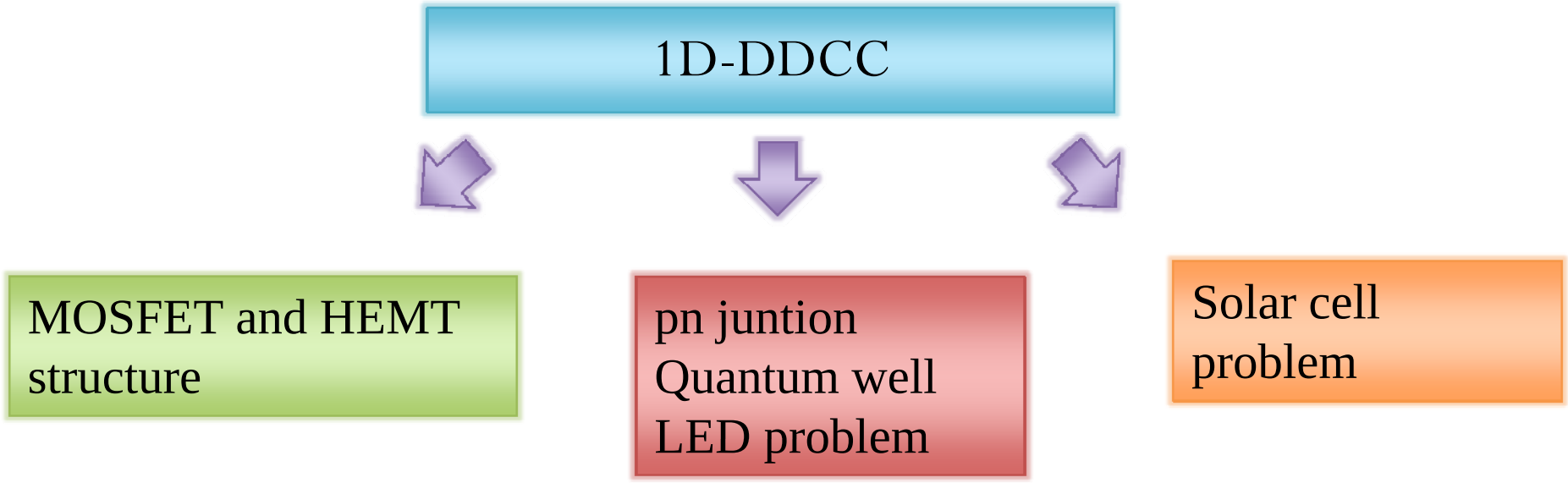
1D- DDCC Program

1. The program can solve Poisson, Schrodinger, Drift-diffusion equation self-consistently.
2. The Slotboom variable and Scharfetter-Gummel variable are used. (different verions). The current version is using Slotboom variable.
3. Consideration of Polarization charge is included.
4. The generation and recombination mechanism is included.



Running the 1D-ddcc program

- In the command line of unix or MS-DOS
- Type

ddcc.exe inputfilename.inp

"Input filename" can be changed to any name you like end with .inp

In the package, you should find an example file end with *.inp e.g.
algan32gan.inp or gan-ingan-gan.inp .

/home2/students/ddcc For student in class
/home/epaper/1D-DDCC For my students

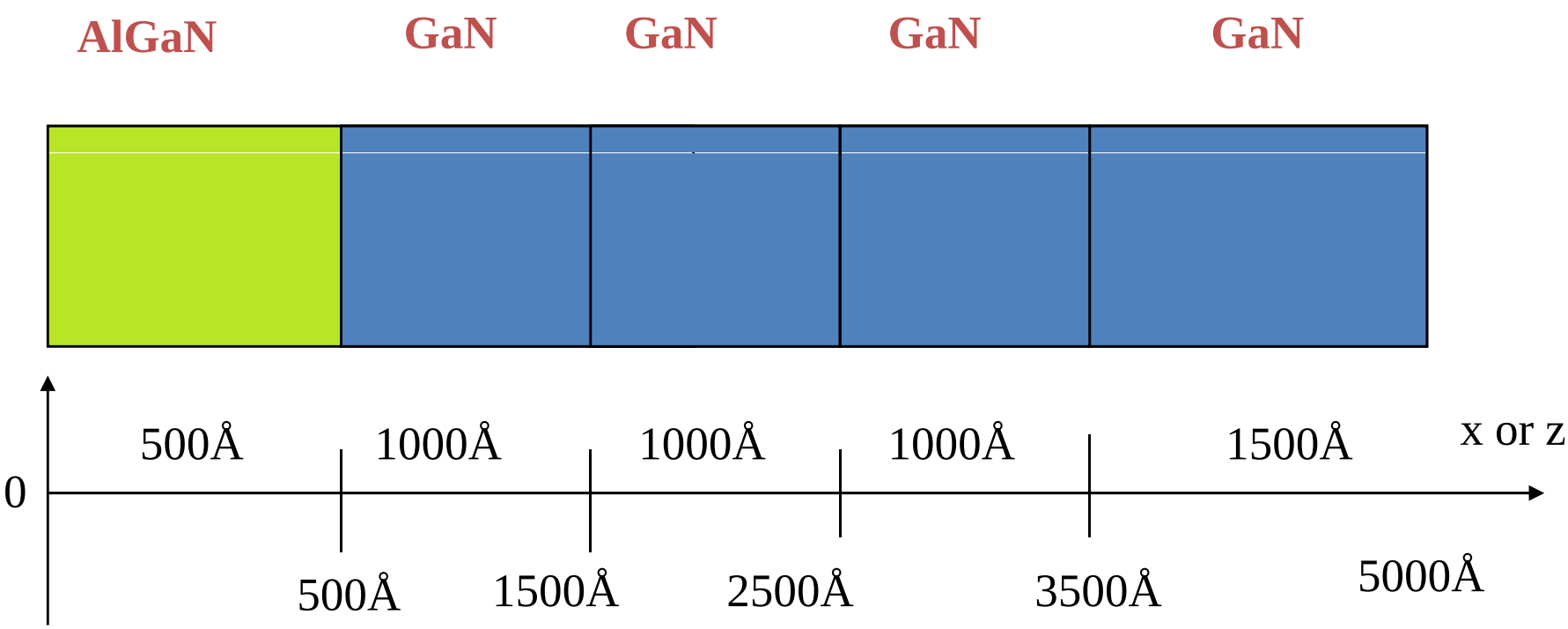
In your home directory , type
mkdir 1D-ddcc
cd 1D-ddcc
cp /home2/students/ddcc/* ./ Copy all the example files to the directory

Content of input filename

$totallayer
5

We use 5 layers. The layer numbers can range from at least 3 to 65535. However, if the materials have the same properties, it is not necessary to use so many layers.

Important: $totallayer must be assigned in the first input parameter (beginning of the input file.



In the program, the junction starts from 0 to the total thickness 5000Å we set. Left side starting from 0 is usually the top layer or the gate contact. Right hand side with larger x values is the bottom side as the source contact in most cases.

$calltunnel → If we want to calculate the tunneling current or not. Defaut is no (remove this command).

$tunnellays 1 → If we want to use WKB approximation to calculate the tunneling current, we need to set the tunneling layer number.

$ivnfile algan32-vg0.0.ivn → Filename to save current information of each bias point.

$wvinpfile algan32-vg0.0.wv → Filename to save the wave function when the schrodinger solver is used and confined states are found.

$n2dresfile algan32-vg0.0.n2d → Filename to save the n2d for multipoint's cases. Work with Monte Carlo program

$gatebias
0.000 0.500 0.100

Gate voltage Start at 0V

Gate voltage end at 0.5V

ΔV_G step size

Note $\Delta V_G \neq 0$ in any case

$outfile
algan32-gan.out → Output file tag: can be any characters is than 40 letters.

$maxsteps
1500 → Maximum iteration steps to get converge. If total iteration steps are larger than this value, the program will stop and output the unconverged results.

$Schottky
1.6800 Schottky barrier height at the top contact

It will not be used in floating gate condition

$body-V
0.1 Schottky barrier height at the bottom

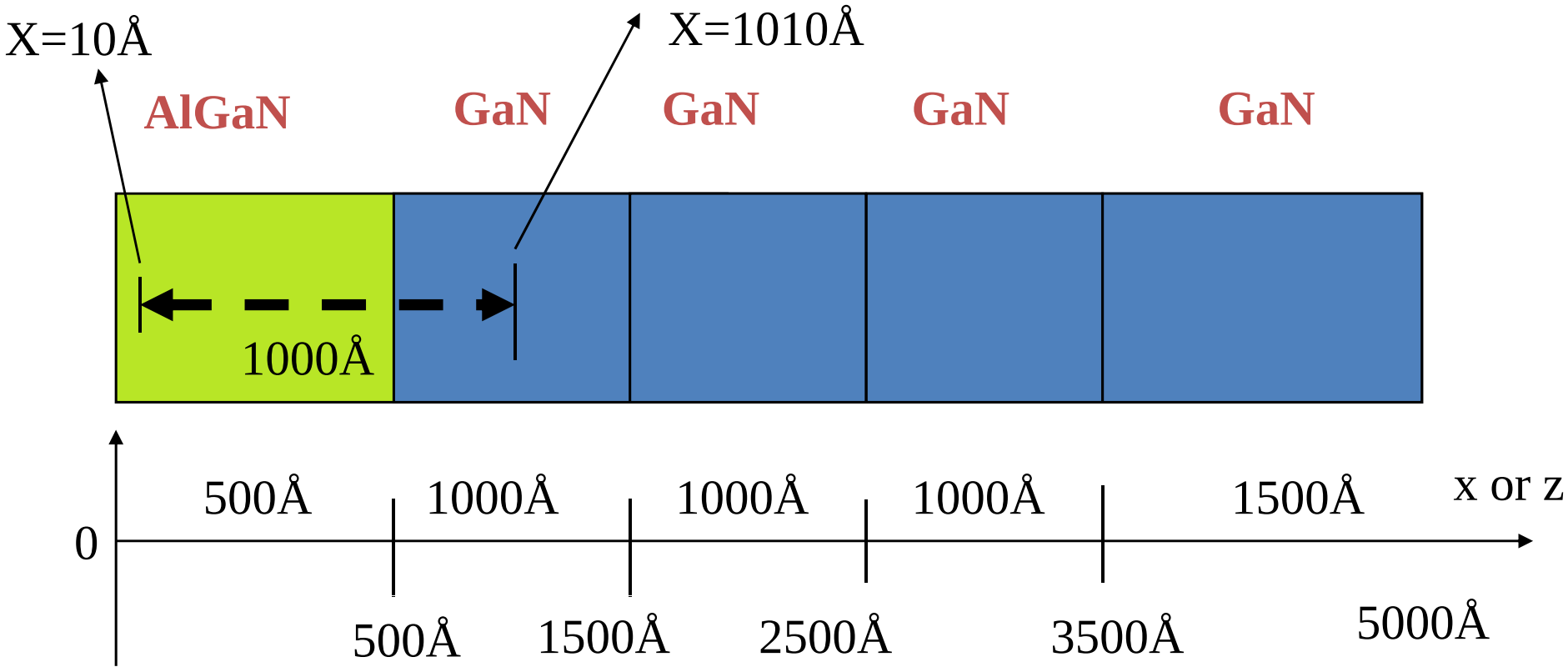
$error
1.0e-5 error tolerance for the program to get converged → Default is 1e-5 without setting.

$QMdepth
1000.0 Q-M solution depth

$QMstart
10.0 Q-M solution depth

Region to solve the Schrödinger equation.

Solving the Schrödinger equation will require a lot of time and memory. Therefore, we only solve the Schrödinger equation in the confined regions



If we set the totally number equal to five, the following parameters need to be set to five as well.

$totallayer
5

$thickness
500.0
1000.0
1000.0
1000.0
1500.0

$3Dmass
0.2459 0.6000 0.6000 Layer 1
0.2000 0.6000 0.6000 Layer 5
m^*_e m^*_{hh} m^*_{lh}
$2Dmass
0.2000 0.2000 0.6000 0.6000 Layer 2
0.2000 0.2000 0.6000 0.6000 Layer 3
0.2000 0.2000 0.6000 0.6000 Layer 4
$m_{e\perp}$ $m_{e\|}$ m^*_{hh} m^*_{lh}

$bandgap
4.2700 Layer 1 (top) eV
3.4000 Layer 2
3.4000 Layer 3
3.4000 Layer 4
3.4000 Layer 5 (bottom)

ε dielectric constant

$diconst
10.010 Layer 1 (top)
10.400 Layer 2
10.400 Layer 3
10.400 Layer 4
10.400 Layer 5 (bottom)

$dEc/dEg
0.6300 Layers' 1-2 Interface
0.6300 Layers' 2-3 Interface
0.6300 Layers' 3-4 Interface
0.6300 Layers' 4-5 Interface
0.6300 Layers' 5-6 Interface

$taunp
6.500E-09 6.500E-09
6.500E-09 6.500E-09
6.500E-09 6.500E-09
6.500E-09 6.500E-09
6.500E-09 6.500E-09

$mobility
0.500E+03 0.200E+03
1.500E+03 0.500E+03
1.500E+03 0.500E+03
1.500E+03 0.500E+03
1.500E+03 0.500E+03

Only the words with red color need to be typied formally. The word with black color is not necessary to be put in the input file. They are only for illustration.

Mobility and Shockley Read Hall recombination parameters. Only need to be set well if we want to calculate the current.

Shockley Read Hall recombination mechanism

$$R = \frac{pn - n_i^2}{\tau_{n0}\left(p + n_i exp\left(\frac{E_i - E_t}{K_B T}\right)\right) + \tau_{p0}\left(n + n_i exp\left(\frac{E_t - E_i}{K_B T}\right)\right)}$$

$$J_n = \mu_n n(z)\frac{\partial E_{\mathrm{fn}}(z)}{\partial z}$$

$$J_p = \mu_p p(z)\frac{\partial E_{\mathrm{fp}}(z)}{\partial z},$$

$$\frac{\partial J_n}{\partial z} = qR$$

$$\frac{\partial J_p}{\partial z} = -qR,$$

```
$taunp
6.500E-09  6.500E-09
6.500E-09  6.500E-09
6.500E-09  6.500E-09
6.500E-09  6.500E-09
6.500E-09  6.500E-09
```

```
$mobility
0.500E+03  0.200E+03
1.500E+03  0.500E+03
1.500E+03  0.500E+03
1.500E+03  0.500E+03
1.500E+03  0.500E+03
```

τ_n τ_p μ_n μ_p

In this input, these parameters will not be used since we do not calculate the drift-diffusion equation in this case.

If we change the total layer to 7, all this parameters need to set to 7 columns

$totallayer
7

$thickness
500.0
1000.0
1000.0
1000.0
500.0
500.0
500.0

$3Dmass
0.2459 0.6000 0.6000 Layer 1
0.2000 0.6000 0.6000 Layer 7

m^*_e m^*_{hh} m^*_{lh}

$2Dmass
0.2000 0.2000 0.6000 0.6000 Layer 2
0.2000 0.2000 0.6000 0.6000 Layer 3
0.2000 0.2000 0.6000 0.6000 Layer 4
0.2000 0.2000 0.6000 0.6000 Layer 5
0.2000 0.2000 0.6000 0.6000 Layer 6

$m_{e\perp}$ $m_{e\parallel}$ m^*_{hh} m^*_{lh}

$bandgap
4.2700 Layer 1 (top) eV
3.4000 Layer 2
3.4000 Layer 3
3.4000 Layer 4
3.4000 Layer 5
3.4000 Layer 6
3.4000 Layer 7 (bottom)

ε dielectric constant

$diconst
10.010 Layer 1 (top)
10.400 Layer 2
10.400 Layer 3
10.400 Layer 4
10.400 Layer 5
10.400 Layer 6
10.400 Layer 7 (bottom)

$dEc/dEg
0.6300 Layers' 1-2 Interface
0.6300 Layers' 2-3 Interface
0.6300 Layers' 3-4 Interface
0.6300 Layers' 4-5 Interface
0.6300 Layers' 5-6 Interface
0.6300 Layers' 6-7 Interface
0.6300 Layers' 7-8 Interface

$taunp

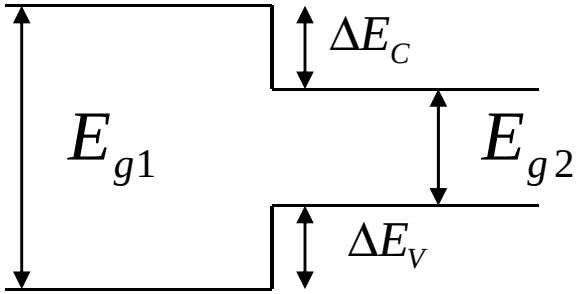
6.500E-09	6.500E-09
6.500E-09	6.500E-09
6.500E-09	6.500E-09
6.500E-09	6.500E-09
6.500E-09	6.500E-09
6.500E-09	6.500E-09
6.500E-09	6.500E-09

$mobility

0.500E+03	0.200E+03
1.500E+03	0.500E+03
1.500E+03	0.500E+03
1.500E+03	0.500E+03
1.500E+03	0.500E+03
1.500E+03	0.500E+03
1.500E+03	0.500E+03

Conduction band offset

```
$dEc/dEg
0.6300  Layers' 1-2 Interface
0.6300  Layers' 2-3 Interface
0.6300  Layers' 3-4 Interface
0.6300  Layers' 4-5 Interface
0.6300  Layers' 5-6 Interface
```

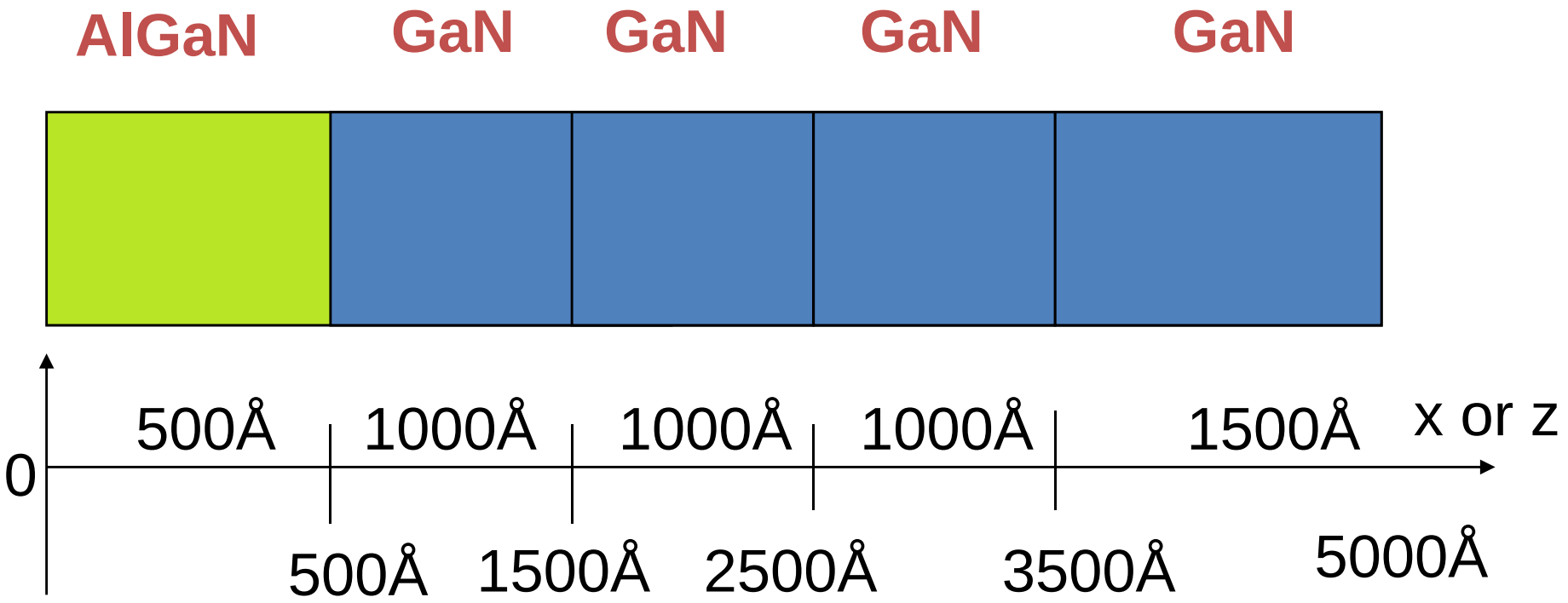


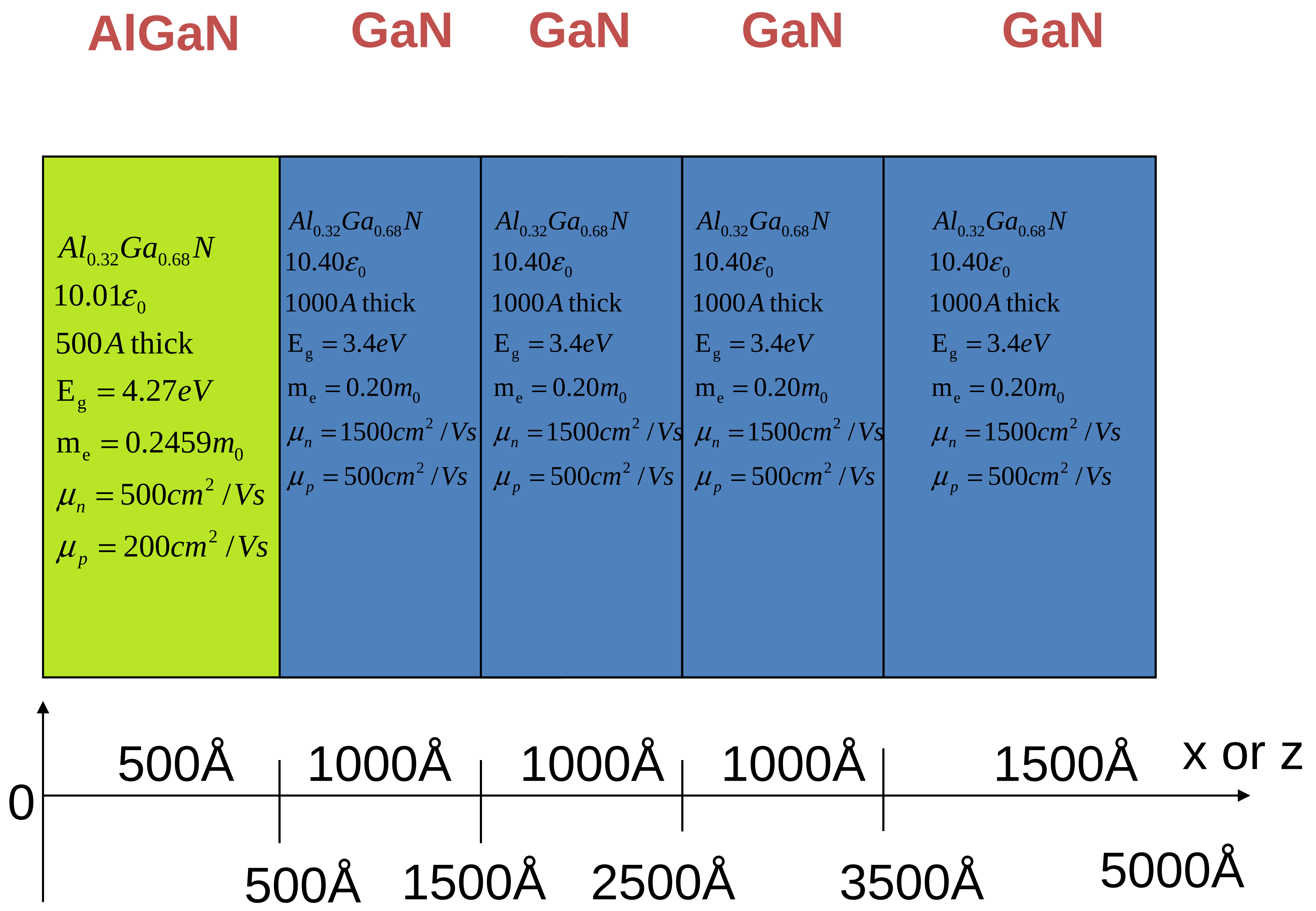
$$\Delta E_g = E_{g1} - E_{g2}$$

$$\Delta E_c / \Delta E_g = 0.63$$

dummy parameters

No meaning and not to be used in the program




AlGaN
GaN
GaN
GaN
GaN
$Al_{0.32}Ga_{0.68}N$
$10.01\varepsilon_0$
$500A$ thick
$E_g = 4.27eV$
$m_e = 0.2459m_0$
$\mu_n = 500cm^2/Vs$
$\mu_p = 200cm^2/Vs$
$Al_{0.32}Ga_{0.68}N$
$10.40\varepsilon_0$
$1000A$ thick
$E_g = 3.4eV$
$m_e = 0.20m_0$
$\mu_n = 1500cm^2/Vs$
$\mu_p = 500cm^2/Vs$
$Al_{0.32}Ga_{0.68}N$
$10.40\varepsilon_0$
$1000A$ thick
$E_g = 3.4eV$
$m_e = 0.20m_0$
$\mu_n = 1500cm^2/Vs$
$\mu_p = 500cm^2/Vs$
$Al_{0.32}Ga_{0.68}N$
$10.40\varepsilon_0$
$1000A$ thick
$E_g = 3.4eV$
$m_e = 0.20m_0$
$\mu_n = 1500cm^2/Vs$
$\mu_p = 500cm^2/Vs$
$Al_{0.32}Ga_{0.68}N$
$10.40\varepsilon_0$
$1000A$ thick
$E_g = 3.4eV$
$m_e = 0.20m_0$
$\mu_n = 1500cm^2/Vs$
$\mu_p = 500cm^2/Vs$
500Å
1000Å
1000Å
1000Å
1500Å
x or z
0
500Å
1500Å
2500Å
3500Å
5000Å

$doping

3 Number of contiguous doping regions

500.0	**1.00E+16**	**25.0**	Region 1
2000.0	**1.00E+17**	**25.0**	Region 2
2500.0	**1.00E+18**	**25.0**	Region 3

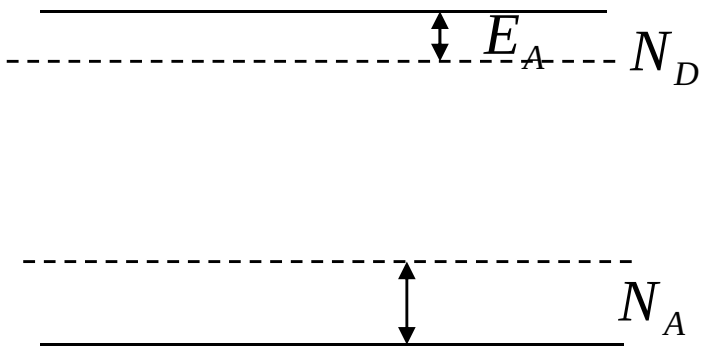
thickness N_D or N_A activation

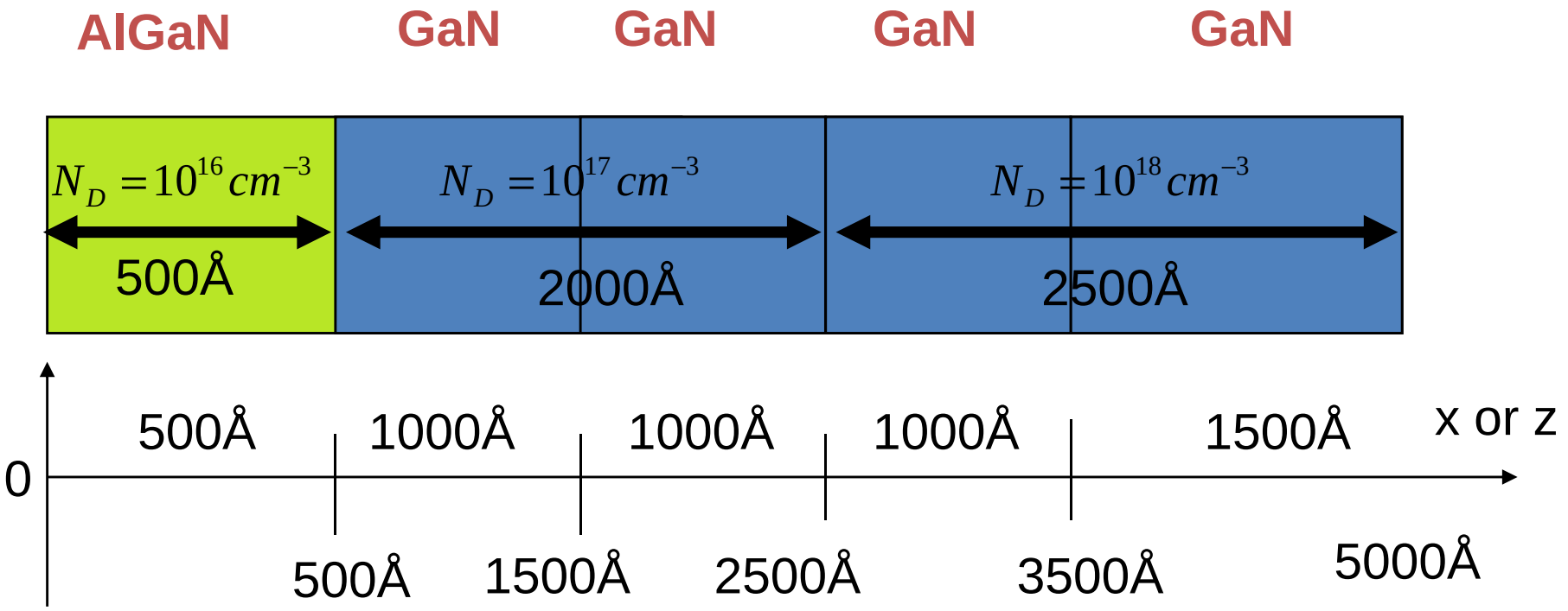
$+: N_D$ energy

$-: N_A$ E_A (meV)

$$N_d^* = N_d \frac{1}{1 + 2e^{(E_f - E_c - E_d)/k_B T}}$$

$$N_a^* = N_a \frac{1}{1 + 4e^{(E_a + E_v - E_f)/k_B T}};$$





$background

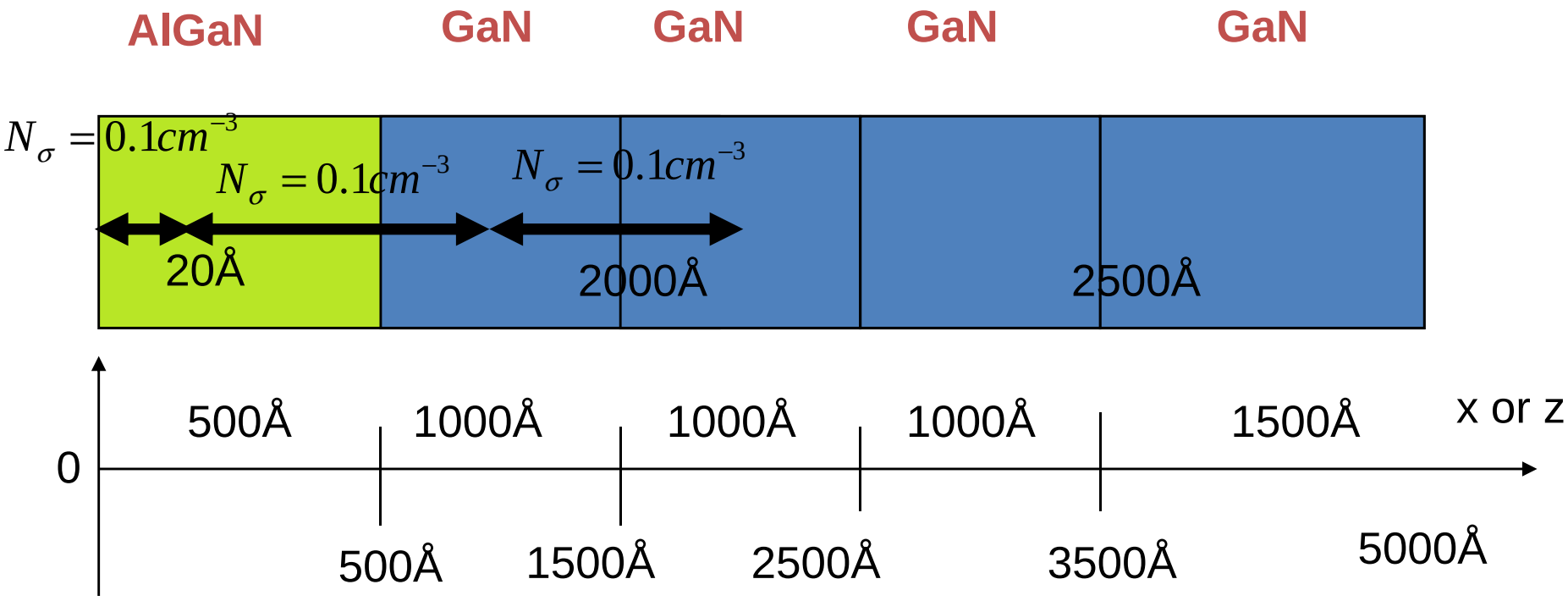
3 Number of contiguous background fixed charges (format = i2)

20.0 0.100E+00 Region 1

980.0 0.100E+00 Region 2

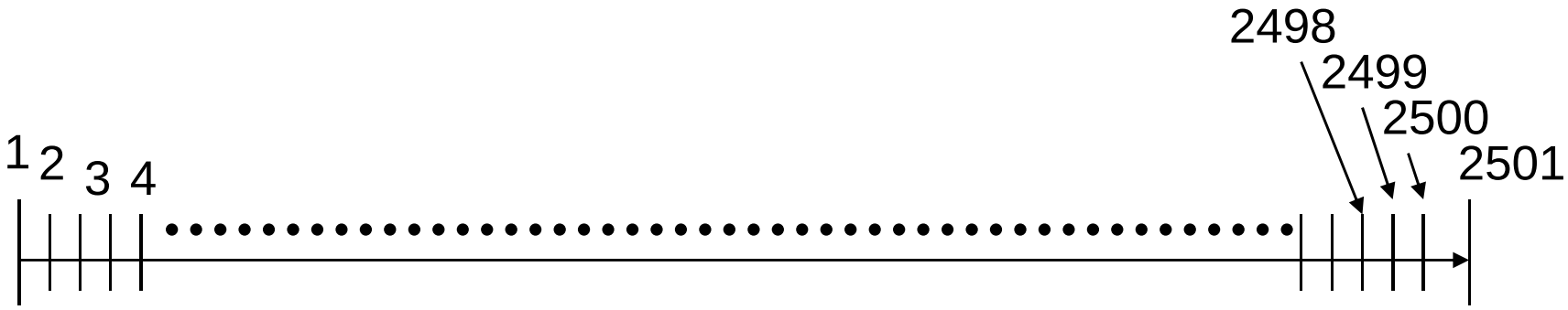
1000.0 0.100E+00 Region 3

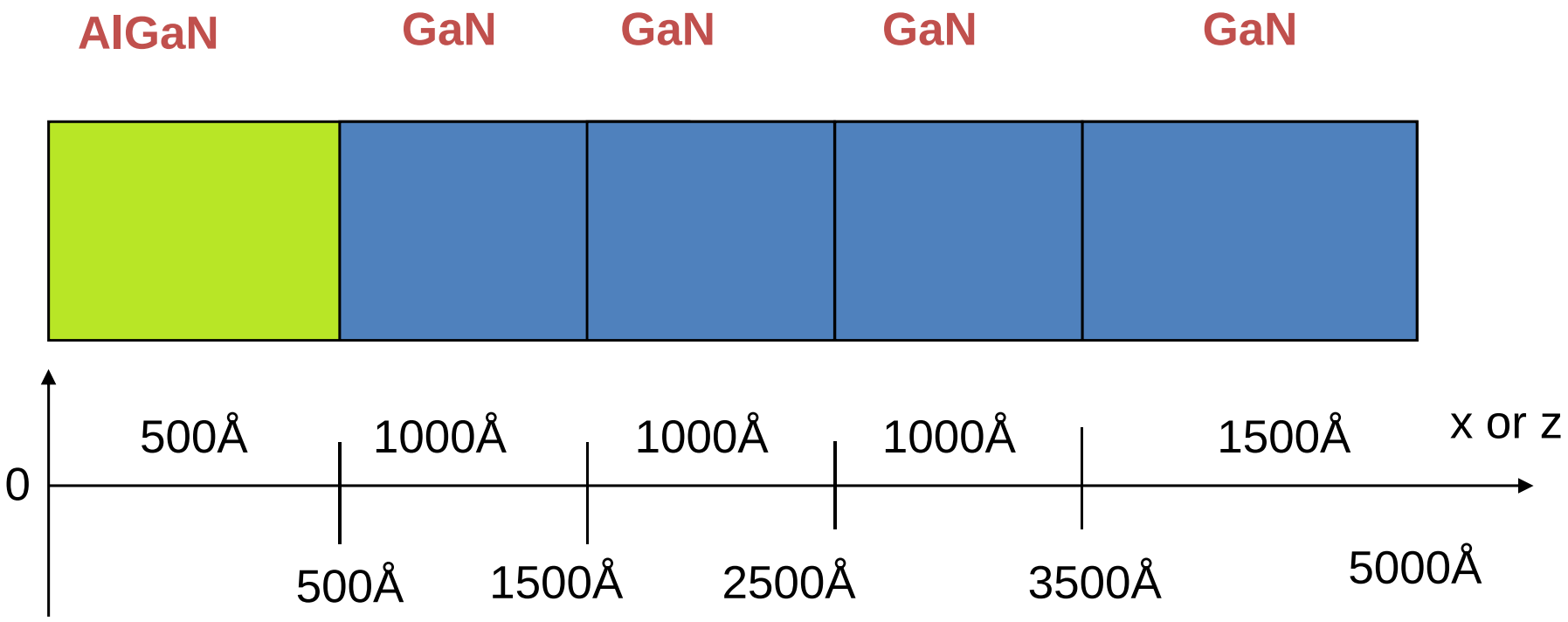
The back fixed charges can be used to represent the back ground impurities, interface charges, etc. Here we set it to be very small so that the effect can be neglected



$calcgrid
2501 Number of grid points

In this case, total thickness is 5000Å and calcgrid is 2501, dz=(5000)/(2501-1)=2Å

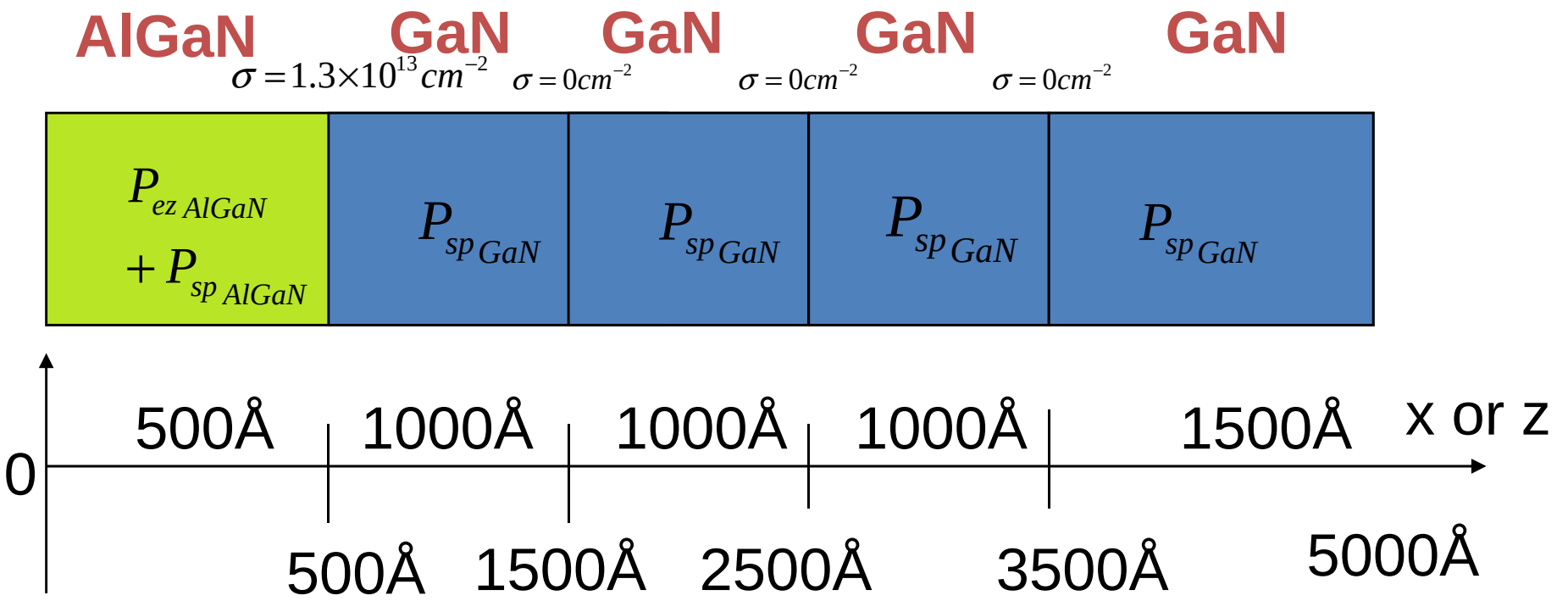




$piezcharge
1.300E+13 Piezelectric charge density - 1-2 Interface
0.000E+00 Layers' 2-3 Interface
0.000E+00 Layers' 3-4 Interface
0.000E+00 Layers' 4-5 Interface

$$\Delta P_1 = \left(P_{sp1} + P_{ez1}\right) - \left(P_{sp2} + P_{ez2}\right)$$

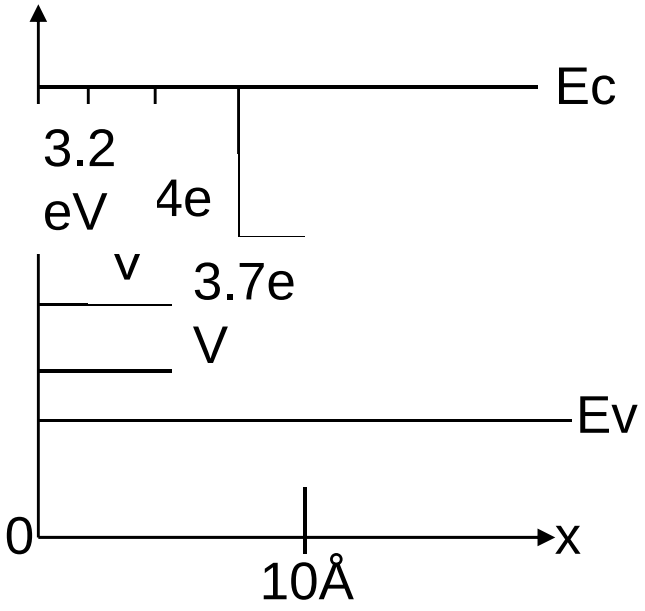
$$\Delta P_1 = \left(P_{sp2} + P_{ez2}\right) - \left(P_{sp3} + P_{ez3}\right)$$

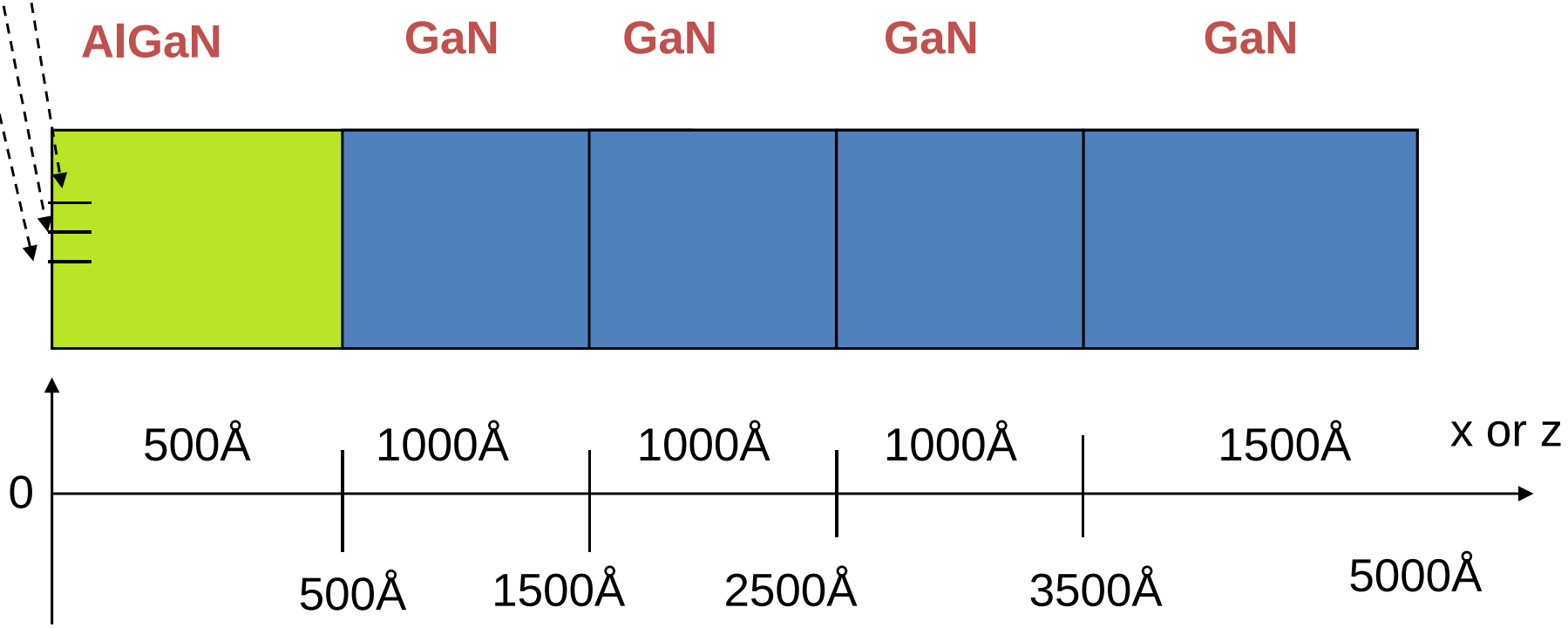


lx Å	rx Å	trapNT cm^-3	traplevel eV	degeneracy	taun (s)	taup (s)
$traps						
3			number of states			
0.0	**10.0**	**-3.00E+20**	**3.200**	**1**	**1.0E-08**	**1.0E-08**
0.0	**10.0**	**-3.00E+20**	**3.400**	**1**	**1.0E-08**	**1.0E-08**
0.0	**10.0**	**-3.00E+20**	**3.700**	**1**	**1.0E-08**	**1.0E-08**

donar like traps

τ_n and τ_p are related to trap density and cross section. Please see the document attached below





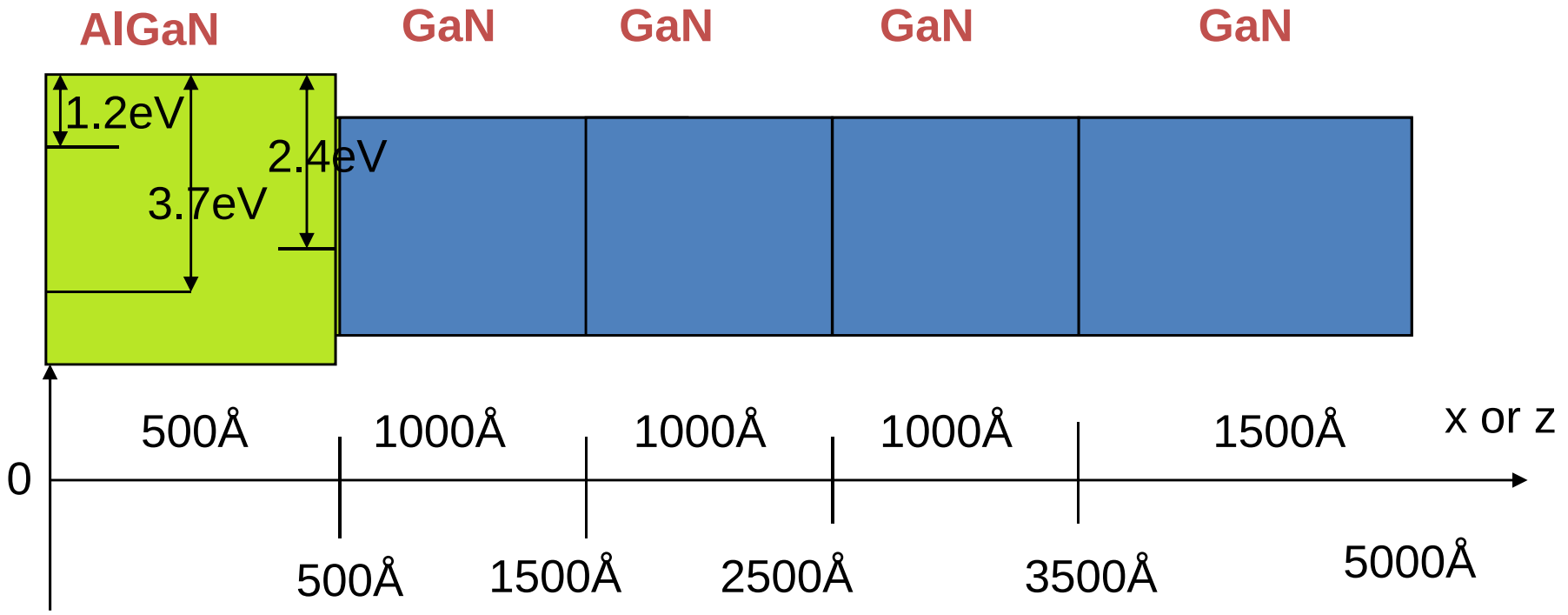
For example

donar like trap (set as negative), behave as negative charges after trap an electron

degeneracy of traps, usually set as 1

```
$traps
3
0.0 10.0  -3.00E+20   1.200   1   1.0E-08   1.0E-08
480.0 500.0  3.00E+20   2.400   1   1.0E-08   1.0E-08
0.0 100.0  3.00E+19   3.700   1   1.0E-08   1.0E-08
```

acceptor like trap (set value as positive), behave as positive charges after trapping a hole.



$float-gate → Use the floating gate condition. If we use float gate condition, this term should be set.

$nodriftdi → Don't calculate drift-diffusion equation.

$iffermibol → Use boltzmann approximation. Default is using Fermi-Dirac approximation.

$ifshockley → Consider the nonradiative SRH recombination

$schrodnodd →

1. Solve the Poisson-and Drift –diffusion until they convergse.
2. Then Set Efn(x) and Efp(x) as known values.
3. Solve the Poisson-Schrodinger equation self-consistently.

If this term is not set, the program will solve Poisson, Drift-diffusion, and Schrodinger equation simutaneously and iteratively.

For the solar cell problem (New function)

$ifsolargen
100000.000

####################3
use am1.5 solar spectrum
the absorption coefficient alpha 0
I = I0 * exp (- alpha0*(E-Eg)^0.5/E * dx)
#############

$solarstrength
1.000

#########
solar strength, 1.00 means one sun
500.00 mean 500 sun, used for concentrator

########

$ifsolarspectrum
Solarspeam1.5.xxx
2000 → File line size

(optional) If you don't want to use am1.5 spectrum, change the spectrum file.

Output File

- algan32-gan.out.vg_ 0.00-cb.res

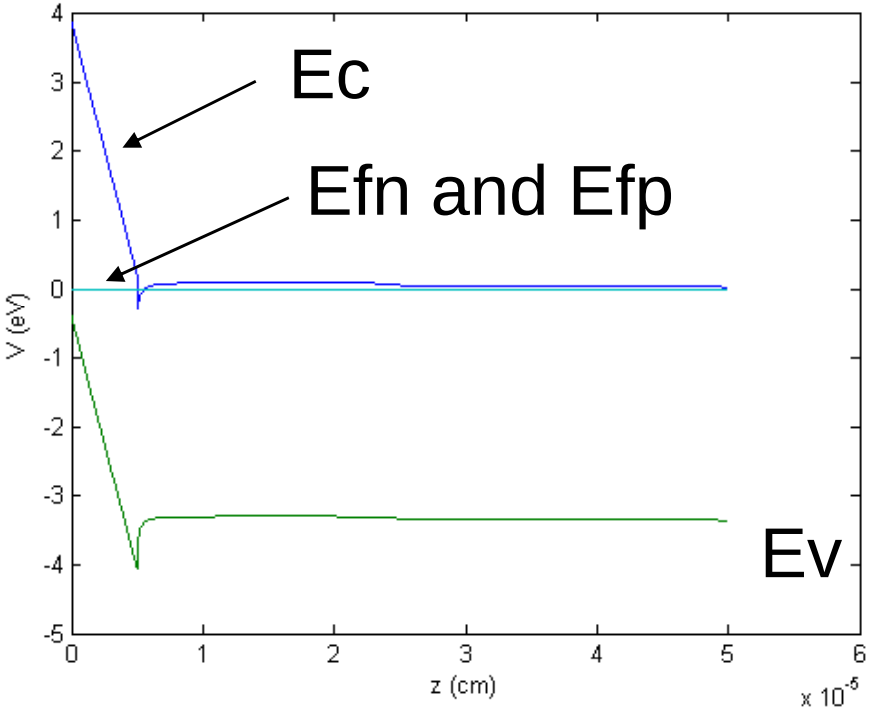
Direct recombination rate

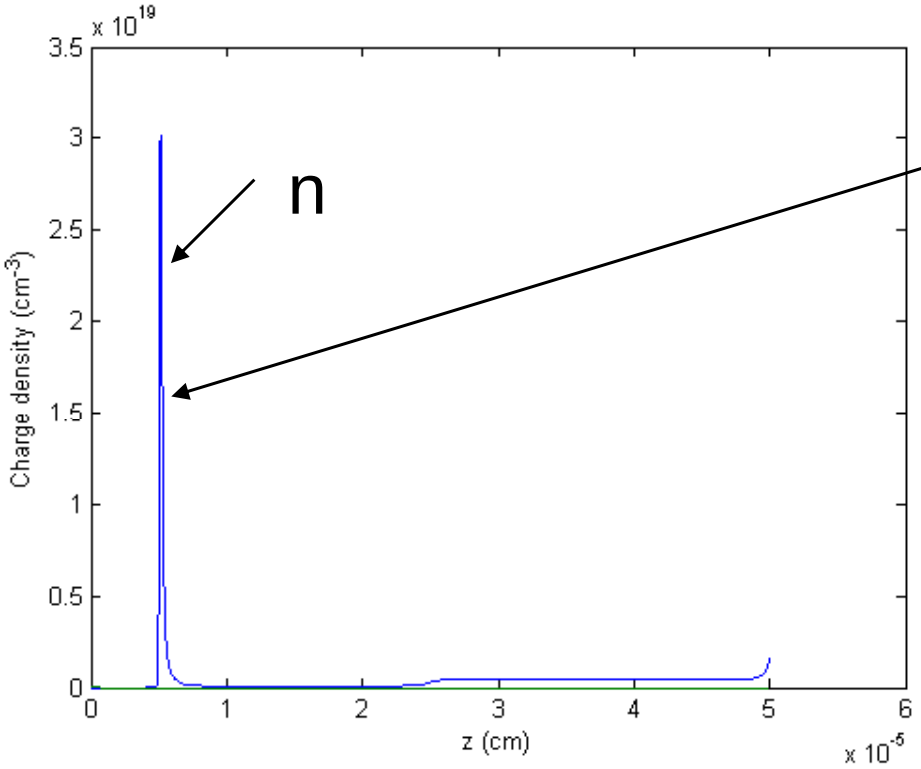
position(cm)	E_c	E_v	E_{fn}	E_{fp}	n	p	J_n	J_p	
0.00000E+00	3.85149E+00	-4.18511E-01	0.00000E+00	0.00000E+00	6.03885E-47	2.17167E+12	0.00000E+00	0.00000E+00	0.00000E+00
2.00000E-08	3.83784E+00	-4.32165E-01	0.00000E+00	0.00000E+00	1.02398E-46	1.28071E+12	0.00000E+00	0.00000E+00	0.00000E+00
4.00000E-08	3.82415E+00	-4.45851E-01	0.00000E+00	0.00000E+00	1.73931E-46	7.54314E+11	0.00000E+00	0.00000E+00	0.00000E+00
6.00000E-08	3.81029E+00	-4.59714E-01	0.00000E+00	0.00000E+00	2.97312E-46	4.41267E+11	0.00000E+00	0.00000E+00	0.00000E+00

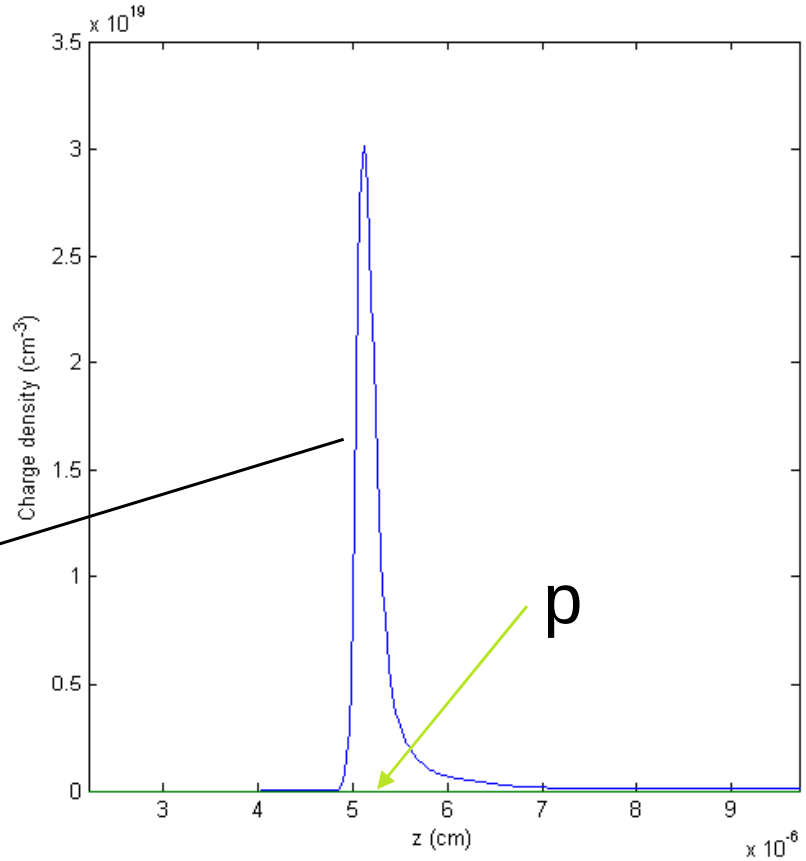
Electron and hole current and the radiative recombination

In Matlab, if you execute plotall.m and type

plotall('algan32-gan.out.vg_ 0.00-cb.res')


Ec
Efn and Efp
Ev
V (eV)
z (cm)
x 10^-5


n
x 10^19
Charge density (cm^-3)
z (cm)
x 10^-5

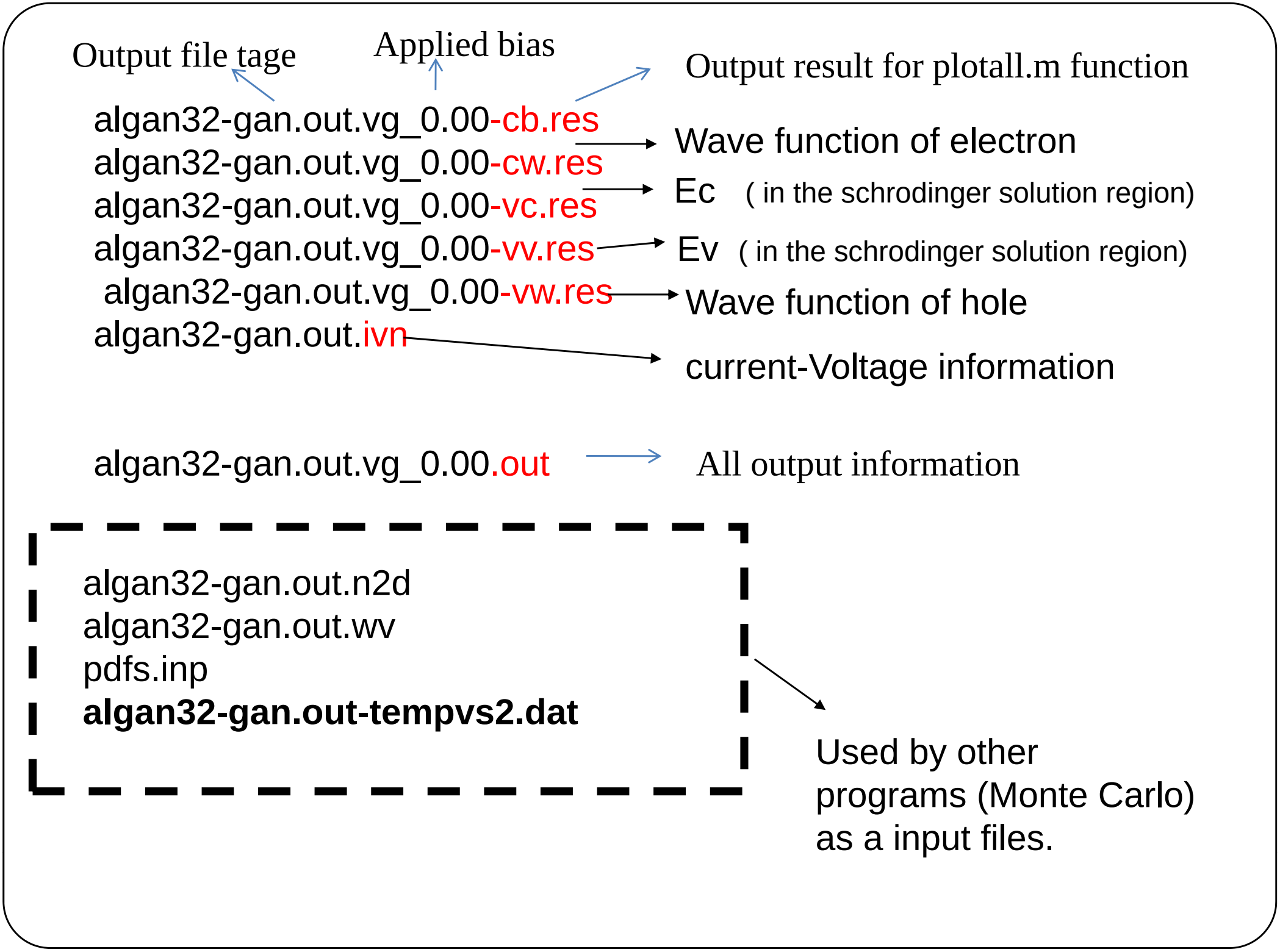

p
x 10^19
Charge density (cm^-3)
z (cm)
x 10^-6

Iv Information of the tunneling current and drift-diffusion current

The current information is save in $ivn, For Example, **algan32-vg0.0.ivn**

If you calculate the current in the device, you can plot out the IV-date by typing

Plotiv('algan32-vg0.0.ivn') **in matlab with plotiv.m file**


Output file tage
Applied bias
Output result for plotall.m function
algan32-gan.out.vg_0.00-cb.res
algan32-gan.out.vg_0.00-cw.res
algan32-gan.out.vg_0.00-vc.res
algan32-gan.out.vg_0.00-vv.res
algan32-gan.out.vg_0.00-vw.res
algan32-gan.out.ivn
Wave function of electron
Ec (in the schrodinger solution region)
Ev (in the schrodinger solution region)
Wave function of hole
current-Voltage information
algan32-gan.out.vg_0.00.out
All output information
algan32-gan.out.n2d
algan32-gan.out.wv
pdfs.inp
algan32-gan.out-tempvs2.dat
Used by other programs (Monte Carlo) as a input files.

Output format of the file end with *-cb.res

yrwu@node19: ~/ddcc

GNU nano 2.0.9 File: GaN-InGaN-GaN-4-1.out.vg_3.50-cb.res

0.00000E+00	-1.00000E-01	-3.50000E+00	-3.50000E+00	-3.50000E+00	1.70377E-39	1.78473E+19	2.66302E+03	8.91849E+02	3.04078E-30	0.00000E+00	0.00000E+00	0.00000E+00	-1.00000E-01	-3.50000E+00
1.00000E-08	-1.04037E-01	-3.50404E+00	-3.66635E-01	-3.50000E+00	8.69996E+13	1.57504E+19	2.66302E+03	8.91849E+02	1.37028E+23	0.00000E+00	0.00000E+00	0.00000E+00	-1.04037E-01	-3.50404E+00
2.00000E-08	-1.07801E-01	-3.50780E+00	-3.50594E-01	-3.50000E+00	1.87127E+14	1.39800E+19	2.66302E+03	8.91849E+02	2.61603E+23	0.00000E+00	0.00000E+00	0.00000E+00	-1.07801E-01	-3.50780E+00
3.00000E-08	-1.11321E-01	-3.51132E+00	-3.41868E-01	-3.50000E+00	3.00526E+14	1.24750E+19	2.66302E+03	8.91848E+02	3.74907E+23	0.00000E+00	0.00000E+00	0.00000E+00	-1.11321E-01	-3.51132E+00
4.00000E-08	-1.14624E-01	-3.51462E+00	-3.36077E-01	-3.50000E+00	4.27196E+14	1.11916E+19	2.66302E+03	8.91847E+02	4.78100E+23	0.00000E+00	0.00000E+00	0.00000E+00	-1.14624E-01	-3.51462E+00
5.00000E-08	-1.17732E-01	-3.51773E+00	-3.31858E-01	-3.50000E+00	5.67290E+14	1.00901E+19	2.66302E+03	8.91846E+02	5.72403E+23	0.00000E+00	0.00000E+00	0.00000E+00	-1.17732E-01	-3.51773E+00
6.00000E-08	-1.20665E-01	-3.52066E+00	-3.28608E-01	-3.50000E+00	7.20438E+14	9.13675E+18	2.66303E+03	8.91845E+02	6.58246E+23	0.00000E+00	0.00000E+00	0.00000E+00	-1.20665E-01	-3.52066E+00
7.00000E-08	-1.23439E-01	-3.52344E+00	-3.26009E-01	-3.50000E+00	8.87025E+14	8.30974E+18	2.66303E+03	8.91844E+02	7.37094E+23	0.00000E+00	0.00000E+00	0.00000E+00	-1.23439E-01	-3.52344E+00
8.00000E-08	-1.26069E-01	-3.52607E+00	-3.23872E-01	-3.50000E+00	1.06653E+15	7.58768E+18	2.66303E+03	8.91843E+02	8.09251E+23	0.00000E+00	0.00000E+00	0.00000E+00	-1.26069E-01	-3.52607E+00
9.00000E-08	-1.28567E-01	-3.52857E+00	-3.22079E-01	-3.50000E+00	1.25916E+15	6.95438E+18	2.66303E+03	8.91841E+02	8.75669E+23	0.00000E+00	0.00000E+00	0.00000E+00	-1.28567E-01	-3.52857E+00
1.00000E-07	-1.30944E-01	-3.53094E+00	-3.20548E-01	-3.49999E+00	1.46459E+15	6.39621E+18	2.66303E+03	8.91840E+02	9.36781E+23	0.00000E+00	0.00000E+00	0.00000E+00	-1.30944E-01	-3.53094E+00
1.10000E-07	-1.33210E-01	-3.53321E+00	-3.19224E-01	-3.49999E+00	1.68250E+15	5.90336E+18	2.66303E+03	8.91838E+02	9.93238E+23	0.00000E+00	0.00000E+00	0.00000E+00	-1.33210E-01	-3.53321E+00
1.20000E-07	-1.35374E-01	-3.53537E+00	-3.18066E-01	-3.49999E+00	1.91302E+15	5.46437E+18	2.66303E+03	8.91837E+02	1.04535E+24	0.00000E+00	0.00000E+00	0.00000E+00	-1.35374E-01	-3.53537E+00
1.30000E-07	-1.37442E-01	-3.53744E+00	-3.17042E-01	-3.49999E+00	2.15622E+15	5.07398E+18	2.66304E+03	8.91835E+02	1.09406E+24	0.00000E+00	0.00000E+00	0.00000E+00	-1.37442E-01	-3.53744E+00
1.40000E-07	-1.39423E-01	-3.53942E+00	-3.16131E-01	-3.49999E+00	2.41165E+15	4.72439E+18	2.66304E+03	8.91833E+02	1.13936E+24	0.00000E+00	0.00000E+00	0.00000E+00	-1.39423E-01	-3.53942E+00
1.50000E-07	-1.41323E-01	-3.54132E+00	-3.15313E-01	-3.49999E+00	2.67874E+15	4.41031E+18	2.66304E+03	8.91831E+02	1.18141E+24	0.00000E+00	0.00000E+00	0.00000E+00	-1.41323E-01	-3.54132E+00
1.60000E-07	-1.43145E-01	-3.54315E+00	-3.14575E-01	-3.49999E+00	2.95762E+15	4.12716E+18	2.66304E+03	8.91829E+02	1.22066E+24	0.00000E+00	0.00000E+00	0.00000E+00	-1.43145E-01	-3.54315E+00

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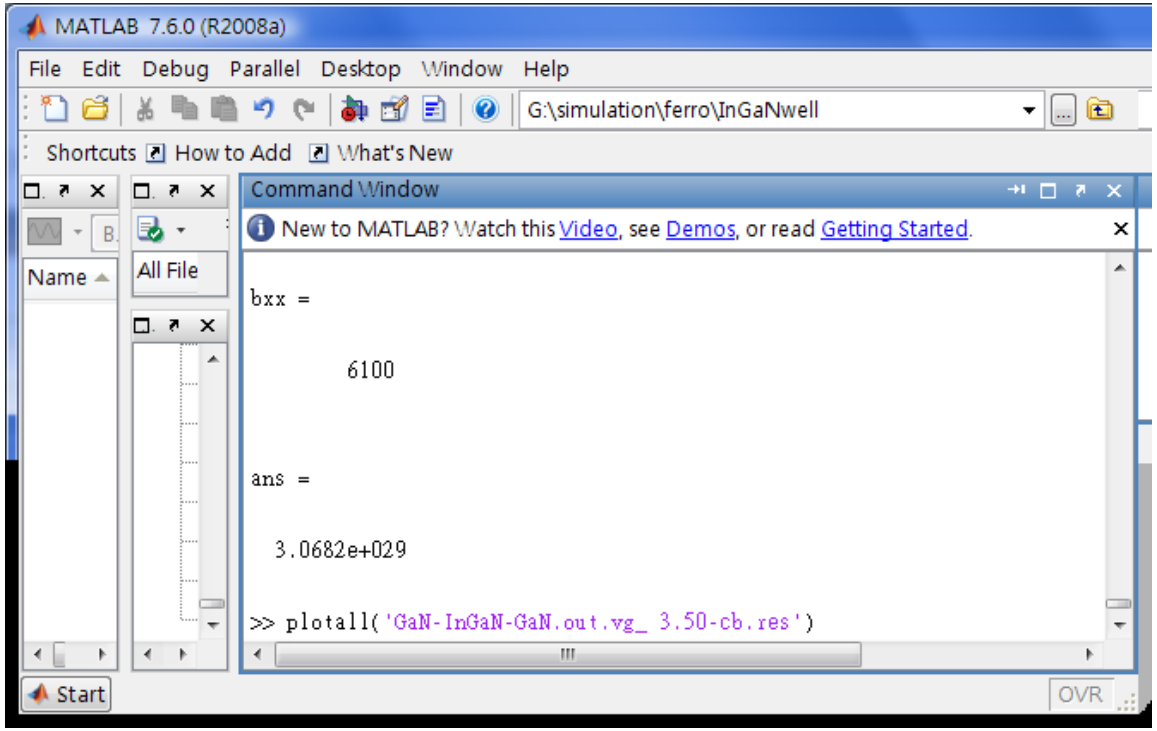
Z , Ec , Ev, Efn, Efp, n , P , Jn , Jp , rad, nonrad , Auger,Rsp, Eb, Ebh , generation rate



To output the result, in matlab, please type

plotall('*-cb.res')

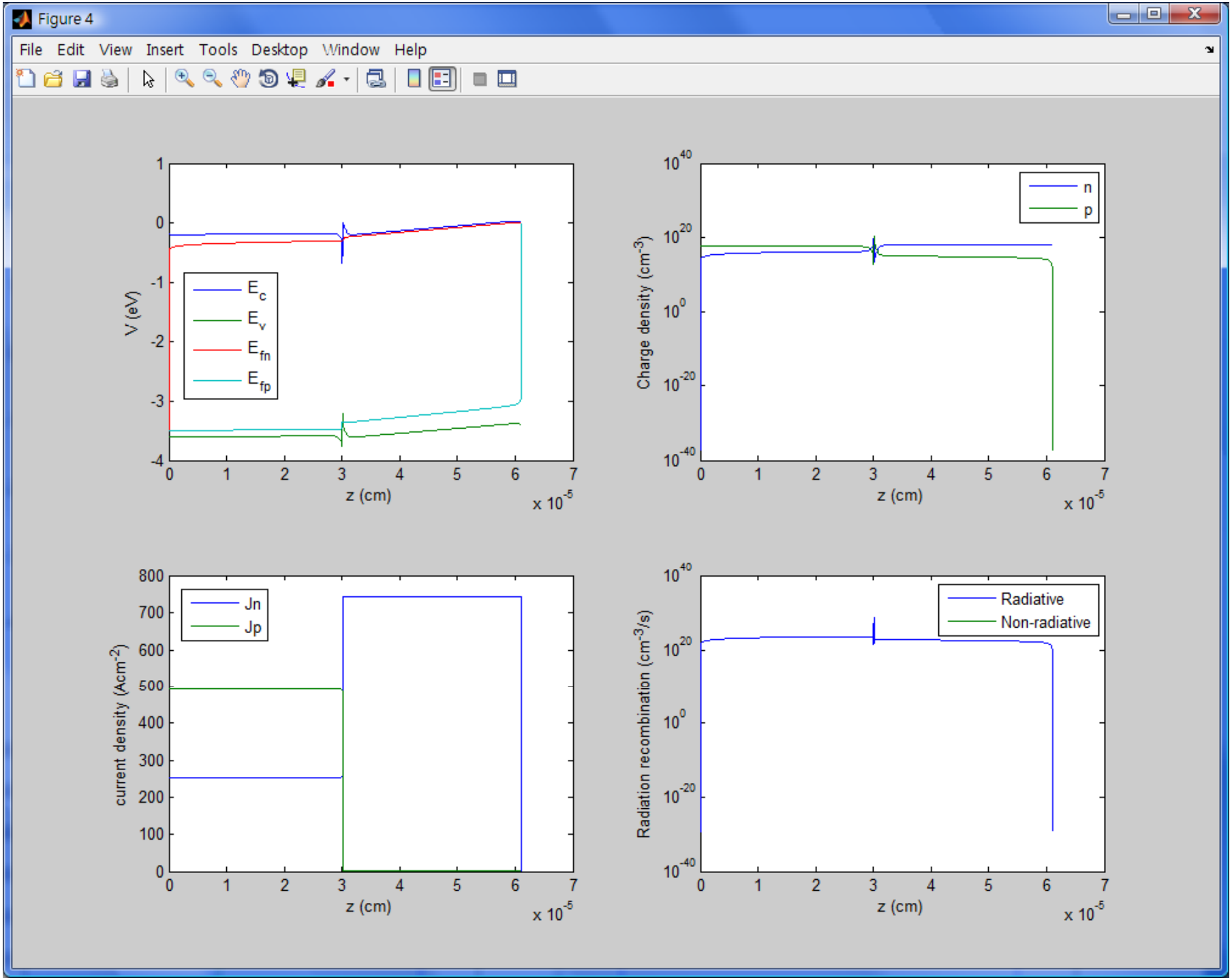


Figure 4
File Edit View Insert Tools Desktop Window Help
V (eV)
z (cm)
x 10^-5
E_c
E_v
E_fn
E_fp
Charge density (cm^-3)
n
p
current density (Acm^-2)
Jn
Jp
Radiation recombination (cm^-3/s)
Radiative
Non-radiative

File output ended with *-cw.res and *-vw.res

yrwu@node19: ~/ddcc

GNU nano 2.0.9 File: GaN-InGaN-GaN-4-1.out.vg_3.50-vw.res

```
0.0000000000E+00    0.5282974219E-08    0.1199647088E-06    0.3782628897E-06    0.4989241998E-07    0.1116779909E-05    0.1266157534E-05
0.1000000000E-07    0.7760597500E-08    0.1796771561E-06    0.5716491747E-06    0.7597877224E-07    0.1711935606E-05    0.1949925883E-05
0.2000000000E-07    0.9110592105E-08    0.2141770727E-06    0.6863308136E-06    0.9178782597E-07    0.2079287889E-05    0.2377356002E-05
0.3000000000E-07    0.9885351222E-08    0.2351911649E-06    0.7580467334E-06    0.1018922648E-06    0.2318439300E-05    0.2659168834E-05
0.4000000000E-07    0.1034082832E-07    0.2483196199E-06    0.8040675186E-06    0.1085218537E-06    0.2478300341E-05    0.2849979821E-05
0.5000000000E-07    0.1061199467E-07    0.2566356282E-06    0.8340252107E-06    0.1129359975E-06    0.2586775720E-05    0.2981154803E-05
0.6000000000E-07    0.1077455253E-07    0.2619455112E-06    0.8536920018E-06    0.1159011037E-06    0.2661058142E-05    0.3072178215E-05
0.7000000000E-07    0.1087237164E-07    0.2653519258E-06    0.8666691951E-06    0.1179037517E-06    0.2712218654E-05    0.3135716107E-05
0.8000000000E-07    0.1093134418E-07    0.2675430836E-06    0.8752583827E-06    0.1192609005E-06    0.2747582153E-05    0.3180236773E-05
0.9000000000E-07    0.1096691442E-07    0.2689543581E-06    0.8809526495E-06    0.1201823921E-06    0.2772079729E-05    0.3211505584E-05
0.1000000000E-06    0.1098835223E-07    0.2698634937E-06    0.8847298346E-06    0.1208086193E-06    0.2789069027E-05    0.3233495268E-05
0.1100000000E-06    0.1100124212E-07    0.2704486154E-06    0.8872342800E-06    0.1212341624E-06    0.2800853826E-05    0.3248965697E-05
0.1200000000E-06    0.1100895592E-07    0.2708243442E-06    0.8888922749E-06    0.1215230333E-06    0.2809023005E-05    0.3259844909E-05
0.1300000000E-06    0.1101353210E-07    0.2710645949E-06    0.8899865883E-06    0.1217186888E-06    0.2814676268E-05    0.3267485031E-05
0.1400000000E-06    0.1101620403E-07    0.2712170978E-06    0.8907051116E-06    0.1218506929E-06    0.2818576588E-05    0.3272836853E-05
0.1500000000E-06    0.1101771827E-07    0.2713127004E-06    0.8911728328E-06    0.1219391860E-06    0.2821254190E-05    0.3276570195E-05
0.1600000000E-06    0.1101852678E-07    0.2713713498E-06    0.8914729550E-06    0.1219979013E-06    0.2823077971E-05    0.3279157547E-05
0.1700000000E-06    0.1101890322E-07    0.2714059479E-06    0.8916608901E-06    0.1220362089E-06    0.2824304777E-05    0.3280932498E-05
0.1800000000E-06    0.1101901321E-07    0.2714248405E-06    0.8917735492E-06    0.1220605041E-06    0.2825113524E-05    0.3282130704E-05
0.1900000000E-06    0.1101895698E-07    0.2714334257E-06    0.8918355214E-06    0.1220751525E-06    0.2825628878E-05    0.3282918703E-05
```

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^X Exit ^J Justify ^W Where Is ^V Next Page ^U UnCut Text ^T To Spell

Position (z)

First wave funciton

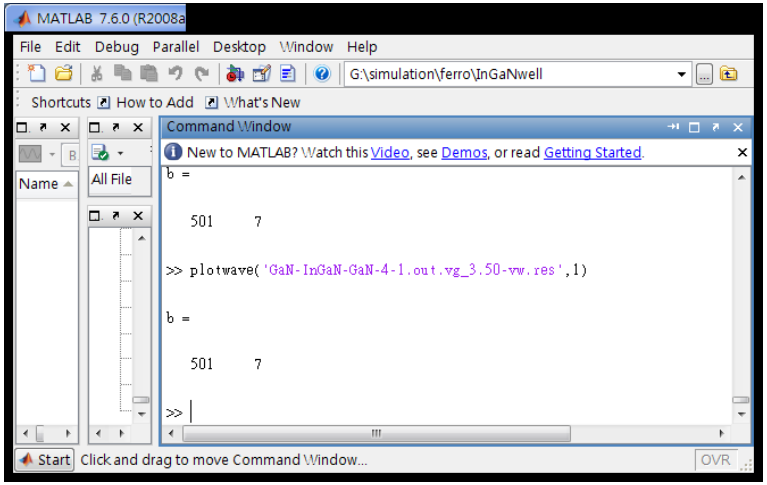
Second wave funciton

Third to the maximum confined state number……

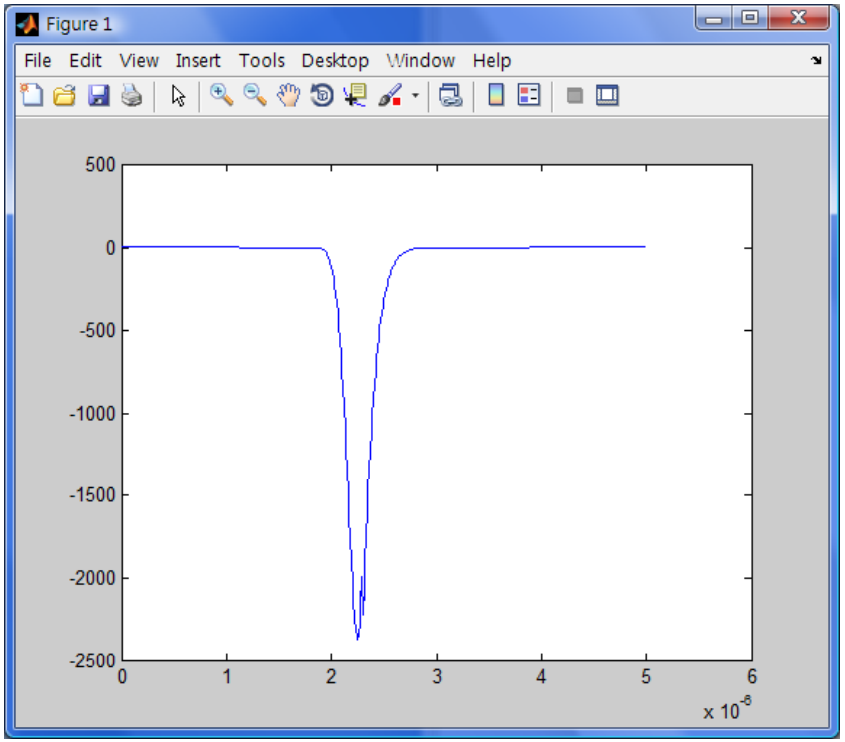
In the matlab, type

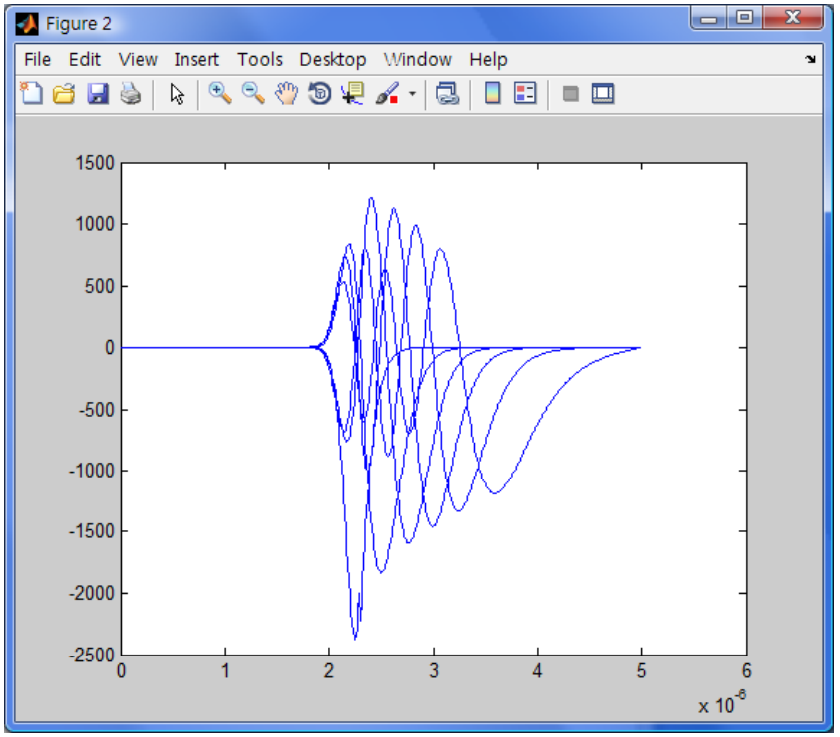
plotwave(‘*-cb.res or *-vw.res’, 1)

Subband number



Plot of hole wave function





Output of current and voltage (I-V)

yrwu@node19: ~/ferro/test

GNU nano 2.2.2 File: pnjunction.ivn

ate-Voltage	Schottky-bar	Error	totalcurrent-l	totalcurrent-r	tunnel-jn	tunnel-jp	drift-diff-l-jn	drift-diff-l-jp	drift-diff-r-jn	drift-diff-r-jp	$
-1.000	1.400	-8.8530656E-07	-2.6278672E+00	-2.6278367E+00	0.0000000E+00	0.0000000E+00	9.5200031E-01	-3.5798676E+00	-2.9209419E+00	2.9310516E-01	100$
-0.900	1.400	-2.3520439E-08	-2.6254485E+00	-2.6254171E+00	0.0000000E+00	0.0000000E+00	9.5302619E-01	-3.5784747E+00	-2.9199155E+00	2.9449845E-01	100$
-0.800	1.400	-2.3520461E-08	-2.6229615E+00	-2.6229357E+00	0.0000000E+00	0.0000000E+00	9.5407477E-01	-3.5770363E+00	-2.9188689E+00	2.9593317E-01	100$
-0.700	1.400	-2.4245221E-08	-2.6204093E+00	-2.6203784E+00	0.0000000E+00	0.0000000E+00	9.5514834E-01	-3.5755576E+00	-2.9177905E+00	2.9741209E-01	100$
-0.600	1.400	-2.3520443E-08	-2.6177781E+00	-2.6177503E+00	0.0000000E+00	0.0000000E+00	9.5624876E-01	-3.5740268E+00	-2.9166890E+00	2.9893873E-01	100$
-0.500	1.400	-2.3520459E-08	-2.6150700E+00	-2.6150381E+00	0.0000000E+00	0.0000000E+00	9.5737853E-01	-3.5724486E+00	-2.9155551E+00	3.0051694E-01	100$
-0.400	1.400	-2.4902207E-08	-2.6122725E+00	-2.6122422E+00	0.0000000E+00	0.0000000E+00	9.5853987E-01	-3.5708124E+00	-2.9143935E+00	3.0215127E-01	100$
-0.300	1.400	7.7099674E-08	-2.6093759E+00	-2.6093492E+00	0.0000000E+00	0.0000000E+00	9.5973614E-01	-3.5691121E+00	-2.9131960E+00	3.0384678E-01	100$
-0.200	1.400	3.2923558E-08	-2.6063819E+00	-2.6063517E+00	0.0000000E+00	0.0000000E+00	9.6097023E-01	-3.5673521E+00	-2.9119612E+00	3.0560946E-01	100$
-0.100	1.400	-2.3520438E-08	-2.6032634E+00	-2.6032344E+00	0.0000000E+00	0.0000000E+00	9.6224741E-01	-3.5655108E+00	-2.9106807E+00	3.0744630E-01	100$
0.000	1.400	-2.3520461E-08	-2.6000194E+00	-2.5999900E+00	0.0000000E+00	0.0000000E+00	9.6357181E-01	-3.5635912E+00	-2.9093555E+00	3.0936553E-01	100$
0.100	1.400	3.7818312E-08	-2.5966285E+00	-2.5965966E+00	0.0000000E+00	0.0000000E+00	9.6495142E-01	-3.5615799E+00	-2.9079735E+00	3.1137688E-01	100$
0.200	1.400	-2.3520448E-08	-2.5930674E+00	-2.5930372E+00	0.0000000E+00	0.0000000E+00	9.6639307E-01	-3.5594604E+00	-2.9065295E+00	3.1349232E-01	100$
0.300	1.400	7.7110800E-08	-2.5893131E+00	-2.5892869E+00	0.0000000E+00	0.0000000E+00	9.6790810E-01	-3.5572212E+00	-2.9050133E+00	3.1572643E-01	100$
0.400	1.400	7.7098301E-08	-2.5853389E+00	-2.5853123E+00	0.0000000E+00	0.0000000E+00	9.6951080E-01	-3.5548492E+00	-2.9034098E+00	3.1809745E-01	100$
0.500	1.400	-2.3520453E-08	-2.5810961E+00	-2.5810677E+00	0.0000000E+00	0.0000000E+00	9.7121982E-01	-3.5523159E+00	-2.9016965E+00	3.2062881E-01	100$
0.600	1.400	-2.3520438E-08	-2.5765252E+00	-2.5764985E+00	0.0000000E+00	0.0000000E+00	9.7306330E-01	-3.5495885E+00	-2.8998496E+00	3.2335111E-01	100$

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^X Exit ^J Justify ^W Where Is ^V Next Page ^U UnCut Text ^T To Spell

Vg

Φ_B

Error, convergence

Total current of left side and right side (should be the same)

Electron Tunnel Current (disabled)

hole Tunnel Current (disabled)

Electron current at top contact (1st layer

hole current at top contact (1st layer

Electron current at buttom contact (1st layer

hole current at buttom contact (1st layer

- algan32-gan.out.vg_ 0.00.out

Total output file, all information is listed here

Input file information

Heavy hole density in each layer

Light hole density in each layer

electron density in each layer

carrier density obtained by Schrödinger solver with confined states

```
Simulation gatevoltage =  0.00000E+00 V
--------layerthickness----------
 5.00000E-06   1.50000E-05   2.50000E-05   3.50000E-05   5.00000E-05
--------effmass----------
Heavy hole          6.00000E-01   6.00000E-01   6.00000E-01   6.00000E-01   6.00000E-01
Light hole          6.00000E-01   6.00000E-01   6.00000E-01   6.00000E-01   6.00000E-01
eletron  in-plane   2.45900E-01   2.00000E-01   2.00000E-01   2.00000E-01   2.00000E-01
eletron  out-plane  2.45900E-01   2.00000E-01   2.00000E-01   2.00000E-01   2.00000E-01
------------------------------
 0.00000E+00   0.00000E+00   0.00000E+00   8.61553E+12   NaN
------------------------------
------------------------------
tunneling current =  0.00000E+00 1/cm^2/s
Output the fraction of phi in each layer
      band layer eigen value      qn       fraction
================================================
heavy hole 2DEG
eigenvalue
layer, 2DEG
   1
   2
   3
   4
   5
================================================
light hole 2DEG
eigenvalue
layer, 2DEG
   1
   2
   3
   4
   5
================================================
electron   2DEG
eigenvalue    -0.08324211    0.02074200    0.05848915
layer, 2DEG   7.58376E+12   8.16067E+11   2.15707E+11
   1       0.0396009748  0.0161195038  0.0082074449
   2       0.9603990252  0.9838804962  0.9917925551
   3       0.0000000000  0.0000000000  0.0000000000
   4       0.0000000000  0.0000000000  0.0000000000
   5       0.0000000000  0.0000000000  0.0000000000
================================================
   Total 2DEG distribution in each layer 1, heavy hole 2, light hole 3,electron
  0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
  0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00   0.00000E+00
  3.15249E+11   8.30028E+12   0.00000E+00   0.00000E+00   0.00000E+00
================================================
Simulation gatevoltage =  0.00000E+00 V
Output the potential profile o
```

Second section, output the potential information

```
================================================
Simulation gatevoltage =  0.00000E+00 V
Output the potential profile o
 2.00000E-08  3.85149E+00 -4.18511E-01  0.00000E+00  0.00000E+00  3.85046E+00 -4.19536E-01  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E
 4.00000E-08  3.83784E+00 -4.32165E-01  0.00000E+00  0.00000E+00  3.83717E+00 -4.32827E-01  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E
 6.00000E-08  3.82415E+00 -4.45851E-01  0.00000E+00  0.00000E+00  3.82368E+00 -4.46320E-01  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E
 8.00000E-08  3.81029E+00 -4.59714E-01  0.00000E+00  0.00000E+00  3.81001E+00 -4.59994E-01  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E
 1.00000E-07  3.79612E+00 -4.73878E-01  0.00000E+00  0.00000E+00  3.79603E+00 -4.73973E-01  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E
```

x E_c E_V E_{fn} E_{fp} E_c E_V E_{fn} E_{fp} J_n J_p

Band structure which are obtained by solving Poisson and Schrodinger equation self-consistently.

Band structure which only solves . Poisson equation.

Radiatve recombination

Non-radiative recombination

Auger recombination rates

Third section – output the charge information

Simulation gatevoltage = 0.00000E+00 V
Output the total charge concentration of each grid points
1 4.04905E+11 1.03480E+05
2 9.36764E+12 3.67963E-42
3 9.86514E+11 4.20935E-42
4 4.51496E+12 8.25626E-43
5 7.34294E+12 1.16088E-42

Carrier density in each layer

Output the total charge distribution

2.00000E-08	6.03885E-47	2.17167E+12	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
4.00000E-08	1.02398E-46	1.28071E+12	0.00000E+00	0.00000E+00	-5.78259E+09	-1.32466E+13	-1.44537E+18	0.00000E+00	0.00000E+00	0.00000E+00
6.00000E-08	1.73931E-46	7.54314E+11	0.00000E+00	0.00000E+00	-9.81749E+09	-2.24896E+13	-2.44569E+18	0.00000E+00	0.00000E+00	0.00000E+00
8.00000E-08	2.97312E-46	4.41267E+11	0.00000E+00	0.00000E+00	-1.67818E+10	-3.84432E+13	-4.15656E+18	0.00000E+00	0.00000E+00	0.00000E+00
1.00000E-07	5.14254E-46	2.55121E+11	0.00000E+00	0.00000E+00	-2.90255E+10	-6.64907E+13	-7.11717E+18	0.00000E+00	0.00000E+00	0.00000E+00
1.20000E-07	7.65810E-05	8.18452E+10	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1.40000E-07	9.93335E-05	8.18452E+10	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1.60000E-07	1.03480E-04	4.64482E+10	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
1.80000E-07	1.04622E-04	2.63255E+10	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2.00000E-07	1.05308E-04	1.49202E+10	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2.20000E-07	1.05929E-04	8.45596E+09	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2.40000E-07	1.06545E-04	4.79456E+09	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00
2.60000E-07	1.07165E-04	2.71764E+09	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00

x

n

p

J_n

J_p

Trapped charges at level 1

Trapped charges at level 2

Trapped charges at level 3

Dummy output, will be removed for this revision 10

Fourth section – output the wavefunction obtained by Schrödinger solver

Simulation gatevoltage = 0.00000E+00 V

Output the wave function 1 for

```
 1  0.12000E-06
 1  0.14000E-06
 1  0.16000E-06
 1  0.18000E-06
 1  0.20000E-06
.......
 2  0.12000E-06
 2  0.14000E-06
 2  0.16000E-06
.......
 3  0.12000E-06   0.38254E-09  0.59909E-08  0.14632E-07
 3  0.14000E-06   0.43426E-09  0.68192E-08  0.16672E-07
 3  0.16000E-06   0.44280E-09  0.69589E-08  0.17018E-07
 3  0.18000E-06   0.44511E-09  0.69968E-08  0.17113E-07
 3  0.20000E-06   0.44651E-09  0.70195E-08  0.17169E-07
 ...
```

Wave function for heavy hole, denoted as 1

Note. In this case, there is no confined states for holes and three confined states of electrons.

Electron or hole

Position x

Wave function of level 1

Wave function of level 2

Wave function of level 2

Plot of electron wave function in this case