cm^2
column #3: electron concentration per cm^2 in layer 1
column #4: electron concentration per cm^2 in layer 2
...
column #n: electron concentration per cm^2 in layer n-2

APPENDIX E: ADDING MATERIAL SUBROUTINES

Adding new material capabilities is a fairly simple task involving changes to one subroutine, BANDX, and the addition of a routine to define the new material's parameters. These subroutines, as well as the original material subroutines ALGAAS and CDHGTE, are all contained in the file with the main program to facilitate modifications. The routines ALGAAS and CDHGTE can be used as guides for new material definitions. The changes to BANDX involve simple expansion of block if statements to allow more material cases.

The appropriate lines to modify in BANDX are marked with the comment line:

```
c mmm insert new material definitions here mmm
```

APPENDIX F: DEFINING MATERIAL PARAMETERS BY LAYERS

While creating a new material subroutine is a way to permanently add new material definitions, new material parameters can also be defined layer by layer in the input deck. All the material parameters used by FISH1D (i.e. bandgaps and conduction band effective masses for the L, Γ , and X valleys, valence band effective mass, dielectric constant, and electron affinity) can be specified for each layer in a device. These new definitions are entered into the simulation by setting SEMI=USERMAT in the MATTER card and adding one MATDEF card for every layer with different material parameters in the structure to be simulated. If every parameter is not known for a particular layer or if just a few parameters in an already existing material subroutine wish to be changed, the key DEFSUB can be set to default unknown parameters to a specified FISH1D material subroutine (i.e. ALGAAS, GESI, ZNSE, ect.). If DEFSUB is left unset, all parameters must be specified or an error will occur. If DEFSUB is set for each layer, but differs from layer to layer, ELCAFF, the electron affinity, must be set for every layer in the device (since FISH1D presently has no method for determining the relative electron affinities between different material systems). Of course, this rule also applies if DEFSUB is left unset for some layers--ELCAFF must be set for every layer. Any violation of this condition will invoke an input error message or undoubtedly cause erroneous results (be careful!).

To use this option, create the input deck as before (excluding the XMOLE key in the MATTER card) and make the following adjustments/additions:

- (1) Set SEMI=USERMAT in the MATTER card.
- (2) Create a MATDEF card for each layer with different material properties, (i.e. if two layers are silicon, differing only in doping and thickness, only one MATDEF card needs to be specified). Number the MATDEF cards consecutively by setting the key MATNO={integer between 1-10} in each card (note: MATNO must occur as the first key in each MATDEF statement or an error will occur). Define material properties using the key definitions on the following page. If and only if every MATDEF card uses the same DEFSUB (default FISH1D material subroutine) go to step (3), else make sure ELCAFF (electron affinity) is assigned for each MATDEF card and skip to step (4).
- (3) If DEFSUB is the same for every MATDEF card, the electron affinity can be assigned automatically by setting AFFSET=DEFAULT in the MATTER card (thereby eliminating the need to set ELCAFF in the MATDEF cards). This option is especially useful when modifying just one or two parameters in a device involving only one FISH1D material system. For instance, the bandgap of the base in a

$\text{Ge}_x\text{Si}_{1-x}$ HBT can be assigned a value according to experimental results, bypassing the GESI subroutine bandgap value while using all other values defined by GESI.

(4) Create string $\text{LAYMAT}=\text{x}_1/\text{x}_2/\text{x}_3/\dots/\text{x}_i/\dots/\text{x}_n$ in the MATTER card where the x_i 's correspond to the MATNO of the MATDEF card associated with each layer (denoted by the subscript i) in the actual n -layer device. For instance, in a four layer device, $\text{LAYMAT}=1/2/1/3$ corresponds to using the material properties of MATDEF card $\text{MATNO}=1$ in the first and third layers of the actual device, the properties of MATDEF card $\text{MATNO}=2$ in the second layer, and the properties of MATDEF card $\text{MATNO}=3$ in the fourth. The thickness corresponding to the layers should be accounted for by the $\text{XHJ}(i)$ string in the MATTER card.

Example input decks using the MATDEF definition option are given following the key descriptions on the next page.

MATDEF

The MATDEF card allows material parameters to be defined separately for each layer in a device. Before using this card, the instructions on the preceding two pages should be read.

The MATDEF keys are:

MATNO

Assigns a reference number for each MATDEF card. The material parameters corresponding to each MATDEF card are then referenced by this number in the MATTER card LAYMAT key (see examples). The MATNO key must be assigned for each MATDEF card and must be placed before all other MATDEF keys. Allowable MATNO values are integers between 1 and 10. Default value: MATNO=-1.

DEFSUB

Defines the FISH1D material subroutine which will assign "default" material parameters to those left unspecified in the MATDEF card. Unless all material parameters are assigned in the MATDEF card, this key must be set. Allowable values are the names of the current FISH1D material subroutines. Default value: DEFSUB='UNSET'

MOLFRC

The mole fraction of the FISH1D material system defined by DEFSUB. Allowable values are between 0 and 1. Default value: MOLFRC=0.0

BANDGG

The bandgap of the Γ valley in eV. Default value: BANDGG=-1.

BANDGX

The bandgap of the X valley in eV. Default value: BANDGX=-1.

BANDGL

The bandgap of the L valley in eV. Default value: BANDGL=-1.

EFFMAG

The density-of-states effective mass of electrons in the Γ conduction band valley as a fraction of m_0 . Default value: EFFMAG=-1.

EFFMAX

The density-of-states effective mass of electrons in the X conduction band valley as a fraction of m_0 . Default value: EFFMAX=-1.

EFFMAL

The density-of-states effective mass of electrons in the L conduction band valley as a fraction of m_0 . Default value: EFFMAL=-1.

EFFMAV

The density-of-states effective mass of holes in the valence band as a fraction of m_0 . Default value: EFFMAV=-1.

DIECON

The relative dielectric constant (unitless). Default value: DIECON=-1.

ELCAFF

The electron affinity in eV. This key must be set unless every MATDEF card in the input deck assigns the same DEFSUB. Default value: ELCAFF=-1.

ADDITIONS TO THE MATTER CARD

Use of the MATDEF card also requires the subsequent additions/alterations to the MATTER card:

XMOLE(i)

This card must be omitted and replaced with LAYMAT(i).

LAYMAT(i)

An array of integers that specifies which MATDEF card defines the material parameters for each layer of the device. MATDEF card material parameters are assigned to a layer in the actual device by placing the MATNO of the MATDEF card in the element of the LAYMAT(i) corresponding to the XHJ(i) element (see MATTER card) of the layer. Consequently, the LAYMAT(i) array length must correspond to XHJ(i) array length. The same MATNO can be specified more than once in the LAYMAT(i) array if the material definitions of a given MATDEF apply to several layers in the actual device. Examples are given on the next page. Default value: LAYMAT(i)=1.

AFFSET

When the DEFSUB is set identically in all MATDEF cards, AFFSET may be set to DEFAULT indicating that the electron affinities of all layers are to be computed by the FISH1D material subroutine specified in the DEFSUB keys. If the DEFSUB are not the same for all MATDEF cards, or not specified for some, this option must be left unset (or erroneous answers will result). Default value: AFFSET='UNSET'

EXAMPLE INPUT DECKS USING THE "MATDEF" OPTION

- 1) Compute the equilibrium solution for a $\text{Ge}_{.31}\text{Si}_{.69}$ base HBT and redefine the base bandgap. Notice that there are only two MATDEF cards, because the collector and emitter are both normal silicon (remember, MOLFRFC defaults to 0.0 if not specified, therefore the subroutine GESI ($\text{Ge}_x\text{Si}_{1-x}$) gives just Si parameters for $x=0.0$). Notice also that AFFSET is allowed to be set to DEFAULT (resulting in the automatic computation of the electron affinity) only because DEFSUB is defined identically (to GESI) in both MATDEF cards.

```
*title HBT (IEEE Elec. Dev. Lett., vol. 10, no. 2, pg. 52)
grid
device length=1.6
doping xstep=.41/.43/1.6
+ nastep=0.0/7.e18/0.0
+ ndstep=1.4e17/0.0/3.e16
matter xhj=.41/.43/1.6
+ semi=usermat
+ affset=default
+ laymat=1/2/1
model decfrc=0.0
compute
matdef matno=1 defsub=gesi
matdef matno=2 defsub=gesi molfrc=0.31 bandgx=.884
print vgprrt=0.0 tabprt=true jstep=2
plot type=eband/mole/electron/doping xmin=.25 xmax=.65
save
```

- 2) In this example, the equilibrium solution for a Ge_4Si_6 quantum well structure is computed using the subroutine SILICON instead of GESI with $x=0$. Since the DEFSUB keys of the two MATDEF cards differ, ELCAFF, the electron affinity, must be specified in both cards. Consequently, AFFSET is left at its default setting, UNSET.

```
*title Quantum well (Appl. Phys. Lett., vol. 53, no. 3, pg. 204)
grid
device length=.424 temp=-196
doping xstep=.185/.2/.205/.209/.214/.239/.424
+ nastep=5.e18/0.0/0.0/0.0/0.0/0.0/5.e18
matter xhj=.2/.205/.209/.214/.424
+ semi=usermat
+ laymat=1/2/1/2/1
compute
matdef matno=1 defsub=gesi molfrc=.4 elcaff=4.05
matdef matno=2 defsub=silicon elcaff=4.05
print
plot type=eband/mole/electron/doping xmin=.17 xmax=.24
save
```

- 3) In this example, the equilibrium solution of a Ge_5Si_5 channel BICFET is calculated with the material parameters of one layer completely specified by a MATDEF card. Notice that the bandgaps of the Γ and L valleys are arbitrarily set 1 eV higher than the X valley. Also notice that the effective masses of these valleys are set arbitrarily small. This is an example of avoiding specifying every parameter exactly without significantly altering the solution.

```
*title BICFET (IEEE Elec. Dev. Lett., vol. 10, no. 1, pg. 14)
grid
solve
device length=.5
doping xstep=.1/.135/.138/.150/.41/.5
+ nastep=0.0/0.0/1.e19/0.0/0.0/0.0
+ ndstep=3.e19/1.e18/0.0/1.e17/1.e17/3.e19
matter xhj=.1/.135/.140/.150/.41/.5
+ semi=usermat
+ laymat=1/3/1/2/1/1
model decfrc=0.0
contact
bias
compute
matdef matno=1 defsub=silicon elcaff=4.05
matdef matno=2 defsub=gesi molfrc=0.47 bandgx=.814 elcaff=4.05
matdef matno=3 bandgg=2.124 bandgx=1.124 bandgl=2.124
+ effmag=1.17e-13 effmax=1.18 effmal=1.17e-13 effmav=.8098
+ diecon=11.8 elcaff=4.05
print vgprrt=0.0 tabprt=true jstep=2
plot type=eband/efield/mole/electron/holes/doping xmin=.13 xmax=.16
save
save
```

In the above example, if several values in the MATDEF card MATNO=3 were left unspecified, an error message of "*** x more parameter(s) need to be set if DEF-SUB not specified ***" would occur in the output file, with x being the number of parameters left unset. If ELCAFF were unset in any of the layers, the above error message would be joined with "***** ELCAFF MUST BE SET! *****".

APPENDIX G: USING FISH1D AT PURDUE

1) WHERE TO FISH

FISH1D has been installed on the ei machine and it will also run on the en machine, although it has not been installed there.

2) HOW TO FISH

To run FISH1D on ei, first create an input deck as described earlier in this manual and enter it into a file. This file can be given any name, for example *infile*. The output file created by FISH1D can also be given any name, for example *outfile*. To run a simulation, type (in your shell):

```
fish1d < infile > outfile
```

If a data dump was requested, additional files ending in ".dat" will be created. See Appendix D for the format of these files. If plots were requested, files ending in ".plot" will be created.

3) HOW TO PRODUCE PLOTS

A. FROM FISH1D ".plot" FILES

If plots were requested on the PLOT card, ".plot" files have been created. These ".plot" files correspond to the PLOT card input strings as follows:

d.plot	-----	DOPING
mo.plot	-----	MOLE
v.plot	-----	POTENT
e.plot	-----	EFIELD
n.plot	-----	ELECTRON
p.plot	-----	HOLES
ec.plot	-----	EC
ev.plot	-----	EV
eb.plot	-----	EBAND
ns.plot	-----	NSQUARE
cv.plot1 and cv.plot2	----	CV (C and $\frac{1}{C^2}$, respectively)

In addition, if profiling was requested, then the file pf.plot will be created. To send these plots to a Printronix printer, use the command:

gplp -XX plotfile

where XX is the printer code and *plotfile* is the ".plot" file. Since this process can be tedious, an interactive shell file exists which simplifies this task. It is on the ei machine and can be copied from:

/b/doddp/bin/fplt

B. USING THE MONDANE GRAPHICS PACKAGE

The data files created by FISH1D can be used as input files to the Mondane graphics package, which allows plots to be displayed on the crt screen or sent to a laser printer, among other features. Using the Mondane graphics package requires a initial investment in setting up a Mondane directory with datafile definitions, but the enhanced features make it well worth the effort. A complete explanation of how to set up this directory is beyond the scope of this manual. On line help is available for Mondane using the command:

help mondane

Shell files have been written to simplify the use of Mondane once the definitions are in place. Direct questions to Paul Dodd (login doddp).

4) SOURCE CODE

The source code for FISH1D can be copied from:

en: /b/hetsim/Fish1d/Release

The code in this directory is needed if the user wants to define a doping profile using the UDEFINE feature of FISH1D. Compilation instructions are included in the comment block at the the beginning of the main program.

APPENDIX H: FISH1D INSTALLATION NOTES

FISH1D was written in standard FORTRAN 77, and it is configured to run under the UNIX operating system. At Purdue FISH1D runs on a Gould NP-1 and also on a Gould PN9080, computers with a double precision wordlength of 64 bits. FISH1D will not run without modifications on some systems, for example the VAX 11/780 running UNIX, due to their inability to represent very large and very small real numbers. The NP-1 and PN9080 allow manipulation of numbers on the order of $10^{\pm 74}$. Various users have modified FISH1D to run on different systems- from mainframes to the IBM Personal Computer. These notes give some basic guidelines for installation of FISH1D on other computers.

One subroutine library is used: CRC, an in-house plotting package which is very similar to the CALCOMP plotting library. Six FISH1D subroutines (DO PLOT, NSPLOT, CVPLOT, NAPPT, LGAXIS, and GRAPH) contain calls to CRC routines. FISH1D will store all calculated data on request, however. This data is stored in ASCII format in columns (see Appendix D for precise structure of data files). This data can then be processed easily with an external plotting package. For this reason it is recommended that if the CRC routines are not available, the user should delete all plotting routines from FISH1D itself and do plots externally. This will typically allow more plotting flexibility, particularly if any massaging of data is desired.

Any subroutines with known machine-dependent code are marked with the comment line:

```
c zzz machine-dependent code zzz
```

A brief description of each machine-dependent routine follows.

CVPLOT, DO PLOT, NAPPT, NSPLOT

These three subroutine use the CRC routines FNAME and PLOTS to name and initialize plot output files.

GRAPH

This subroutine produces plots using CRC routines.

LGAXIS

This subroutine produces a vertical logarithmic axis using CRC routines.

REXP

This function is used to prevent underflow of exponentials. When $\exp(x)$ underflows, 0.0 is returned. The value of x_{\min} , the most negative argument permitted by the exponential, is machine-dependent.

WHEN

This subroutine returns the current date and time using the external system library routine FDATE.

APPENDIX I: FORMULATION OF POISSON'S EQUATION FOR COMPOSITIONALLY NONUNIFORM SEMICONDUCTORS

Preface

In this appendix, Poisson's equation for semiconductor heterostructures is derived and expressed in a form convenient for numerical solution. Multiple conduction band valleys, carrier degeneracy, conduction band nonparabolicity and impurity deionization are each treated. Since the results are similar to those long used for homostructure device analysis, proven numerical solution methods are directly applicable. FISH1D is based on the formulation developed here.

I.1 INTRODUCTION

Solving Poisson's equation is often the first step in semiconductor device analysis. When Boltzmann statistics are assumed for an equilibrium semiconductor with uniform material composition, Poisson's equation takes the form [1]:

$$\nabla^2 V = \frac{-q}{\kappa_S \epsilon_0} (n_i e^{-qV/kT} - n_i e^{qV/kT} + N_D^+ - N_A^-). \quad (I1)$$

Equation (I1), the so-called Poisson-Boltzmann equation, is in a form convenient for device analysis and is routinely solved under a variety of conditions [2-4]. It is our purpose in this appendix to discuss a generalization of (I1) valid for compositionally nonuniform semiconductors.

Poisson's equation for semiconductors with nonuniform material composition was presented some years ago [5], but the formulation bore little resemblance to (I1) (so well-developed solution methods could not be directly applied) and involved several assumptions that limited its validity. A simplified solution technique based on the depletion approximation has also been reported [6] and applied to device analysis [7], but, since the method is not generally valid, specialized techniques may be required for some applications [8]. A generalization of (I1) to semiconductor heterostructures would, however, be widely applicable and readily solved.

In a previous paper, a generalization of (I1) was developed for semiconductors with nonuniform composition [9]. The purpose of this appendix is to extend that work to realistically model III-V heterostructures. Specifically, we treat: 1) multiple conduction band valleys, 2) carrier degeneracy in multiple valleys, 3) nonparabolic conduction bands, and 4) incomplete ionization of dopants. These extensions are motivated by the observation that each of the above-listed effects is important in III-V semiconductors such as GaAs:AlGaAs (see for example [10] and [11]). The resulting Poisson equation is similar in form to (I1) and is easily solved by methods similar to those employed to

solve (II). No discussion of numerical solution strategies or examples of computations are included in this appendix; the topics will be treated in a subsequent publication.

I.2 PROBLEM FORMULATION

Our goal is to express Poisson's equation,

$$\nabla \cdot \vec{D} = q(p - n + N_D^+ - N_A^-), \quad (I2)$$

in terms of the unknown electrostatic potential and known parameters that describe the semiconductor doping and composition. We begin by writing the conduction and valence band edges in a semiconductor with nonuniform composition as [12]

$$E_C(\vec{r}) = E_0 - \chi(\vec{r}) - qV'(\vec{r}) \quad (I3)$$

and

$$E_V(\vec{r}) = E_C(\vec{r}) - E_G(\vec{r}), \quad (I4)$$

where E_0 is a constant and V' the electrostatic potential. The spatial variation in the band edges arises both from the macroscopic electrostatic potential and from the spatially varying composition described by χ and E_G . Equations (I3) and (I4) show that the band edges are not parallel to $-qV'(\vec{r})$ as they are in a homostructure (nor is the intrinsic level). If E_0 is identified with the field-free vacuum level, then χ is the electron affinity and the so-called Anderson model results [13]. Since the ability of this model to predict measured band discontinuities is limited [14,15], we adjust $\chi(\vec{r})$ to produce band discontinuities in agreement with measured values.

The electron and hole densities in a heterostructure are related to the band edges (I3) and (4) by

$$n = N_C(\vec{r}) \tilde{F}_{1/2}(\eta_C) \quad (I5)$$

and

$$p = N_V(\vec{r}) \tilde{F}_{1/2}(\eta_V), \quad (I6)$$

where

$$\eta_C = (F_n - E_C)/kT \quad (I7)$$

and

$$\eta_V = (E_V - F_p)/kT, \quad (I8)$$

with F_n and F_p being the quasi-Fermi levels for electrons and holes. The Fermi-Dirac integral, $\tilde{F}_{1/2}(\eta)$ reduces to the exponential for nondegenerate semiconductors (i.e. $\eta \ll 0$). For III-V semiconductors such as $Al_xGa_{1-x}As$, in which three conduction band valleys are considered, the electron density is the sum of three terms similar to (I5).

The carrier densities, (I5) and (I6), can be expressed in terms of the electrostatic potential by use of (I3), (I4), (I7), and (I8). When the result is then inserted in (I2), the desired equation results.

I.3 DERIVATION

In this section, Poisson's equation is formulated under simplifying assumptions; extensions required to model III-V heterostructures accurately are the subject of the following section.

When Boltzmann statistics are assumed, the electron density (I5) becomes

$$n_B = N_C e^{(F_n - E_0 + \chi + qV')/kT}, \quad (I9)$$

where the subscript B indicates that Boltzmann statistics were assumed. The constant E_0 may be eliminated by evaluating (I9) in a reference material to obtain

$$n_B = n_r \frac{N_C}{N_{Cr}} e^{(F_n - F_{nr} + \chi - \chi_r + qV' - qV'_r)/kT}, \quad (I10)$$

where a subscript r denotes a value in the reference material. Equation (I10) is further simplified by specifying the reference material to be in equilibrium ($F_n = E_F$) and intrinsic ($n_r = n_{ir}$). If we let $V = V' - V'_r$, then

$$n_B = n_{ir} e^{q(V + V_n - \phi_n)/kT}, \quad (I11)$$

where

$$qV_n(\vec{r}) = \chi(\vec{r}) - \chi_r + kT \ln(N_C(\vec{r})/N_{Cr}) \quad (I12)$$

and

$$q\phi_n = (E_F - F_n). \quad (I13)$$

A corresponding development for holes leads to

$$p_B = n_{ir} e^{-q(V - V_p - \phi_p)/kT}, \quad (I14)$$

where

$$qV_p(\vec{r}) = - \left[\chi(\vec{r}) - \chi_r + E_G(\vec{r}) - E_{Gr} - kT \ln(N_V(\vec{r})/N_{Vr}) \right] \quad (I15)$$

and

$$q\phi_p = (E_F - F_p). \quad (I16)$$

A differential equation for $V(\vec{r})$ results when (I11) and (I14) are inserted in (I2). The result,

$$\nabla \cdot (\kappa_S \nabla V) = \frac{-q}{\epsilon_0} \left[n_{ir} e^{-q(V-V_p-\phi_p)/kT} - n_{ir} e^{q(V+V_n-\phi_n)/kT} + N_D^+ - N_A^- \right] \quad (I17)$$

is the desired generalization of (I1) to semiconductor heterostructures; a similar expression has been presented previously [9]. We now extend (I17) to include effects important in III-V heterostructures.

I.4 EXTENSIONS

In this section we extend the result presented above by considering in turn Fermi-Dirac statistics, conduction-band nonparabolicity, multiple conduction bands, and impurity deionization. To account for degenerate carrier statistics yet retain a Boltzmann-like form, we write (I5) as

$$n = \gamma_{1/2}(\eta_C) N_C e^{\eta_C}, \quad (I18)$$

where the activity coefficient,

$$\gamma_{1/2}(\eta_C) = \frac{\tilde{F}_{1/2}(\eta_C)}{e^{\eta_C}}, \quad (I19)$$

reduces to unity when nondegenerate statistics apply. Following the procedure outlined in Sec. I.3, we now obtain,

$$n = \gamma_{1/2}(\eta_C) n_{ir} e^{q(V+V_n-\phi_n)/kT}, \quad (I20)$$

the generalization of (I11) to degenerate carrier statistics. Since (I18) and (I20) may be equated to find

$$\eta_C = q(V+V_n-\phi_n)/kT - \ln(N_C/n_{ir}), \quad (I21)$$

(I20) relates the electron density to the electrostatic potential and known parameters. Following the same steps for holes, we find:

$$p = \gamma_{1/2}(\eta_V) n_{ir} e^{-q(V-V_p-\phi_p)/kT}, \quad (I22)$$

where $\gamma_{1/2}(\eta_V)$ is defined in the same manner as (I19).

The above-described technique for treating Fermi-Dirac statistics differs somewhat from that used in [9]. In the present treatment, degeneracy is accounted for by the activity coefficients; formerly it was included in the band parameters. Although either technique may be used, we have found it convenient to separate Fermi-Dirac statistics from the band parameters when treating multiple conduction band valleys.

In GaAs, nonparabolicity of the Γ conduction band produces a significant increase in the effective density-of-states [11]. When nonparabolicity is considered, (I5) becomes [11]

$$n = N_C \left[\tilde{F}_{1/2}(\eta_C) - \frac{15\alpha kT}{4E_C} \tilde{F}_{3/2}(\eta_C) \right], \quad (I23)$$

where α (which is < 0) is the nonparabolicity coefficient. In this case, (I20) is modified to

$$n = n_{ir} \left[\gamma_{1/2}(\eta_C) - \frac{15\alpha kT}{4E_C} \gamma_{3/2}(\eta_C) \right] e^{q(V+V_n-\phi_n)/kT}, \quad (I24)$$

where $\gamma_{3/2}$ has the form given by (I19) but with $\tilde{F}_{3/2}$ replacing $\tilde{F}_{1/2}$.

For a material such as $Al_xGa_{1-x}As$, three conduction band valleys (Γ , L and X) must be considered [10]. If, to simplify the algebra, we ignore nonparabolicity, then the density of electrons in the Γ band is

$$n_\Gamma = \gamma_{1/2}(\eta_{C\Gamma}) N_{C\Gamma} e^{\eta_{C\Gamma}} = \gamma_{1/2}(\eta_{C\Gamma}) N_{C\Gamma} e^{(I_C - E_{C\Gamma})/kT} e^{\eta_C}, \quad (I25)$$

where $E_{C\Gamma}$ is the minimum of the Γ conduction band and E_C is the lowest of $\$E$ sub {C GAMMA}, $\sim E$ sub {CL}, \sim and $\sim E$ sub CX\$. When similar expressions for the L and X bands are added, we find the total electron density to be

$$n = \left[\gamma_{1/2}(\eta_{C\Gamma}) N'_{C\Gamma} + \gamma_{1/2}(\eta_{CL}) N'_{CL} + \gamma_{1/2}(\eta_{CX}) N'_{CX} \right] e^{\eta_C}, \quad (I26)$$

where

$$N'_{C\Gamma} = N_{C\Gamma} e^{(I_C - E_{C\Gamma})/kT}, \text{ etc.} \quad (I27)$$

Beginning with (I26) instead of (I18), we find instead of (I20),

$$n = n_{ir} \left[\gamma_{1/2}(\eta_{C\Gamma}) e^{qV_{n\Gamma}/kT} + \gamma_{1/2}(\eta_{CL}) e^{qV_{nL}/kT} + \gamma_{1/2}(\eta_{CX}) e^{qV_{nX}/kT} \right] e^{q(V-\phi_n)/kT} \quad (I28)$$

the extension of (I20) to include three conduction band valleys. There are now three separate band parameters defined by

$$qV_{n\Gamma} = (\chi - \chi_r) + kT \ln(N'_{C\Gamma}/N'_{Cr}) \quad (I29)$$

and similar expressions for V_{nL} and V_{nX} . In (I29) χ is measured to the lowest conduction band minimum and

$$N'_{Cr} = N'_{C\Gamma} + N'_{CL} + N'_{CX}. \quad (I30)$$

For nondegenerate statistics, the three separate band parameters may be combined in a single parameter, but this is not possible for degenerate statistics. Nonparabolicity is readily incorporated in (I28) in the manner indicated by (I24).

Impurity de-ionization is an important factor in materials like $Al_xGa_{1-x}As$ for which the carrier binding energy increases with aluminum fraction [10]. The ionized donor concentration may be written as [16]

$$N_D^+ = \frac{N_D}{1 + g_D \exp(F_n - E_D)/kT} \quad (I31)$$

if the donor level communicates solely with the conduction band. Our task is to express (I31) in terms of the electrostatic potential. We begin by writing

$$e^{(F_n - E_D)/kT} = e^{(\eta_C + E_{CD})/kT}, \quad (I32)$$

where $E_{CD} = E_C - E_D$ is the binding energy of the donor. Now e^{η_C} may be eliminated using (I26) to obtain

$$e^{(F_n - E_D)/kT} = \frac{n e^{E_{CD}/kT}}{[\gamma_{1/2}(\eta_{Cr})N'_{Cr} + \gamma_{1/2}(\eta_{Cl})N'_{Cl} + \gamma_{1/2}(\eta_{Cx})N'_{Cx}]} \quad (I33)$$

Then using (I28) for n we find

$$e^{(F_n - E_D)/kT} = \frac{n_{ir}}{N'_{Cr}} e^{(\chi - \chi_r + E_{CD})/kT} e^{q(V - \phi_n)/kT}, \quad (I34)$$

When (I34) is substituted into (I31), the result,

$$N_D^+ = \frac{N_D}{1 + n_B/n_1}, \quad (I35)$$

is obtained. The parameter n_1

$$n_1 = \frac{(N'_{Cr} + N'_{Cl} + N'_{Cx}) e^{-E_{CD}/kT}}{g_D} \quad (I36)$$

describes the donor level. It should be stressed that although n_B (given by (I11)) is the electron density that would have resulted by assuming Boltzmann statistics, (I35) is valid for both degenerate and nondegenerate carrier statistics.

The corresponding expressions for the ionized acceptor density are

$$N_A^- = \frac{N_A}{1 + p_B/p_1}, \quad (I37)$$

where

$$p_1 = \frac{N_V}{g_A} e^{-E_{AV}/kT}. \quad (I38)$$

This completes the derivation of Poisson's equation for semiconductor heterostructures. Referring to (I2), we observe that p , n , N_D^+ , and N_A^- have each been related to the electrostatic potential and known material parameters by (I22), (I28), (I35), and (I37), which are valid for both degenerate and nondegenerate carrier statistics.

I.V SUMMARY

The solution to Poisson's equation finds many applications in semiconductor device analysis. Our goal in this appendix has been to formulate Poisson's equation for compositionally nonuniform III-V semiconductors in a form convenient for numerical solution. Each of the terms in (I2), p , n , N_D^+ , and N_A^- was related to the electrostatic potential V and to the nonuniform material composition (via (I22), (I28), (I35), and (I37)). Except for the addition of band parameters to describe the nonuniform composition, the results are much like those for semiconductor homostructures [3]. Consequently, well-developed techniques for the numerical solution of Poisson's equation are directly applicable [2-4]. The results of this work should find application in the analysis of heterostructure devices for which quantum confinement effects [17] are not pronounced.

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