Appendix C GAIN Examples

In this appendix, the use of the GAIN program is demonstrated for ten material systems. Each section below contains an example of how GAIN is used with one of these material systems.

C.1. Material system #1: AlGaAs/ AlGaAs

This is a simulation of a five-layer laser structure that contains a single quantum well (QW), two separated confinement heterostructure (SCH) layers, and two cladding layers as shown in Fig. C.1.1.

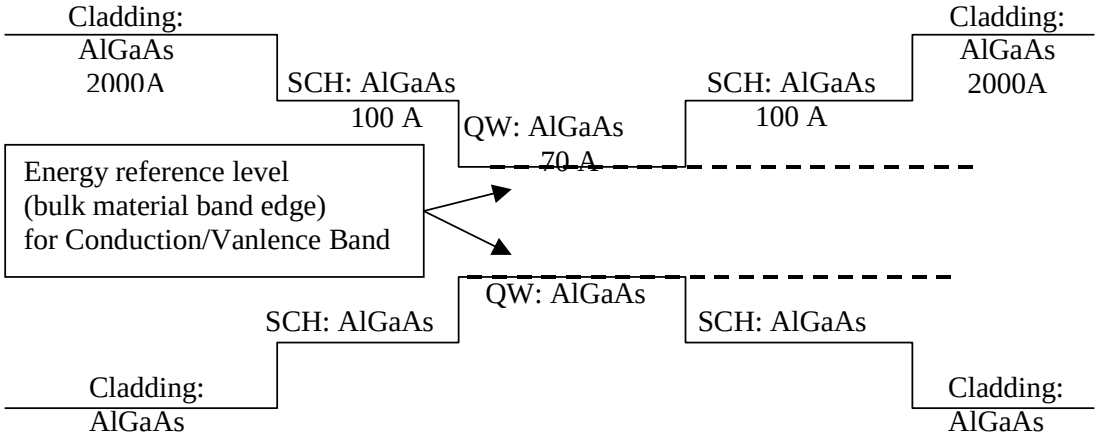

Figure C.1.1. Energy band diagram for the simple quantum well structure

C.1.1. Calculation of material compositions and energy band edges.

The first step of the GAIN program is to calculate the material compositions and energy band edges of the each layer. The user is asked to enter the photoluminescence wavelength, thickness, and strain of the QW, SCH, and cladding layers. After these parameters are input, the GAIN program generates two output files: cbandeg.dat and vbandeg.dat, containing the material compositions, and the conduction band edges and valence band edges respectively. The detailed explanation is provided in Chapter 2 of this manual.

a) The input parameters to the GAIN program in this step islisted in Table. C.4.1.

Table C.4.1. Input parameters to the GAIN program in this step.

Layer	λ (um)	Strain	Thickness (Å)
QW ($Al_xGa_{1-x}As$)	0.87	------	50
SCH ($Al_xGa_{1-x}As$)	0.74	------	60
Cladding ($Al_xGa_{1-x}As$)	0.58		100

b) The steps in using the GAIN program to calculate the material compositions and energy band edges are listed in Table C.1.2

Table C.1.2. steps to run the GAIN program for necessary parameters.

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

1

 ENTER 1 FOR AlGaAs/AlGaAs
      2 FOR InGaAsP/InGaAsP/InP
      3 FOR InGaAs/InGaAsP/InP
      4 FOR InGaAlAs/InGaAlAs/InP
      5 FOR GaInP/(AlGa)0.5In0.5P/AlInP
      6 FOR InGaAs/AlGaAs/AlGaAs
      7 FOR InGaAs/InGaAsP/Ga0.51In0.49P(MATCHED GaAs)
      8 FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
      9 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/InP
     10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(matched InP)
     11 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/AlAsxSb1-x
     12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs (dilute N)
     13 FOR In(1-x)Ga(x)As(y)P(1-y)/GaAs
     14 FOR EXIT, BACK TO MAIN PAGE!
1
 INPUT THE LAYER # FOR GRIN STRUCTURE(STEP)
 STEP N=
2
  INPUT THE WELL WAVELENGTH (um)
0.87
  INPUT THE BARRIER WAVELENGTH (um)
0.74
  INPUT THE CLADDING WAVELENGTH (um)
0.58
  BANDGAP ENERGY OF QUANTUM WELL=   1.42528735632184       eV
  INPUT CLADDING, BARRIER,QUANTUM WELL WIDTH (A)
100 60 50

  WRITE CONDUCTION BAND PARAMETERS INTO CBANDEG.DAT

  WRITE VALENCE BAND PARAMETERS INTO VBANDEG.DAT
  INPUT 1 FOR NEW CALCULATION
       2 FOR EXIT
  INPUT =?
2

 ENTER 1 FOR AlGaAs/AlGaAs
      2 FOR InGaAsP/InGaAsP/InP
      3 FOR InGaAs/InGaAsP/InP
      4 FOR InGaAlAs/InGaAlAs/InP
```

```
 5 FOR GaInP/(AlGa)0.5In0.5P/AlInP
 6 FOR InGaAs/AlGaAs/AlGaAs
 7 FOR InGaAs/InGaAsP/Ga0.51In0.49P(MATCHED GaAs)
 8 FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
 9 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/InP
10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(matched InP)
11 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/AlAsxSb1-x
12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs (dilute N)
13 FOR In(1-x)Ga(x)As(y)P(1-y)/GaAs
14 FOR EXIT, BACK TO MAIN PAGE!
14
 THIS PROGRAM STOP HERE!, BACK TO MAIN PAGE
```

c) The output files, cbandeg.dat and vbandeg.dat are explained in Table C.1.3.

Table C.1.3. Material compositions and band offsets:

a) cbandeg.dat for conduction band

```
*************************************************************************
 QW strain   lattice constant
0.000000E+00  0.565311E-09
                        material compositions
 layer thickness,          Al                    conduction band edges
  0.10000000E+03  0.56115438E+00  0.0000000  0.4632184   cladding layer
  0.60000000E+02  0.20182492E+00  0.0000000  0.1627524   SCH layer
  0.50000000E+02  0.10323627E-02  0.0000000  0.0000000   quantum well
  0.60000000E+02  0.20182492E+00  0.0000000  0.1627524   SCH layer
  0.10000000E+03  0.56115438E+00  0.0000000  0.4632184   cladding layer
*************************************************************************
```

b) vbandeg.dat for valence band

```
************************************************** **********************
 QW strain   lattice constant
0.000000E+00  0.565311E-09
                        material compositions
 layer thickness,          Al                    valence band edges
  0.10000000E+03  0.56115438E+00  0.0000000  -0.2494253   cladding layer
  0.60000000E+02  0.20182492E+00  0.0000000  -0.0876359   SCH layer
  0.50000000E+02  0.10323627E-02  0.0000000   0.0000000   quantum well
  0.60000000E+02  0.20182492E+00  0.0000000  -0.0876359   SCH layer
  0.10000000E+03  0.56115438E+00  0.0000000  -0.2494253   cladding layer
*************************************************************************
```

C.1.2. Energy level calculations

After the calculation of the material compositions and energy band edges, the GAIN program calculates energy levels in the conduction band and valence bands. The detailed explanations are discussed in Chapter 3 of this manual.

a) The steps of how to calculate the energy levels are shown in Table C.1.4.

Table C.4.4. Steps to calculate the energy levels

i) Steps to calculate the conduction band energy levels

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

2
 INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
 INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
 INPUT N=
5
 INPUT THE LOWEST POTENTIAL LAYER(1st Q-WELL) IC= ?
3
 INPUT THE SELECTED CENTER LAYER OF STRUCTURE ICR=
3
 ******************************************************
  INPUT I=1  FOR AlGaAs
       I=2  FOR InGaAsP
       I=3  FOR In1-xGaxAs/InGaAsP/InP
       I=4  FOR InGaAlAs/InGaAlAs
       I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
       I=6  FOR InGaAs/AlGaAs/AlGaAs
       I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
       I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
       I=9  FOR InzGa1-zAs/AlxGayIn1-x-yAs/InP
       I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
       I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
       I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
       I=13 FOR InGaAs/In(1-y)Ga(x)As(y)P(1-y)/GaAs
  INPUT I= ?
 ******************************************************
1
ENERGY EIGENVALUE===>  0.639537366786E-01 ERROR= .4682221E-14
ENERGY EIGENVALUE===>  0.192116584232E+00 ERROR= .4043667E-14
ENERGY EIGENVALUE===>  0.241763368724E+00 ERROR= .2926458E-14
ENERGY EIGENVALUE===>  0.310657613785E+00 ERROR= .2317973E-14
ENERGY EIGENVALUE===>  0.426765405664E+00 ERROR= .1485678E-14

 FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
 SKIP INPUT I==> 2
 I=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
0.639537366786E-01
 INPUT THE NAME OF OUTPUT FILE
cb1.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.82988859E-04
 CONFINEMENT FACTOR OF    2 th LAYER = 0.95857126E-01
 CONFINEMENT FACTOR OF    3 th LAYER = 0.80811977E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.95857126E-01
```

```
 CONFINEMENT FACTOR OF    5 th LAYER = 0.82988859E-04
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
1
  INPUT THE EIGENVALUE
  EIGEN VALUE=
0.192116584232E+00
  INPUT THE NAME OF OUTPUT FILE
cb2.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.66304726E-02
 CONFINEMENT FACTOR OF    2 th LAYER = 0.39546197E+00
 CONFINEMENT FACTOR OF    3 th LAYER = 0.19581511E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.39546197E+00
 CONFINEMENT FACTOR OF    5 th LAYER = 0.66304726E-02
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
2
```

ii) Steps to calculate the heavy hole energy levels

```
 ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT
3
  INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
  INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
  INPUT N=
5
  INPUT THE HIGHEST POTENTIAL(1st Q-WELL) LAYER IC= ?
3
  INPUT THE SELECTED CENTER OF THE STRUCTURE ICR=?
3
 ********************************************************
   INPUT I=1  FOR AlGaAs
        I=2  FOR InGaAsP
        I=3  FOR In(1-x)Ga(x)As/InGaAsP/InP
        I=4  FOR InGaAlAs/InGaAlAs
        I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
        I=6  FOR InGaAs/AlGaAs/AlGaAs
        I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
        I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
        I=9  FOR In(z)Ga(1-z)As/AlxGayIn1-x-yAs/InP
        I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
        I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
        I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
        I=13 FOR InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
   INPUT I= ?
 ********************************************************
1
 ********************************************************

  DOES THE STRUCTURE STRAIN OR STRAIN-COMPENSATED?
```

```
 IF STRAIN ONLY INPUT 1, STRAIN-COMPENSATED INPUT 2
 INPUT SELECT = ?

1
 ENERGY EIGENVALUE===> -0.238975151109E+00 ERROR= .3120685E-14
 ENERGY EIGENVALUE===> -0.197312089899E+00 ERROR= .4405413E-14
 ENERGY EIGENVALUE===> -0.166878855802E+00 ERROR= .2808856E-14
 ENERGY EIGENVALUE===> -0.139814196248E+00 ERROR= .4012646E-14
 ENERGY EIGENVALUE===> -0.111477421547E+00 ERROR= .3853459E-14
 ENERGY EIGENVALUE===> -0.102378800292E+00 ERROR= .1062527E-14
 ENERGY EIGENVALUE===> -0.681164844294E-01 ERROR= .2446502E-14
 ENERGY EIGENVALUE===> -0.188139816633E-01 ERROR= .1912450E-14

 FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
 SKIP INPUT I==> 2
 I=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
-0.188139816633E-01
 INPUT THE NAME OF OUTPUT FILE
hh1.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.38718131E-06
 CONFINEMENT FACTOR OF    2 th LAYER = 0.35292976E-01
 CONFINEMENT FACTOR OF    3 th LAYER = 0.92941327E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.35292976E-01
 CONFINEMENT FACTOR OF    5 th LAYER = 0.38718131E-06
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
-0.681164844294E-01
 INPUT THE NAME OF OUTPUT FILE
hh2.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.68925350E-04
 CONFINEMENT FACTOR OF    2 th LAYER = 0.18086577E+00
 CONFINEMENT FACTOR OF    3 th LAYER = 0.63813061E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.18086577E+00
 CONFINEMENT FACTOR OF    5 th LAYER = 0.68925350E-04
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
2
```

iii) Steps to calculate the light hole energy levels

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

4
 INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
```

```
 INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
 INPUT N=
5
 INPUT THE HIGHEST POTENTIAL(1st Q-WELL) LAYER IC= ?
3
 INPUT THE SELECTED CENTER OF THE STRUCTURE ICR=?
3
 ********************************************************
  INPUT I=1  FOR AlGaAs
      I=2  FOR InGaAsP
      I=3  FOR In(1-x)Ga(x)As/InGaAsP/InP
      I=4  FOR InGaAlAs/InGaAlAs
      I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
      I=6  FOR InGaAs/AlGaAs/AlGaAs
      I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
      I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
      I=9  FOR In(z)Ga(1-z)As/AlxGayIn1-x-yAs/InP
      I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
      I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
      I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
      I=13 FOR InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
  INPUT I= ?
 ********************************************************
1
 ********************************************************

 DOES THE STRUCTURE STRAIN OR STRAIN-COMPENSATED?
 IF STRAIN ONLY INPUT 1, STRAIN-COMPENSATED INPUT 2
 INPUT SELECT = ?

1
 ENERGY EIGENVALUE===> -0.205954300457E+00 ERROR= .3173697E-14
 ENERGY EIGENVALUE===> -0.149979763519E+00 ERROR= .2832057E-14
 ENERGY EIGENVALUE===> -0.114996860133E+00 ERROR= .2360129E-14
 ENERGY EIGENVALUE===> -0.415229761969E-01 ERROR= .2788797E-14

 FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
 SKIP INPUT I==> 2
 I=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
-0.415229761969E-01
 INPUT THE NAME OF OUTPUT FILE
lh1.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.38818584E-03
 CONFINEMENT FACTOR OF    2 th LAYER = 0.12463156E+00
 CONFINEMENT FACTOR OF    3 th LAYER = 0.74996051E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.12463156E+00
 CONFINEMENT FACTOR OF    5 th LAYER = 0.38818584E-03
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
-0.114996860133E+00
```

```
 INPUT THE NAME OF OUTPUT FILE
lh2.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.13841264E-01
 CONFINEMENT FACTOR OF    2 th LAYER = 0.41302518E+00
 CONFINEMENT FACTOR OF    3 th LAYER = 0.14626712E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.41302518E+00
 CONFINEMENT FACTOR OF    5 th LAYER = 0.13841264E-01
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
2
```

b) The main output file from this part of GAIN program is energy.dat, containing all the energy levels as shown in Table C.1.5. After the energy eigen values are calculated, the GAIN program asks the user whether he would like to check the wave envelope function or not. We suggest that the user check the wave envelope functions of the first and second energy levels for conduction and valence bands. The plots of the envelope functions are shown in Fig. C.1.2, Fig. C.1.3, Fig C.1.4.

Table C.1.5. output file energy.dat

```
 CONDUCTION BAND ENERGY===>  0.639537366786E-01 ERROR= .4682221E-14

 CONDUCTION BAND ENERGY===>  0.192116584232E+00 ERROR= .4043667E-14

 CONDUCTION BAND ENERGY===>  0.241763368724E+00 ERROR= .2926458E-14

 CONDUCTION BAND ENERGY===>  0.310657613785E+00 ERROR= .2317973E-14

 CONDUCTION BAND ENERGY===>  0.426765405664E+00 ERROR= .1485678E-14

 HEAVY HOLE ENERGY===> -0.238975151109E+00 ERROR= .3120685E-14

 HEAVY HOLE ENERGY===> -0.197312089899E+00 ERROR= .4405413E-14

 HEAVY HOLE ENERGY===> -0.166878855802E+00 ERROR= .2808856E-14

 HEAVY HOLE ENERGY===> -0.139814196248E+00 ERROR= .4012646E-14

 HEAVY HOLE ENERGY===> -0.111477421547E+00 ERROR= .3853459E-14

 HEAVY HOLE ENERGY===> -0.102378800292E+00 ERROR= .1062527E-14

 HEAVY HOLE ENERGY===> -0.681164844294E-01 ERROR= .2446502E-14

 HEAVY HOLE ENERGY===> -0.188139816633E-01 ERROR= .1912450E-14

 LIGHT HOLE ENERGY===> -0.205954300457E+00 ERROR= .3173697E-14

 LIGHT HOLE ENERGY===> -0.149979763519E+00 ERROR= .2832057E-14

 LIGHT HOLE ENERGY===> -0.114996860133E+00 ERROR= .2360129E-14

 LIGHT HOLE ENERGY===> -0.415229761969E-01 ERROR= .2788797E-14
```

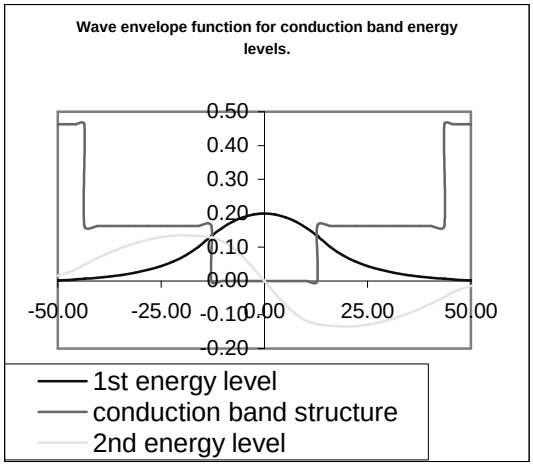

Fig. C.1.2. Wave envelop functions for energy levels in conduction band

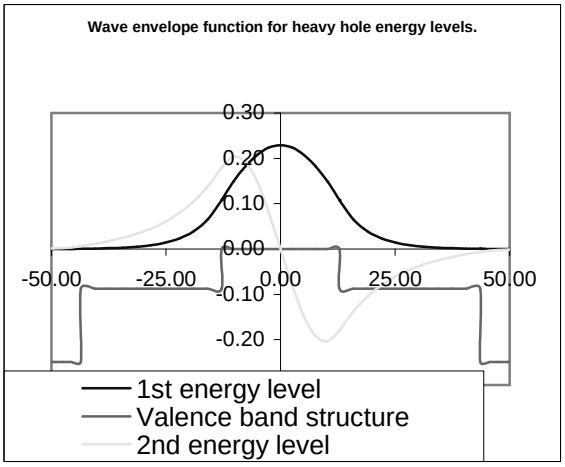

Fig. C.1.3. Wave envelop functions for heavy hole energy levels

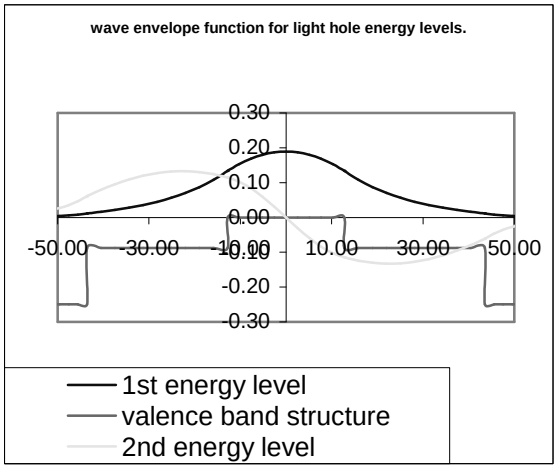

Fig. C.1.4. Wave envelop functions for light hole energy levels

C.1.3. Computation of Gain and Laser Characteristics

This is the last step of simulations using the GAIN program. With the previous calculated material composition, energy band edges, energy levels, and other parameters like material loss and Auger coefficient, the GAIN program can simulate the threshold current, threshold current density, slope efficiency, optical gain and mode gain as functions of wavelengths and photo energies, and L-I curve. The details are explained in Chapter 4 of the manual.

In this part of GAIN program, the input file needs to be constructed with the results of the previous steps and according to the laser design. In this example, single quantum well structure is used to simulate a three-QW laser. For the two-quantum-well laser with a ridge length of 750 μm and ridge width of 3 μm, the input file is shown in Table C.1.6. The detailed steps of simulations are listed in Table C.1.7. The main output files: L-I curve, optical gain as a function of the wavelength, and mode gain vs. current density are plotted in Fig. C.1.5, Fig. C.1.6, and Fig. C.1.7.

a) The input file:

Table C.1.6. Input file for gain and threshold current calculation

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c    1. Input the compositions, width of well, effective index        c
c      and lasing wavelength.                                         c
c    Ex: xx,xz,qy,xy,lx,n,lam                                         c
c    for different materials the following are the forms of inputs.   c
c                                                                     c
c    w -- > well, b -- > barrier  cxz and cxy for cladding.            c
c                                                                     c
c    a.  AlxGa1-xAs : xx (Al w) xz (Al b) qy (0) xy (0)               c
c    b.  In1-xGaxAsyP1-y : xx (Ga w) xz (Ga b) qy (As w) xy (As b)    c
c    c.  In1-xGaxAs/InGaAsP : xx (Ga w) xz (Ga b) qy (0) xy (As b)    c
c    d.  AlxGayIn1-x-yAs/InP : xx (Ga w) xz (Ga b) qy (Al w) xy (Al b)c
c    e.                                                               c
c    f.  InxGa1-xAs/AlGaAs : xx (In w) xz (0) qy (0) xy (Al b)        c
c    g.                                                               c
c    h.  AlyInxGa1-x-yAs/AlGaAs : xx (Al w) xz (al b) qy (In w) xz (0)c
c    i.  In1-xGaxAs/AlGaInAs : xx (In w) xz (0) qy (Al b) xy (Ga b)   c
c    j.  In(y)Ga(1-y)As(x)N(1-x) :xx(As w),xz(As, b),qy(In w),xy(In b)c
c    k.  InGaAs/InGaAsP/GaAs: xx (In w), (0), xz(Ga w) xy (As b)
c    2. Input the energy gap,temperature, barrier band edges(both bands)
c    Ex: eg,temp,ec,ev                                                c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
0.10323627E-02 0.20182492E+00  0  0  6.0  3.50  0.82
1.42528735632184 298 0.1627524 0.0876359
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c    3. Input the ist level sub-band energy levels.                   c
c    Ex: ec1,eh1,el1                                                  c
c                                                                     c
```

```
c     4. Input the material loss, reflectivities, number of quantum     c
c        wells and beta(for spontaneous emission).                      c
c     Ex: alpha,r1,r2,mm,beta.                                          c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
0.639537366786E-01  0.188139816633E-01  0.415229761969E-01  1  0.681164844294E-01  1
12.0d0  0.30   0.30   1  5.D-5
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c     5. Input the cavity length, ridge width, internal efficiency      c
c        Auger, strain(except AlGaAs,put 0) and confinement factor.     c
c     Ex: cl,cw,etha,ca,es,confine                                      c
c                                                                       c
c     6. Input the cladding composition and band edges.                 c
c     Ex: cxz,cxy,ecc,evv                                               c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
750.D-4  3D-4  0.96  1.00d-29   0.01  0.009834488
0.56115438E+00 0.0  0.4632184  0.2494253
```

b) The steps for these calculations mentioned are listed in Table C.1.7

Table C.1.7. The steps for the gain and threshold current density calculations

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

5
  THE INPUT FILE NAME=
in1_sys1_new.tex
  SELECT MATERIAL=?
  1--AlGaAs
  2--InGaAsP
  3--In1-zGazAs/InGaAsP/InP
  4-- InGaAlAs
  5--GaInP/AlzGawIn1-z-wP/Al0.5In0.5P
  6-- InxGa1-xAs/AlxGa1-xAs/AlGaAs
  7--In1-xGaxAs/InGaAsP/GaxIn1-xP(X=0.51) MATCHED TO GaAs
  8--AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
  9--InzGa1-zAs/AlxGayIn1-x-yAs/InP
  10-- InGaAlAs/InGaAlAs/AlAsSb
  11--InzGa1-zAs/AlxGayIn1-x-yAs/AlAsSb
  12--In(y)Ga(1-y)As(x)N(1-x)/GaAs
  13--InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
  INPUT SELECTION
1
 INPUT MODE = ? FOR TE--> MODE =1, FOR TM--> MODE =2
  INPUT TE OR TM ?
1
 IF EL1 BELOW EH1 THEN SELECT 1, OTHERWISE SELECT 2
  SELECTION=?
1
  ************************************************
 CALCULATE THE EFFECTIVE MASS
```

```
 ************************************************
 FOR QUASI-FERMI LEVEL SELECT=1,
 FOR READ EXISTING QUASI-FERMI LEVEL SELECT=2
 SELECT=?
1

 J(LEAKAGE)=0.537974D+00 A/cm^2  N=0.239674D+19 1/cm^3
 J(LEAKAGE)=0.554846D+00 A/cm^2  N=0.241654D+19 1/cm^3
 J(LEAKAGE)=0.572232D+00 A/cm^2  N=0.243634D+19 1/cm^3
 J(LEAKAGE)=0.590147D+00 A/cm^2  N=0.245614D+19 1/cm^3
…….
J(LEAKAGE)=0.215349D+04 A/cm^2  N=0.788120D+19 1/cm^3
 J(LEAKAGE)=0.221784D+04 A/cm^2  N=0.790100D+19 1/cm^3
 J(LEAKAGE)=0.228410D+04 A/cm^2  N=0.792080D+19 1/cm^3
 J(LEAKAGE)=0.235231D+04 A/cm^2  N=0.794060D+19 1/cm^3
 J(LEAKAGE)=0.242253D+04 A/cm^2  N=0.796040D+19 1/cm^3
 J(LEAKAGE)=0.249481D+04 A/cm^2  N=0.798020D+19 1/cm^3
 J(LEAKAGE)=0.256922D+04 A/cm^2  N=0.800000D+19 1/cm^3
 ************************************************
 G(J) PARAMETERS FROM SINGLE WELL
 Go=0.218113D+02 1/cm  Jo=0.303353D+03 A/cm^2

 G(N) PARAMETERS FROM SINGLE WELL
 NGo=0.221783D+04 1/cm  XNo=0.136717D+19 1/cm^3

 Jtr=0.111597D+03 A/cm^2  NTR=0.502953D+18 1/cm^3


 THE OPTIMUM NUMBER OF QUANTUM WELL FOLLOWS THE ARTICLE
 BY McIlory et al. IEEE JQE-21 1985.

 THE OPTIMUM NUMBER OF QUANTUM WELL Nopt =          2
 INPUT Nopt(CAN BE DIFFERENT FROM ABOVE CALCULATION)=?
2
  NUMBER OF QUANTUM WELL(MAY OR MAY NOT BE Nopt)=?
2

  ************************************************
  ************************************************
  1ST CHECK USE SINGLE WELL TIMES # OF WELLS
  ************************************************
  ************************************************
  2ND CHECK FOLLOWS FORMULA BY McIlory IN IEEE
  JOURNAL OF QUANTUM ELECTRONIC QE-21 1985.
  ************************************************
  Gth=  28.0530 1/cm Nth=0.176316D+19 1/cm^3 IY=   85
  1ST CHECK Jth=   806.35405951 A/cm^2
  2ND CHECK Jth=   631.98567 A/cm^2

  1ST CHECK Ith=0.181430D+02 mA NUMBER OF WELLS=  2
  2ND CHECK Ith=0.142197D+02 mA

 ************************************************
CALCULATE THE P-I RELATION

NDATA=        316
```

```
 ************************************************
 CALCULATE THE SLOPE: mW/mA Y=A+BX
 CONSTANT A=  -7.3929014   SLOPE B=   0.4074803

 ************************************************
 INPUT POWER PO FOR THE LINEWIDTH, PO=0 FOR STOP
 INPUT PO=    mW
0
 INPUT 1 FOR THE DYNAMIC CALCULATION. 2 FOR SKIP
 INPUT =
2
  K-FACTOR= 0.35774 nS  MAXIUM FREQ.= 24.8387 GHz

  ************************************************
  INPUT 1 FOR CALCULATE THE GAIN(E) RELATION.

  INPUT 2 FOR CALCULATE THE LINEWIDTH ENHENCEMENT
  FACTOR AND PHOTON ENERGY RELATION

  INPUT 3 FOR EXIT THE PROGRAM

 THE INPUT # IS
1
 INPUT FERMILEVELS IN C-BAND, V-BAND, AND CARRIER DENSITY
0.139680787212E+00 -0.953800948086E-02 0.200075187970E+19
 CALCULATE THE CONVOLUTION GAIN(E) COEFFICIENT
  ************************************************
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(LAMBDA)
COGLa.txt
  ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(LAMBDA)
CMGLa.txt
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(E)
COGEa.txt
  ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(E)
CMGEa.txt
  ************************************************
 INPUT 1 FOR REPEAT THE G(E) CALCULATION
 INPUT 2 FOR REPEAT THE ALPHA(E) CALCULATION
 INPUT 3 FOR EXIT
1
  ************************************************
  INPUT 1 FOR CALCULATE THE GAIN(E) RELATION.

  INPUT 2 FOR CALCULATE THE LINEWIDTH ENHENCEMENT
  FACTOR AND PHOTON ENERGY RELATION

  INPUT 3 FOR EXIT THE PROGRAM

 THE INPUT # IS
1
 INPUT FERMILEVELS IN C-BAND, V-BAND, AND CARRIER DENSITY
0.160216100041E+00 -0.259237429430E-02 0.251553884712E+19
 CALCULATE THE CONVOLUTION GAIN(E) COEFFICIENT
  ************************************************
```

```
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(LAMBDA)
COGLb.txt
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(LAMBDA)
CMGLb.txt
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(E)
COGEb.txt
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(E)
CMGEb.txt
 ************************************************
 INPUT 1 FOR REPEAT THE G(E) CALCULATION
 INPUT 2 FOR REPEAT THE ALPHA(E) CALCULATION
 INPUT 3 FOR EXIT
3
ENTER 1 FOR THE NECESSARY PARAMETERS
     2 FOR THE ENERGY VALUES OF CONDUCTION BAND
     3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
     4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
     5 FOR THE LASER G-J AND G(LAMBDA)
     6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
     7 FOR EXIT

7
```

c) The Output characteristics of designed laser from step 5 are summarized in Table C.1.7.

Table C.1.7 Characteristics of the designed laser

Optimized number of QWs (Nopt)	2
Number of QWs	2
Slope efficiency (%)	40.75
Jth (A/cm^2)	806.35 - 1st check, for matching threshold conditions 631.99 – 2nd check, using McIlory method
Ith (mA)	18.14 - 1st check, for matching threshold conditions 14.22 - 2nd check, using McIlory method
Peak λ at operating temperature (um)	0.819 um for carrier density of 2.0E18 /cm3 0.819 um for carrier density of 2.5E18 /cm3
Peak material gain (1/cm)	3619.36/cm for carrier density of 2.0E18 /cm3 4386.09 /cm for carrier density of 2.5E18 /cm3

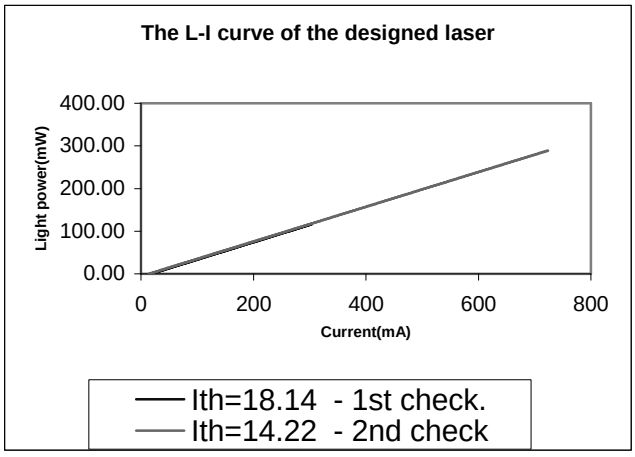

Fig. C.1.5. L-I curve of the laser

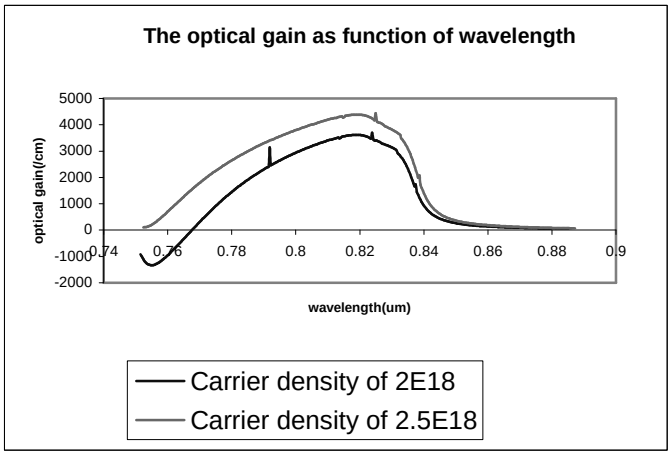

Fig. C.1.6. Optical gain-λ curve of the laser

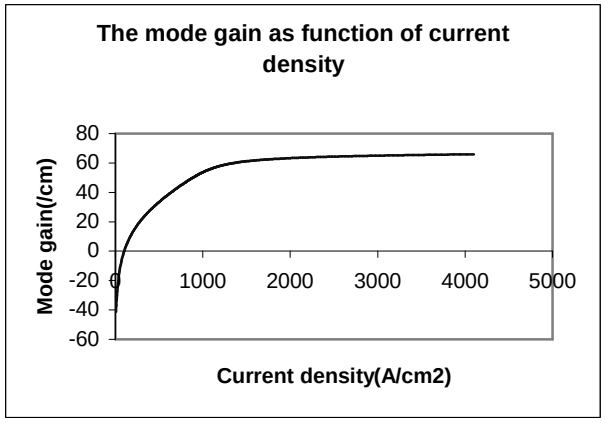

Fig. C.1.7. Mode gain as a function of current density (J)

C.2 Material system #2: InGaAs/InGaAlAs/InP

This is a simulation of a seventeen-layer laser structure that contains four quantum wells (QW), two separated confinement heterostructure (SCH) layers, and two cladding layers as shown in Fig. C.2.1. This device is a real one for research purpose. We will see the characteristics of this device.

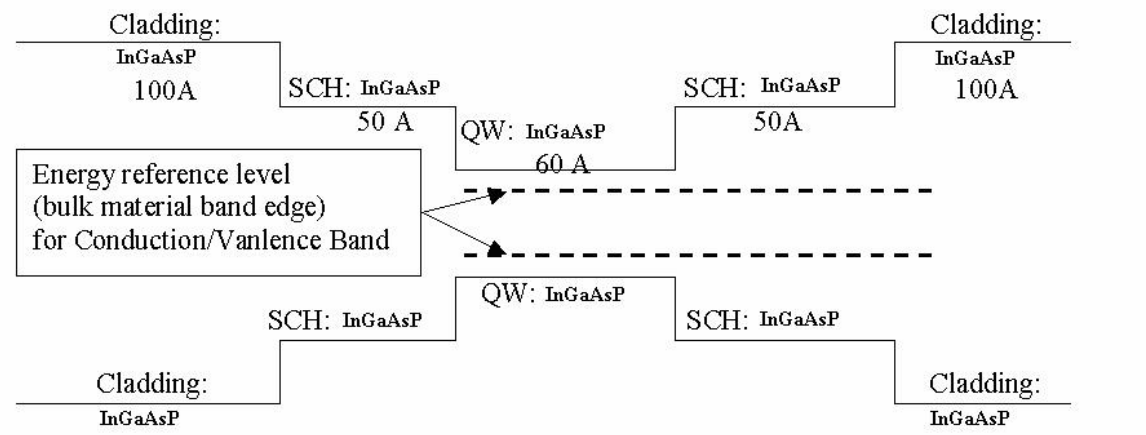

Figure C.2.2. Energy band diagram for the simple quantum well structure

C.2.1. Calculation of material compositions and energy band edges.

The first step of the GAIN program is to calculate the material compositions and energy band edges of the each layer. The user is asked to enter the photoluminescence wavelength, thickness, and strain of the QW, SCH, and cladding layers. After these parameters are input, the GAIN program generates two output files: cbandeg.dat and vbandeg.dat, containing the material compositions, and the conduction band edges and valence band edges respectively. The detailed explanation is provided in Chapter 2 of this manual.

a) The input parameters to the GAIN program in this step are listed in Table. C.2.1.

Table C.2.1. Input parameters to the GAIN program in this step.

Layer	λ (um)	Strain	Thickness (Å)
QW ($Ga_{1-x}In_xAs_yP_{1-y}$)	1.525	-0.012	60
SCH ($Ga_{1-x}In_xAs_yP_{1-y}$)	1.28		50
Cladding ($Ga_{1-x}In_xAs_yP_{1-y}$)	0.98		100

b) The steps in using the GAIN program to calculate the material compositions and energy band edges are listed in Table C.2.2

Table C.2.2. steps to run the GAIN program for necessary parameters.

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT
1

 ENTER 1 FOR AlGaAs/AlGaAs
      2 FOR InGaAsP/InGaAsP/InP
      3 FOR InGaAs/InGaAsP/InP
      4 FOR InGaAlAs/InGaAlAs/InP
      5 FOR GaInP/(AlGa)0.5In0.5P/AlInP
      6 FOR InGaAs/AlGaAs/AlGaAs
      7 FOR InGaAs/InGaAsP/Ga0.51In0.49P(MATCHED GaAs)
      8 FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
      9 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/InP
     10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(matched InP)
     11 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/AlAsxSb1-x
     12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs (dilute N)
     13 FOR In(1-x)Ga(x)As(y)P(1-y)/GaAs
     14 FOR EXIT, BACK TO MAIN PAGE!
2
 INPUT THE LAYER # FOR GRIN STRUCTURE(STEP)
 STEP N=
2
  INPUT THE WELL WAVELENGTH (um)
1.525
  INPUT THE BARRIER WAVELENGTH (um)
1.28
  INPUT THE CLADDING WAVELENGTH (um)
98
  BANDGAP ENERGY OF QUANTUM WELL=   0.683804000019804
  INPUT CLADDING, BARRIER,QUANTUM WELL WIDTH (A)
100 50 60

  In1-xGaxAsyP1-y, in output read Ga first then AsIN OUTPUT READ Ga FIRST THEN As

    FOR InGaAsP, only compress strain (~1.5%) available
    INPUT EX
-0.012

    FOR LATTICE MATCHED BARRIER SELECT --> 1
    FOR STRAIN COMPENSATED SELECT -- 2

    INPUT SELECTION===> ?
1

WRITE CONDUCTION BAND PARAMETERS INTO CBANDEG.DAT

  WRITE VALENCE BAND PARAMETERS INTO VBANDEG.DAT
  INPUT 1 FOR NEW CALCULATION, 2 FOR EXIT
  I= ?
2
```

```
 ENTER 1 FOR AlGaAs/AlGaAs
     2 FOR InGaAsP/InGaAsP/InP
     3 FOR InGaAs/InGaAsP/InP
     4 FOR InGaAlAs/InGaAlAs/InP
     5 FOR GaInP/(AlGa)0.5In0.5P/AlInP
     6 FOR InGaAs/AlGaAs/AlGaAs
     7 FOR InGaAs/InGaAsP/Ga0.51In0.49P(MATCHED GaAs)
     8 FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
     9 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/InP
    10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(matched InP)
    11 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/AlAsxSb1-x
    12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs (dilute N)
    13 FOR In(1-x)Ga(x)As(y)P(1-y)/GaAs
    14 FOR EXIT, BACK TO MAIN PAGE!
14
 THIS PROGRAM STOP HERE!, BACK TO MAIN PAGE
```

c) The output files, cbandeg.dat and vbandeg.dat are explained in Table C.2.3.

Table C.2.3. Material compositions and band offsets:

a) cbandeg.dat for conduction band

```
*************************************************************************
 QW strain   lattice constant
-.120000E-01  0.593923E-09
                          material compositions
   layer thickness,          Ga              Al      conduction band edges
   0.10000000E+03  0.50731155E-01   0.1116804   0.1763546      cladding layer
   0.50000000E+02  0.25335652E+00   0.5501187   0.0606978      SCH layer
   0.60000000E+02  0.10405969E+00   0.5965452   0.0481108      quantum well
   0.50000000E+02  0.25335652E+00   0.5501187   0.0606978      SCH layer
   0.10000000E+03  0.50731155E-01   0.1116804   0.1763546      cladding layer
*************************************************************************
```

b) vbandeg.dat for valence band

```
*************************************************** *********************
 QW strain   lattice constant
-.120000E-01  0.593923E-09
                          material compositions
  layer thickness,          Ga              Al      valence band edges
   0.10000000E+03  0.50731155E-01   0.1116804   -0.2758368      cladding layer
   0.50000000E+02  0.25335652E+00   0.5501187   -0.0949375      SCH layer
   0.60000000E+02  0.10405969E+00   0.5965452   -0.0240554      quantum well
   0.50000000E+02  0.25335652E+00   0.5501187   -0.0949375      SCH layer
   0.10000000E+03  0.50731155E-01   0.1116804   -0.2758368      cladding layer
*************************************************************************
```

C.2.2. Energy level calculations

After the calculation of the material compositions and energy band edges, the GAIN program calculates energy levels in the conduction band and valence bands. The detailed explanations are discussed in Chapter 3 of this manual.

a) The steps of how to calculate the energy levels are shown in Table C.2.4.

Table C.2.4. Steps to calculate the energy levels

i) Steps to calculate the conduction band energy levels

```
ENTER 1 FOR THE NECESSARY PARAMETERS

      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT
2
 INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
 INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
 INPUT N=
5
 INPUT THE LOWEST POTENTIAL LAYER(1st Q-WELL) IC= ?
3
 INPUT THE SELECTED CENTER LAYER OF STRUCTURE ICR=
3
 *******************************************************
  INPUT I=1  FOR AlGaAs

       I=2  FOR InGaAsP
      I=3  FOR In1-xGaxAs/InGaAsP/InP
      I=4  FOR InGaAlAs/InGaAlAs
      I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
      I=6  FOR InGaAs/AlGaAs/AlGaAs
      I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
      I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
      I=9  FOR InzGa1-zAs/AlxGayIn1-x-yAs/InP
      I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
      I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
      I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
      I=13 FOR InGaAs/In(1-y)Ga(x)As(y)P(1-y)/GaAs
  INPUT I= ?
 *******************************************************
2
 ENERGY EIGENVALUE===>  0.670294366291E-01 ERROR= .3576162E-14
 ENERGY EIGENVALUE===>  0.101465108959E+00 ERROR= .3081508E-14
 ENERGY EIGENVALUE===>  0.155412249439E+00 ERROR= .2750090E-14

 FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
 SKIP INPUT I==> 2
 I=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
0.670294366291E-01
 INPUT THE NAME OF OUTPUT FILE
```

```
cb1.txt
CONFINEMENT FACTOR OF    1 th LAYER = 0.11124994E-01
 CONFINEMENT FACTOR OF    2 th LAYER = 0.18768431E+00
 CONFINEMENT FACTOR OF    3 th LAYER = 0.60238139E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.18768431E+00
 CONFINEMENT FACTOR OF    5 th LAYER = 0.11124994E-01
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
1
  INPUT THE EIGENVALUE
  EIGEN VALUE=
0.101465108959
  INPUT THE NAME OF OUTPUT FILE
cb2.txt
CONFINEMENT FACTOR OF    1 th LAYER = 0.46526184E-01
 CONFINEMENT FACTOR OF    2 th LAYER = 0.36258718E+00
 CONFINEMENT FACTOR OF    3 th LAYER = 0.18177326E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.36258718E+00
 CONFINEMENT FACTOR OF    5 th LAYER = 0.46526184E-01
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
2
```

ii) Steps to calculate the heavy hole energy levels

```
 ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND

      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT
3
  INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
  INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
  INPUT N=
5
  INPUT THE HIGHEST POTENTIAL(1st Q-WELL) LAYER IC= ?
3
  INPUT THE SELECTED CENTER OF THE STRUCTURE ICR=?
3
 ******************************************************
   INPUT I=1  FOR AlGaAs
       I=2  FOR InGaAsP
       I=3  FOR In(1-x)Ga(x)As/InGaAsP/InP
       I=4  FOR InGaAlAs/InGaAlAs
       I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
       I=6  FOR InGaAs/AlGaAs/AlGaAs
       I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
       I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
       I=9  FOR In(z)Ga(1-z)As/AlxGayIn1-x-yAs/InP
       I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
       I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
       I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
```

```
      I=13 FOR InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
  INPUT I= ?
 ********************************************************
2
 ********************************************************

  DOES THE STRUCTURE STRAIN OR STRAIN-COMPENSATED?
  IF STRAIN ONLY INPUT 1, STRAIN-COMPENSATED INPUT 2
  INPUT SELECT = ?
1
  ENERGY EIGENVALUE===> -0.266289655713E+00 ERROR= .2082626E-14
  ENERGY EIGENVALUE===> -0.220090610686E+00 ERROR= .2912430E-14
  ENERGY EIGENVALUE===> -0.186287733747E+00 ERROR= .4671376E-14
  ENERGY EIGENVALUE===> -0.140850401092E+00 ERROR= .8911599E-14
  ENERGY EIGENVALUE===> -0.122228608502E+00 ERROR= .4338441E-14
  ENERGY EIGENVALUE===> -0.101432618035E+00 ERROR= .1307382E-14
  ENERGY EIGENVALUE===> -0.428488013474E-01 ERROR= .2038714E-14
  ENERGY EIGENVALUE===>  0.509274076994E-02 ERROR= .2348418E-14

  FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
  SKIP INPUT I==> 2
  I=?
1
  INPUT THE EIGENVALUE
  EIGEN VALUE=
0.509274076994E-02
  INPUT THE NAME OF OUTPUT FILE
hh1.txt
CONFINEMENT FACTOR OF    1 th LAYER = 0.43858757E-06
 CONFINEMENT FACTOR OF    2 th LAYER = 0.19049653E-01
 CONFINEMENT FACTOR OF    3 th LAYER = 0.96189982E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.19049653E-01
 CONFINEMENT FACTOR OF    5 th LAYER = 0.43858757E-06
  SELECT=?
1
  INPUT THE EIGENVALUE
  EIGEN VALUE=
-0.428488013474E-01
  INPUT THE NAME OF OUTPUT FILE
hh2.txt
CONFINEMENT FACTOR OF    1 th LAYER = 0.18387626E-04
 CONFINEMENT FACTOR OF    2 th LAYER = 0.90457734E-01
 CONFINEMENT FACTOR OF    3 th LAYER = 0.81904776E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.90457734E-01
 CONFINEMENT FACTOR OF    5 th LAYER = 0.18387626E-04
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
2
```

iii) Steps to calculate the light hole energy levels

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND

      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
```

```
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT
4
 INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
 INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
 INPUT N=
5
 INPUT THE HIGHEST POTENTIAL(1st Q-WELL) LAYER IC= ?
3
 INPUT THE SELECTED CENTER OF THE STRUCTURE ICR=?
3
 *******************************************************
  INPUT I=1  FOR AlGaAs

       I=2  FOR InGaAsP
      I=3  FOR In(1-x)Ga(x)As/InGaAsP/InP
      I=4  FOR InGaAlAs/InGaAlAs
      I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
      I=6  FOR InGaAs/AlGaAs/AlGaAs
      I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
      I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
      I=9  FOR In(z)Ga(1-z)As/AlxGayIn1-x-yAs/InP
      I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
      I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
      I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
      I=13 FOR InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
  INPUT I= ?
 *******************************************************
2
 *******************************************************

  DOES THE STRUCTURE STRAIN OR STRAIN-COMPENSATED?
  IF STRAIN ONLY INPUT 1, STRAIN-COMPENSATED INPUT 2
  INPUT SELECT = ?
1
  ENERGY EIGENVALUE===> -0.235564886491E+00 ERROR= .4251760E-14
  ENERGY EIGENVALUE===> -0.159589791816E+00 ERROR= .2633269E-14
  ENERGY EIGENVALUE===> -0.968705335737E-01 ERROR= .1268730E-14

  FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
  SKIP INPUT I==> 2
  I=?
1
  INPUT THE EIGENVALUE
  EIGEN VALUE=
-0.968705335737E-01
  INPUT THE NAME OF OUTPUT FILE
lh1.txt
CONFINEMENT FACTOR OF    1 th LAYER = 0.83034669E-02
 CONFINEMENT FACTOR OF    2 th LAYER = 0.20626333E+00
 CONFINEMENT FACTOR OF    3 th LAYER = 0.57086641E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.20626333E+00
 CONFINEMENT FACTOR OF    5 th LAYER = 0.83034669E-02
```

```
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
-0.159589791816E+00
 INPUT THE NAME OF OUTPUT FILE
lh2.txt
CONFINEMENT FACTOR OF    1 th LAYER = 0.44635531E-01
 CONFINEMENT FACTOR OF    2 th LAYER = 0.39731088E+00
 CONFINEMENT FACTOR OF    3 th LAYER = 0.11610718E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.39731088E+00
 CONFINEMENT FACTOR OF    5 th LAYER = 0.44635531E-01
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
2
```

b) The main output file from this part of GAIN program is energy.dat, containing all the energy levels as shown in Table C.2.5. After the energy eigen values are calculated, the GAIN program asks the user whether he would like to check the wave envelope function or not. We suggest that the user check the wave envelope functions of the first and second energy levels for conduction and valence bands. The plots of the envelope functions are shown in Fig. C.2.2, Fig. C.2.3, Fig C.2.4.

Table C.2.5 Output file energy.dat

```
 CONDUCTION BAND ENERGY===>  0.670294366291E-01 ERROR= .3576162E-14

 CONDUCTION BAND ENERGY===>  0.101465108959E+00 ERROR= .3081508E-14

 CONDUCTION BAND ENERGY===>  0.155412249439E+00 ERROR= .2750090E-14

 HEAVY HOLE ENERGY===> -0.266289655713E+00 ERROR= .2082626E-14

 HEAVY HOLE ENERGY===> -0.220090610686E+00 ERROR= .2912430E-14

 HEAVY HOLE ENERGY===> -0.186287733747E+00 ERROR= .4671376E-14

 HEAVY HOLE ENERGY===> -0.140850401092E+00 ERROR= .8911599E-14

 HEAVY HOLE ENERGY===> -0.122228608502E+00 ERROR= .4338441E-14

 HEAVY HOLE ENERGY===> -0.101432618035E+00 ERROR= .1307382E-14

 HEAVY HOLE ENERGY===> -0.428488013474E-01 ERROR= .2038714E-14

 HEAVY HOLE ENERGY===>  0.509274076994E-02 ERROR= .2348418E-14

 LIGHT HOLE ENERGY===> -0.235564886491E+00 ERROR= .4251760E-14

 LIGHT HOLE ENERGY===> -0.159589791816E+00 ERROR= .2633269E-14

 LIGHT HOLE ENERGY===> -0.968705335737E-01 ERROR= .1268730E-14
```

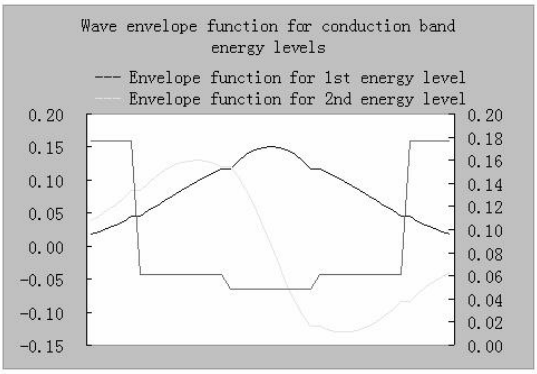

Fig. C.2.2. Wave envelop functions for energy levels in conduction band

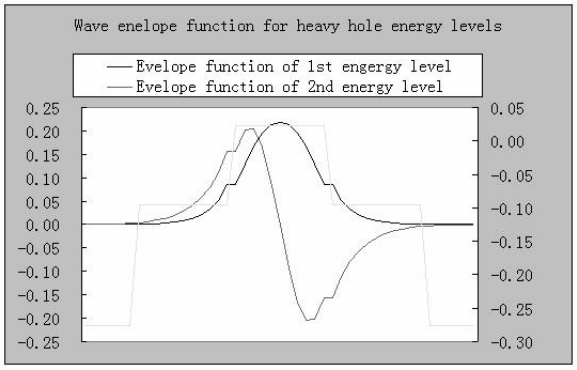

Fig. C.2.3. Wave envelope functions for heavy hole energy levels. There is some rounding error with plot

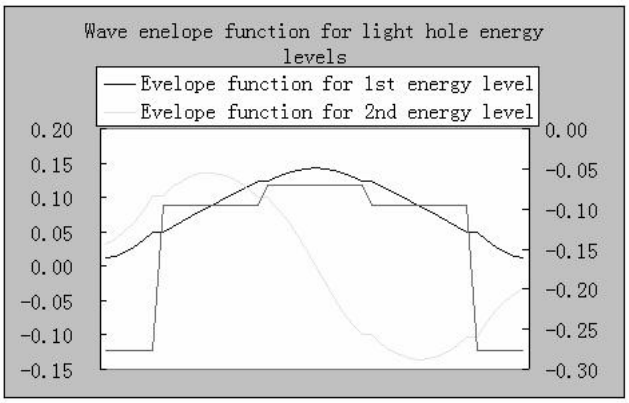

Fig. C.2.4. Wave envelope functions for light hole energy levels

C.2.3 Computation of Gain and Laser Characteristics

This is the last step of simulations using the GAIN program. With the previous calculated material composition, energy band edges, energy levels, and other parameters like material loss and Auger coefficient, the GAIN program can simulate the threshold current, threshold current density, slope efficiency, optical gain and mode gain as functions of wavelengths and photon energies, and L-I curve. The details are explained in Chapter 4 of the manual.

In this part of GAIN program, the input file needs to be constructed with the results of the previous steps and according to the laser design. In this example, single quantum well structure is used to simulate a three-QW laser. For the three-quantum-well laser with a ridge length of 750 μm and ridge width of 3 μm, the input file is shown in Table C.2.6. The detailed steps of simulations are listed in Table C.2.7. The main output files: L-I curve, optical gain as a function of the wavelength, and mode gain vs. current density are plotted in Fig. C.2.5, Fig. C.2.6, and Fig. C.2.7.

a) The input file:

Table C.2.6. Input file for gain and threshold current calculation

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c    1. Input the compositions, width of well, effective index       c
c      and lasing wavelength.                                        c
c    Ex: xx,xz,qy,xy,lx,n,lam                                        c
c    for different materials the following are the forms of inputs.  c
c                                                                    c
c    w -- > well, b -- > barrier  cxz and cxy for cladding.          c
c                                                                    c
c    a.  AlxGa1-xAs : xx (Al w) xz (Al b) qy (0) xy (0)              c
c    b.  In1-xGaxAsyP1-y : xx (Ga w) xz (Ga b) qy (As w) xy (As b)   c
c    c.  In1-xGaxAs/InGaAsP : xx (Ga w) xz (Ga b) qy (0) xy (As b)   c
c    d.  AlxGayIn1-x-yAs/InP : xx (Ga w) xz (Ga b) qy (Al w) xy (Al b)c
c    e.                                                              c
c    f.  InxGa1-xAs/AlGaAs : xx (In w) xz (0) qy (0) xy (Al b)       c
c    g.                                                              c
c    h.  AlyInxGa1-x-yAs/AlGaAs : xx (Al w) xz (al b) qy (In w) xz (0)c
c    i.  In1-xGaxAs/AlGaInAs : xx (In w) xz (0) qy (Al b) xy (Ga b)  c
c    j.  In(y)Ga(1-y)As(x)N(1-x) :xx(As w),xz(As, b),qy(In w),xy(In b)c
c    k.  InGaAs/InGaAsP/GaAs: xx (In w), (0), xz(Ga w) xy (As b)
c    2. Input the energy gap,temperature, barrier band edges(both bands)
c    Ex: eg,temp,ec,ev                                               c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
0.10405969 0.25335652 0.5965452 0.5501187 6.0 3.348741 1.31
0.94656 298 0.0606978  0.0949375
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c    3. Input the ist level sub-band energy levels.                  c
c    Ex: ec1,eh1,el1                                                 c
c                                                                    c
```

```
c     4. Input the material loss, reflectivities, number of quantum     c
c        wells and beta(for spontaneous emission).                      c
c     Ex: alpha,r1,r2,mm,beta.                                          c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
0.0670294366291  -0.509274076994E-02  0.096870533574  0.101465108959   0.0428488013474
0.159589791816
12.0d0  0.30   0.30   1  5.D-5
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c     5. Input the cavity length, ridge width, internal efficiency      c
c        Auger, strain(except AlGaAs,put 0) and confinement factor.     c
c     Ex: cl,cw,etha,ca,es,confine                                      c
c                                                                       c
c     6. Input the cladding composition and band edges.                 c
c     Ex: cxz,cxy,ecc,evv                                               c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
750.D-4  3D-4  0.96  1.00d-29   0.000  0.009834488
0.050731155     0.1116804   0.1763546 0.2758368
```

b) The steps for these calculations mentioned are listed in Table C.2.7

Table C.2.7. The steps for the gain and threshold current density calculations

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

5
  THE INPUT FILE NAME=
in1.tex
  SELECT MATERIAL=?
  1--AlGaAs
  2--InGaAsP
  3--In1-zGazAs/InGaAsP/InP
  4-- InGaAlAs
  5--GaInP/AlzGawIn1-z-wP/Al0.5In0.5P
  6-- InxGa1-xAs/AlxGa1-xAs/AlGaAs
  7--In1-xGaxAs/InGaAsP/GaxIn1-xP(X=0.51) MATCHED TO GaAs
  8--AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
  9--InzGa1-zAs/AlxGayIn1-x-yAs/InP
  10-- InGaAlAs/InGaAlAs/AlAsSb
  11--InzGa1-zAs/AlxGayIn1-x-yAs/AlAsSb
  12--In(y)Ga(1-y)As(x)N(1-x)/GaAs
  13--InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
  INPUT SELECTION
2
 INPUT MODE = ? FOR TE--> MODE =1, FOR TM--> MODE =2
  INPUT TE OR TM ?
1
 IF EL1 BELOW EH1 THEN SELECT 1, OTHERWISE SELECT 2
  SELECTION=?
1
  ************************************************
```

```
 CALCULATE THE EFFECTIVE MASS
  ************************************************
  FOR QUASI-FERMI LEVEL SELECT=1,
  FOR READ EXISTING QUASI-FERMI LEVEL SELECT=2
  SELECT=?
1

 J(LEAKAGE)=0.522156D-01 A/cm^2  N=0.328772D+19 1/cm^3
 J(LEAKAGE)=0.544163D-01 A/cm^2  N=0.330752D+19 1/cm^3
 J(LEAKAGE)=0.567097D-01 A/cm^2  N=0.332732D+19 1/cm^3
 J(LEAKAGE)=0.590996D-01 A/cm^2  N=0.334712D+19 1/cm^3
…….

  J(LEAKAGE)=0.685423D+04 A/cm^2  N=0.788120D+19 1/cm^3
  J(LEAKAGE)=0.689811D+04 A/cm^2  N=0.790100D+19 1/cm^3
  J(LEAKAGE)=0.694207D+04 A/cm^2  N=0.792080D+19 1/cm^3
  J(LEAKAGE)=0.698612D+04 A/cm^2  N=0.794060D+19 1/cm^3
  J(LEAKAGE)=0.703024D+04 A/cm^2  N=0.796040D+19 1/cm^3
  J(LEAKAGE)=0.707444D+04 A/cm^2  N=0.798020D+19 1/cm^3
  J(LEAKAGE)=0.711872D+04 A/cm^2  N=0.800000D+19 1/cm^3
*****************************************************
G(J) PARAMETERS FROM SINGLE WELL
  G(J) PARAMETERS FROM SINGLE WELL
  Go=0.704410D+01 1/cm  Jo=0.147036D+03 A/cm^2

  G(N) PARAMETERS FROM SINGLE WELL
  NGo=0.716265D+03 1/cm  XNo=0.126817D+19 1/cm^3

  Jtr=0.540917D+02 A/cm^2  NTR=0.466534D+18 1/cm^3

  THE OPTIMUM NUMBER OF QUANTUM WELL FOLLOWS THE ARTICLE
  BY McIlory et al. IEEE JQE-21 1985.

  THE OPTIMUM NUMBER OF QUANTUM WELL Nopt =          4
  INPUT Nopt(CAN BE DIFFERENT FROM ABOVE CALCULATION)=?
4
  NUMBER OF QUANTUM WELL(MAY OR MAY NOT BE Nopt)=?
4

    ************************************************
  ************************************************
  1ST CHECK USE SINGLE WELL TIMES # OF WELLS
  ************************************************
  ************************************************
  2ND CHECK FOLLOWS FORMULA BY McIlory IN IEEE
  JOURNAL OF QUANTUM ELECTRONIC QE-21 1985.
  ************************************************
  Gth=  28.0530 1/cm Nth=0.629724D+19 1/cm^3 IY=  314
   1ST CHECK Jth=  5406.36686808 A/cm^2
   2ND CHECK Jth=   612.65148 A/cm^2

   1ST CHECK Ith=0.121643D+03 mA NUMBER OF WELLS=  4
   2ND CHECK Ith=0.137847D+02 mA

  ************************************************
 CALCULATE THE P-I RELATION
```

```
 NDATA=         87
  ************************************************
  CALCULATE THE SLOPE: mW/mA Y=A+BX
  CONSTANT A= -32.6181898   SLOPE B=   0.2681463

  ************************************************
  INPUT POWER PO FOR THE LINEWIDTH, PO=0 FOR STOP
  INPUT PO=    mW
0
 INPUT 1 FOR THE DYNAMIC CALCULATION. 2 FOR SKIP
 INPUT =
2
  K-FACTOR= 0.58163 nS  MAXIUM FREQ.= 15.2773 GHz

  ************************************************
  INPUT 1 FOR CALCULATE THE GAIN(E) RELATION.

  INPUT 2 FOR CALCULATE THE LINEWIDTH ENHENCEMENT
  FACTOR AND PHOTONN ENERGY RELATION

  INPUT 3 FOR EXIT THE PROGRAM

 THE INPUT # IS
1
 INPUT FERMILEVELS IN C-BAND, V-BAND, AND CARRIER DENSITY
0.117426601301  -0.161989946432E-01 0.209974937343E+19
 CALCULATE THE CONVOLUTION GAIN(E) COEFFICIENT
  ************************************************
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(LAMBDA)
ol1.txt
  ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(LAMBDA)
ml1.txt
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(E)
oe1.txt
  ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(E)
me1.txt
  ************************************************
 INPUT 1 FOR REPEAT THE G(E) CALCULATION
 INPUT 2 FOR REPEAT THE ALPHA(E) CALCULATION
 INPUT 3 FOR EXIT
1
  ************************************************
  INPUT 1 FOR CALCULATE THE GAIN(E) RELATION.

  INPUT 2 FOR CALCULATE THE LINEWIDTH ENHENCEMENT
  FACTOR AND PHOTONN ENERGY RELATION

  INPUT 3 FOR EXIT THE PROGRAM

 THE INPUT # IS
1
 INPUT FERMILEVELS IN C-BAND, V-BAND, AND CARRIER DENSITY
0.138679340946 -0.441266076305E-02 0.301052631579E+19
```

```
 CALCULATE THE CONVOLUTION GAIN(E) COEFFICIENT
  ************************************************
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(LAMBDA)
ol2.txt
  ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(LAMBDA)
ml2.txt
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(E)
oe2.txt
  ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(E)
me2.txt
  ************************************************
 INPUT 1 FOR REPEAT THE G(E) CALCULATION
 INPUT 2 FOR REPEAT THE ALPHA(E) CALCULATION
 INPUT 3 FOR EXIT
3
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT
7
```

c) The Output characteristics of designed laser from step 5 are summarized in Table C.2.7.

Table C.2.7 Characteristics of the designed laser

Optimized number of QWs (Nopt)	4
Number of QWs	4
Slope efficiency (%)	26.8
Jth (A/cm^2)	5406.4 - 1st check, for matching threshold conditions 612.7 – 2nd check, using McIlory method
Ith (mA)	121 mA - 1st check, for matching threshold conditions 13.7 mA - 2nd check, using McIlory method
Peak λ at operating temperature (um)	1.21 um for carrier density of 2.0E19 /cm3 1.18 um for carrier density of 3.0E19 /cm3
Peak material gain (1/cm)	2362 /cm for carrier density of 2.0E19 /cm3 3360 /cm for carrier density of 3.0E19 /cm3

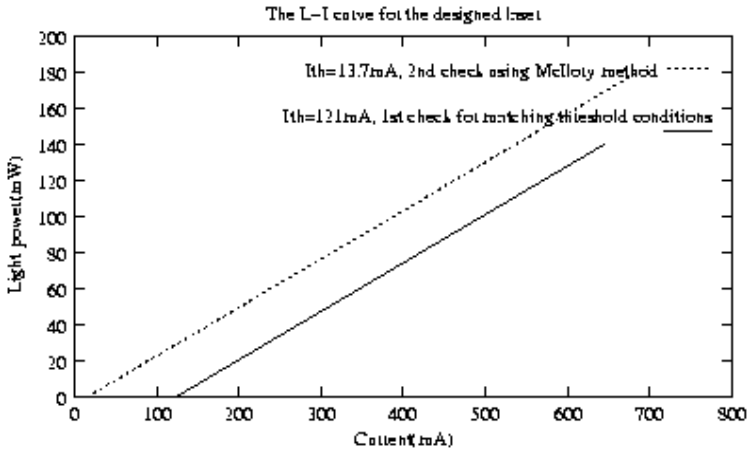

Fig. C.2.5. L-I curve of the laser

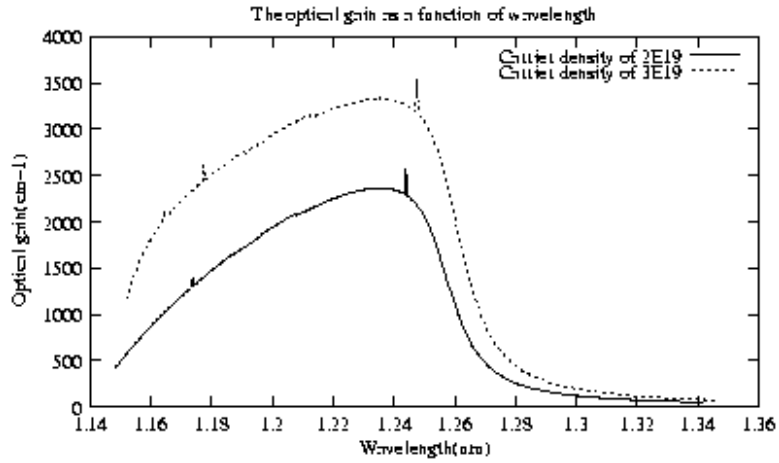

Fig. C.2.6. Optical gain-λ curve of the laser

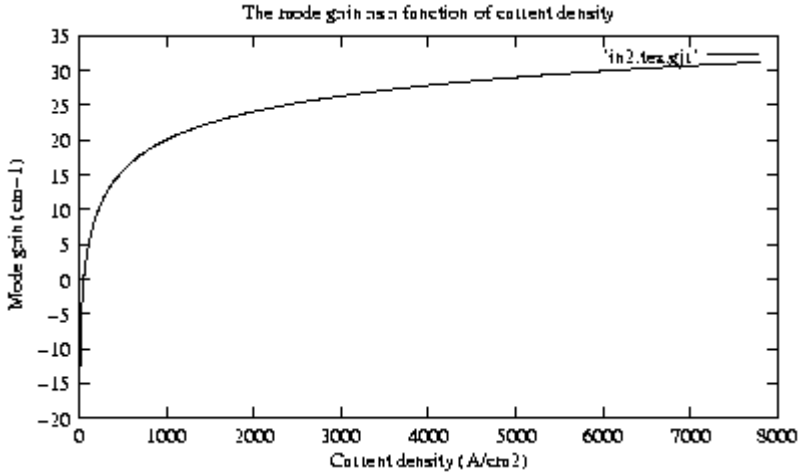

Fig. C.2.7. Mode gain as a function of current density (J)

C.3. Material system #3: InGaAs/InGaAsP/InP

This is a simulation of a five-layer laser structure that contains a single quantum well (QW), two separated confinement heterostructure (SCH) layers, and two cladding layers as shown in Fig. C.3.1.

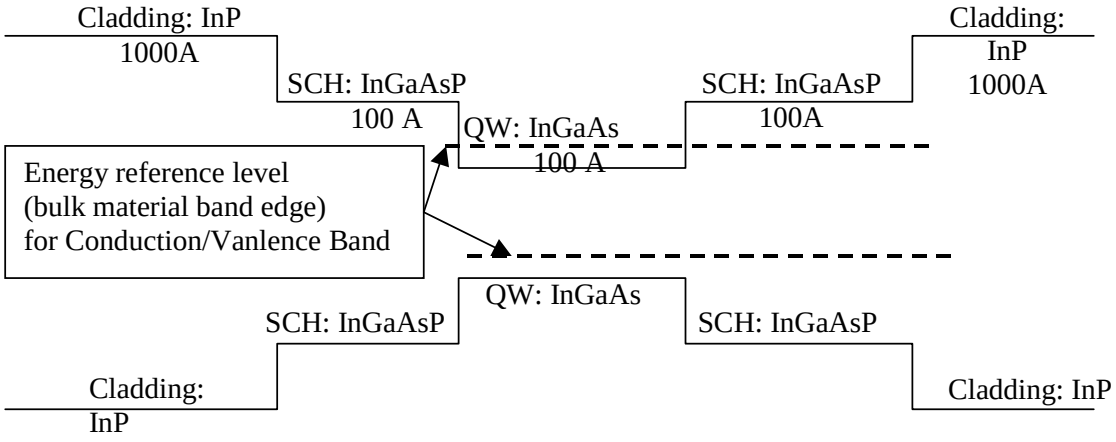

Figure C.3.3. Energy band diagram for the simple quantum well structure

C.3.1. Calculation of material compositions and energy band edges.

The first step of the GAIN program is to calculate the material compositions and energy band edges of the each layer. The user is asked to enter the photoluminescence wavelength, thickness, and strain of the QW, SCH, and cladding layers. After these parameters are input, the GAIN program generates two output files: cbandeg.dat and vbandeg.dat, containing the material compositions, and the conduction band edges and valence band edges respectively. The detailed explanation is provided in Chapter 2 of this manual.

a) The input parameters to the GAIN program in this step is listed in Table. C.3.1.

Table C.3.1. Input parameters to the GAIN program in this step.

Layer	λ (um)	Strain	Thickness (Å)
QW (InGaAs)	1.56	0.003507	100
SCH ($In_{1-x}Ga_xAs_yP_{1-y}$)	1.21	0	100
Cladding (InP)	0.9185		1000

b) The steps in using the GAIN program to calculate the material compositions and energy band edges are listed in Table C.3.2

Table C.3.2. steps to run the GAIN program for necessary parameters.

ENTER 1 **FOR THE NECESSARY PARAMETERS**
2 FOR THE ENERGY VALUES OF CONDUCTION BAND

```
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

1

 ENTER 1 FOR AlGaAs/AlGaAs
      2 FOR InGaAsP/InGaAsP/InP
      3 FOR InGaAs/InGaAsP/InP
      4 FOR InGaAlAs/InGaAlAs/InP
      5 FOR GaInP/(AlGa)0.5In0.5P/AlInP
      6 FOR InGaAs/AlGaAs/AlGaAs
      7 FOR InGaAs/InGaAsP/Ga0.51In0.49P(MATCHED GaAs)
      8 FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
      9 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/InP
     10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(matched InP)
     11 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/AlAsxSb1-x
     12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs (dilute N)
     13 FOR In(1-x)Ga(x)As(y)P(1-y)/GaAs
     14 FOR EXIT, BACK TO MAIN PAGE!
3
 INPUT THE LAYER # FOR GRIN STRUCTURE(STEP)
 STEP N=
2
  INPUT THE WELL WAVELENGTH (um)
1.56
  INPUT THE BARRIER WAVELENGTH (um)
1.21
  INPUT THE CLADDING WAVELENGTH (um)
0.9185
  BANDGAP ENERGY OF QUANTUM WELL=   0.79487179
  INPUT CLADDING, BARRIER,QUANTUM WELL WIDTH (A)
1000 100 100

  FOR BARRIER IS LATTICE MATCHED SELECT ==>1
  FOR BARRIER IS STRAIN COMPENSATED SELECT ==> 2

  SELECTION IS ===> ?
1

STRAIN FOR In1-xGaxAs= 3.507367375368143E-003

  WRITE CONDUCION BAND PARAMETERS INTO CBANDEG.DAT

  WRITE VALENCE BAND PARAMETERS INTO VBANDEG.DAT
  INPUT 1 FOR NEW CALCULATION,   2 FOR EXIT
  I =?
2

 ENTER 1 FOR AlGaAs/AlGaAs
      2 FOR InGaAsP/InGaAsP/InP
      3 FOR InGaAs/InGaAsP/InP
      4 FOR InGaAlAs/InGaAlAs/InP
      5 FOR GaInP/(AlGa)0.5In0.5P/AlInP
```

```
      6 FOR InGaAs/AlGaAs/AlGaAs
      7 FOR InGaAs/InGaAsP/Ga0.51In0.49P(MATCHED GaAs)
      8 FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
      9 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/InP
     10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(matched InP)
     11 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/AlAsxSb1-x
     12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs (dilute N)
     13 FOR In(1-x)Ga(x)As(y)P(1-y)/GaAs
     14 FOR EXIT, BACK TO MAIN PAGE!
14
 THIS PROGRAM STOP HERE!, BACK TO MAIN PAGE
```

c) The output files, cbandeg.dat and vbandeg.dat are explained in Table C.3.3.

Table C.3.3. Material compositions and band offsets:

a) cbandeg.dat for conduction band

```
**************************************************************************
 QW strain   lattice constant
0.350737E-02 0.584822E-09
                          material compositions
 layer thickness,          Ga              As      conduction band edges
 0.10000000E+04  0.00000000E+00   0.0000000   0.1998462      cladding layer
  0.10000000E+03  0.21142234E+00   0.4603684   0.0827718      SCH layer
  0.10000000E+03  0.51884522E+00   0.0000000  -0.0190298      quantum well
  0.10000000E+03  0.21142234E+00   0.4603684   0.0827718      SCH layer
  0.10000000E+04  0.00000000E+00   0.0000000   0.1998462      cladding layer
**************************************************************************
```

b) vbandeg.dat for valence band

```
************************************************** **********************
 QW strain   lattice constant
 0.350737E-02  0.584822E-09
                          material compositions
 layer thickness,          Ga              As      valence band edges
  0.10000000E+04  0.00000000E+00   0.0000000  -0.3552821      cladding layer
  0.10000000E+03  0.21142234E+00   0.4603684  -0.1471498      SCH layer
  0.10000000E+03  0.51884522E+00   0.0000000   0.0095149      quantum well
  0.10000000E+03  0.21142234E+00   0.4603684  -0.1471498      SCH layer
  0.10000000E+04  0.00000000E+00   0.0000000  -0.3552821      cladding layer
**************************************************************************
```

C.3.2. Energy level calculations

After the calculation of the material compositions and energy band edges, the GAIN program calculates energy levels in the conduction band and valence bands. The detailed explanations are discussed in Chapter 3 of this manual.

a) The steps of how to calculate the energy levels are shown in Table C.3.4.

Table C.3.4. Steps to calculate the energy levels

i) Steps to calculate the conduction band energy levels

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

2
 INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
 INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
 INPUT N=
5
 INPUT THE LOWEST POTENTIAL LAYER(1st Q-WELL) IC= ?
3
 INPUT THE SELECTED CENTER LAYER OF STRUCTURE ICR=
3
 ******************************************************
  INPUT I=1  FOR AlGaAs
       I=2  FOR InGaAsP
       I=3  FOR In1-xGaxAs/InGaAsP/InP
       I=4  FOR InGaAlAs/InGaAlAs
       I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
       I=6  FOR InGaAs/AlGaAs/AlGaAs
       I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
       I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
       I=9  FOR InzGa1-zAs/AlxGayIn1-x-yAs/InP
       I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
       I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
       I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
       I=13 FOR InGaAs/In(1-y)Ga(x)As(y)P(1-y)/GaAs
  INPUT I= ?
 ******************************************************
3
 ENERGY EIGENVALUE===>  0.102677331562E-01 ERROR= .4838213E-14
 ENERGY EIGENVALUE===>  0.829312203346E-01 ERROR= .3134953E-14
 ENERGY EIGENVALUE===>  0.116110587122E+00 ERROR= .1700480E-14
 ENERGY EIGENVALUE===>  0.137409592564E+00 ERROR= .2887171E-14
 ENERGY EIGENVALUE===>  0.193078448219E+00 ERROR= .2186428E-14

 FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
 SKIP INPUT I==> 2
 I=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
0.0102677331562

 INPUT THE NAME OF OUTPUT FILE
cb1.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.23125143E-04
 CONFINEMENT FACTOR OF    2 th LAYER = 0.60295889E-01
 CONFINEMENT FACTOR OF    3 th LAYER = 0.87936197E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.60295889E-01
```

```
 CONFINEMENT FACTOR OF    5 th LAYER = 0.23125143E-04
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
1
  INPUT THE EIGENVALUE
  EIGEN VALUE=
0.0829312203346
  INPUT THE NAME OF OUTPUT FILE
cb2.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.30920015E-02
 CONFINEMENT FACTOR OF    2 th LAYER = 0.29765260E+00
 CONFINEMENT FACTOR OF    3 th LAYER = 0.39851080E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.29765260E+00
 CONFINEMENT FACTOR OF    5 th LAYER = 0.30920015E-02
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
2
```

ii) Steps to calculate the heavy hole energy levels

```
 ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT
3
  INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
  INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
  INPUT N=
5
  INPUT THE HIGHEST POTENTIAL(1st Q-WELL) LAYER IC= ?
3
  INPUT THE SELECTED CENTER OF THE STRUCTURE ICR=?
3
 ********************************************************
   INPUT I=1  FOR AlGaAs
        I=2  FOR InGaAsP
        I=3  FOR In(1-x)Ga(x)As/InGaAsP/InP
        I=4  FOR InGaAlAs/InGaAlAs
        I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
        I=6  FOR InGaAs/AlGaAs/AlGaAs
        I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
        I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
        I=9  FOR In(z)Ga(1-z)As/AlxGayIn1-x-yAs/InP
        I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
        I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
        I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
        I=13 FOR InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
   INPUT I= ?
 ********************************************************
3
 ********************************************************

  DOES THE STRUCTURE STRAIN OR STRAIN-COMPENSATED?
```

```
 IF STRAIN ONLY INPUT 1, STRAIN-COMPENSATED INPUT 2
 INPUT SELECT = ?

1

 ENERGY EIGENVALUE===> -0.345448893969E+00 ERROR= .5479616E-14
 ENERGY EIGENVALUE===> -0.313421614966E+00 ERROR= .4977968E-14
 ENERGY EIGENVALUE===> -0.286023116439E+00 ERROR= .3741431E-14
 ENERGY EIGENVALUE===> -0.265617316582E+00 ERROR= .4216452E-14
 ENERGY EIGENVALUE===> -0.234960966106E+00 ERROR= .1892574E-14
 ENERGY EIGENVALUE===> -0.220233112417E+00 ERROR= .3492980E-14
 ENERGY EIGENVALUE===> -0.198687987806E+00 ERROR= .2194434E-14
 ENERGY EIGENVALUE===> -0.182167124769E+00 ERROR= .5669799E-14
 ENERGY EIGENVALUE===> -0.173478187551E+00 ERROR= .3761173E-14
 ENERGY EIGENVALUE===> -0.156637644140E+00 ERROR= .4590558E-14
 ENERGY EIGENVALUE===> -0.154444131718E+00 ERROR= .2538691E-14
 ENERGY EIGENVALUE===> -0.127480216412E+00 ERROR= .2519639E-14
 ENERGY EIGENVALUE===> -0.758643937665E-01 ERROR= .2498963E-14
 ENERGY EIGENVALUE===> -0.356919987894E-01 ERROR= .2709770E-14
 ENERGY EIGENVALUE===> -0.109370594171E-01 ERROR= .2119172E-14

 FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
 SKIP INPUT I==> 2
 I=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
-0.0109370594171
 INPUT THE NAME OF OUTPUT FILE
hh1.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.18195603E-12
 CONFINEMENT FACTOR OF    2 th LAYER = 0.48861990E-02
 CONFINEMENT FACTOR OF    3 th LAYER = 0.99022760E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.48861990E-02
 CONFINEMENT FACTOR OF    5 th LAYER = 0.18195603E-12
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
-0.0356919987894
 INPUT THE NAME OF OUTPUT FILE
hh2.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.60477885E-11
 CONFINEMENT FACTOR OF    2 th LAYER = 0.20535375E-01
 CONFINEMENT FACTOR OF    3 th LAYER = 0.95892925E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.20535375E-01
 CONFINEMENT FACTOR OF    5 th LAYER = 0.60477885E-11
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
2
```

iii) Steps to calculate the light hole energy levels

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
```

```
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

4
 INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
 INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
 INPUT N=
5
 INPUT THE HIGHEST POTENTIAL(1st Q-WELL) LAYER IC= ?
3
 INPUT THE SELECTED CENTER OF THE STRUCTURE ICR=?
3
 ********************************************************
  INPUT I=1  FOR AlGaAs
       I=2  FOR InGaAsP
       I=3  FOR In(1-x)Ga(x)As/InGaAsP/InP
       I=4  FOR InGaAlAs/InGaAlAs
       I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
       I=6  FOR InGaAs/AlGaAs/AlGaAs
       I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
       I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
       I=9  FOR In(z)Ga(1-z)As/AlxGayIn1-x-yAs/InP
       I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
       I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
       I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
       I=13 FOR InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
  INPUT I= ?
 ********************************************************
3
 ********************************************************

 DOES THE STRUCTURE STRAIN OR STRAIN-COMPENSATED?
 IF STRAIN ONLY INPUT 1, STRAIN-COMPENSATED INPUT 2
 INPUT SELECT = ?

1
 ENERGY EIGENVALUE===> -0.324350665429E+00 ERROR= .2529748E-14
 ENERGY EIGENVALUE===> -0.268485842580E+00 ERROR= .4118834E-14
 ENERGY EIGENVALUE===> -0.200300476894E+00 ERROR= .3413517E-14
 ENERGY EIGENVALUE===> -0.181133391050E+00 ERROR= .2018955E-14
 ENERGY EIGENVALUE===> -0.116983827560E+00 ERROR= .3183911E-14
 ENERGY EIGENVALUE===> -0.161551734944E-01 ERROR= .3222829E-14

 FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
 SKIP INPUT I==> 2
 I=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
-0.0161551734944
 INPUT THE NAME OF OUTPUT FILE
lh1.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.28197495E-05
```

```
 CONFINEMENT FACTOR OF    2 th LAYER = 0.39958233E-01
 CONFINEMENT FACTOR OF    3 th LAYER = 0.92007789E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.39958233E-01
 CONFINEMENT FACTOR OF    5 th LAYER = 0.28197495E-05
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
1
  INPUT THE EIGENVALUE
  EIGEN VALUE=
-0.116983827560
  INPUT THE NAME OF OUTPUT FILE
lh2.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.39043702E-03
 CONFINEMENT FACTOR OF    2 th LAYER = 0.19969312E+00
 CONFINEMENT FACTOR OF    3 th LAYER = 0.59983288E-01
 CONFINEMENT FACTOR OF    4 th LAYER = 0.19969312E+00
 CONFINEMENT FACTOR OF    5 th LAYER = 0.39043702E-03
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
2
```

b) The main output file from this part of GAIN program is energy.dat, containing all the energy levels as shown in Table C.3.5. After the energy eigen values are calculated, the GAIN program asks the user whether he would like to check the wave envelope function or not. We suggest that the user check the wave envelope functions of the first and second energy levels for conduction and valence bands. The plots of the envelope functions are shown in Fig. C.3.2, Fig. C.3.3, Fig C.3.4.

Table C.3.5. output file energy.dat

```
 CONDUCTION BAND ENERGY===>  0.132273196491E+00 ERROR= .1825400E-14

 CONDUCTION BAND ENERGY===>  0.338026920933E+00 ERROR= .2075989E-14

 CONDUCTION BAND ENERGY===>  0.438393858497E+00 ERROR= .1374688E-14

 CONDUCTION BAND ENERGY===>  0.500546559386E+00 ERROR= .1783885E-14

 HEAVY HOLE ENERGY===> -0.190388140560E+00 ERROR= .3376657E-14

 HEAVY HOLE ENERGY===> -0.178205351549E+00 ERROR= .2794590E-14

 HEAVY HOLE ENERGY===> -0.146868929570E+00 ERROR= .1933278E-14

 HEAVY HOLE ENERGY===> -0.649012884792E-01 ERROR= .1722105E-14

 HEAVY HOLE ENERGY===> -0.584031671619E-02 ERROR= .1782035E-14

 LIGHT HOLE ENERGY===> -0.224692198534E+00 ERROR= .5190988E-14

 LIGHT HOLE ENERGY===> -0.169366776608E+00 ERROR= .3378719E-14

 LIGHT HOLE ENERGY===> -0.978425419323E-01 ERROR= .2045359E-14
```

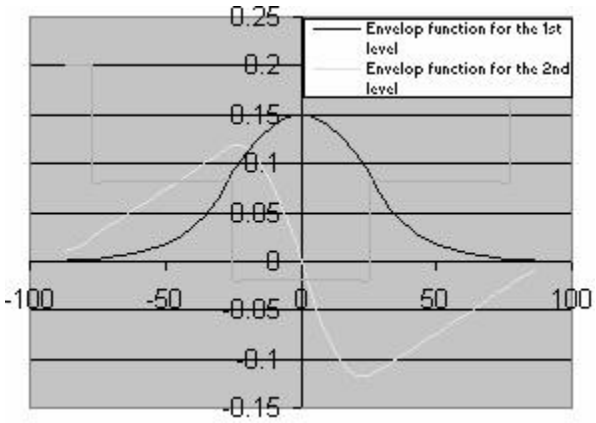

Fig. C.3.2. Wave envelop functions for energy levels in conduction band

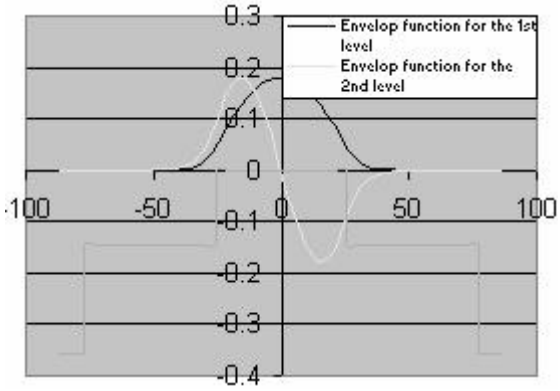

Fig. C.3.3. Wave envelop functions for heavy hole energy levels

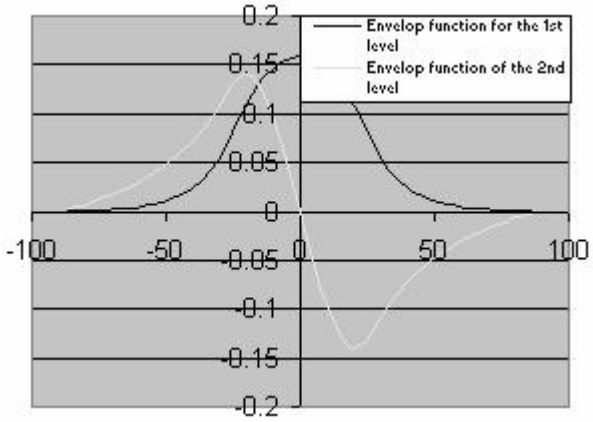

Fig. C.3.4. Wave envelop functions for light hole energy levels

C.3.3. Computation of Gain and Laser Characteristics

This is the last step of simulations using the GAIN program. With the previous calculated material composition, energy band edges, energy levels, and other parameters like material loss and Auger coefficient, the GAIN program can simulate the threshold current, threshold current density, slope efficiency, optical gain and mode gain as functions of wavelengths and photo energies, and L-I curve. The details are explained in Chapter 4 of the manual.

In this part of GAIN program, the input file needs to be constructed with the results of the previous steps and according to the laser design. In this example, a tensile single-quantum-well laser with a ridge length of 750μm and ridge width of 3 μm, the input file is shown in Table C.3.6. The detailed steps of simulations are listed in Table C.3.7. The main output files: L-I curve, optical gain as a function of the wavelength, and mode gain vs. current density are plotted in Fig. C.3.5, Fig. C.3.6, and Fig. C.3.7.

a) The input file:

Table C.3.6. Input file for gain and threshold current calculation

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c    1. Input the compositions, width of well, effective index         c
c       and lasing wavelength.                                         c
c    Ex: xx,xz,qy,xy,lx,n,lam                                          c
c    for different materials the following are the forms of inputs.    c
c                                                                      c
c    w -- > well, b -- > barrier  cxz and cxy for cladding.             c
c                                                                      c
c    a.  AlxGa1-xAs : xx (Al w) xz (Al b) qy (0) xy (0)                c
c    b.  In1-xGaxAsyP1-y : xx (Ga w) xz (Ga b) qy (As w) xy (As b)     c
c    c.  In1-xGaxAs/InGaAsP : xx (Ga w) xz (Ga b) qy (0) xy (As b)     c
c    d.  AlxGayIn1-x-yAs/InP : xx (Ga w) xz (Ga b) qy (Al w) xy (Al b)c
c    e.                                                                c
c    f.  InxGa1-xAs/AlGaAs : xx (In w) xz (0) qy (0) xy (Al b)         c
c    g.                                                                c
c    h.  AlyInxGa1-x-yAs/AlGaAs : xx (Al w) xz (al b) qy (In w) xz (0)c
c    i.  In1-xGaxAs/AlGaInAs : xx (In w) xz (0) qy (Al b) xy (Ga b)    c
c                                                                      c
c                                                                      c
c    2. Input the energy gap,temperature, barrier band edges(both bands)c
c    Ex: eg,temp,ec,ev                                                 c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
0.51884522 0.21142234 0.0 0.4603684 10.0 3.32 1.55
0.79487179 298 0.10718016 0.1566647
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c    3. Input the ist level sub-band energy levels.                    c
c    Ex: ec1,eh1,el1                                                   c
c                                                                      c
c    4. Input the material loss, reflectivities, number of quantum     c
```

```
c       wells and beta(for spontaneous emission).                    c
c     Ex: alpha,r1,r2,mm,beta.                                       c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
0.0102677331562   0.0109370594171   0.0161551734944   0.0829312203346   0.0356919987894
0.116983827560
10.0d0 0.3000 0.300 1 5.D-5
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c     5. Input the cavity length, ridge width, internal efficiency     c
c        Auger, strain(except AlGaAs,put 0) and confinement factor.    c
c     Ex: cl,cw,etha,ca,es,confine                                    c
c                                                                     c
c     6. Input the cladding composition and band edges.               c
c     Ex: cxz,cxy,ecc,evv                                             c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
500.D-4 3D-4 0.97 3.10d-29 0.0 0.018
0.00 0.00  0.218876 0.364797
```

b) The steps for these calculations mentioned are listed in Table C.3.7

Table C.3.7. The steps for the gain and threshold current density calculations

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

5
 THE INPUT FILE NAME=
in1.tex
 SELECT MATERIAL=?
 1--AlGaAs
 2--InGaAsP
 3--In1-zGazAs/InGaAsP/InP
 4-- InGaAlAs
 5--GaInP/AlzGawIn1-z-wP/Al0.5In0.5P
 6-- InxGa1-xAs/AlxGa1-xAs/AlGaAs
 7--In1-xGaxAs/InGaAsP/GaxIn1-xP(X=0.51) MATCHED TO GaAs
 8--AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
 9--InzGa1-zAs/AlxGayIn1-x-yAs/InP
 10-- InGaAlAs/InGaAlAs/AlAsSb
 11--InzGa1-zAs/AlxGayIn1-x-yAs/AlAsSb
 12--In(y)Ga(1-y)As(x)N(1-x)/GaAs
 13--InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
 INPUT SELECTION
3
 INPUT MODE = ? FOR TE--> MODE =1, FOR TM--> MODE =2
 INPUT TE OR TM ?
1
 IF EL1 BELOW EH1 THEN SELECT 1, OTHERWISE SELECT 2
 SELECTION=?
1
 ************************************************
 CALCULATE THE EFFECTIVE MASS
```

```
 ************************************************
 FOR QUASI-FERMI LEVEL SELECT=1,
 FOR READ EXISTING QUASI-FERMI LEVEL SELECT=2
 SELECT=?
1

 J(LEAKAGE)=0.104958D+03 A/cm^2  N=0.328772D+19 1/cm^3
 J(LEAKAGE)=0.108158D+03 A/cm^2  N=0.330752D+19 1/cm^3
 J(LEAKAGE)=0.111439D+03 A/cm^2  N=0.332732D+19 1/cm^3
 J(LEAKAGE)=0.114800D+03 A/cm^2  N=0.334712D+19 1/cm^3
…….
J(LEAKAGE)=0.245553D+05A/cm^2  N=0.788120D+19 1/cm^3
J(LEAKAGE)=0.246733D+05A/cm^2  N=0.790100D+19 1/cm^3
J(LEAKAGE)=0.247912D+05A/cm^2  N=0.792080D+19 1/cm^3
J(LEAKAGE)=0.249092D+05A/cm^2  N=0.794060D+19 1/cm^3
J(LEAKAGE)=0.250272D+05A/cm^2  N=0.796040D+19 1/cm^3
J(LEAKAGE)=0.251453D+05 A/cm^2  N=0.798020D+19 1/cm^3
J(LEAKAGE)=0.252633D+05 A/cm^2  N=0.800000D+19 1/cm^3
************************************************
G(J) PARAMETERS FROM SINGLE WELL
 Go=0.178866D+02 1/cm    Jo=0.967184D+02 A/cm^2

 G(N) PARAMETERS FROM SINGLE WELL
 NGo=0.993699D+03 1/cm  XNo=0.951378D+18 1/cm^3

 Jtr=0.355807D+02 A/cm^2  NTR=0.349993D+18 1/cm^3


 THE OPTIMUM NUMBER OF QUANTUM WELL FOLLOWS THE ARTICLE
 BY McIlory et al. IEEE JQE-21 1985.

 THE OPTIMUM NUMBER OF QUANTUM WELL Nopt =          2
 INPUT Nopt(CAN BE DIFFERENT FROM ABOVE CALCULATION)=?
2
 NUMBER OF QUANTUM WELL(MAY OR MAY NOT BE Nopt)=?
1

 ************************************************
 ************************************************
 1ST CHECK USE SINGLE WELL TIMES # OF WELLS
 ************************************************
 ************************************************
 2ND CHECK FOLLOWS FORMULA BY McIlory IN IEEE
 JOURNAL OF QUANTUM ELECTRONIC QE-21 1985.
 ************************************************
 Gth=  34.0795 1/cm Nth=0.174336D+19 1/cm^3 IY=   84
  1ST CHECK Jth=   472.08528249 A/cm^2
  2ND CHECK Jth=   271.03897 A/cm^2

  1ST CHECK Ith=0.708128D+01 mA NUMBER OF WELLS=  2
  2ND CHECK Ith=0.406558D+01 mA

 ************************************************
 CALCULATE THE P-I RELATION

 NDATA=        317
```

```
 ************************************************
 CALCULATE THE SLOPE: mW/mA Y=A+BX
 CONSTANT A=  -1.9085326   SLOPE B=   0.2695181

 ************************************************
 INPUT POWER PO FOR THE LINEWIDTH, PO=0 FOR STOP
 INPUT PO=    mW
0
 INPUT 1 FOR THE DYNAMIC CALCULATION. 2 FOR SKIP
 INPUT =
2
 K-FACTOR= 0.25771 nS  MAXIUM FREQ.= 34.4792 GHz

 ************************************************
 INPUT 1 FOR CALCULATE THE GAIN(E) RELATION.

 INPUT 2 FOR CALCULATE THE LINEWIDTH ENHENCEMENT
 FACTOR AND PHOTON ENERGY RELATION

 INPUT 3 FOR EXIT THE PROGRAM

 THE INPUT # IS
1
 INPUT FERMILEVELS IN C-BAND, V-BAND, AND CARRIER DENSITY
0.136951476602 0.00757985775700 0.200075187970E+19
 CALCULATE THE CONVOLUTION GAIN(E) COEFFICIENT
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(LAMBDA)
ol1.txt
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(LAMBDA)
ml1.txt
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(E)
oe1.txt
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(E)
me1.txt
 ************************************************
 INPUT 1 FOR REPEAT THE G(E) CALCULATION
 INPUT 2 FOR REPEAT THE ALPHA(E) CALCULATION
 INPUT 3 FOR EXIT
1
 ************************************************
 INPUT 1 FOR CALCULATE THE GAIN(E) RELATION.

 INPUT 2 FOR CALCULATE THE LINEWIDTH ENHENCEMENT
 FACTOR AND PHOTON ENERGY RELATION

 INPUT 3 FOR EXIT THE PROGRAM

 THE INPUT # IS
1
 INPUT FERMILEVELS IN C-BAND, V-BAND, AND CARRIER DENSITY
0.292773620684 -0.223794117473E-01 0.301052631579E+19
 CALCULATE THE CONVOLUTION GAIN(E) COEFFICIENT
 ************************************************
```

```
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(LAMBDA)
ol2.txt
  ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(LAMBDA)
ml2.txt
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(E)
oe2.txt
  ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(E)
me2.txt
  ************************************************
 INPUT 1 FOR REPEAT THE G(E) CALCULATION
 INPUT 2 FOR REPEAT THE ALPHA(E) CALCULATION
 INPUT 3 FOR EXIT
3
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

7
```

c) The Output characteristics of designed laser from step 5 are summarized in Table C.3.7.

Table C.3.7 Characteristics of the designed laser

Optimized number of QWs (Nopt)	2
Number of QWs	1
Slope efficiency (%)	26.9581
Jth (A/cm^2)	472.085- 1st check, for matching threshold conditions 271.03897 – 2nd check, using McIlory method
Ith (mA)	7.08128mA - 1st check, for matching threshold conditions 4.06558mA - 2nd check, using McIlory method
Peak λ at operating temperature (um)	1.53509 um for carrier density of 2.0E18 /cm3 1.530496 um for carrier density of 3.0E18 /cm3
Peak material gain (1/cm)	3405.979 /cm for carrier density of 2.0E18 /cm3 4379.23 /cm for carrier density of 3.0E18 /cm3

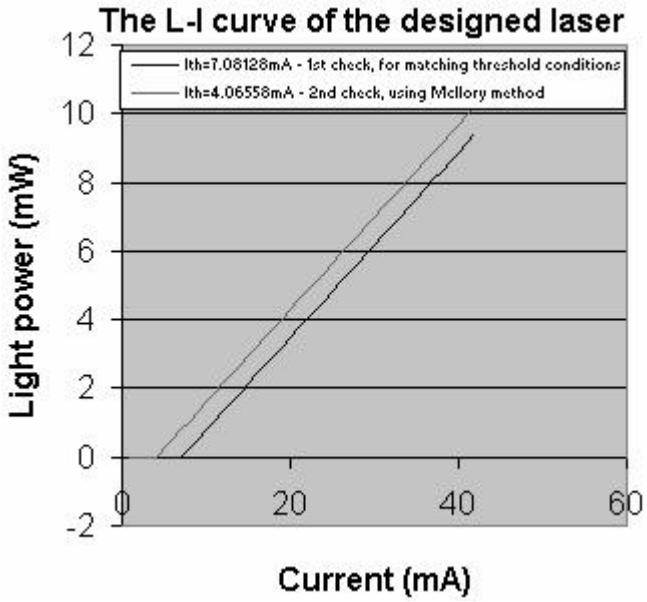

Fig. C.3.5. L-I curve of the laser

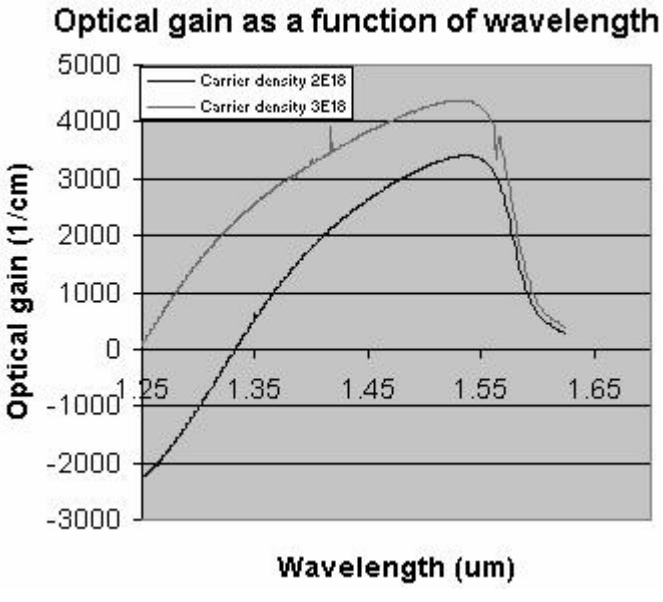

Fig. C.3.6. Optical gain-λ curve of the laser

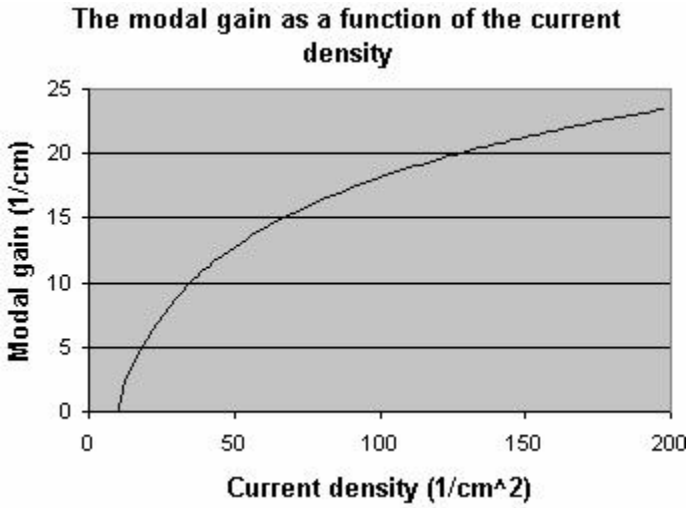

Fig. C.3.7. Mode gain as a function of current density (J)

C.4. Material system #4: InGaAlAs/InGaAlAs/InP

This is a simulation of a five-layer laser structure that contains a single quantum well (QW), two separated confinement heterostructure (SCH) layers, and two cladding layers as shown in Fig. C.4.1.

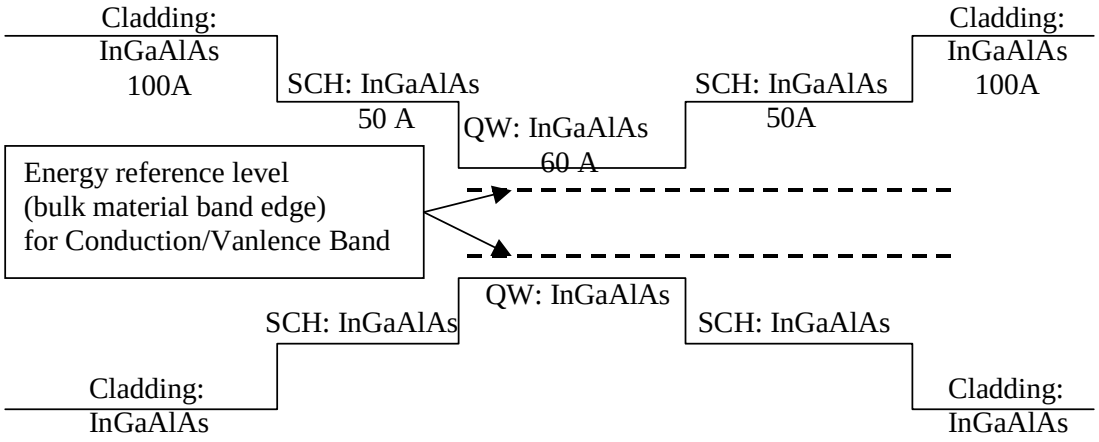

Figure C.4.4. Energy band diagram for the single quantum well structure

C.4.1. Calculation of material compositions and energy band edges.

The first step of the GAIN program is to calculate the material compositions and energy band edges of the each layer. The user is asked to enter the photoluminescence wavelength, thickness, and strain of the QW, SCH, and cladding layers. After these parameters are input, the GAIN program generates two output files: cbandeg.dat and vbandeg.dat, containing the material compositions, and the conduction band edges and valence band edges respectively. The detailed explanation is provided in Chapter 2 of this manual.

a) The input parameters to the GAIN program in this step are listed in Table. C.4.1.

Table C.4.1. Input parameters to the GAIN program in this step.

Layer	λ (um)	Strain	Thickness (Å)
QW ($Ga_xAl_yIn_{1-x-y}As$)	1.813385122	-0.011705	60
SCH ($Ga_xAl_yIn_{1-x-y}As$)	1.023516108	0.0087769	50
Cladding ($Ga_xAl_yIn_{1-x-y}As$)	0.828002068		100

b) The steps in using the GAIN program to calculate the material compositions and energy band edges are listed in Table C.4.2

Table C.4.2. steps to run the GAIN program for necessary parameters.

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

1

 ENTER 1 FOR AlGaAs/AlGaAs
      2 FOR InGaAsP/InGaAsP/InP
      3 FOR InGaAs/InGaAsP/InP
      4 FOR InGaAlAs/InGaAlAs/InP
      5 FOR GaInP/(AlGa)0.5In0.5P/AlInP
      6 FOR InGaAs/AlGaAs/AlGaAs
      7 FOR InGaAs/InGaAsP/Ga0.51In0.49P(MATCHED GaAs)
      8 FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
      9 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/InP
     10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(matched InP)
     11 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/AlAsxSb1-x
     12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs (dilute N)
     13 FOR In(1-x)Ga(x)As(y)P(1-y)/GaAs
     14 FOR EXIT, BACK TO MAIN PAGE!
4
 INPUT THE LAYER # FOR GRIN STRUCTURE(STEP)
 STEP N=
2
  INPUT THE WELL WAVELENGTH (um)
1.813385122
  INPUT THE BARRIER WAVELENGTH (um)
1.023516108
  INPUT THE CLADDING WAVELENGTH (um)
0.828002068
  BANDGAP ENERGY OF QUANTUM WELL=   0.683804000019804
  INPUT CLADDING, BARRIER,QUANTUM WELL WIDTH (A)
100 50 60

  FOR AlyGaxIn(1-x-y)As, in output read Ga first then Al

  IF ONE OF THE COMPONENTS IN ACTIVE REGION IS ZERO,
  YOU HAVE TO TRY ANOTHER INITIAL GUESS FOR
  BOTH WAVELENGTH AND STRAIN

  INPUT STRAIN
-0.011704948

  FOR Eg relation from Dr. Chuang,s book input 1,
 for Industrial experimental formula input 2

  INPUT ==--> ?
1

  FOR BARRIER IS LATTICE MATCHED SELECT ==>1
  FOR BARRIER IS STRAIN COMPENSATED SELECT ==> 2
```

```
 SELECTION IS ===> ?
2

 FOR Eg relation from Dr. Chuang,s book input 1,
for Industrial experimental formula input 2

 INPUT =--> ?
1
 INPUT STRAIN==>?
0.008776922

 WRITE CONDUCTION BAND PARAMETERS INTO CBANDEG.DAT

 WRITE VALENCE BAND PARAMETERS INTO VBANDEG.DAT
 INPUT 1 FOR NEW CALCULATION
     2 FOR EXIT
 INPUT =?
2

ENTER 1 FOR AlGaAs/AlGaAs
     2 FOR InGaAsP/InGaAsP/InP
     3 FOR InGaAs/InGaAsP/InP
     4 FOR InGaAlAs/InGaAlAs/InP
     5 FOR GaInP/(AlGa)0.5In0.5P/AlInP
     6 FOR InGaAs/AlGaAs/AlGaAs
     7 FOR InGaAs/InGaAsP/Ga0.51In0.49P(MATCHED GaAs)
     8 FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
     9 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/InP
    10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(matched InP)
    11 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/AlAsxSb1-x
    12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs (dilute N)
    13 FOR In(1-x)Ga(x)As(y)P(1-y)/GaAs
    14 FOR EXIT, BACK TO MAIN PAGE!
14
 THIS PROGRAM STOP HERE!, BACK TO MAIN PAGE
```

c) The output files, cbandeg.dat and vbandeg.dat are explained in Table C.4.3.

Table C.4.3. Material compositions and band offsets:

a) cbandeg.dat for conduction band

```
**************************************************************************
 QW strain   lattice constant
-.117049E-01  0.593758E-09
                        material compositions
 layer thickness,          Ga              Al      conduction band edges
  0.10000000E+03  0.00000000E+00  0.4829333  0.5859193     cladding layer
  0.50000000E+02  0.34879557E+00  0.2505339  0.3327401     SCH layer
  0.60000000E+02  0.21964924E+00  0.0801355  0.0538058     quantum well
  0.50000000E+02  0.34879557E+00  0.2505339  0.3327401     SCH layer
  0.10000000E+03  0.00000000E+00  0.4829333  0.5859193     cladding layer
**************************************************************************
```

b) vbandeg.dat for valence band

```
************************************************** ********************
```

```
 QW strain   lattice constant
-.117049E-01  0.593758E-09
                          material compositions
 layer thickness,          Ga              Al       valence band edges
  0.10000000E+03  0.00000000E+00  0.4829333  -0.2278575   cladding layer
  0.50000000E+02  0.34879557E+00  0.2505339  -0.1241536   SCH layer
  0.60000000E+02  0.21964924E+00  0.0801355  -0.0269029   quantum well
  0.50000000E+02  0.34879557E+00  0.2505339  -0.1241536   SCH layer
  0.10000000E+03  0.00000000E+00  0.4829333  -0.2278575   cladding layer
*************************************************************************
```

C.4.2. Energy level calculations

After the calculation of the material compositions and energy band edges, the GAIN program calculates energy levels in the conduction band and valence bands. The detailed explanations are discussed in Chapter 3 of this manual.

a) The steps of how to calculate the energy levels are shown in Table C.4.4.

Table C.4.4. Steps to calculate the energy levels

i) Steps to calculate the conduction band energy levels

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

2
 INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
 INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
 INPUT N=
5
 INPUT THE LOWEST POTENTIAL LAYER(1st Q-WELL) IC= ?
3
 INPUT THE SELECTED CENTER LAYER OF STRUCTURE ICR=
3
 ******************************************************
  INPUT I=1  FOR AlGaAs
       I=2  FOR InGaAsP
       I=3  FOR In1-xGaxAs/InGaAsP/InP
       I=4  FOR InGaAlAs/InGaAlAs
       I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
       I=6  FOR InGaAs/AlGaAs/AlGaAs
       I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
       I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
       I=9  FOR InzGa1-zAs/AlxGayIn1-x-yAs/InP
       I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
       I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
       I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
```

```
       I=13 FOR InGaAs/In(1-y)Ga(x)As(y)P(1-y)/GaAs
  INPUT I= ?
 ******************************************************
4
 ENERGY EIGENVALUE===>  0.132273196491E+00 ERROR= .1825400E-14
 ENERGY EIGENVALUE===>  0.338026920933E+00 ERROR= .2075989E-14
 ENERGY EIGENVALUE===>  0.438393858497E+00 ERROR= .1374688E-14
 ENERGY EIGENVALUE===>  0.500546559386E+00 ERROR= .1783885E-14

 FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
 SKIP INPUT I==> 2
 I=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
0.132273196491
 INPUT THE NAME OF OUTPUT FILE
cb1.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.58761391E-04
 CONFINEMENT FACTOR OF    2 th LAYER = 0.60148156E-01
 CONFINEMENT FACTOR OF    3 th LAYER = 0.87958617E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.60148156E-01
 CONFINEMENT FACTOR OF    5 th LAYER = 0.58761391E-04
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
0.338026920933
 INPUT THE NAME OF OUTPUT FILE
cb2.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.56890043E-02
 CONFINEMENT FACTOR OF    2 th LAYER = 0.28761534E+00
 CONFINEMENT FACTOR OF    3 th LAYER = 0.41339131E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.28761534E+00
 CONFINEMENT FACTOR OF    5 th LAYER = 0.56890043E-02
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
2
```

ii) Steps to calculate the heavy hole energy levels

```
 ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT
3
 INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
 INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
 INPUT N=
5
 INPUT THE HIGHEST POTENTIAL(1st Q-WELL) LAYER IC= ?
3
```

```
 INPUT THE SELECTED CENTER OF THE STRUCTURE ICR=?
3
 ******************************************************
  INPUT I=1  FOR AlGaAs
       I=2  FOR InGaAsP
       I=3  FOR In(1-x)Ga(x)As/InGaAsP/InP
       I=4  FOR InGaAlAs/InGaAlAs
       I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
       I=6  FOR InGaAs/AlGaAs/AlGaAs
       I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
       I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
       I=9  FOR In(z)Ga(1-z)As/AlxGayIn1-x-yAs/InP
       I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
       I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
       I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
       I=13 FOR InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
  INPUT I= ?
 ******************************************************
4
 ******************************************************

  DOES THE STRUCTURE STRAIN OR STRAIN-COMPENSATED?
  IF STRAIN ONLY INPUT 1, STRAIN-COMPENSATED INPUT 2
  INPUT SELECT = ?

2
  INPUT BARRIER STRAIN =?
0.008776922
  ENERGY EIGENVALUE===> -0.190388140560E+00 ERROR= .3376657E-14
  ENERGY EIGENVALUE===> -0.178205351549E+00 ERROR= .2794590E-14
  ENERGY EIGENVALUE===> -0.146868929570E+00 ERROR= .1933278E-14
  ENERGY EIGENVALUE===> -0.649012884792E-01 ERROR= .1722105E-14
  ENERGY EIGENVALUE===> -0.584031671619E-02 ERROR= .1782035E-14

  FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
  SKIP INPUT I==> 2
  I=?
1
  INPUT THE EIGENVALUE
  EIGEN VALUE=
-0.584031671619E-02
  INPUT THE NAME OF OUTPUT FILE
hh1.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.10778777E-06
 CONFINEMENT FACTOR OF    2 th LAYER = 0.15062630E-01
 CONFINEMENT FACTOR OF    3 th LAYER = 0.96987452E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.15062630E-01
 CONFINEMENT FACTOR OF    5 th LAYER = 0.10778777E-06
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
1
  INPUT THE EIGENVALUE
  EIGEN VALUE=
-0.649012884792E-01
  INPUT THE NAME OF OUTPUT FILE
hh2.txt
```

```
 CONFINEMENT FACTOR OF    1 th LAYER = 0.51712890E-05
 CONFINEMENT FACTOR OF    2 th LAYER = 0.68039794E-01
 CONFINEMENT FACTOR OF    3 th LAYER = 0.86391007E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.68039794E-01
 CONFINEMENT FACTOR OF    5 th LAYER = 0.51712890E-05
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
2
```

iii) Steps to calculate the light hole energy levels

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

4
  INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
  INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
  INPUT N=
5
  INPUT THE HIGHEST POTENTIAL(1st Q-WELL) LAYER IC= ?
3
  INPUT THE SELECTED CENTER OF THE STRUCTURE ICR=?
3
 *********************************************************
   INPUT I=1  FOR AlGaAs
        I=2  FOR InGaAsP
        I=3  FOR In(1-x)Ga(x)As/InGaAsP/InP
        I=4  FOR InGaAlAs/InGaAlAs
        I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
        I=6  FOR InGaAs/AlGaAs/AlGaAs
        I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
        I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
        I=9  FOR In(z)Ga(1-z)As/AlxGayIn1-x-yAs/InP
        I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
        I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
        I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
        I=13 FOR InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
   INPUT I= ?
 *********************************************************
4
 *********************************************************

  DOES THE STRUCTURE STRAIN OR STRAIN-COMPENSATED?
  IF STRAIN ONLY INPUT 1, STRAIN-COMPENSATED INPUT 2
  INPUT SELECT = ?

2
  INPUT BARRIER STRAIN =?
0.008776922
  ENERGY EIGENVALUE===> -0.224692198534E+00 ERROR= .5190988E-14
  ENERGY EIGENVALUE===> -0.169366776608E+00 ERROR= .3378719E-14
```

```
 ENERGY EIGENVALUE===> -0.978425419323E-01 ERROR= .2045359E-14

 FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
 SKIP INPUT I==> 2
 I=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
-0.978425419323E-01
 INPUT THE NAME OF OUTPUT FILE
lh1.txt
 CONFINEMENT FACTOR OF   1 th LAYER = 0.10863305E-01
 CONFINEMENT FACTOR OF   2 th LAYER = 0.19796026E+00
 CONFINEMENT FACTOR OF   3 th LAYER = 0.58235288E+00
 CONFINEMENT FACTOR OF   4 th LAYER = 0.19796026E+00
 CONFINEMENT FACTOR OF   5 th LAYER = 0.10863305E-01
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
-0.169366776608
 INPUT THE NAME OF OUTPUT FILE
lh2.txt
 CONFINEMENT FACTOR OF   1 th LAYER = 0.90021097E-01
 CONFINEMENT FACTOR OF   2 th LAYER = 0.36387798E+00
 CONFINEMENT FACTOR OF   3 th LAYER = 0.92201838E-01
 CONFINEMENT FACTOR OF   4 th LAYER = 0.36387798E+00
 CONFINEMENT FACTOR OF   5 th LAYER = 0.90021097E-01
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
2
```

b) The main output file from this part of GAIN program is energy.dat, containing all the energy levels as shown in Table C.4.5. After the energy eigen values are calculated, the GAIN program asks the user whether he would like to check the wave envelope function or not. We suggest that the user check the wave envelope functions of the first and second energy levels for conduction and valence bands. The plots of the envelope functions are shown in Fig. C.4.2, Fig. C.4.3, Fig C.4.4.

Table C.4.5. output file energy.dat

```
 CONDUCTION BAND ENERGY===>  0.132273196491E+00 ERROR= .1825400E-14

 CONDUCTION BAND ENERGY===>  0.338026920933E+00 ERROR= .2075989E-14

 CONDUCTION BAND ENERGY===>  0.438393858497E+00 ERROR= .1374688E-14

 CONDUCTION BAND ENERGY===>  0.500546559386E+00 ERROR= .1783885E-14

 HEAVY HOLE ENERGY===> -0.190388140560E+00 ERROR= .3376657E-14

 HEAVY HOLE ENERGY===> -0.178205351549E+00 ERROR= .2794590E-14

 HEAVY HOLE ENERGY===> -0.146868929570E+00 ERROR= .1933278E-14
```

HEAVY HOLE ENERGY===> -0.649012884792E-01 ERROR= .1722105E-14

HEAVY HOLE ENERGY===> -0.584031671619E-02 ERROR= .1782035E-14

LIGHT HOLE ENERGY===> -0.224692198534E+00 ERROR= .5190988E-14

LIGHT HOLE ENERGY===> -0.169366776608E+00 ERROR= .3378719E-14

LIGHT HOLE ENERGY===> -0.978425419323E-01 ERROR= .2045359E-14

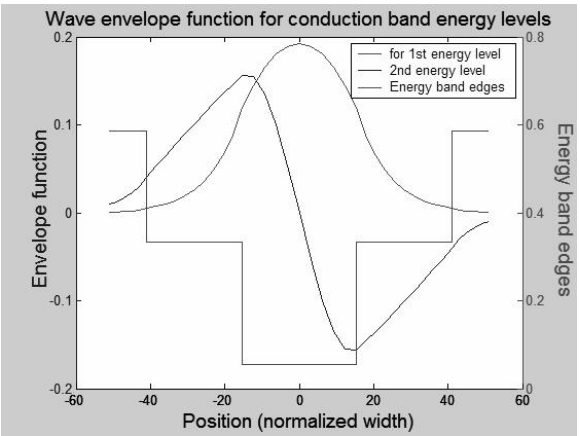

Fig. C.4.2. Wave envelope functions for energy levels in conduction band

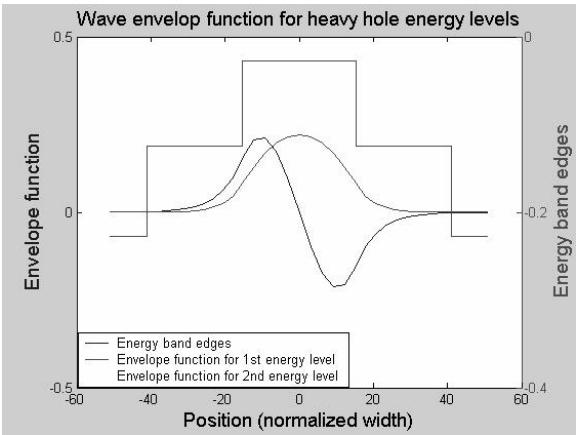

Fig. C.4.3. Wave envelope functions for heavy hole energy levels

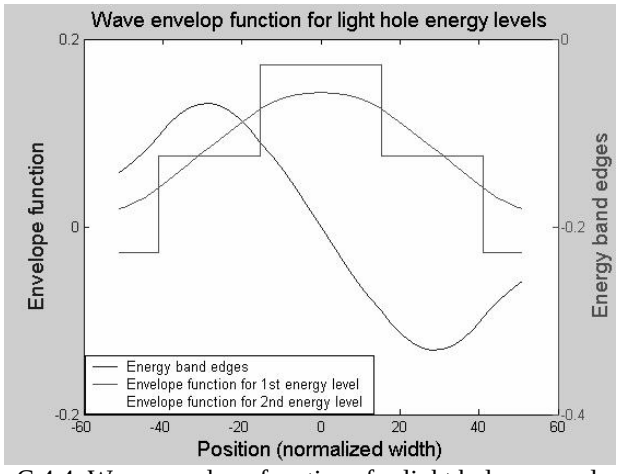

Fig. C.4.4. Wave envelope functions for light hole energy levels

C.4.3. Simulations of Gain and Laser properties

This is the last step of simulations using the GAIN program. With the previous calculated material composition, energy band edges, energy levels, and other parameters like material loss and Auger coefficient, the GAIN program can simulate the threshold current, threshold current density, slope efficiency, optical gain and mode gain as functions of wavelengths and photon energies, and L-I curve. The details are explained in Chapter 4 of the manual.

In this part of GAIN program, the input file needs to be constructed with the results of the previous steps and according to the laser design. In this example, single quantum well structure is used to simulate a three-QW laser. For the three-quantum-well laser with a ridge length of 750 μm and ridge width of 3 μm, the input file is shown in Table C.4.6. The detailed steps of simulations are listed in Table C.4.7. The main output files: L-I curve, optical gain as a function of the wavelength, and mode gain vs. current density are plotted in Fig. C.4.5, Fig. C.4.6, and Fig. C.4.7.

a) The input file:

Table C.4.6. Input file for gain and threshold current calculation

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c    1. Input the compositions, width of well, effective index       c
c      and lasing wavelength.                                        c
c    Ex: xx,xz,qy,xy,lx,n,lam                                        c
c    for different materials the following are the forms of inputs.  c
c                                                                    c
c    w -- > well, b -- > barrier  cxz and cxy for cladding.          c
c                                                                    c
c    a.  AlxGa1-xAs : xx (Al w) xz (Al b) qy (0) xy (0)              c
c    b.  In1-xGaxAsyP1-y : xx (Ga w) xz (Ga b) qy (As w) xy (As b)   c
c    c.  In1-xGaxAs/InGaAsP : xx (Ga w) xz (Ga b) qy (0) xy (As b)   c
c    d.  AlxGayIn1-x-yAs/InP : xx (Ga w) xz (Ga b) qy (Al w) xy (Al b)c
c    e.                                                              c
c    f.  InxGa1-xAs/AlGaAs : xx (In w) xz (0) qy (0) xy (Al b)       c
c    g.                                                              c
c    h.  AlyInxGa1-x-yAs/AlGaAs : xx (Al w) xz (al b) qy (In w) xz (0)c
c    i.  In1-xGaxAs/AlGaInAs : xx (In w) xz (0) qy (Al b) xy (Ga b)  c
c    j.  In(y)Ga(1-y)As(x)N(1-x) :xx(As w),xz(As, b),qy(In w),xy(In b)c
c    k.  InGaAs/InGaAsP/GaAs: xx (In w), (0), xz(Ga w) xy (As b)
c    2. Input the energy gap,temperature, barrier band edges(both bands)
c    Ex: eg,temp,ec,ev                                               c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
0.21964924 0.34879557  0.0801355  0.2505339  6.0  3.218741  1.5
0.683804 298 0.3327401 0.1241536
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c    3. Input the ist level sub-band energy levels.                  c
c    Ex: ec1,eh1,el1                                                 c
c                                                                    c
```

```
c     4. Input the material loss, reflectivities, number of quantum     c
c        wells and beta(for spontaneous emission).                      c
c     Ex: alpha,r1,r2,mm,beta.                                          c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
0.132273291719  0.584032029186E-02  0.978425521147E-01  1  1  1
12.0d0  0.30   0.30   1  5.D-5
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c     5. Input the cavity length, ridge width, internal efficiency      c
c        Auger, strain(except AlGaAs,put 0) and confinement factor.     c
c     Ex: cl,cw,etha,ca,es,confine                                      c
c                                                                       c
c     6. Input the cladding composition and band edges.                 c
c     Ex: cxz,cxy,ecc,evv                                               c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
750.D-4  3D-4  0.96  1.00d-29   0.000  0.009834488
0.48 0.0  0.5859193  0.2278575
```

b) The steps for these calculations mentioned are listed in Table C.4.7

Table C.4.7. The steps for the gain and threshold current density calculations

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

5
 THE INPUT FILE NAME=
in1.tex
 SELECT MATERIAL=?
 1--AlGaAs
 2--InGaAsP
 3--In1-zGazAs/InGaAsP/InP
 4-- InGaAlAs
 5--GaInP/AlzGawIn1-z-wP/Al0.5In0.5P
 6-- InxGa1-xAs/AlxGa1-xAs/AlGaAs
 7--In1-xGaxAs/InGaAsP/GaxIn1-xP(X=0.51) MATCHED TO GaAs
 8--AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
 9--InzGa1-zAs/AlxGayIn1-x-yAs/InP
 10-- InGaAlAs/InGaAlAs/AlAsSb
 11--InzGa1-zAs/AlxGayIn1-x-yAs/AlAsSb
 12--In(y)Ga(1-y)As(x)N(1-x)/GaAs
 13--InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
 INPUT SELECTION
4
 INPUT MODE = ? FOR TE--> MODE =1, FOR TM--> MODE =2
 INPUT TE OR TM ?
1
 IF EL1 BELOW EH1 THEN SELECT 1, OTHERWISE SELECT 2
 SELECTION=?
1
 ************************************************
 CALCULATE THE EFFECTIVE MASS
```

```
 ************************************************
 FOR QUASI-FERMI LEVEL SELECT=1,
 FOR READ EXISTING QUASI-FERMI LEVEL SELECT=2
 SELECT=?
1

 J(LEAKAGE)=0.522156D-01 A/cm^2  N=0.328772D+19 1/cm^3
 J(LEAKAGE)=0.544163D-01 A/cm^2  N=0.330752D+19 1/cm^3
 J(LEAKAGE)=0.567097D-01 A/cm^2  N=0.332732D+19 1/cm^3
 J(LEAKAGE)=0.590996D-01 A/cm^2  N=0.334712D+19 1/cm^3
…….
J(LEAKAGE)=0.654295D+03 A/cm^2  N=0.788120D+19 1/cm^3
J(LEAKAGE)=0.678642D+03 A/cm^2  N=0.790100D+19 1/cm^3
J(LEAKAGE)=0.703785D+03 A/cm^2  N=0.792080D+19 1/cm^3
J(LEAKAGE)=0.729743D+03 A/cm^2  N=0.794060D+19 1/cm^3
J(LEAKAGE)=0.756533D+03 A/cm^2  N=0.796040D+19 1/cm^3
J(LEAKAGE)=0.784174D+03 A/cm^2  N=0.798020D+19 1/cm^3
J(LEAKAGE)=0.812685D+03 A/cm^2  N=0.800000D+19 1/cm^3
************************************************
G(J) PARAMETERS FROM SINGLE WELL
 Go=0.158181D+02 1/cm  Jo=0.954942D+02 A/cm^2

 G(N) PARAMETERS FROM SINGLE WELL
 NGo=0.160843D+04 1/cm  XNo=0.911779D+18 1/cm^3

 Jtr=0.351304D+02 A/cm^2  NTR=0.335425D+18 1/cm^3


 THE OPTIMUM NUMBER OF QUANTUM WELL FOLLOWS THE ARTICLE
 BY McIlory et al. IEEE JQE-21 1985.

 THE OPTIMUM NUMBER OF QUANTUM WELL Nopt =          2
 INPUT Nopt(CAN BE DIFFERENT FROM ABOVE CALCULATION)=?
2
 NUMBER OF QUANTUM WELL(MAY OR MAY NOT BE Nopt)=?
3

 ************************************************
 ************************************************
 1ST CHECK USE SINGLE WELL TIMES # OF WELLS
 ************************************************
 ************************************************
 2ND CHECK FOLLOWS FORMULA BY McIlory IN IEEE
 JOURNAL OF QUANTUM ELECTRONIC QE-21 1985.
 ************************************************
 Gth=  28.0530 1/cm Nth=0.170376D+19 1/cm^3 IY=   82
  1ST CHECK Jth=   381.42697085 A/cm^2
  2ND CHECK Jth=   213.82690 A/cm^2

  1ST CHECK Ith=0.858211D+01 mA NUMBER OF WELLS=  2
  2ND CHECK Ith=0.481111D+01 mA

 ************************************************
 CALCULATE THE P-I RELATION

 NDATA=        319
```

```
 ************************************************
 CALCULATE THE SLOPE: mW/mA Y=A+BX
 CONSTANT A=  -1.8744106   SLOPE B=   0.2184091

 ************************************************
 INPUT POWER PO FOR THE LINEWIDTH, PO=0 FOR STOP
 INPUT PO=    mW
0
 INPUT 1 FOR THE DYNAMIC CALCULATION. 2 FOR SKIP
 INPUT =
2
 K-FACTOR= 0.33294 nS  MAXIUM FREQ.= 26.6891 GHz

 ************************************************
 INPUT 1 FOR CALCULATE THE GAIN(E) RELATION.

 INPUT 2 FOR CALCULATE THE LINEWIDTH ENHENCEMENT
 FACTOR AND PHOTON ENERGY RELATION

 INPUT 3 FOR EXIT THE PROGRAM

 THE INPUT # IS
1
 INPUT FERMILEVELS IN C-BAND, V-BAND, AND CARRIER DENSITY
0.238566456069 -0.666558305734E-02 0.200075187970E+19
 CALCULATE THE CONVOLUTION GAIN(E) COEFFICIENT
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(LAMBDA)
ol1.txt
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(LAMBDA)
ml1.txt
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(E)
oe1.txt
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(E)
me1.txt
 ************************************************
 INPUT 1 FOR REPEAT THE G(E) CALCULATION
 INPUT 2 FOR REPEAT THE ALPHA(E) CALCULATION
 INPUT 3 FOR EXIT
1
 ************************************************
 INPUT 1 FOR CALCULATE THE GAIN(E) RELATION.

 INPUT 2 FOR CALCULATE THE LINEWIDTH ENHENCEMENT
 FACTOR AND PHOTON ENERGY RELATION

 INPUT 3 FOR EXIT THE PROGRAM

 THE INPUT # IS
1
 INPUT FERMILEVELS IN C-BAND, V-BAND, AND CARRIER DENSITY
0.292773620684 -0.223794117473E-01 0.301052631579E+19
 CALCULATE THE CONVOLUTION GAIN(E) COEFFICIENT
 ************************************************
```

```
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(LAMBDA)
ol2.txt
  ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(LAMBDA)
ml2.txt
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(E)
oe2.txt
  ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(E)
me2.txt
  ************************************************
 INPUT 1 FOR REPEAT THE G(E) CALCULATION
 INPUT 2 FOR REPEAT THE ALPHA(E) CALCULATION
 INPUT 3 FOR EXIT
3
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

7
```

c) The Output characteristics of designed laser from step 5 are summarized in Table C.4.7.

Table C.4.7 Characteristics of the designed laser

Optimized number of QWs (Nopt)	2
Number of QWs	3
Slope efficiency (%)	21.84
Jth (A/cm^2)	381.4 - 1st check, for matching threshold conditions 213.8 – 2nd check, using McIlory method
Ith (mA)	8.58 mA - 1st check, for matching threshold conditions 4. 81 mA - 2nd check, using McIlory method
Peak λ at operating temperature (um)	1.52 um for carrier density of 2.0E18 /cm3 1.53 um for carrier density of 3.0E18 /cm3
Peak material gain (1/cm)	3160.1 /cm for carrier density of 2.0E18 /cm3 2115.6 /cm for carrier density of 3.0E18 /cm3

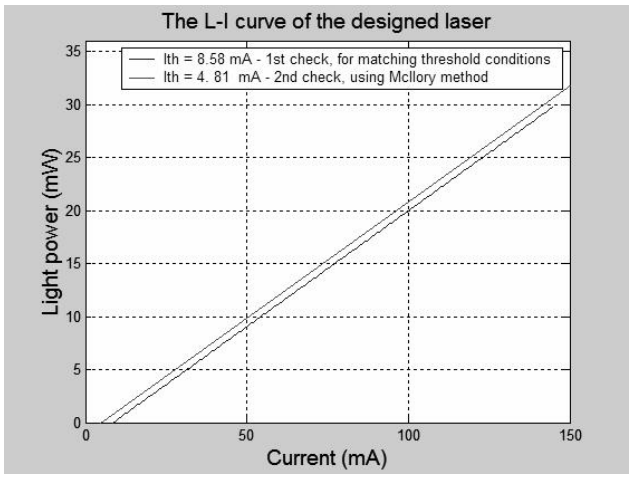

Fig. C.4.5. L-I curve of the laser

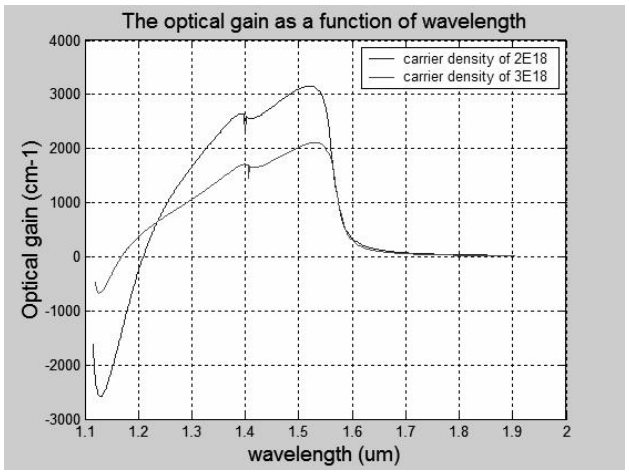

Fig. C.4.6. Optical gain-λ curve of the laser

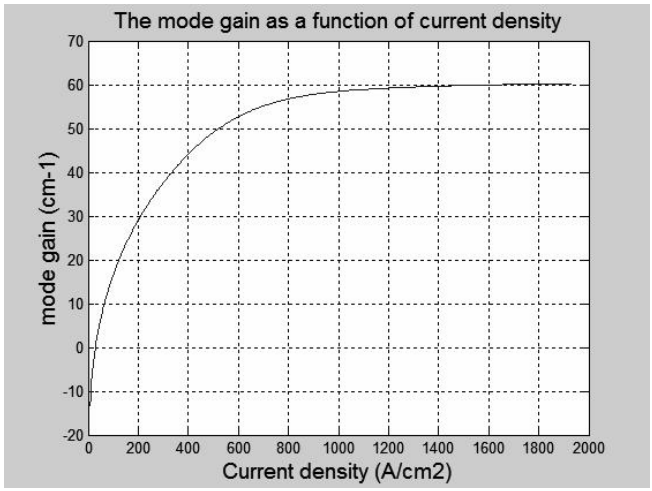

Fig. C.4.7. Mode gain as a function of current density (J)

C.5. Material system #*5:* GaInP/$Al_zGa_wIn_{1-z-w}P/Al_{0.5}In_{0.5}P$

This is a simulation of a five-layer laser structure that contains a single quantum well (QW), two separated confinement heterostructure (SCH) layers, and two cladding layers as shown in Fig. C.5.1.

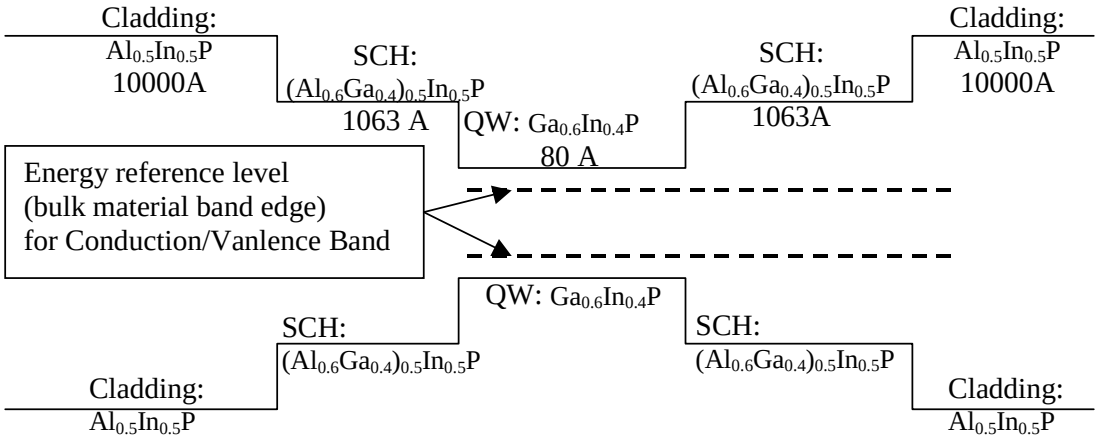

Figure C.5.5. Energy band diagram for the simple quantum well structure

C.5.1. Calculation of material compositions and energy band edges.

The first step of the GAIN program is to calculate the material compositions and energy band edges of the each layer. The user is asked to enter the photoluminescence wavelength, thickness, and strain of the QW, SCH, and cladding layers. After these parameters are input, the GAIN program generates two output files: cbandeg.dat and vbandeg.dat, containing the material compositions, and the conduction band edges and valence band edges respectively. The detailed explanation is provided in Chapter 2 of this manual.

a) The input parameters to the GAIN program in this step islisted in Table. C.5.1.

Table C.5.1. Input parameters to the GAIN program in this step.

Layer	λ (um)	Strain	Thickness (Å)
QW ($Ga_{0.6}In_{0.4}P$)	0.63	-0.0027	80
SCH ($(Al_{0.6}Ga_{0.4})_{0.5}In_{0.5}P$)	0.545	0	1063
Cladding ($Al_{0.5}In_{0.5}P$)	0.491	0	10000

b) The steps in using the GAIN program to calculate the material compositions and energy band edges are listed in Table C.5.2

Table C.5.2. steps to run the GAIN program for necessary parameters.

ENTER 1 FOR THE NECESSARY PARAMETERS 2 FOR THE ENERGY VALUES OF CONDUCTION BAND

```
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

1

 ENTER 1 FOR AlGaAs/AlGaAs
      2 FOR InGaAsP/InGaAsP/InP
      3 FOR InGaAs/InGaAsP/InP
      4 FOR InGaAlAs/InGaAlAs/InP
      5 FOR GaInP/(AlGa)0.5In0.5P/AlInP
      6 FOR InGaAs/AlGaAs/AlGaAs
      7 FOR InGaAs/InGaAsP/Ga0.51In0.49P(MATCHED GaAs)
      8 FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
      9 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/InP
     10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(matched InP)
     11 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/AlAsxSb1-x
     12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs (dilute N)
     13 FOR In(1-x)Ga(x)As(y)P(1-y)/GaAs
     14 FOR EXIT, BACK TO MAIN PAGE!
5

  Ga(x)In(1-x)P/AlGaInP/AlGaInP(matched to GaAs)
  If x=0.5 then GaInP(Eg=1.891eV) lattice matched to GaAs

  The barrier region can be latticed matched to GaAs
  or strained composition.

  In QW region x->Ga, y->0
  Both barrier(SCH) and cladding, X->Ga, Y->Al

 INPUT THE LAYER # FOR GRIN STRUCTURE(STEP)
 STEP N=
2
  INPUT THE WELL WAVELENGTH (um)
0.63
  INPUT THE BARRIER WAVELENGTH (um)
0.545
  INPUT THE CLADDING WAVELENGTH (um)
0.491
  BANDGAP ENERGY OF QUANTUM WELL=    1.96825396825397       eV
  INPUT CLADDING, BARRIER,QUANTUM WELL WIDTH (A)
10000 1063 80
  For AlGaInP lattice matched to GaAs select -->1
  For AlGaInP lattice mismatch select --> 2

  SELECTION ===> ?
1
  STRAIN FOR GaInP   2.714641526427632E-003

  WRITE CONDUCTION BAND PARAMETERS INTO CBANDEG.DAT

  WRITE VALENCE BAND PARAMETERS INTO VBANDEG.DAT
  INPUT 1 FOR NEW CALCULATION, 2 FOR EXIT
```

```
 I= ?
2

 ENTER 1 FOR AlGaAs/AlGaAs
      2 FOR InGaAsP/InGaAsP/InP
      3 FOR InGaAs/InGaAsP/InP
      4 FOR InGaAlAs/InGaAlAs/InP
      5 FOR GaInP/(AlGa)0.5In0.5P/AlInP
      6 FOR InGaAs/AlGaAs/AlGaAs
      7 FOR InGaAs/InGaAsP/Ga0.51In0.49P(MATCHED GaAs)
      8 FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
      9 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/InP
     10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(matched InP)
     11 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/AlAsxSb1-x
     12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs (dilute N)
     13 FOR In(1-x)Ga(x)As(y)P(1-y)/GaAs
     14 FOR EXIT, BACK TO MAIN PAGE!
14
 THIS PROGRAM STOP HERE!, BACK TO MAIN PAGE
```

c) The output files, cbandeg.dat and vbandeg.dat are explained in Table C.5.3.

Table C.5.3. Material compositions and band offsets:

a) cbandeg.dat for conduction band

```
*************************************************************************
 QW strain   lattice constant
 0.271464E-02  0.563795E-09
                        material compositions AlyGaxIn1-x-yP
 layer thickness,          Ga              Al      conduction band edges
  0.10000000E+05  -0.44739897E-02   0.5044740   0.1950215      cladding layer
  0.10630000E+04   0.20063165E+00   0.2993683   0.1074414      SCH layer
  0.80000000E+02   0.55257950E+00   0.0000000  -0.0142929      quantum well
  0.10630000E+04   0.20063165E+00   0.2993683   0.1074414      SCH layer
  0.10000000E+05  -0.44739897E-02   0.5044740   0.1950215      cladding layer
*************************************************************************
```

b) vbandeg.dat for valence band

```
*************************************************** ********************
 QW strain   lattice constant
 0.271464E-02  0.563795E-09
                        material compositions AlyGaxIn1-x-yP
 layer thickness,          Ga              Al      valence band edges
  0.10000000E+05  -0.44739897E-02   0.5044740  -0.3621828      cladding layer
  0.10630000E+04   0.20063165E+00   0.2993683  -0.1995340      SCH layer
  0.80000000E+02   0.55257950E+00   0.0000000   0.0071464      quantum well
  0.10630000E+04   0.20063165E+00   0.2993683  -0.1995340      SCH layer
  0.10000000E+05  -0.44739897E-02   0.5044740  -0.3621828      cladding layer
*************************************************************************
```

C.5.2. Energy level calculations

After the calculation of the material compositions and energy band edges, the GAIN program calculates energy levels in the conduction band and valence bands. The detailed explanations are discussed in Chapter 3 of this manual.

a) The steps of how to calculate the energy levels are shown in Table C.5.4.

Table C.5.4. Steps to calculate the energy levels

i) Steps to calculate the conduction band energy levels

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

2
 INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
 INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
 INPUT N=
5
 INPUT THE LOWEST POTENTIAL LAYER(1st Q-WELL) IC= ?
3
 INPUT THE SELECTED CENTER LAYER OF STRUCTURE ICR=
3
 ******************************************************
  INPUT I=1  FOR AlGaAs
       I=2  FOR InGaAsP
       I=3  FOR In1-xGaxAs/InGaAsP/InP
       I=4  FOR InGaAlAs/InGaAlAs
       I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
       I=6  FOR InGaAs/AlGaAs/AlGaAs
       I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
       I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
       I=9  FOR InzGa1-zAs/AlxGayIn1-x-yAs/InP
       I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
       I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
       I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
       I=13 FOR InGaAs/In(1-y)Ga(x)As(y)P(1-y)/GaAs
  INPUT I= ?
 ******************************************************
5

 ENERGY EIGENVALUE===>  0.961974438375E-02 ERROR=
.2786910E-14
 ENERGY EIGENVALUE===>  0.743662554277E-01 ERROR= .2580380E-14
 ENERGY EIGENVALUE===>  0.107675191040E+00 ERROR= .4266368E-14
 ENERGY EIGENVALUE===>  0.107688174734E+00 ERROR= .2463437E-14
 ENERGY EIGENVALUE===>  0.108376258685E+00 ERROR= .6317963E-14
 ENERGY EIGENVALUE===>  0.108428037338E+00 ERROR= .1442872E-14
 ENERGY EIGENVALUE===>  0.109543687391E+00 ERROR= .2900562E-14
 ENERGY EIGENVALUE===>  0.109659654907E+00 ERROR= .1483391E-14
```

```
 ENERGY EIGENVALUE===>  0.111175954839E+00 ERROR= .2524093E-14
 ENERGY EIGENVALUE===>  0.111380963353E+00 ERROR= .1915930E-14
 ENERGY EIGENVALUE===>  0.113270939913E+00 ERROR= .2521982E-14
 ENERGY EIGENVALUE===>  0.113589356334E+00 ERROR= .2292240E-14
 ENERGY EIGENVALUE===>  0.115825939696E+00 ERROR= .2102730E-14
 ENERGY EIGENVALUE===>  0.116281876661E+00 ERROR= .1980838E-14
 ENERGY EIGENVALUE===>  0.118837702628E+00 ERROR= .2070679E-14
 ENERGY EIGENVALUE===>  0.119455372783E+00 ERROR= .1414132E-14
 ENERGY EIGENVALUE===>  0.122302488065E+00 ERROR= .2748183E-14
 ENERGY EIGENVALUE===>  0.123106599250E+00 ERROR= .1286513E-14
 ENERGY EIGENVALUE===>  0.126216164546E+00 ERROR= .2382521E-14
 ENERGY EIGENVALUE===>  0.127232254643E+00 ERROR= .1318435E-14
 ENERGY EIGENVALUE===>  0.130574357571E+00 ERROR= .3582667E-14
 ENERGY EIGENVALUE===>  0.131828958191E+00 ERROR= .2236097E-14
 ENERGY EIGENVALUE===>  0.135372648300E+00 ERROR= .2832335E-14
 ENERGY EIGENVALUE===>  0.136893165876E+00 ERROR= .2662248E-14
 ENERGY EIGENVALUE===>  0.140606801955E+00 ERROR= .2075560E-14
 ENERGY EIGENVALUE===>  0.142421018041E+00 ERROR= .2486680E-14
 ENERGY EIGENVALUE===>  0.146272964900E+00 ERROR= .2509426E-14
 ENERGY EIGENVALUE===>  0.148408090543E+00 ERROR= .1416510E-14
 ENERGY EIGENVALUE===>  0.152367710782E+00 ERROR= .3201183E-14
 ENERGY EIGENVALUE===>  0.154848978871E+00 ERROR= .2597122E-14
 ENERGY EIGENVALUE===>  0.158887734556E+00 ERROR= .1766965E-14
 ENERGY EIGENVALUE===>  0.161736541616E+00 ERROR= .2628242E-14
 ENERGY EIGENVALUE===>  0.165828843460E+00 ERROR= .2472018E-14
 ENERGY EIGENVALUE===>  0.169060333436E+00 ERROR= .1986998E-14
 ENERGY EIGENVALUE===>  0.173183433744E+00 ERROR= .3017043E-14
 ENERGY EIGENVALUE===>  0.176802685912E+00 ERROR= .1597014E-14
 ENERGY EIGENVALUE===>  0.180933567715E+00 ERROR= .2328795E-14
 ENERGY EIGENVALUE===>  0.184925313643E+00 ERROR= .2516799E-14
 ENERGY EIGENVALUE===>  0.189021845141E+00 ERROR= .1893777E-14
 ENERGY EIGENVALUE===>  0.193267857341E+00 ERROR= .2992086E-14

 FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
 SKIP INPUT I==> 2
 I=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
0.00962
 INPUT THE NAME OF OUTPUT FILE
v1
 CONFINEMENT FACTOR OF    1 th LAYER = 0.19880306E-80
 CONFINEMENT FACTOR OF    2 th LAYER = 0.37682916E+00
 CONFINEMENT FACTOR OF    3 th LAYER = 0.11196418E-24
 CONFINEMENT FACTOR OF    4 th LAYER = 0.62317084E+00
 CONFINEMENT FACTOR OF    5 th LAYER = 0.19880985E-80
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
0.07437
 INPUT THE NAME OF OUTPUT FILE
v2
 CONFINEMENT FACTOR OF    1 th LAYER = 0.15868871E-32
```

```
 CONFINEMENT FACTOR OF    2 th LAYER = 0.15724277E+00
 CONFINEMENT FACTOR OF    3 th LAYER = 0.68556334E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.15719389E+00
 CONFINEMENT FACTOR OF    5 th LAYER = 0.15863938E-32
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
2
```

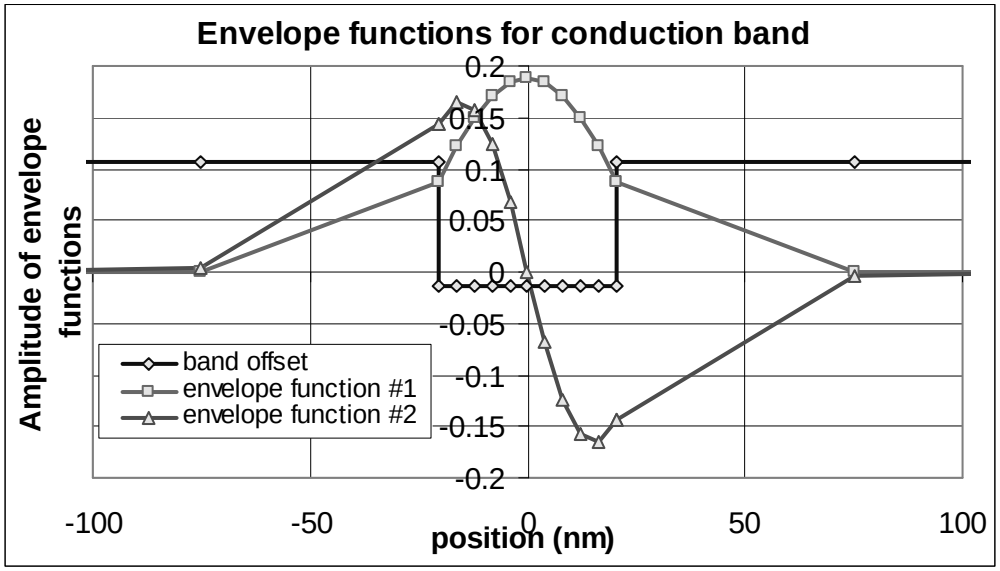

Fig. C.5.2 Envelope functions for conduction band

ii) Steps to calculate the heavy hole energy levels

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

3
  INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
  INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
  INPUT N=
5
  INPUT THE HIGHEST POTENTIAL(1st Q-WELL) LAYER IC= ?
3
  INPUT THE SELECTED CENTER OF THE STRUCTURE ICR=?
3
 ********************************************************
   INPUT I=1  FOR AlGaAs
        I=2  FOR InGaAsP
        I=3  FOR In(1-x)Ga(x)As/InGaAsP/InP
        I=4  FOR InGaAlAs/InGaAlAs
        I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
        I=6  FOR InGaAs/AlGaAs/AlGaAs
        I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
```

```
      I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
      I=9  FOR In(z)Ga(1-z)As/AlxGayIn1-x-yAs/InP
      I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
      I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
      I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
      I=13 FOR InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
  INPUT I= ?
 ******************************************************
5
 ******************************************************

  DOES THE STRUCTURE STRAIN OR STRAIN-COMPENSATED?
  IF STRAIN ONLY INPUT 1, STRAIN-COMPENSATED INPUT 2
  INPUT SELECT = ?

1
  ENERGY EIGENVALUE===> -0.361192916606E+00 ERROR= .2318346E-14
  ENERGY EIGENVALUE===> -0.358485532473E+00 ERROR= .4956447E-14
  ENERGY EIGENVALUE===> -0.354716248972E+00 ERROR= .5526373E-14
  ENERGY EIGENVALUE===> -0.351913554427E+00 ERROR= .5317960E-14
  ENERGY EIGENVALUE===> -0.348266207154E+00 ERROR= .2918676E-14
  ENERGY EIGENVALUE===> -0.345413437374E+00 ERROR= .3749323E-14
  ENERGY EIGENVALUE===> -0.341928545612E+00 ERROR= .3487911E-14
  ENERGY EIGENVALUE===> -0.339023804865E+00 ERROR= .4983602E-14
  ENERGY EIGENVALUE===> -0.335719117586E+00 ERROR= .2977748E-14
  ENERGY EIGENVALUE===> -0.332757485607E+00 ERROR= .2663835E-14
  ENERGY EIGENVALUE===> -0.329642979500E+00 ERROR= .4769990E-14
  ENERGY EIGENVALUE===> -0.326621008574E+00 ERROR= .2474339E-14
  ENERGY EIGENVALUE===> -0.323701256646E+00 ERROR= .4188658E-14
  ENERGY EIGENVALUE===> -0.320618410761E+00 ERROR= .4940924E-14
  ENERGY EIGENVALUE===> -0.317893261288E+00 ERROR= .3395574E-14
  ENERGY EIGENVALUE===> -0.314752486888E+00 ERROR= .2722462E-14
  ENERGY EIGENVALUE===> -0.312217533281E+00 ERROR= .3080726E-14
  ENERGY EIGENVALUE===> -0.309025316890E+00 ERROR= .3714707E-14
  ENERGY EIGENVALUE===> -0.306672506150E+00 ERROR= .3651204E-14
  ENERGY EIGENVALUE===> -0.303438526815E+00 ERROR= .4852848E-14
  ENERGY EIGENVALUE===> -0.301256950156E+00 ERROR= .2606583E-14
  ENERGY EIGENVALUE===> -0.297993433199E+00 ERROR= .3079430E-14
  ENERGY EIGENVALUE===> -0.295970220156E+00 ERROR= .3775307E-14
  ENERGY EIGENVALUE===> -0.292691130035E+00 ERROR= .5023247E-14
  ENERGY EIGENVALUE===> -0.290812329627E+00 ERROR= .4216785E-14
  ENERGY EIGENVALUE===> -0.287532544737E+00 ERROR= .2473812E-14
  ENERGY EIGENVALUE===> -0.285783893576E+00 ERROR= .3723957E-14
  ENERGY EIGENVALUE===> -0.282518476130E+00 ERROR= .5303396E-14
  ENERGY EIGENVALUE===> -0.280885995969E+00 ERROR= .4570210E-14
  ENERGY EIGENVALUE===> -0.277649621354E+00 ERROR= .3537788E-14
  ENERGY EIGENVALUE===> -0.276120032911E+00 ERROR= .4293540E-14
  ENERGY EIGENVALUE===> -0.272926595561E+00 ERROR= .3632004E-14
  ENERGY EIGENVALUE===> -0.271487567178E+00 ERROR= .2909894E-14
  ENERGY EIGENVALUE===> -0.268349946744E+00 ERROR= .3976899E-14
  ENERGY EIGENVALUE===> -0.266990212090E+00 ERROR= .4204415E-14
  ENERGY EIGENVALUE===> -0.263920167090E+00 ERROR= .1103405E-13
  ENERGY EIGENVALUE===> -0.262629549143E+00 ERROR= .1689306E-14
  ENERGY EIGENVALUE===> -0.259637701783E+00 ERROR= .3319052E-14
  ENERGY EIGENVALUE===> -0.258407076018E+00 ERROR= .3786958E-14
  ENERGY EIGENVALUE===> -0.255502955805E+00 ERROR= .1151041E-13
```

```
ENERGY EIGENVALUE===> -0.254324178366E+00 ERROR= .4380337E-14
ENERGY EIGENVALUE===> -0.251516299101E+00 ERROR= .1407601E-13
ENERGY EIGENVALUE===> -0.250382118475E+00 ERROR= .2547440E-14
ENERGY EIGENVALUE===> -0.247678070270E+00 ERROR= .9114289E-14
ENERGY EIGENVALUE===> -0.246582034966E+00 ERROR= .2802900E-14
ENERGY EIGENVALUE===> -0.243988578824E+00 ERROR= .4761360E-14
ENERGY EIGENVALUE===> -0.242924949068E+00 ERROR= .2434459E-14
ENERGY EIGENVALUE===> -0.240448105895E+00 ERROR= .3480106E-14
ENERGY EIGENVALUE===> -0.239411774399E+00 ERROR= .4274582E-14
ENERGY EIGENVALUE===> -0.237056903110E+00 ERROR= .6999869E-14
ENERGY EIGENVALUE===> -0.236043328190E+00 ERROR= .3901435E-14
ENERGY EIGENVALUE===> -0.233815189170E+00 ERROR= .4571935E-14
ENERGY EIGENVALUE===> -0.232820342717E+00 ERROR= .2810531E-14
ENERGY EIGENVALUE===> -0.230723143380E+00 ERROR= .3910965E-14
ENERGY EIGENVALUE===> -0.229743476197E+00 ERROR= .1968086E-14
ENERGY EIGENVALUE===> -0.227780895151E+00 ERROR= .4565070E-14
ENERGY EIGENVALUE===> -0.226813322769E+00 ERROR= .2321745E-14
ENERGY EIGENVALUE===> -0.224988508124E+00 ERROR= .5484183E-14
ENERGY EIGENVALUE===> -0.224030421380E+00 ERROR= .1919168E-14
ENERGY EIGENVALUE===> -0.222345957410E+00 ERROR= .1879845E-14
ENERGY EIGENVALUE===> -0.221395263540E+00 ERROR= .1827758E-14
ENERGY EIGENVALUE===> -0.219853098509E+00 ERROR= .4186959E-14
ENERGY EIGENVALUE===> -0.218908299959E+00 ERROR= .3620360E-14
ENERGY EIGENVALUE===> -0.217509627335E+00 ERROR= .2453680E-14
ENERGY EIGENVALUE===> -0.216569946120E+00 ERROR= .3220033E-14
ENERGY EIGENVALUE===> -0.215315033070E+00 ERROR= .3463684E-14
ENERGY EIGENVALUE===> -0.214380586860E+00 ERROR= .2219382E-14
ENERGY EIGENVALUE===> -0.213268550022E+00 ERROR= .2777570E-14
ENERGY EIGENVALUE===> -0.212340580018E+00 ERROR= .2743067E-14
ENERGY EIGENVALUE===> -0.211369121597E+00 ERROR= .4226083E-14
ENERGY EIGENVALUE===> -0.210450259232E+00 ERROR= .3692444E-14
ENERGY EIGENVALUE===> -0.209615397194E+00 ERROR= .3171740E-14
ENERGY EIGENVALUE===> -0.208709935933E+00 ERROR= .4209780E-14
ENERGY EIGENVALUE===> -0.208005786497E+00 ERROR= .1814778E-14
ENERGY EIGENVALUE===> -0.207119900601E+00 ERROR= .3397305E-14
ENERGY EIGENVALUE===> -0.206538587407E+00 ERROR= .3003403E-14
ENERGY EIGENVALUE===> -0.205680423359E+00 ERROR= .3543397E-14
ENERGY EIGENVALUE===> -0.205212178908E+00 ERROR= .2834381E-14
ENERGY EIGENVALUE===> -0.204391753956E+00 ERROR= .3372802E-14
ENERGY EIGENVALUE===> -0.204025235404E+00 ERROR= .1580920E-14
ENERGY EIGENVALUE===> -0.203254121238E+00 ERROR= .3043020E-14
ENERGY EIGENVALUE===> -0.202976896095E+00 ERROR= .2298392E-14
ENERGY EIGENVALUE===> -0.202267732184E+00 ERROR= .3884085E-14
ENERGY EIGENVALUE===> -0.202066832823E+00 ERROR= .1442648E-14
ENERGY EIGENVALUE===> -0.201432770625E+00 ERROR= .3171156E-14
ENERGY EIGENVALUE===> -0.201295200743E+00 ERROR= .2947302E-14
ENERGY EIGENVALUE===> -0.200749395757E+00 ERROR= .5270798E-14
ENERGY EIGENVALUE===> -0.200662501388E+00 ERROR= .1723172E-14
ENERGY EIGENVALUE===> -0.200217740582E+00 ERROR= .3038427E-14
ENERGY EIGENVALUE===> -0.200169410122E+00 ERROR= .1957778E-14
ENERGY EIGENVALUE===> -0.199837910396E+00 ERROR= .3248494E-14
ENERGY EIGENVALUE===> -0.199816614058E+00 ERROR= .1532467E-14
ENERGY EIGENVALUE===> -0.199609981468E+00 ERROR= .5295449E-14
ENERGY EIGENVALUE===> -0.199604685919E+00 ERROR= .1312598E-14
ENERGY EIGENVALUE===> -0.148632604544E+00 ERROR= .2080935E-14
ENERGY EIGENVALUE===> -0.876451923558E-01 ERROR= .2306744E-14
```

ENERGY EIGENVALUE===> -0.412267198395E-01 ERROR= .2280033E-14

ENERGY EIGENVALUE===> -0.126212972547E-01 ERROR= .1971012E-14

```
 FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
 SKIP INPUT I==> 2
 I=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
-0.01262
 INPUT THE NAME OF OUTPUT FILE
v1
 CONFINEMENT FACTOR OF    1 th LAYER = 0.52282888-137
 CONFINEMENT FACTOR OF    2 th LAYER = 0.34694604E-02
 CONFINEMENT FACTOR OF    3 th LAYER = 0.99306255E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.34679900E-02
 CONFINEMENT FACTOR OF    5 th LAYER = 0.52260731-137
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
-0.04123
 INPUT THE NAME OF OUTPUT FILE
v2
 CONFINEMENT FACTOR OF    1 th LAYER = 0.10877571-125
 CONFINEMENT FACTOR OF    2 th LAYER = 0.14859493E-01
 CONFINEMENT FACTOR OF    3 th LAYER = 0.97028911E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.14851394E-01
 CONFINEMENT FACTOR OF    5 th LAYER = 0.10871642-125
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
2
```

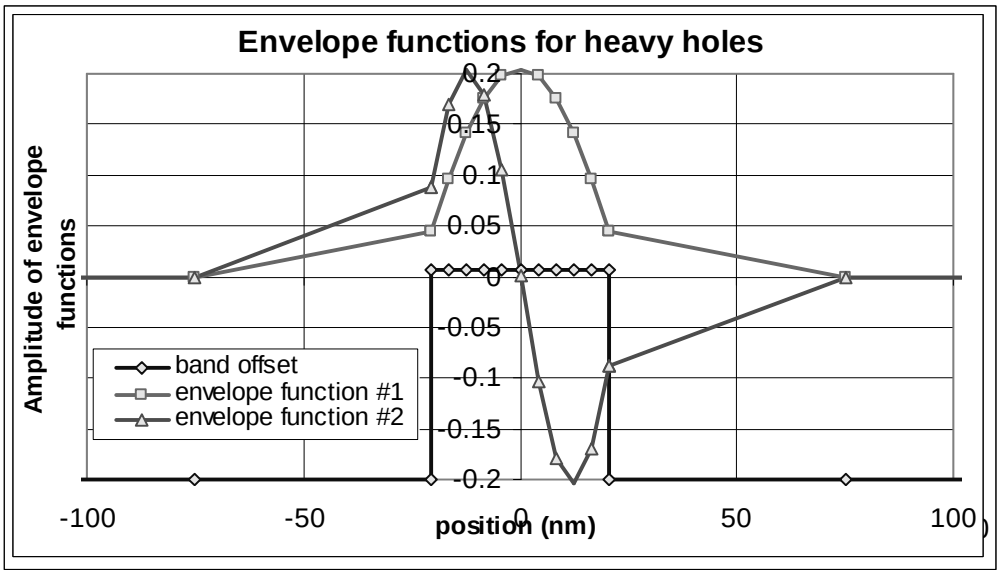

Fig. C.5.3. Envelope functions for heavy holes

iii) Steps to calculate the light hole energy levels

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

4
 INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
 INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
 INPUT N=
5
 INPUT THE HIGHEST POTENTIAL(1st Q-WELL) LAYER IC= ?
3
 INPUT THE SELECTED CENTER OF THE STRUCTURE ICR=?
3
 ********************************************************
  INPUT I=1  FOR AlGaAs
       I=2  FOR InGaAsP
       I=3  FOR In(1-x)Ga(x)As/InGaAsP/InP
       I=4  FOR InGaAlAs/InGaAlAs
       I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
       I=6  FOR InGaAs/AlGaAs/AlGaAs
       I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
       I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
       I=9  FOR In(z)Ga(1-z)As/AlxGayIn1-x-yAs/InP
       I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
       I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
       I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
       I=13 FOR InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
  INPUT I= ?
 ********************************************************
5
 ********************************************************

 DOES THE STRUCTURE STRAIN OR STRAIN-COMPENSATED?
 IF STRAIN ONLY INPUT 1, STRAIN-COMPENSATED INPUT 2
 INPUT SELECT = ?

1
 ENERGY EIGENVALUE===> -0.355569923291E+00 ERROR= .2120444E-14
 ENERGY EIGENVALUE===> -0.350213432069E+00 ERROR= .2426284E-14
 ENERGY EIGENVALUE===> -0.342922783182E+00 ERROR= .3165783E-14
 ENERGY EIGENVALUE===> -0.337911435179E+00 ERROR= .5718315E-14
 ENERGY EIGENVALUE===> -0.330625015453E+00 ERROR= .2861106E-14
 ENERGY EIGENVALUE===> -0.326008761019E+00 ERROR= .4734580E-14
 ENERGY EIGENVALUE===> -0.318798731413E+00 ERROR= .1888460E-14
 ENERGY EIGENVALUE===> -0.314568675940E+00 ERROR= .1013061E-13
 ENERGY EIGENVALUE===> -0.307483438965E+00 ERROR= .3719772E-14
 ENERGY EIGENVALUE===> -0.303617431871E+00 ERROR= .5426840E-14
 ENERGY EIGENVALUE===> -0.296698810286E+00 ERROR= .1928970E-14
 ENERGY EIGENVALUE===> -0.293170593472E+00 ERROR= .4117972E-14
```

ENERGY EIGENVALUE===> -0.286456711046E+00 ERROR= .2087373E-14
ENERGY EIGENVALUE===> -0.283239553955E+00 ERROR= .5116587E-14
ENERGY EIGENVALUE===> -0.276765133426E+00 ERROR= .4002561E-14
ENERGY EIGENVALUE===> -0.273833711271E+00 ERROR= .3188520E-14
ENERGY EIGENVALUE===> -0.267629853353E+00 ERROR= .2473219E-13
ENERGY EIGENVALUE===> -0.264961286499E+00 ERROR= .4783343E-14
ENERGY EIGENVALUE===> -0.259055249198E+00 ERROR= .1445075E-13
ENERGY EIGENVALUE===> -0.256629650468E+00 ERROR= .2986270E-14
ENERGY EIGENVALUE===> -0.251044756020E+00 ERROR= .4368280E-14
ENERGY EIGENVALUE===> -0.248845466028E+00 ERROR= .3916633E-14
ENERGY EIGENVALUE===> -0.243601143953E+00 ERROR= .3203893E-14
ENERGY EIGENVALUE===> -0.241614764042E+00 ERROR= .3829278E-14
ENERGY EIGENVALUE===> -0.236726707646E+00 ERROR= .2318723E-14
ENERGY EIGENVALUE===> -0.234942997591E+00 ERROR= .4144951E-14
ENERGY EIGENVALUE===> -0.230423413478E+00 ERROR= .3722336E-14
ENERGY EIGENVALUE===> -0.228835088921E+00 ERROR= .1889767E-14
ENERGY EIGENVALUE===> -0.224693035843E+00 ERROR= .7133531E-14
ENERGY EIGENVALUE===> -0.223295471814E+00 ERROR= .2689170E-14
ENERGY EIGENVALUE===> -0.219537311510E+00 ERROR= .3510794E-14
ENERGY EIGENVALUE===> -0.218328128086E+00 ERROR= .1768869E-14
ENERGY EIGENVALUE===> -0.214958149620E+00 ERROR= .2491797E-14
ENERGY EIGENVALUE===> -0.213936616153E+00 ERROR= .2951357E-14
ENERGY EIGENVALUE===> -0.210957957871E+00 ERROR= .5197287E-14
ENERGY EIGENVALUE===> -0.210124090200E+00 ERROR= .3596255E-14
ENERGY EIGENVALUE===> -0.207540190458E+00 ERROR= .2365701E-14
ENERGY EIGENVALUE===> -0.206893309508E+00 ERROR= .1630595E-14
ENERGY EIGENVALUE===> -0.204710293790E+00 ERROR= .2473877E-14
ENERGY EIGENVALUE===> -0.204246638588E+00 ERROR= .1699402E-14
ENERGY EIGENVALUE===> -0.202477269514E+00 ERROR= .4978716E-14
ENERGY EIGENVALUE===> -0.202186039835E+00 ERROR= .1133236E-14
ENERGY EIGENVALUE===> -0.200855776105E+00 ERROR= .3613962E-14
ENERGY EIGENVALUE===> -0.200713061214E+00 ERROR= .2681968E-14
ENERGY EIGENVALUE===> -0.199867089971E+00 ERROR= .4376218E-14
ENERGY EIGENVALUE===> -0.199828822046E+00 ERROR= .2747680E-14
ENERGY EIGENVALUE===> -0.194053584736E+00 ERROR= .2807414E-14

ENERGY EIGENVALUE===> -0.921176591126E-01 ERROR= .2804206E-14

ENERGY EIGENVALUE===> -0.113712309471E-01 ERROR= .2367096E-14

FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
SKIP INPUT I==> 2
I=?
1
INPUT THE EIGENVALUE
EIGEN VALUE=
-0.01137
INPUT THE NAME OF OUTPUT FILE
v1
CONFINEMENT FACTOR OF 1 th LAYER = 0.74617117-109
CONFINEMENT FACTOR OF 2 th LAYER = 0.42705762E+00
CONFINEMENT FACTOR OF 3 th LAYER = 0.60268078E-39
CONFINEMENT FACTOR OF 4 th LAYER = 0.57294238E+00
CONFINEMENT FACTOR OF 5 th LAYER = 0.74606910-109
INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2

```
 SELECT=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
-0.09212
 INPUT THE NAME OF OUTPUT FILE
v2
 CONFINEMENT FACTOR OF    1 th LAYER = 0.15954161E-52
 CONFINEMENT FACTOR OF    2 th LAYER = 0.75010282E-01
 CONFINEMENT FACTOR OF    3 th LAYER = 0.84999032E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.74999400E-01
 CONFINEMENT FACTOR OF    5 th LAYER = 0.15951847E-52
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
2
```

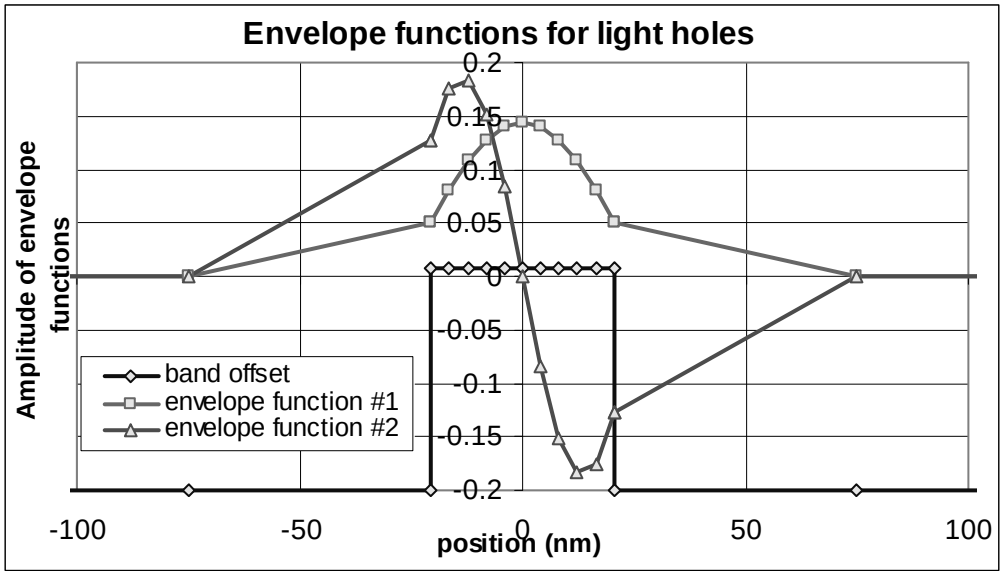

Fig. C.5.4. Envelope functions for light holes

b) The main output file from this part of GAIN program is energy.dat, containing all the energy levels as shown in Table C.5.5. After the energy eigen values are calculated, the GAIN program asks the user whether he would like to check the wave envelope function or not. We suggest that the user check the wave envelope functions of the first and second energy levels for conduction and valence bands.

Table C.5.5. output file energy.dat

```
CONDUCTION BAND ENERGY===>  0.961974438375E-02 ERROR= .2786910E-14

 CONDUCTION BAND ENERGY===>  0.743662554277E-01 ERROR= .2580380E-14

 CONDUCTION BAND ENERGY===>  0.107675191040E+00 ERROR= .4266368E-14

 CONDUCTION BAND ENERGY===>  0.107688174734E+00 ERROR= .2463437E-14

 CONDUCTION BAND ENERGY===>  0.108376258685E+00 ERROR= .6317963E-14

 CONDUCTION BAND ENERGY===>  0.108428037338E+00 ERROR= .1442872E-14
```

CONDUCTION BAND ENERGY===> 0.109543687391E+00 ERROR= .2900562E-14

CONDUCTION BAND ENERGY===> 0.109659654907E+00 ERROR= .1483391E-14

CONDUCTION BAND ENERGY===> 0.111175954839E+00 ERROR= .2524093E-14

CONDUCTION BAND ENERGY===> 0.111380963353E+00 ERROR= .1915930E-14

CONDUCTION BAND ENERGY===> 0.113270939913E+00 ERROR= .2521982E-14

CONDUCTION BAND ENERGY===> 0.113589356334E+00 ERROR= .2292240E-14

CONDUCTION BAND ENERGY===> 0.115825939696E+00 ERROR= .2102730E-14

CONDUCTION BAND ENERGY===> 0.116281876661E+00 ERROR= .1980838E-14

CONDUCTION BAND ENERGY===> 0.118837702628E+00 ERROR= .2070679E-14

CONDUCTION BAND ENERGY===> 0.119455372783E+00 ERROR= .1414132E-14

CONDUCTION BAND ENERGY===> 0.122302488065E+00 ERROR= .2748183E-14

CONDUCTION BAND ENERGY===> 0.123106599250E+00 ERROR= .1286513E-14

CONDUCTION BAND ENERGY===> 0.126216164546E+00 ERROR= .2382521E-14

CONDUCTION BAND ENERGY===> 0.127232254643E+00 ERROR= .1318435E-14

CONDUCTION BAND ENERGY===> 0.130574357571E+00 ERROR= .3582667E-14

CONDUCTION BAND ENERGY===> 0.131828958191E+00 ERROR= .2236097E-14

CONDUCTION BAND ENERGY===> 0.135372648300E+00 ERROR= .2832335E-14

CONDUCTION BAND ENERGY===> 0.136893165876E+00 ERROR= .2662248E-14

CONDUCTION BAND ENERGY===> 0.140606801955E+00 ERROR= .2075560E-14

CONDUCTION BAND ENERGY===> 0.142421018041E+00 ERROR= .2486680E-14

CONDUCTION BAND ENERGY===> 0.146272964900E+00 ERROR= .2509426E-14

CONDUCTION BAND ENERGY===> 0.148408090543E+00 ERROR= .1416510E-14

CONDUCTION BAND ENERGY===> 0.152367710782E+00 ERROR= .3201183E-14

CONDUCTION BAND ENERGY===> 0.154848978871E+00 ERROR= .2597122E-14

CONDUCTION BAND ENERGY===> 0.158887734556E+00 ERROR= .1766965E-14

CONDUCTION BAND ENERGY===> 0.161736541616E+00 ERROR= .2628242E-14

CONDUCTION BAND ENERGY===> 0.165828843460E+00 ERROR= .2472018E-14

CONDUCTION BAND ENERGY===> 0.169060333436E+00 ERROR= .1986998E-14

CONDUCTION BAND ENERGY===> 0.173183433744E+00 ERROR= .3017043E-14

CONDUCTION BAND ENERGY===> 0.176802685912E+00 ERROR= .1597014E-14

CONDUCTION BAND ENERGY===> 0.180933567715E+00 ERROR= .2328795E-14

CONDUCTION BAND ENERGY===> 0.184925313643E+00 ERROR= .2516799E-14

CONDUCTION BAND ENERGY===> 0.189021845141E+00 ERROR= .1893777E-14

CONDUCTION BAND ENERGY===> 0.193267857341E+00 ERROR= .2992086E-14

HEAVY HOLE ENERGY===> -0.361192916606E+00 ERROR= .2318346E-14

HEAVY HOLE ENERGY===> -0.358485532473E+00 ERROR= .4956447E-14

HEAVY HOLE ENERGY===> -0.354716248972E+00 ERROR= .5526373E-14

HEAVY HOLE ENERGY===> -0.351913554427E+00 ERROR= .5317960E-14

HEAVY HOLE ENERGY===> -0.348266207154E+00 ERROR= .2918676E-14

HEAVY HOLE ENERGY===> -0.345413437374E+00 ERROR= .3749323E-14

HEAVY HOLE ENERGY===> -0.341928545612E+00 ERROR= .3487911E-14

HEAVY HOLE ENERGY===> -0.339023804865E+00 ERROR= .4983602E-14

HEAVY HOLE ENERGY===> -0.335719117586E+00 ERROR= .2977748E-14

HEAVY HOLE ENERGY===> -0.332757485607E+00 ERROR= .2663835E-14

HEAVY HOLE ENERGY===> -0.329642979500E+00 ERROR= .4769990E-14

HEAVY HOLE ENERGY===> -0.326621008574E+00 ERROR= .2474339E-14

HEAVY HOLE ENERGY===> -0.323701256646E+00 ERROR= .4188658E-14

HEAVY HOLE ENERGY===> -0.320618410761E+00 ERROR= .4940924E-14

HEAVY HOLE ENERGY===> -0.317893261288E+00 ERROR= .3395574E-14

HEAVY HOLE ENERGY===> -0.314752486888E+00 ERROR= .2722462E-14

HEAVY HOLE ENERGY===> -0.312217533281E+00 ERROR= .3080726E-14

HEAVY HOLE ENERGY===> -0.309025316890E+00 ERROR= .3714707E-14

HEAVY HOLE ENERGY===> -0.306672506150E+00 ERROR= .3651204E-14

HEAVY HOLE ENERGY===> -0.303438526815E+00 ERROR= .4852848E-14

HEAVY HOLE ENERGY===> -0.301256950156E+00 ERROR= .2606583E-14

HEAVY HOLE ENERGY===> -0.297993433199E+00 ERROR= .3079430E-14

HEAVY HOLE ENERGY===> -0.295970220156E+00 ERROR= .3775307E-14

HEAVY HOLE ENERGY===> -0.292691130035E+00 ERROR= .5023247E-14

HEAVY HOLE ENERGY===> -0.290812329627E+00 ERROR= .4216785E-14

HEAVY HOLE ENERGY===> -0.287532544737E+00 ERROR= .2473812E-14

HEAVY HOLE ENERGY===> -0.285783893576E+00 ERROR= .3723957E-14

HEAVY HOLE ENERGY===> -0.282518476130E+00 ERROR= .5303396E-14

HEAVY HOLE ENERGY===> -0.280885995969E+00 ERROR= .4570210E-14

HEAVY HOLE ENERGY===> -0.277649621354E+00 ERROR= .3537788E-14

HEAVY HOLE ENERGY===> -0.276120032911E+00 ERROR= .4293540E-14

HEAVY HOLE ENERGY===> -0.272926595561E+00 ERROR= .3632004E-14

HEAVY HOLE ENERGY===> -0.271487567178E+00 ERROR= .2909894E-14

HEAVY HOLE ENERGY===> -0.268349946744E+00 ERROR= .3976899E-14

HEAVY HOLE ENERGY===> -0.266990212090E+00 ERROR= .4204415E-14

HEAVY HOLE ENERGY===> -0.263920167090E+00 ERROR= .1103405E-13

HEAVY HOLE ENERGY===> -0.262629549143E+00 ERROR= .1689306E-14

HEAVY HOLE ENERGY===> -0.259637701783E+00 ERROR= .3319052E-14

HEAVY HOLE ENERGY===> -0.258407076018E+00 ERROR= .3786958E-14

HEAVY HOLE ENERGY===> -0.255502955805E+00 ERROR= .1151041E-13

HEAVY HOLE ENERGY===> -0.254324178366E+00 ERROR= .4380337E-14

HEAVY HOLE ENERGY===> -0.251516299101E+00 ERROR= .1407601E-13

HEAVY HOLE ENERGY===> -0.250382118475E+00 ERROR= .2547440E-14

HEAVY HOLE ENERGY===> -0.247678070270E+00 ERROR= .9114289E-14

HEAVY HOLE ENERGY===> -0.246582034966E+00 ERROR= .2802900E-14

HEAVY HOLE ENERGY===> -0.243988578824E+00 ERROR= .4761360E-14

HEAVY HOLE ENERGY===> -0.242924949068E+00 ERROR= .2434459E-14

HEAVY HOLE ENERGY===> -0.240448105895E+00 ERROR= .3480106E-14

HEAVY HOLE ENERGY===> -0.239411774399E+00 ERROR= .4274582E-14

HEAVY HOLE ENERGY===> -0.237056903110E+00 ERROR= .6999869E-14

HEAVY HOLE ENERGY===> -0.236043328190E+00 ERROR= .3901435E-14

HEAVY HOLE ENERGY===> -0.233815189170E+00 ERROR= .4571935E-14

HEAVY HOLE ENERGY===> -0.232820342717E+00 ERROR= .2810531E-14

HEAVY HOLE ENERGY===> -0.230723143380E+00 ERROR= .3910965E-14

HEAVY HOLE ENERGY===> -0.229743476197E+00 ERROR= .1968086E-14

HEAVY HOLE ENERGY===> -0.227780895151E+00 ERROR= .4565070E-14

HEAVY HOLE ENERGY===> -0.226813322769E+00 ERROR= .2321745E-14

HEAVY HOLE ENERGY===> -0.224988508124E+00 ERROR= .5484183E-14

HEAVY HOLE ENERGY===> -0.224030421380E+00 ERROR= .1919168E-14

HEAVY HOLE ENERGY===> -0.222345957410E+00 ERROR= .1879845E-14

HEAVY HOLE ENERGY===> -0.221395263540E+00 ERROR= .1827758E-14

HEAVY HOLE ENERGY===> -0.219853098509E+00 ERROR= .4186959E-14

HEAVY HOLE ENERGY===> -0.218908299959E+00 ERROR= .3620360E-14

HEAVY HOLE ENERGY===> -0.217509627335E+00 ERROR= .2453680E-14

HEAVY HOLE ENERGY===> -0.216569946120E+00 ERROR= .3220033E-14

HEAVY HOLE ENERGY===> -0.215315033070E+00 ERROR= .3463684E-14

HEAVY HOLE ENERGY===> -0.214380586860E+00 ERROR= .2219382E-14

HEAVY HOLE ENERGY===> -0.213268550022E+00 ERROR= .2777570E-14

HEAVY HOLE ENERGY===> -0.212340580018E+00 ERROR= .2743067E-14

HEAVY HOLE ENERGY===> -0.211369121597E+00 ERROR= .4226083E-14

HEAVY HOLE ENERGY===> -0.210450259232E+00 ERROR= .3692444E-14

HEAVY HOLE ENERGY===> -0.209615397194E+00 ERROR= .3171740E-14

HEAVY HOLE ENERGY===> -0.208709935933E+00 ERROR= .4209780E-14

HEAVY HOLE ENERGY===> -0.208005786497E+00 ERROR= .1814778E-14

HEAVY HOLE ENERGY===> -0.207119900601E+00 ERROR= .3397305E-14

HEAVY HOLE ENERGY===> -0.206538587407E+00 ERROR= .3003403E-14

HEAVY HOLE ENERGY===> -0.205680423359E+00 ERROR= .3543397E-14

HEAVY HOLE ENERGY===> -0.205212178908E+00 ERROR= .2834381E-14

HEAVY HOLE ENERGY===> -0.204391753956E+00 ERROR= .3372802E-14

HEAVY HOLE ENERGY===> -0.204025235404E+00 ERROR= .1580920E-14

HEAVY HOLE ENERGY===> -0.203254121238E+00 ERROR= .3043020E-14

HEAVY HOLE ENERGY===> -0.202976896095E+00 ERROR= .2298392E-14

HEAVY HOLE ENERGY===> -0.202267732184E+00 ERROR= .3884085E-14

HEAVY HOLE ENERGY===> -0.202066832823E+00 ERROR= .1442648E-14

HEAVY HOLE ENERGY===> -0.201432770625E+00 ERROR= .3171156E-14

HEAVY HOLE ENERGY===> -0.201295200743E+00 ERROR= .2947302E-14

HEAVY HOLE ENERGY===> -0.200749395757E+00 ERROR= .5270798E-14

HEAVY HOLE ENERGY===> -0.200662501388E+00 ERROR= .1723172E-14

HEAVY HOLE ENERGY===> -0.200217740582E+00 ERROR= .3038427E-14

HEAVY HOLE ENERGY===> -0.200169410122E+00 ERROR= .1957778E-14

HEAVY HOLE ENERGY===> -0.199837910396E+00 ERROR= .3248494E-14

HEAVY HOLE ENERGY===> -0.199816614058E+00 ERROR= .1532467E-14

HEAVY HOLE ENERGY===> -0.199609981468E+00 ERROR= .5295449E-14

HEAVY HOLE ENERGY===> -0.199604685919E+00 ERROR= .1312598E-14

HEAVY HOLE ENERGY===> -0.148632604544E+00 ERROR= .2080935E-14

HEAVY HOLE ENERGY===> -0.876451923558E-01 ERROR= .2306744E-14

HEAVY HOLE ENERGY===> -0.412267198395E-01 ERROR= .2280033E-14

HEAVY HOLE ENERGY===> -0.126212972547E-01 ERROR= .1971012E-14

LIGHT HOLE ENERGY===> -0.355569923291E+00 ERROR= .2120444E-14

LIGHT HOLE ENERGY===> -0.350213432069E+00 ERROR= .2426284E-14

LIGHT HOLE ENERGY===> -0.342922783182E+00 ERROR= .3165783E-14

LIGHT HOLE ENERGY===> -0.337911435179E+00 ERROR= .5718315E-14

LIGHT HOLE ENERGY===> -0.330625015453E+00 ERROR= .2861106E-14

LIGHT HOLE ENERGY===> -0.326008761019E+00 ERROR= .4734580E-14

LIGHT HOLE ENERGY===> -0.318798731413E+00 ERROR= .1888460E-14

LIGHT HOLE ENERGY===> -0.314568675940E+00 ERROR= .1013061E-13

LIGHT HOLE ENERGY===> -0.307483438965E+00 ERROR= .3719772E-14

LIGHT HOLE ENERGY===> -0.303617431871E+00 ERROR= .5426840E-14

LIGHT HOLE ENERGY===> -0.296698810286E+00 ERROR= .1928970E-14

LIGHT HOLE ENERGY===> -0.293170593472E+00 ERROR= .4117972E-14

LIGHT HOLE ENERGY===> -0.286456711046E+00 ERROR= .2087373E-14

LIGHT HOLE ENERGY===> -0.283239553955E+00 ERROR= .5116587E-14

LIGHT HOLE ENERGY===> -0.276765133426E+00 ERROR= .4002561E-14

LIGHT HOLE ENERGY===> -0.273833711271E+00 ERROR= .3188520E-14

LIGHT HOLE ENERGY===> -0.267629853353E+00 ERROR= .2473219E-13

LIGHT HOLE ENERGY===> -0.264961286499E+00 ERROR= .4783343E-14

LIGHT HOLE ENERGY===> -0.259055249198E+00 ERROR= .1445075E-13

LIGHT HOLE ENERGY===> -0.256629650468E+00 ERROR= .2986270E-14

LIGHT HOLE ENERGY===> -0.251044756020E+00 ERROR= .4368280E-14

LIGHT HOLE ENERGY===> -0.248845466028E+00 ERROR= .3916633E-14

LIGHT HOLE ENERGY===> -0.243601143953E+00 ERROR= .3203893E-14

LIGHT HOLE ENERGY===> -0.241614764042E+00 ERROR= .3829278E-14

LIGHT HOLE ENERGY===> -0.236726707646E+00 ERROR= .2318723E-14

LIGHT HOLE ENERGY===> -0.234942997591E+00 ERROR= .4144951E-14

LIGHT HOLE ENERGY===> -0.230423413478E+00 ERROR= .3722336E-14

LIGHT HOLE ENERGY===> -0.228835088921E+00 ERROR= .1889767E-14

LIGHT HOLE ENERGY===> -0.224693035843E+00 ERROR= .7133531E-14

LIGHT HOLE ENERGY===> -0.223295471814E+00 ERROR= .2689170E-14

LIGHT HOLE ENERGY===> -0.219537311510E+00 ERROR= .3510794E-14

LIGHT HOLE ENERGY===> -0.218328128086E+00 ERROR= .1768869E-14

LIGHT HOLE ENERGY===> -0.214958149620E+00 ERROR= .2491797E-14

LIGHT HOLE ENERGY===> -0.213936616153E+00 ERROR= .2951357E-14

LIGHT HOLE ENERGY===> -0.210957957871E+00 ERROR= .5197287E-14

LIGHT HOLE ENERGY===> -0.210124090200E+00 ERROR= .3596255E-14

LIGHT HOLE ENERGY===> -0.207540190458E+00 ERROR= .2365701E-14

LIGHT HOLE ENERGY===> -0.206893309508E+00 ERROR= .1630595E-14

LIGHT HOLE ENERGY===> -0.204710293790E+00 ERROR= .2473877E-14

LIGHT HOLE ENERGY===> -0.204246638588E+00 ERROR= .1699402E-14

LIGHT HOLE ENERGY===> -0.202477269514E+00 ERROR= .4978716E-14

LIGHT HOLE ENERGY===> -0.202186039835E+00 ERROR= .1133236E-14

LIGHT HOLE ENERGY===> -0.200855776105E+00 ERROR= .3613962E-14

LIGHT HOLE ENERGY===> -0.200713061214E+00 ERROR= .2681968E-14

LIGHT HOLE ENERGY===> -0.199867089971E+00 ERROR= .4376218E-14

LIGHT HOLE ENERGY===> -0.199828822046E+00 ERROR= .2747680E-14

LIGHT HOLE ENERGY===> -0.194053584736E+00 ERROR= .2807414E-14

LIGHT HOLE ENERGY===> -0.921176591126E-01 ERROR= .2804206E-14

LIGHT HOLE ENERGY===> -0.113712309471E-01 ERROR= .2367096E-14

C.5.3. Computation of Gain and Laser Characteristics

This is the last step of simulations using the GAIN program. With the previous calculated material composition, energy band edges, energy levels, and other parameters like material loss and Auger coefficient, the GAIN program can simulate the threshold current, threshold current density, slope efficiency, optical gain and mode gain as functions of wavelengths and photo energies, and L-I curve. The details are explained in Chapter 4 of the manual, and the basic theory is discussed in Appendix C.

In this part of GAIN program, the input file needs to be constructed with the results of the previous steps and according to the laser design. In this example, single quantum well structure is used with a ridge length of 500 μm and ridge width of 5 μm, the input file is shown in Table C.5.6. The detailed steps of simulations are listed in Table C.5.7. The main output files: L-I curve, optical gain as a function of the wavelength, and mode gain vs. current density are plotted in Fig. C.5.5, Fig. C.5.6, and Fig. C.5.7.

a) The input file:

Table C.5.6. Input file for gain and threshold current calculation

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c    1. Input the compositions, width of well, effective index       c
c      and lasing wavelength.                                        c
c    Ex: xx,xz,qy,xy,lx,n,lam                                        c
c    for different materials the following are the forms of inputs.  c
c                                                                    c
c    w -- > well, b -- > barrier  cxz and cxy for cladding.          c
c                                                                    c
c    a.  AlxGa1-xAs : xx (Al w) xz (Al b) qy (0) xy (0)              c
c    b.  In1-xGaxAsyP1-y : xx (Ga w) xz (Ga b) qy (As w) xy (As b)   c
c    c.  In1-xGaxAs/InGaAsP : xx (Ga w) xz (Ga b) qy (0) xy (As b)   c
c    d.  AlxGayIn1-x-yAs/InP : xx (Ga w) xz (Ga b) qy (Al w) xy (Al b)c
c    e.                                                              c
c    f.  InxGa1-xAs/AlGaAs : xx (In w) xz (0) qy (0) xy (Al b)       c
c    g.                                                              c
c    h.  AlyInxGa1-x-yAs/AlGaAs : xx (Al w) xz (al b) qy (In w) xz (0)c
c    i.  InxGa1-xAs/AlGaInAs : xx (In w) xz (0) qy (Al b) xy (Ga b)  c
c    j.  In(y)Ga(1-y)As(x)N(1-x) :xx(As w),xz(As, b),qy(In w),xy(In b)c
c    k.  InGaAs/InGaAsP/GaAs: xx (In w), (0), xz(Ga w) xy (As b)
c    2. Input the energy gap,temperature, barrier band edges(both bands)
c    Ex: eg,temp,ec,ev                                               c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
0.4 0.0E+00 0.3 0.2  8D0 3.329233 0.635d0
1.968 300  0.1074 0.1995
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c    3. Input the ist level sub-band energy levels.                  c
c    Ex: ec1,eh1,el1                                                 c
c                                                                    c
```

```
c     4. Input the material loss, reflectivities, number of quantum     c
c        wells and beta(for spontaneous emission).                      c
c     Ex: alpha,r1,r2,mm,beta.                                          c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
0.00962 0.01262 0.01137 0.07437 0.04123 0.09212
2.0d0  0.300   0.300   1  5.D-5
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c     5. Input the cavity length, ridge width, internal efficiency      c
c        Auger, strain(except AlGaAs,put 0) and confinement factor.     c
c     Ex: cl,cw,etha,ca,es,confine                                      c
c                                                                       c
c     6. Input the cladding composition and band edges.                 c
c     Ex: cxz,cxy,ecc,evv                                               c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
500.D-4  5.0D-4  0.97  1.00d-29   0.0027  0.03028
0.0  0.5  0.195 0.362
```

b) The steps for these calculations mentioned are listed in Table C.5.7

Table C.5.7. The steps for the gain and threshold current density calculations

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

5
 THE INPUT FILE NAME=
RED2
 SELECT MATERIAL=?
 1--AlGaAs
 2--InGaAsP
 3--In1-zGazAs/InGaAsP/InP
 4-- InGaAlAs
 5--GaInP/AlzGawIn1-z-wP/Al0.5In0.5P
 6-- InxGa1-xAs/AlxGa1-xAs/AlGaAs
 7--In1-xGaxAs/InGaAsP/GaxIn1-xP(X=0.51) MATCHED TO GaAs
 8--AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
 9--InzGa1-zAs/AlxGayIn1-x-yAs/InP
 10-- InGaAlAs/InGaAlAs/AlAsSb
 11--InzGa1-zAs/AlxGayIn1-x-yAs/AlAsSb
 12--In(y)Ga(1-y)As(x)N(1-x)/GaAs
 13--InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
 INPUT SELECTION
5
 INPUT MODE = ? FOR TE--> MODE =1, FOR TM--> MODE =2
  INPUT TE OR TM ?
1
 IF EL1 BELOW EH1 THEN SELECT 1, OTHERWISE SELECT 2
  SELECTION=?
1
 ************************************************
 CALCULATE THE EFFECTIVE MASS
```

```
 ************************************************
 FOR QUASI-FERMI LEVEL SELECT=1,
 FOR READ EXISTING QUASI-FERMI LEVEL SELECT=2
 SELECT=?
1

…….
 J(LEAKAGE)=0.235638D+05 A/cm^2  N=0.792080D+19 1/cm^3
 J(LEAKAGE)=0.238799D+05 A/cm^2  N=0.794060D+19 1/cm^3
 J(LEAKAGE)=0.241994D+05 A/cm^2  N=0.796040D+19 1/cm^3
 J(LEAKAGE)=0.245222D+05 A/cm^2  N=0.798020D+19 1/cm^3
 J(LEAKAGE)=0.248484D+05 A/cm^2  N=0.800000D+19 1/cm^3
 ************************************************
 G(J) PARAMETERS FROM SINGLE WELL
 Go=0.279835D+02 1/cm  Jo=0.595524D+03 A/cm^2

 G(N) PARAMETERS FROM SINGLE WELL
 NGo=0.924158D+03 1/cm  XNo=0.213935D+19 1/cm^3

 Jtr=0.219081D+03 A/cm^2  NTR=0.787022D+18 1/cm^3


 THE OPTIMUM NUMBER OF QUANTUM WELL FOLLOWS THE ARTICLE
 BY McIlory et al. IEEE JQE-21 1985.

 THE OPTIMUM NUMBER OF QUANTUM WELL Nopt =          1
 INPUT Nopt(CAN BE DIFFERENT FROM ABOVE CALCULATION)=?
1
 NUMBER OF QUANTUM WELL(MAY OR MAY NOT BE Nopt)=?
1

 ************************************************
 ************************************************
 1ST CHECK USE SINGLE WELL TIMES # OF WELLS
 ************************************************
 ************************************************
 2ND CHECK FOLLOWS FORMULA BY McIlory IN IEEE
 JOURNAL OF QUANTUM ELECTRONIC QE-21 1985.
 ************************************************
 Gth=  26.0795 1/cm Nth=0.206015D+19 1/cm^3 IY=  100
  1ST CHECK Jth=   559.67770378 A/cm^2
  2ND CHECK Jth=   613.94244 A/cm^2

  1ST CHECK Ith=0.139919D+02 mA NUMBER OF WELLS=  1
  2ND CHECK Ith=0.153486D+02 mA

 ************************************************
 CALCULATE THE P-I RELATION

 NDATA=        301
 ************************************************
 CALCULATE THE SLOPE: mW/mA Y=A+BX
 CONSTANT A= -12.2471182   SLOPE B=   0.8752979

 ************************************************
 INPUT POWER PO FOR THE LINEWIDTH, PO=0 FOR STOP
```

```
 INPUT PO=    mW
0
 INPUT 1 FOR THE DYNAMIC CALCULATION. 2 FOR SKIP
 INPUT =
2
 K-FACTOR= 0.23795 nS  MAXIUM FREQ.= 37.3426 GHz

 ************************************************
 INPUT 1 FOR CALCULATE THE GAIN(E) RELATION.

 INPUT 2 FOR CALCULATE THE LINEWIDTH ENHENCEMENT
 FACTOR AND PHOTON ENERGY RELATION

 INPUT 3 FOR EXIT THE PROGRAM

 THE INPUT # IS
1
 INPUT FERMILEVELS IN C-BAND, V-BAND, AND CARRIER DENSITY
0.0908 0.00389 3E18
 CALCULATE THE CONVOLUTION GAIN(E) COEFFICIENT
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(LAMBDA)
gl3
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(LAMBDA)
glm3
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(E)
ge3
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(E)
gem3
 ************************************************
 INPUT 1 FOR REPEAT THE G(E) CALCULATION
 INPUT 2 FOR REPEAT THE ALPHA(E) CALCULATION
 INPUT 3 FOR EXIT
1
 ************************************************
 INPUT 1 FOR CALCULATE THE GAIN(E) RELATION.

 INPUT 2 FOR CALCULATE THE LINEWIDTH ENHENCEMENT
 FACTOR AND PHOTON ENERGY RELATION

 INPUT 3 FOR EXIT THE PROGRAM

 THE INPUT # IS
1
 INPUT FERMILEVELS IN C-BAND, V-BAND, AND CARRIER DENSITY
0.0332 -0.0289 1E18
 CALCULATE THE CONVOLUTION GAIN(E) COEFFICIENT
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(LAMBDA)
gl1
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(LAMBDA)
glm1
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(E)
```

```
ge1
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(E)
gem1
 ************************************************
 INPUT 1 FOR REPEAT THE G(E) CALCULATION
 INPUT 2 FOR REPEAT THE ALPHA(E) CALCULATION
 INPUT 3 FOR EXIT
1
 ************************************************
  INPUT 1 FOR CALCULATE THE GAIN(E) RELATION.

  INPUT 2 FOR CALCULATE THE LINEWIDTH ENHENCEMENT
  FACTOR AND PHOTON ENERGY RELATION

  INPUT 3 FOR EXIT THE PROGRAM

 THE INPUT # IS
1
 INPUT FERMILEVELS IN C-BAND, V-BAND, AND CARRIER DENSITY
0.132 0.0214 5E18
 CALCULATE THE CONVOLUTION GAIN(E) COEFFICIENT
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(LAMBDA)
gl5
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(LAMBDA)
glm5
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(E)
ge5
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(E)
gem5
 ************************************************
 INPUT 1 FOR REPEAT THE G(E) CALCULATION
 INPUT 2 FOR REPEAT THE ALPHA(E) CALCULATION
 INPUT 3 FOR EXIT
3
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

7
```

c) The Output characteristics of designed laser from step 5 are summarized in Table C.5.7.

Table C.5.7 Characteristics of the designed laser

Optimized number of QWs (Nopt)	2
Number of QWs	3
Slope efficiency (%)	21.84

Jth (A/cm^2)	560 - 1st check, for matching threshold conditions 614 – 2nd check, using McIlory method
Ith (mA)	14.0 mA - 1st check, for matching threshold conditions 15.3 mA - 2nd check, using McIlory method
Peak λ at operating temperature (um)	631 nm for carrier density of 3.0E18 /cm3 631 nm for carrier density of 5.0E18 /cm3
Peak material gain (1/cm)	3152 /cm for carrier density of 2.0E18 /cm3 4808 /cm for carrier density of 2.0E18 /cm3

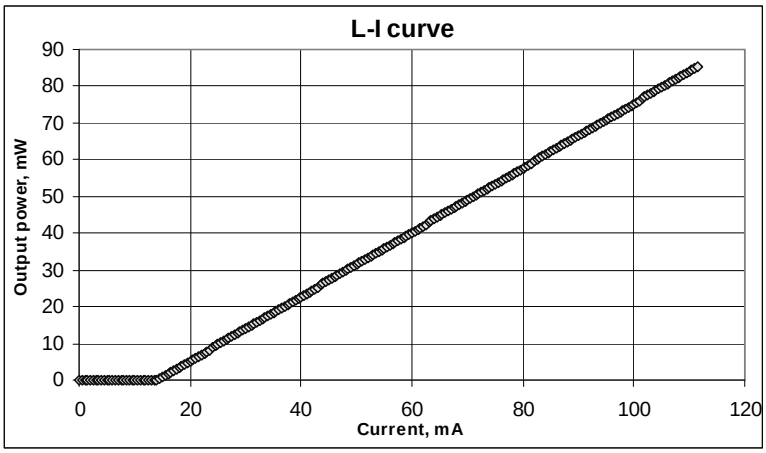

Fig. C.5.5. L-I curve of the laser

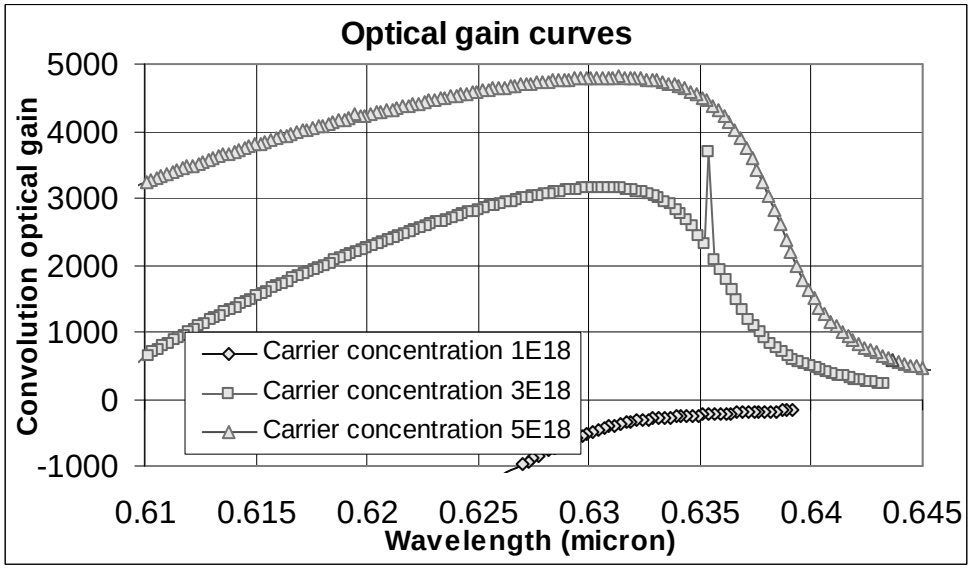

Fig. C.5.6. Optical gain-λ curve of the laser

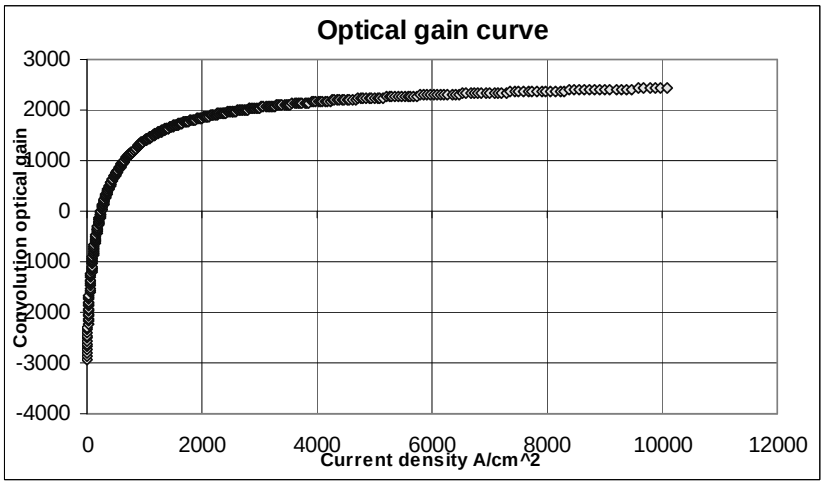

Fig. C.5.7. Mode gain as a function of current density (J)

C.6. Material system #6: InGaAs/AlGaAs/AlGaAs

This is a simulation of a five-layer laser structure that contains a single compressively strained quantum well (QW), two separated confinement heterostructure (SCH) layers, and two cladding layers as shown in Fig. C.6.1.

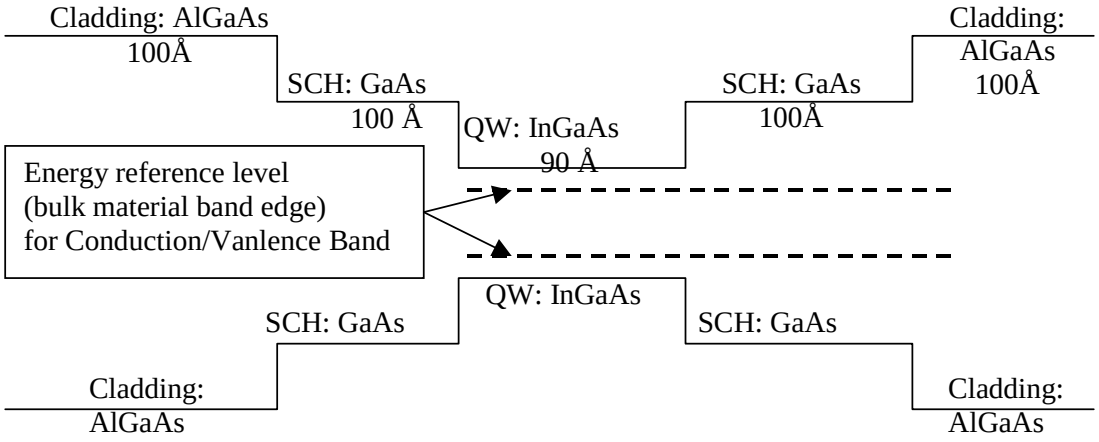

Figure C.6.6. Energy band diagram for the single quantum well structure

C.6.1. Calculation of material compositions and energy band edges.

The first step of the GAIN program is to calculate the material compositions and energy band edges of the each layer. The user is asked to enter the photoluminescence wavelength, thickness, and strain of the QW, SCH, and cladding layers. After these parameters are input, the GAIN program generates two output files: cbandeg.dat and vbandeg.dat, containing the material compositions, and the conduction band edges and valence band edges respectively. The detailed explanation is provided in Chapter 2 of this manual.

a) The input parameters to the GAIN program in this step are listed in Table. C.6.1.

Table C.6.1. Input parameters to the GAIN program in this step.

Layer	λ (um)	Strain	Thickness (Å)
QW ($In_xGa_{1-x}As_{1-y}$)	1.06	-0.0119285	90
SCH ($Al_xGa_{1-x}As_{1-y}$)	0.871	-	100
Cladding ($Al_xGa_{1-x}As_{1-y}$)	0.6665	-	100

b) The steps in using the GAIN program to calculate the material compositions and energy band edges are listed in Table C.6.2

Table C.6.2. Steps to run the GAIN program for necessary parameters.

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

1

 ENTER 1 FOR AlGaAs/AlGaAs
      2 FOR InGaAsP/InGaAsP/InP
      3 FOR InGaAs/InGaAsP/InP
      4 FOR InGaAlAs/InGaAlAs/InP
      5 FOR GaInP/(AlGa)0.5In0.5P/AlInP
```

6 FOR InGaAs/AlGaAs/AlGaAs

```
      7 FOR InGaAs/InGaAsP/Ga0.51In0.49P(MATCHED GaAs)
      8 FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
      9 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/InP
     10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(matched InP)
     11 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/AlAsxSb1-x
     12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs (dilute N)
     13 FOR In(1-x)Ga(x)As(y)P(1-y)/GaAs
     14 FOR EXIT, BACK TO MAIN PAGE!
6
 INPUT THE LAYER # FOR GRIN STRUCTURE(STEP)
 STEP N=
2
  INPUT THE WELL WAVELENGTH (um)
1.06
  INPUT THE BARRIER WAVELENGTH (um)
0.871
  INPUT THE CLADDING WAVELENGTH (um)
0.6665
  BANDGAP ENERGY OF QUANTUM WELL=    1.16981132075472       eV
  INPUT CLADDING, BARRIER,QUANTUM WELL WIDTH (A)
100 100 90
  STRAIN FOR InGaAs/AlGaAs IS  -1.192854285325509E-002

  WRITE CONDUCTION BAND PARAMETERS INTO CBANDEG.DAT

  WRITE VALENCE BAND PARAMETERS INTO VBANDEG.DAT
  INPUT 1 FOR NEW CALCULATION, 2 FOR EXIT
  I= ?
2

 ENTER 1 FOR AlGaAs/AlGaAs
      2 FOR InGaAsP/InGaAsP/InP
      3 FOR InGaAs/InGaAsP/InP
      4 FOR InGaAlAs/InGaAlAs/InP
      5 FOR GaInP/(AlGa)0.5In0.5P/AlInP
      6 FOR InGaAs/AlGaAs/AlGaAs
      7 FOR InGaAs/InGaAsP/Ga0.51In0.49P(MATCHED GaAs)
      8 FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
```

```
     9 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/InP
    10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(matched InP)
    11 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/AlAsxSb1-x
    12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs (dilute N)
    13 FOR In(1-x)Ga(x)As(y)P(1-y)/GaAs
    14 FOR EXIT, BACK TO MAIN PAGE!
14
 THIS PROGRAM STOP HERE!, BACK TO MAIN PAGE
```

c) The output files, cbandeg.dat and vbandeg.dat are explained in Table C.6.3.

Table C.6.3. Material compositions and band offsets:

a) cbandeg.dat for conduction band

```
*************************************************************************
 QW strain   lattice constant
 -.119285E-01  0.572074E-09
                        material compositions(see Table C.6.1 for x and y)
 layer thickness,          x                  y      conduction band edges
  0.10000000E+03  0.35001212E+00   0.0000000   0.4143923      cladding layer
  0.10000000E+03  0.00000000E+00   0.0000000   0.1525132      SCH layer
  0.90000000E+02  0.16650773E+00   0.0000000   0.0779318      quantum well
  0.10000000E+03  0.00000000E+00   0.0000000   0.1525132      SCH layer
  0.10000000E+03  0.35001212E+00   0.0000000   0.4143923      cladding layer
*************************************************************************
```

b) vbandeg.dat for valence band

```
*************************************************** ********************
 QW strain   lattice constant
-.119285E-01  0.572074E-09
                        material compositions(see Table C.6.1 for x and y)
 layer thickness,          x                  y     valence band edges
  0.10000000E+03  0.35001212E+00   0.0000000   -0.2762615     cladding layer
  0.10000000E+03  0.00000000E+00   0.0000000   -0.1016755     SCH layer
  0.90000000E+02  0.16650773E+00   0.0000000   -0.0389659     quantum well
  0.10000000E+03  0.00000000E+00   0.0000000   -0.1016755     SCH layer
  0.10000000E+03  0.35001212E+00   0.0000000   -0.2762615     cladding layer
*************************************************************************
```

C.6.2. Energy level calculations

After the calculation of the material compositions and energy band edges, the GAIN program calculates energy levels in the conduction band and valence bands. The detailed explanations are discussed in Chapter 3 of this manual.

a) The steps of how to calculate the energy levels are shown in Table C.6.4.

Table C.6.4. Steps to calculate the energy levels

i) Steps to calculate the conduction band energy levels

```
ENTER 1 FOR THE NECESSARY PARAMETERS
     2 FOR THE ENERGY VALUES OF CONDUCTION BAND
```

```
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

2
 INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
 INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
 INPUT N=
5
 INPUT THE LOWEST POTENTIAL LAYER(1st Q-WELL) IC= ?
3
 INPUT THE SELECTED CENTER LAYER OF STRUCTURE ICR=
3
 ********************************************************
  INPUT I=1  FOR AlGaAs
       I=2  FOR InGaAsP
       I=3  FOR In1-xGaxAs/InGaAsP/InP
       I=4  FOR InGaAlAs/InGaAlAs
       I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
       I=6  FOR InGaAs/AlGaAs/AlGaAs
       I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
       I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
       I=9  FOR InzGa1-zAs/AlxGayIn1-x-yAs/InP
       I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
       I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
       I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
       I=13 FOR InGaAs/In(1-y)Ga(x)As(y)P(1-y)/GaAs
  INPUT I= ?
 ********************************************************
6
 ENERGY EIGENVALUE===>  0.103971205206E+00 ERROR= .2196720E-14
 ENERGY EIGENVALUE===>  0.160339839908E+00 ERROR= .4536506E-14
 ENERGY EIGENVALUE===>  0.188593940032E+00 ERROR= .1502184E-14
 ENERGY EIGENVALUE===>  0.216772324699E+00 ERROR= .1762640E-14
 ENERGY EIGENVALUE===>  0.274768762405E+00 ERROR= .2171751E-14
 ENERGY EIGENVALUE===>  0.325125329658E+00 ERROR= .2457422E-14
 ENERGY EIGENVALUE===>  0.391898735270E+00 ERROR= .3003635E-14
 FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
 SKIP INPUT I==> 2
 I=?
1
 INPUT THE EIGENVALUE
0.103971205206E+00
 INPUT THE NAME OF OUTPUT FILE
cb1.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.30876860E-04
 CONFINEMENT FACTOR OF    2 th LAYER = 0.77269958E-01
 CONFINEMENT FACTOR OF    3 th LAYER = 0.84539833E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.77269958E-01
 CONFINEMENT FACTOR OF    5 th LAYER = 0.30876860E-04
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
1
```

```
 INPUT THE EIGENVALUE
 EIGEN VALUE=
0.160339839908E+00
 INPUT THE NAME OF OUTPUT FILE
cb2.txt
CONFINEMENT FACTOR OF    1 th LAYER = 0.17971109E-02
CONFINEMENT FACTOR OF    2 th LAYER = 0.34495801E+00
CONFINEMENT FACTOR OF    3 th LAYER = 0.30648976E+00
CONFINEMENT FACTOR OF    4 th LAYER = 0.34495801E+00
CONFINEMENT FACTOR OF    5 th LAYER = 0.17971109E-02
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
2
```

ii) Steps to calculate the heavy hole energy levels

```
 ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT
3
 INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
 INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
 INPUT N=
5
 INPUT THE HIGHEST POTENTIAL(1st Q-WELL) LAYER IC= ?
3
 INPUT THE SELECTED CENTER OF THE STRUCTURE ICR=?
3
 *******************************************************
  INPUT I=1  FOR AlGaAs
       I=2  FOR InGaAsP
       I=3  FOR In(1-x)Ga(x)As/InGaAsP/InP
       I=4  FOR InGaAlAs/InGaAlAs
       I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
       I=6  FOR InGaAs/AlGaAs/AlGaAs
       I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
       I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
       I=9  FOR In(z)Ga(1-z)As/AlxGayIn1-x-yAs/InP
       I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
       I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
       I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
       I=13 FOR InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
  INPUT I= ?
 *******************************************************
6
 *******************************************************

 DOES THE STRUCTURE STRAIN OR STRAIN-COMPENSATED?
 IF STRAIN ONLY INPUT 1, STRAIN-COMPENSATED INPUT 2
 INPUT SELECT = ?

1
```

```
ENERGY EIGENVALUE===> -0.276161746518E+00 ERROR= .3213873E-14
ENERGY EIGENVALUE===> -0.249003066242E+00 ERROR= .3486414E-14
ENERGY EIGENVALUE===> -0.228161537631E+00 ERROR= .4497189E-14
ENERGY EIGENVALUE===> -0.203092263186E+00 ERROR= .5310731E-14
ENERGY EIGENVALUE===> -0.180916942916E+00 ERROR= .3511095E-14
ENERGY EIGENVALUE===> -0.165761178280E+00 ERROR= .4162485E-14
ENERGY EIGENVALUE===> -0.143069425545E+00 ERROR= .4250671E-14
ENERGY EIGENVALUE===> -0.133410067391E+00 ERROR= .3870578E-14
ENERGY EIGENVALUE===> -0.118223143065E+00 ERROR= .4899315E-14
ENERGY EIGENVALUE===> -0.110268204173E+00 ERROR= .1851366E-14
ENERGY EIGENVALUE===> -0.105757454777E+00 ERROR= .1558283E-14
ENERGY EIGENVALUE===> -0.699260205944E-01 ERROR= .1407043E-14
ENERGY EIGENVALUE===> -0.320975532071E-01 ERROR= .1616452E-14
ENERGY EIGENVALUE===> -0.777880626765E-02 ERROR= .2132668E-14
 FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
 SKIP INPUT I==> 2
 I=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
-0.777880626765E-02
 INPUT THE NAME OF OUTPUT FILE
hh1.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.10519999E-10
 CONFINEMENT FACTOR OF    2 th LAYER = 0.76950168E-02
 CONFINEMENT FACTOR OF    3 th LAYER = 0.98460997E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.76950168E-02
 CONFINEMENT FACTOR OF    5 th LAYER = 0.10519999E-10
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
-0.320975532071E-01
 INPUT THE NAME OF OUTPUT FILE
hh2.txt
CONFINEMENT FACTOR OF    1 th LAYER = 0.54106617E-09
CONFINEMENT FACTOR OF    2 th LAYER = 0.33991734E-01
CONFINEMENT FACTOR OF    3 th LAYER = 0.93201653E+00
CONFINEMENT FACTOR OF    4 th LAYER = 0.33991734E-01
CONFINEMENT FACTOR OF    5 th LAYER = 0.54106617E-09
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
2
```

iii) Steps to calculate the light hole energy levels

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

4
 INPUT THE NUMBER OF QUANTUM WELLS NUM=?
```

```
1
 INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
 INPUT N=
5
 INPUT THE HIGHEST POTENTIAL(1st Q-WELL) LAYER IC= ?
3
 INPUT THE SELECTED CENTER OF THE STRUCTURE ICR=?
3
 *******************************************************
  INPUT I=1  FOR AlGaAs
      I=2  FOR InGaAsP
      I=3  FOR In(1-x)Ga(x)As/InGaAsP/InP
      I=4  FOR InGaAlAs/InGaAlAs
      I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
      I=6  FOR InGaAs/AlGaAs/AlGaAs
      I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
      I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
      I=9  FOR In(z)Ga(1-z)As/AlxGayIn1-x-yAs/InP
      I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
      I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
      I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
      I=13 FOR InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
  INPUT I= ?
 *******************************************************
6
 *******************************************************

  DOES THE STRUCTURE STRAIN OR STRAIN-COMPENSATED?
  IF STRAIN ONLY INPUT 1, STRAIN-COMPENSATED INPUT 2
  INPUT SELECT = ?

1

ENERGY EIGENVALUE===> -0.241668303016E+00 ERROR= .4759339E-14
ENERGY EIGENVALUE===> -0.204240716400E+00 ERROR= .3625060E-14
ENERGY EIGENVALUE===> -0.163104914064E+00 ERROR= .6006058E-14
ENERGY EIGENVALUE===> -0.133943830987E+00 ERROR= .3084882E-14
ENERGY EIGENVALUE===> -0.117111299716E+00 ERROR= .1442205E-14
ENERGY EIGENVALUE===> -0.914197602868E-01 ERROR= .2400351E-14
  FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
  SKIP INPUT I==> 2
  I=?
1
  INPUT THE EIGENVALUE
  EIGEN VALUE=
-0.914197602868E-01
  INPUT THE NAME OF OUTPUT FILE
lh1.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.29896156E-03
 CONFINEMENT FACTOR OF    2 th LAYER = 0.15044882E+00
 CONFINEMENT FACTOR OF    3 th LAYER = 0.69850443E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.15044882E+00
 CONFINEMENT FACTOR OF    5 th LAYER = 0.29896156E-03
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
1
```

```
 INPUT THE EIGENVALUE
 EIGEN VALUE=
-0.117111299716E+00
 INPUT THE NAME OF OUTPUT FILE
lh2.txt
CONFINEMENT FACTOR OF   1 th LAYER = 0.47451492E-02
CONFINEMENT FACTOR OF   2 th LAYER = 0.42827779E+00
CONFINEMENT FACTOR OF   3 th LAYER = 0.13395411E+00
CONFINEMENT FACTOR OF   4 th LAYER = 0.42827779E+00
CONFINEMENT FACTOR OF   5 th LAYER = 0.47451492E-02
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
2
```

b) The main output file from this part of GAIN program is energy.dat, containing all the energy levels as shown in Table C.6.5. After the energy eigen values are calculated, the GAIN program asks the user whether he would like to check the wave envelope function or not. We suggest that the user check the wave envelope functions of the first and second energy levels for conduction, heavy hole and light-hole bands. The plots of the envelope functions are shown in Fig. C.6.2, Fig. C.6.3, Fig C.6.4.

Table C.6.5. output file energy.dat

```
 CONDUCTION BAND ENERGY===>  0.103971205206E+00 ERROR= .2196720E-14

 CONDUCTION BAND ENERGY===>  0.160339839908E+00 ERROR= .4536506E-14

                                        …….

 HEAVY HOLE ENERGY===> -0.320975532071E-01 ERROR= .1616452E-14

 HEAVY HOLE ENERGY===> -0.777880626765E-02 ERROR= .2132668E-14

                                        ……..

 LIGHT HOLE ENERGY===> -0.117111299716E+00 ERROR= .1442205E-14

 LIGHT HOLE ENERGY===> -0.914197602868E-01 ERROR= .2400351E-14
```

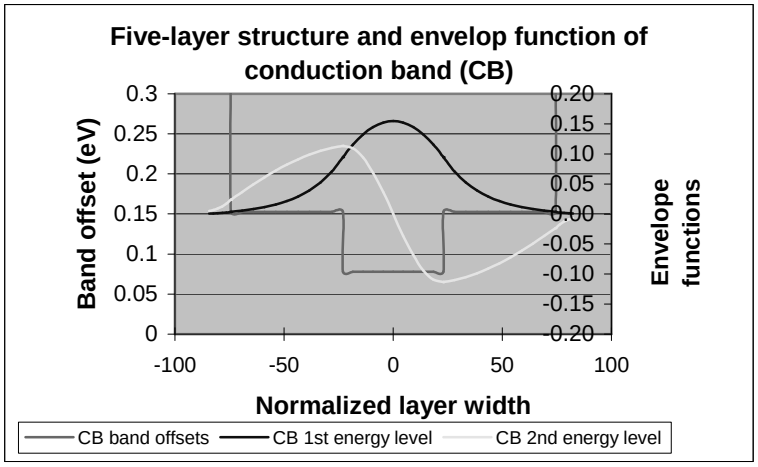

Fig. C.6.2. Wave envelope functions for energy levels in conduction band

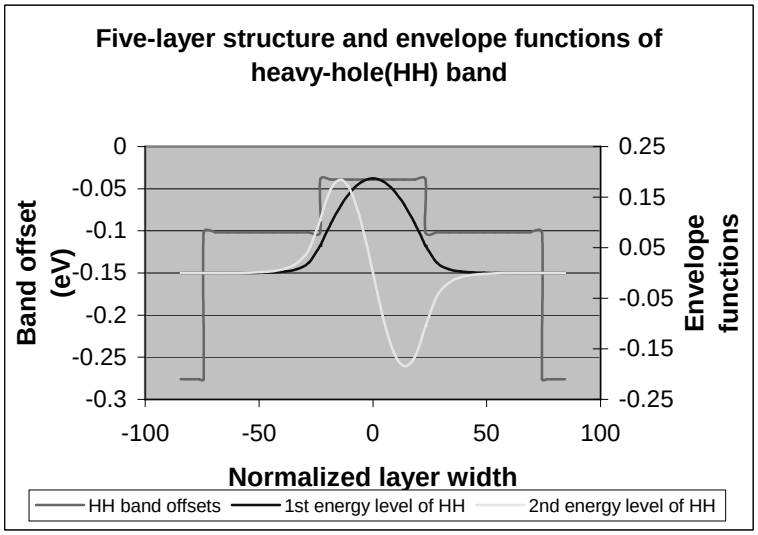

Fig. C.6.3. Wave envelope functions for heavy hole energy levels

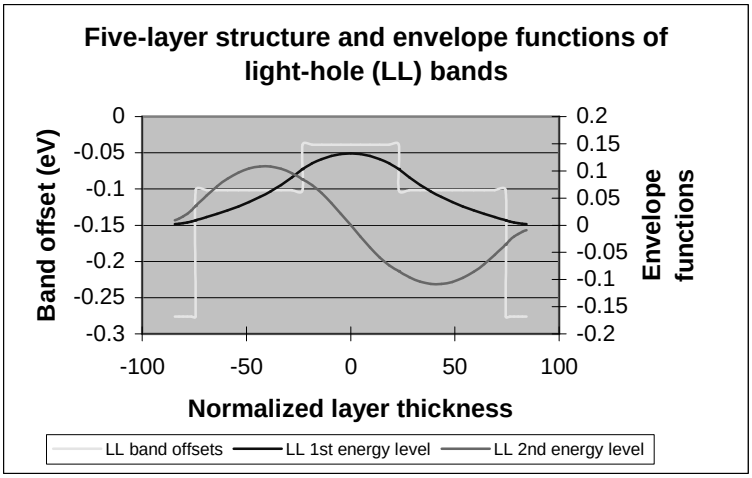

Fig. C.6.4. Wave envelope functions for light hole energy levels

C.6.3. Computation of Gain and Laser Characteristics

This is the last step of simulations using the GAIN program. With the previous calculated material composition, energy band edges, energy levels, and other parameters like material loss and Auger coefficient, the GAIN program can simulate the threshold current, threshold current density, slope efficiency, optical gain and mode gain as functions of wavelengths and photon energies, and L-I curve. The details are explained in Chapter 4 of the manual.

In this part of GAIN program, the input file needs to be constructed with the results of the previous steps and according to the laser design. The input file of material #6 is shown in Table C.6.6. The detailed steps of simulations are listed in Table C.6.7. The main output files: L-I curve, optical gain as a function of the wavelength, and mode gain vs. current density are plotted in Fig. C.6.5, Fig. C.6.6, and Fig. C.6.7.

a) The input file:

Table C.6.6. Input file (mat_13.txt) for gain and threshold current calculation

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c    1. Input the compositions, width of well, effective index                  c
c       and lasing wavelength.                                                  c
c    Ex: xx,xz,qy,xy,lx,n,lam                                                   c
c    for different materials the following are the forms of inputs.             c
c                                                                               c
c    w -- > well, b -- > barrier  cxz and cxy for cladding.                      c
c                                                                               c
c    a.  AlxGa1-xAs : xx (Al w) xz (Al b) qy (0) xy (0)                         c
c    b.  In1-xGaxAsyP1-y : xx (Ga w) xz (Ga b) qy (As w) xy (As b)              c
c    c.  In1-xGaxAs/InGaAsP : xx (Ga w) xz (Ga b) qy (0) xy (As b)              c
c    d.  AlxGayIn1-x-yAs/InP : xx (Ga w) xz (Ga b) qy (Al w) xy (Al b)          c
c    e.                                                                         c
c    f.  InxGa1-xAs/AlGaAs : xx (In w) xz (0) qy (0) xy (Al b)                  c
c    g.                                                                         c
c    h.  AlyInxGa1-x-yAs/AlGaAs : xx (Al w) xz (al b) qy (In w) xz (0)          c
c    i.  In1-xGaxAs/AlGaInAs : xx (In w) xz (0) qy (Al b) xy (Ga b)             c
c    j.  In(y)Ga(1-y)As(x)N(1-x) :xx(As w),xz(As, b),qy(In w),xy(In b)          c
c    k.  InGaAs/InGaAsP/GaAs: xx (In w), (0), xz(Ga w) xy (As b)
c    2. Input the energy gap,temperature, barrier band edges(both bands)
c    Ex: eg,temp,ec,ev                                                          c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
0.16650773E+00  0.0        0.0        0.0        9        3.33          0.975
1.1698              298       0.1525132              0.1016755
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c    3. Input the ist level sub-band energy levels.                             c
c    Ex: ec1,eh1,el1                                                            c
c                                                                               c
c    4. Input the material loss, reflectivities, number of quantum              c
c       wells and beta(for spontaneous emission).                               c
c    Ex: alpha,r1,r2,mm,beta.                                                   c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
0.103971    0.0077788    0.09141976    0.16034    0.03209756    0.1171113
```

```
6.0d0        0.3000          0.300          1          5.D-5
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c     5. Input the cavity length, ridge width, internal efficiency                c
c        Auger, strain(except AlGaAs,put 0) and confinement factor.                c
c     Ex: cl,cw,etha,ca,es,confine                                                 c
c                                                                                  c
c     6. Input the cladding composition and band edges.                            c
c     Ex: cxz,cxy,ecc,evv                                                          c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
1000.D-4        4.0D-4        0.86          1.00d-29        0.000        0.018
0.35001212      0.0       0.4143923   0.2762615
```

b) The steps for these calculations mentioned are listed in Table C.6.7

Table C.6.7. The steps for the gain and threshold current density calculations

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

5
 THE INPUT FILE NAME=
mat_6.tex
 SELECT MATERIAL=?
 1--AlGaAs
 2--InGaAsP
 3--In1-zGazAs/InGaAsP/InP
 4-- InGaAlAs
 5--GaInP/AlzGawIn1-z-wP/Al0.5In0.5P
 6-- InxGa1-xAs/AlxGa1-xAs/AlGaAs
 7--In1-xGaxAs/InGaAsP/GaxIn1-xP(X=0.51) MATCHED TO GaAs
 8--AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
 9--InzGa1-zAs/AlxGayIn1-x-yAs/InP
 10-- InGaAlAs/InGaAlAs/AlAsSb
 11--InzGa1-zAs/AlxGayIn1-x-yAs/AlAsSb
 12--In(y)Ga(1-y)As(x)N(1-x)/GaAs
 13--InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
 INPUT SELECTION
6
 INPUT MODE = ? FOR TE--> MODE =1, FOR TM--> MODE =2
 INPUT TE OR TM ?
1
 IF EL1 BELOW EH1 THEN SELECT 1, OTHERWISE SELECT 2
 SELECTION=?
1
 ************************************************
 CALCULATE THE EFFECTIVE MASS
 ************************************************
 FOR QUASI-FERMI LEVEL SELECT=1,
 FOR READ EXISTING QUASI-FERMI LEVEL SELECT=2
 SELECT=?
1
```

```
…….
J(LEAKAGE)=0.274159D+05 A/cm^2  N=0.780201D+19 1/cm^3
J(LEAKAGE)=0.280129D+05 A/cm^2  N=0.782180D+19 1/cm^3
J(LEAKAGE)=0.286204D+05 A/cm^2  N=0.784160D+19 1/cm^3
J(LEAKAGE)=0.292386D+05 A/cm^2  N=0.786140D+19 1/cm^3
J(LEAKAGE)=0.298675D+05 A/cm^2  N=0.788120D+19 1/cm^3
J(LEAKAGE)=0.305072D+05 A/cm^2  N=0.790100D+19 1/cm^3
J(LEAKAGE)=0.311578D+05 A/cm^2  N=0.792080D+19 1/cm^3
J(LEAKAGE)=0.318195D+05 A/cm^2  N=0.794060D+19 1/cm^3
J(LEAKAGE)=0.324922D+05 A/cm^2  N=0.796040D+19 1/cm^3
J(LEAKAGE)=0.331761D+05 A/cm^2  N=0.798020D+19 1/cm^3
J(LEAKAGE)=0.338712D+05 A/cm^2  N=0.800000D+19 1/cm^3
 ************************************************
   G(J) PARAMETERS FROM SINGLE WELL
 Go=0.348368D+02 1/cm  Jo=0.261496D+03 A/cm^2

 G(N) PARAMETERS FROM SINGLE WELL
 NGo=0.193538D+04 1/cm  XNo=0.134737D+19 1/cm^3

 Jtr=0.961992D+02 A/cm^2  NTR=0.495669D+18 1/cm^3


 THE OPTIMUM NUMBER OF QUANTUM WELL FOLLOWS THE ARTICLE
 BY McIlory et al. IEEE JQE-21 1985.

 THE OPTIMUM NUMBER OF QUANTUM WELL Nopt =          1
 INPUT Nopt(CAN BE DIFFERENT FROM ABOVE CALCULATION)=?
1
 NUMBER OF QUANTUM WELL(MAY OR MAY NOT BE Nopt)=?
1
 ************************************************
 ************************************************
 1ST CHECK USE SINGLE WELL TIMES # OF WELLS
 ************************************************
 ************************************************
 2ND CHECK FOLLOWS FORMULA BY McIlory IN IEEE
 JOURNAL OF QUANTUM ELECTRONIC QE-21 1985.
 ************************************************
  Gth=  18.0397 1/cm Nth=0.753383D+18 1/cm^3 IY=   34
  1ST CHECK Jth=   152.41859383 A/cm^2
  2ND CHECK Jth=   304.06565 A/cm^2

  1ST CHECK Ith=0.609674D+01 mA NUMBER OF WELLS=  1
  2ND CHECK Ith=0.121626D+02 mA

 ************************************************
 CALCULATE THE P-I RELATION

 NDATA=        367
 ************************************************
 CALCULATE THE SLOPE: mW/mA Y=A+BX
 CONSTANT A=  -3.2295952   SLOPE B=   0.3609355

 ************************************************
 INPUT POWER PO FOR THE LINEWIDTH, PO=0 FOR STOP
```

```
 INPUT PO=    mW
0
 INPUT 1 FOR THE DYNAMIC CALCULATION. 2 FOR SKIP
 INPUT =
2
 K-FACTOR= 0.25787 nS  MAXIUM FREQ.= 34.4582 GHz
 ************************************************
 INPUT 1 FOR CALCULATE THE GAIN(E) RELATION.

 INPUT 2 FOR CALCULATE THE LINEWIDTH ENHENCEMENT
 FACTOR AND PHOTON ENERGY RELATION

 INPUT 3 FOR EXIT THE PROGRAM

 THE INPUT # IS
1
INPUT FERMILEVELS IN C-BAND, V-BAND, AND CARRIER DENSITY
0.196827942412E+00 0.314112077552E-02 0.200075187970E+19
 CALCULATE THE CONVOLUTION GAIN(E) COEFFICIENT
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(LAMBDA)
ol1_mat6
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(LAMBDA)
ml1_mat6
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(E)
oe1_mat6
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(E)
me1_mat6
 ************************************************
 INPUT 1 FOR REPEAT THE G(E) CALCULATION
 INPUT 2 FOR REPEAT THE ALPHA(E) CALCULATION
 INPUT 3 FOR EXIT
1
 ************************************************
 INPUT 1 FOR CALCULATE THE GAIN(E) RELATION.

 INPUT 2 FOR CALCULATE THE LINEWIDTH ENHENCEMENT
 FACTOR AND PHOTON ENERGY RELATION

 INPUT 3 FOR EXIT THE PROGRAM

 THE INPUT # IS
1
INPUT FERMILEVELS IN C-BAND, V-BAND, AND CARRIER DENSITY
0.232657297045E+00 0.168447625974E-01  0.299072681704E+19
 CALCULATE THE CONVOLUTION GAIN(E) COEFFICIENT
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(LAMBDA)
ol2_mat6
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(LAMBDA)
ml2_mat6
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(E)
oe2_mat6
```

```
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(E)
me2_mat6
 ************************************************
 INPUT 1 FOR REPEAT THE G(E) CALCULATION
 INPUT 2 FOR REPEAT THE ALPHA(E) CALCULATION
 INPUT 3 FOR EXIT
3

ENTER 1 FOR THE NECESSARY PARAMETERS
     2 FOR THE ENERGY VALUES OF CONDUCTION BAND
     3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
     4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
     5 FOR THE LASER G-J AND G(LAMBDA)
     6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
     7 FOR EXIT

7
```

c) The Output characteristics of designed laser from step 5 are summarized in Table C.6.7.

Table C.6.7 Characteristics of the designed laser

Optimized number of QWs (Nopt)	1
Number of QWs	1
Slope efficiency (%)	36.12
Jth (A/cm^2)	152.42 - 1st check, for matching threshold conditions 304.07 - 2nd check, using McIlory method
Peak λ at operating temperature (um)	0.973 um for carrier density of 2.0E18 /cm3 0.974 um for carrier density of 3.0E18 /cm3
Peak material gain (1/cm)	2724/cm for carrier density of 2.0E18 /cm3 3472 /cm for carrier density of 3.0E18 /cm3

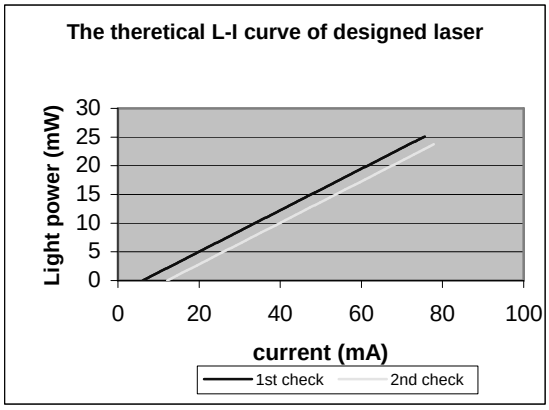

Fig. C.6.5. L-I curve of the laser

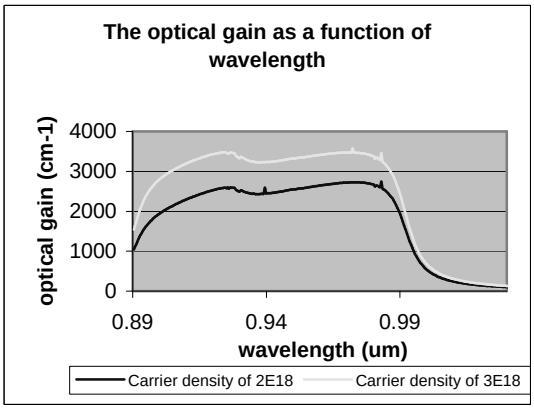

Fig. C.6.6. Optical gain-λ curve of the laser

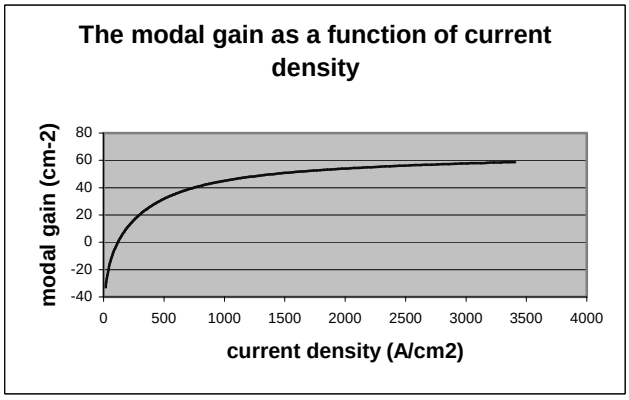

Fig. C.6.7. Mode gain as a function of current density (J)

C.8. Material system #8: AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs

This is a simulation of a five-layer laser structure that contains a single quantum well (QW), two separated confinement heterostructure (SCH) layers, and two cladding layers as shown in Fig. C.8.1.

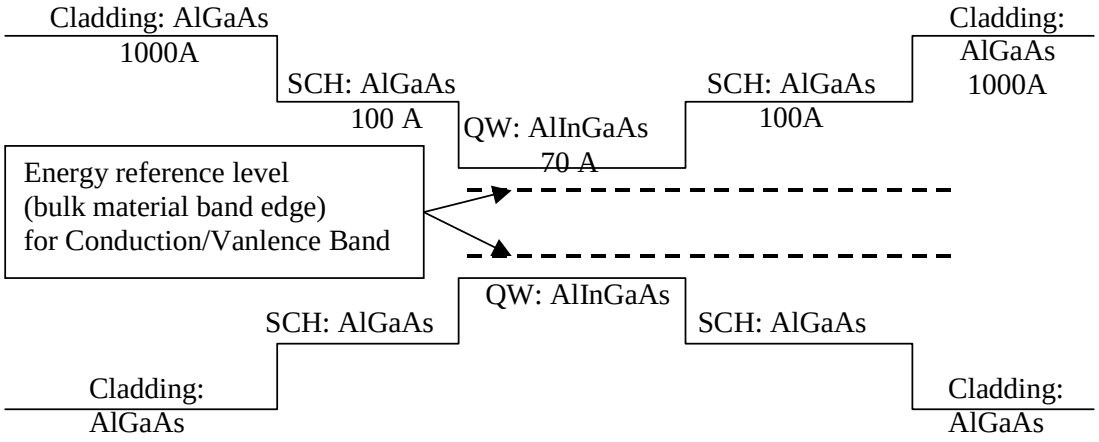

Figure C.8.7. Energy band diagram for the simple quantum well structure

C.8.1. Calculation of material compositions and energy band edges.

The first step of the GAIN program is to calculate the material compositions and energy band edges of the each layer. The user is asked to enter the photoluminescence wavelength, thickness, and strain of the QW, SCH, and cladding layers. After these parameters are input, the GAIN program generates two output files: cbandeg.dat and vbandeg.dat, containing the material compositions, and the conduction band edges and valence band edges respectively. The detailed explanation is provided in Chapter 2 of this manual.

a) The input parameters to the GAIN program in this step is listed in Table. C.8.1.

Table C.4.1. Input parameters to the GAIN program in this step.

Layer	λ (um)	Strain	Thickness (Å)
QW ($Al_yIn_xGa_{1-x-y}As$)	0.9397	-0.016	70
SCH ($Al_zGa_{1-z}As$)	0.74101		100
Cladding ($Al_zGa_{1-z}As$)	0.56		1000

b) The steps in using the GAIN program to calculate the material compositions and energy band edges are listed in Table C.8.2

Table C.8.2. steps to run the GAIN program for necessary parameters.

ENTER 1 **FOR THE NECESSARY PARAMETERS**
2 FOR THE ENERGY VALUES OF CONDUCTION BAND

```
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

1

 ENTER 1 FOR AlGaAs/AlGaAs
      2 FOR InGaAsP/InGaAsP/InP
      3 FOR InGaAs/InGaAsP/InP
      4 FOR InGaAlAs/InGaAlAs/InP
      5 FOR GaInP/(AlGa)0.5In0.5P/AlInP
      6 FOR InGaAs/AlGaAs/AlGaAs
      7 FOR InGaAs/InGaAsP/Ga0.51In0.49P(MATCHED GaAs)
      8 FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
      9 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/InP
     10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(matched InP)
     11 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/AlAsxSb1-x
     12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs (dilute N)
     13 FOR In(1-x)Ga(x)As(y)P(1-y)/GaAs
     14 FOR EXIT, BACK TO MAIN PAGE!
8
 INPUT THE LAYER # FOR GRIN STRUCTURE(STEP)
 STEP N=
2
  INPUT THE WELL WAVELENGTH (um)
0.9397
  INPUT THE BARRIER WAVELENGTH (um)
0.74101
  INPUT THE CLADDING WAVELENGTH (um)
0.56
    BANDGAP ENERGY OF QUANTUM WELL=    1.31957007555603       eV
  INPUT CLADDING, BARRIER,QUANTUM WELL WIDTH (A)
1000 100 70

CALCULATE AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs

  INPUT STRAIN
-0.016

WELL LATTICE =    5.74375727038792       BARRIER LATTICE =
   5.65485994822169
  STRAIN =  -1.572051703847871E-002

  WRITE CONDUCTION BAND PARAMETERS INTO CBANDEG.DAT

  WRITE VALENCE BAND PARAMETERS INTO VBANDEG.DAT
  INPUT 1 FOR NEW CALCULATION, 2 FOR EXIT
  I= ?

2

 ENTER 1 FOR AlGaAs/AlGaAs
      2 FOR InGaAsP/InGaAsP/InP
      3 FOR InGaAs/InGaAsP/InP
```

```
      4 FOR InGaAlAs/InGaAlAs/InP
      5 FOR GaInP/(AlGa)0.5In0.5P/AlInP
      6 FOR InGaAs/AlGaAs/AlGaAs
      7 FOR InGaAs/InGaAsP/Ga0.51In0.49P(MATCHED GaAs)
      8 FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
      9 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/InP
     10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(matched InP)
     11 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/AlAsxSb1-x
     12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs (dilute N)
     13 FOR In(1-x)Ga(x)As(y)P(1-y)/GaAs
     14 FOR EXIT, BACK TO MAIN PAGE!
14
 THIS PROGRAM STOP HERE!, BACK TO MAIN PAGE
```

c) The output files, cbandeg.dat and vbandeg.dat are explained in Table C.8.3.

Table C.8.3. Material compositions and band offsets:

a) cbandeg.dat for conduction band

```
**************************************************************************
 QW strain   lattice constant
 -.157205E-01  0.574376E-09
                        material compositions
 layer thickness,     Al(barrier)In (qw)    Al(qw)     conduction band edges
  0.10000000E+04   0.61015643E+00    0.0000000    0.6084067      cladding layer
  0.10000000E+03   0.19999336E+00    0.0000000    0.2405987      SCH layer
  0.70000000E+02   0.22040026E+00    0.1504008    0.0964814      quantum well
  0.10000000E+03   0.19999336E+00    0.0000000    0.2405987      SCH layer
 0.10000000E+04   0.61015643E+00    0.0000000    0.6084067      cladding layer
**************************************************************************
```

b) vbandeg.dat for valence band

```
************************************************** **********************
 QW strain   lattice constant
-.157205E-01  0.574376E-09
                        material compositions
 layer thickness,     Al(barrier)In (qw)    Al(qw)     valence band edges
  0.10000000E+04   0.61015643E+00    0.0000000   -0.2863090      cladding layer
  0.10000000E+03   0.19999336E+00    0.0000000   -0.1132229      SCH layer
  0.70000000E+02   0.22040026E+00    0.1504008   -0.0482407      quantum well
  0.10000000E+03   0.19999336E+00    0.0000000   -0.1132229      SCH layer
  0.10000000E+04   0.61015643E+00    0.0000000   -0.2863090     cladding layer
**************************************************************************
```

C.8.2. Energy level calculations

After the calculation of the material compositions and energy band edges, the GAIN program calculates energy levels in the conduction band and valence bands. The detailed explanations are discussed in Chapter 3 of this manual.

a) The steps of how to calculate the energy levels are shown in Table C.8.4.

Table C.8.4. Steps to calculate the energy levels

i) Steps to calculate the conduction band energy levels

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

2
 INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
 INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
 INPUT N=
5
 INPUT THE LOWEST POTENTIAL LAYER(1st Q-WELL) IC= ?
3
 INPUT THE SELECTED CENTER LAYER OF STRUCTURE ICR=
3
 ********************************************************
  INPUT I=1  FOR AlGaAs
       I=2  FOR InGaAsP
       I=3  FOR In1-xGaxAs/InGaAsP/InP
       I=4  FOR InGaAlAs/InGaAlAs
       I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
       I=6  FOR InGaAs/AlGaAs/AlGaAs
       I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
       I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
       I=9  FOR InzGa1-zAs/AlxGayIn1-x-yAs/InP
       I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
       I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
       I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
       I=13 FOR InGaAs/In(1-y)Ga(x)As(y)P(1-y)/GaAs
  INPUT I= ?
 ********************************************************
8
 ENERGY EIGENVALUE===>  0.138709276765E+00 ERROR= .4799291E-14
 ENERGY EIGENVALUE===>  0.232901930540E+00 ERROR= .6412287E-14
 ENERGY EIGENVALUE===>  0.276726767247E+00 ERROR= .3711948E-14
 ENERGY EIGENVALUE===>  0.303014125323E+00 ERROR= .1551081E-14
 ENERGY EIGENVALUE===>  0.367974646637E+00 ERROR= .1433712E-14
 ENERGY EIGENVALUE===>  0.425273029859E+00 ERROR= .1640863E-14
 ENERGY EIGENVALUE===>  0.501513800567E+00 ERROR= .2646723E-14
 ENERGY EIGENVALUE===>  0.583662116165E+00 ERROR= .1561274E-14

 FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
 SKIP INPUT I==> 2
 I=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
0.138709276765E+00
 INPUT THE NAME OF OUTPUT FILE
ce1.dat
```

```
CONFINEMENT FACTOR OF    1 th LAYER = 0.21621179E-05
 CONFINEMENT FACTOR OF    2 th LAYER = 0.54850032E-01
 CONFINEMENT FACTOR OF    3 th LAYER = 0.89029561E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.54850032E-01
 CONFINEMENT FACTOR OF    5 th LAYER = 0.21621179E-05
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
1
  INPUT THE EIGENVALUE
  EIGEN VALUE=
0.232901930540E+00
  INPUT THE NAME OF OUTPUT FILE
ce2.dat
  CONFINEMENT FACTOR OF    1 th LAYER = 0.41673581E-03
 CONFINEMENT FACTOR OF    2 th LAYER = 0.29132209E+00
 CONFINEMENT FACTOR OF    3 th LAYER = 0.41652235E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.29132209E+00
 CONFINEMENT FACTOR OF    5 th LAYER = 0.41673581E-03
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
2
```

ii) Steps to calculate the heavy hole energy levels

```
 ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT
3
  INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
  INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
  INPUT N=
5
  INPUT THE HIGHEST POTENTIAL(1st Q-WELL) LAYER IC= ?
3
  INPUT THE SELECTED CENTER OF THE STRUCTURE ICR=?
3
 ******************************************************
   INPUT I=1  FOR AlGaAs
        I=2  FOR InGaAsP
        I=3  FOR In(1-x)Ga(x)As/InGaAsP/InP
        I=4  FOR InGaAlAs/InGaAlAs
        I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
        I=6  FOR InGaAs/AlGaAs/AlGaAs
        I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
        I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
        I=9  FOR In(z)Ga(1-z)As/AlxGayIn1-x-yAs/InP
        I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
        I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
        I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
        I=13 FOR InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
   INPUT I= ?
 ******************************************************
```

```
8
 ******************************************************

  DOES THE STRUCTURE STRAIN OR STRAIN-COMPENSATED?
  IF STRAIN ONLY INPUT 1, STRAIN-COMPENSATED INPUT 2
  INPUT SELECT = ?

1

  ENERGY EIGENVALUE===> -0.284385739775E+00 ERROR= .1839577E-14
  ENERGY EIGENVALUE===> -0.255905460776E+00 ERROR= .2322763E-14
  ENERGY EIGENVALUE===> -0.234841860479E+00 ERROR= .2272918E-14
  ENERGY EIGENVALUE===> -0.206302710392E+00 ERROR= .4324053E-14
  ENERGY EIGENVALUE===> -0.187763267853E+00 ERROR= .5809361E-14
  ENERGY EIGENVALUE===> -0.168383437529E+00 ERROR= .2956487E-14
  ENERGY EIGENVALUE===> -0.149353291457E+00 ERROR= .5093768E-14
  ENERGY EIGENVALUE===> -0.140222438643E+00 ERROR= .2070569E-14
  ENERGY EIGENVALUE===> -0.123256448240E+00 ERROR= .3857883E-14
  ENERGY EIGENVALUE===> -0.120525810269E+00 ERROR= .2284583E-14
  ENERGY EIGENVALUE===> -0.969071742920E-01 ERROR= .2454913E-14
  ENERGY EIGENVALUE===> -0.453040076948E-01 ERROR= .1799212E-14
  ENERGY EIGENVALUE===> -0.972318690802E-02 ERROR= .2326139E-14

  FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
  SKIP INPUT I==> 2
  I=?
1
  INPUT THE EIGENVALUE
  EIGEN VALUE=
-0.972318690802E-02
  INPUT THE NAME OF OUTPUT FILE
hhe1.dat
  CONFINEMENT FACTOR OF    1 th LAYER = 0.63895895E-11
 CONFINEMENT FACTOR OF    2 th LAYER = 0.11454696E-01
 CONFINEMENT FACTOR OF    3 th LAYER = 0.97709061E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.11454696E-01
 CONFINEMENT FACTOR OF    5 th LAYER = 0.63895895E-11
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
1
  INPUT THE EIGENVALUE
  EIGEN VALUE=
-0.649012884792E-01
  INPUT THE NAME OF OUTPUT FILE
hhe2.dat
CONFINEMENT FACTOR OF    1 th LAYER = 0.99899806E-09
 CONFINEMENT FACTOR OF    2 th LAYER = 0.52677815E-01
 CONFINEMENT FACTOR OF    3 th LAYER = 0.89464437E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.52677815E-01
 CONFINEMENT FACTOR OF    5 th LAYER = 0.99899806E-09
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
2
```

iii) Steps to calculate the light hole energy levels

```
ENTER 1 FOR THE NECESSARY PARAMETERS
```

```
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

4
 INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
 INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
 INPUT N=
5
 INPUT THE HIGHEST POTENTIAL(1st Q-WELL) LAYER IC= ?
3
 INPUT THE SELECTED CENTER OF THE STRUCTURE ICR=?
3
 ********************************************************
  INPUT I=1  FOR AlGaAs
       I=2  FOR InGaAsP
       I=3  FOR In(1-x)Ga(x)As/InGaAsP/InP
       I=4  FOR InGaAlAs/InGaAlAs
       I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
       I=6  FOR InGaAs/AlGaAs/AlGaAs
       I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
       I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
       I=9  FOR In(z)Ga(1-z)As/AlxGayIn1-x-yAs/InP
       I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
       I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
       I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
       I=13 FOR InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
  INPUT I= ?
 ********************************************************
8
 ********************************************************

 DOES THE STRUCTURE STRAIN OR STRAIN-COMPENSATED?
 IF STRAIN ONLY INPUT 1, STRAIN-COMPENSATED INPUT 2
 INPUT SELECT = ?
1

 ENERGY EIGENVALUE===> -0.269466833989E+00 ERROR= .5288152E-14
 ENERGY EIGENVALUE===> -0.226547460437E+00 ERROR= .5259840E-14
 ENERGY EIGENVALUE===> -0.186071818477E+00 ERROR= .2292515E-14
 ENERGY EIGENVALUE===> -0.151389428652E+00 ERROR= .1780460E-14
 ENERGY EIGENVALUE===> -0.131943108468E+00 ERROR= .2798805E-14
 ENERGY EIGENVALUE===> -0.110796843027E+00 ERROR= .2434081E-14

 FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
 SKIP INPUT I==> 2
 I=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
-0.110796843027E+00
 INPUT THE NAME OF OUTPUT FILE
```

```
lhe1.dat
CONFINEMENT FACTOR OF    1 th LAYER = 0.70421019E-03
 CONFINEMENT FACTOR OF    2 th LAYER = 0.22417666E+00
 CONFINEMENT FACTOR OF    3 th LAYER = 0.55023826E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.22417666E+00
 CONFINEMENT FACTOR OF    5 th LAYER = 0.70421019E-03  INPUT NEW EIGENVALUE-
-> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
1
  INPUT THE EIGENVALUE
  EIGEN VALUE=
-0.131943108468E+00
  INPUT THE NAME OF OUTPUT FILE
lhe2.dat
CONFINEMENT FACTOR OF    1 th LAYER = 0.59278096E-02
 CONFINEMENT FACTOR OF    2 th LAYER = 0.45844574E+00
 CONFINEMENT FACTOR OF    3 th LAYER = 0.71252902E-01
 CONFINEMENT FACTOR OF    4 th LAYER = 0.45844574E+00
 CONFINEMENT FACTOR OF    5 th LAYER = 0.59278096E-02
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
2
```

b) The main output file from this part of GAIN program is energy.dat, containing all the energy levels as shown in Table C.8.5. After the energy eigen values are calculated, the GAIN program asks the user whether he would like to check the wave envelope function or not. We suggest that the user check the wave envelope functions of the first and second energy levels for conduction and valence bands. The plots of the envelope functions are shown in Fig. C.8.2, Fig. C.8.3, Fig C.8.4.

Table C.8.5. output file energy.dat

```
  CONDUCTION BAND ENERGY===>  0.138709276765E+00 ERROR= .4799291E-14

  CONDUCTION BAND ENERGY===>  0.232901930540E+00 ERROR= .6412287E-14

  CONDUCTION BAND ENERGY===>  0.276726767247E+00 ERROR= .3711948E-14

  CONDUCTION BAND ENERGY===>  0.303014125323E+00 ERROR= .1551081E-14

  CONDUCTION BAND ENERGY===>  0.367974646637E+00 ERROR= .1433712E-14

  CONDUCTION BAND ENERGY===>  0.425273029859E+00 ERROR= .1640863E-14

  CONDUCTION BAND ENERGY===>  0.501513800567E+00 ERROR= .2646723E-14

  CONDUCTION BAND ENERGY===>  0.583662116165E+00 ERROR= .1561274E-14

  HEAVY HOLE ENERGY===> -0.284385739775E+00 ERROR= .1839577E-14

  HEAVY HOLE ENERGY===> -0.255905460776E+00 ERROR= .2322763E-14

  HEAVY HOLE ENERGY===> -0.234841860479E+00 ERROR= .2272918E-14

  HEAVY HOLE ENERGY===> -0.206302710392E+00 ERROR= .4324053E-14
```

HEAVY HOLE ENERGY===> -0.187763267853E+00 ERROR= .5809361E-14

HEAVY HOLE ENERGY===> -0.168383437529E+00 ERROR= .2956487E-14

HEAVY HOLE ENERGY===> -0.149353291457E+00 ERROR= .5093768E-14

HEAVY HOLE ENERGY===> -0.140222438643E+00 ERROR= .2070569E-14

HEAVY HOLE ENERGY===> -0.123256448240E+00 ERROR= .3857883E-14

HEAVY HOLE ENERGY===> -0.120525810269E+00 ERROR= .2284583E-14

HEAVY HOLE ENERGY===> -0.969071742920E-01 ERROR= .2454913E-14

HEAVY HOLE ENERGY===> -0.453040076948E-01 ERROR= .1799212E-14

HEAVY HOLE ENERGY===> -0.972318690802E-02 ERROR= .2326139E-14

LIGHT HOLE ENERGY===> -0.269466833989E+00 ERROR= .5288152E-14

LIGHT HOLE ENERGY===> -0.226547460437E+00 ERROR= .5259840E-14

LIGHT HOLE ENERGY===> -0.186071818477E+00 ERROR= .2292515E-14

LIGHT HOLE ENERGY===> -0.151389428652E+00 ERROR= .1780460E-14

LIGHT HOLE ENERGY===> -0.131943108468E+00 ERROR= .2798805E-14

LIGHT HOLE ENERGY===> -0.110796843027E+00 ERROR= .2434081E-14

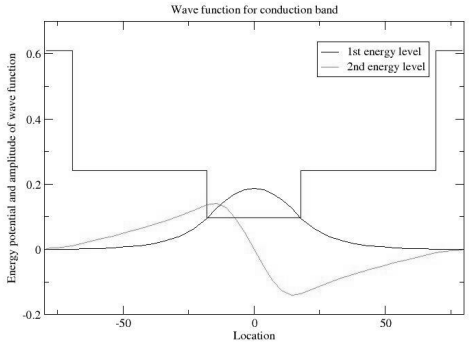

Fig. C.8.2. Wave envelop functions for energy levels in conduction band

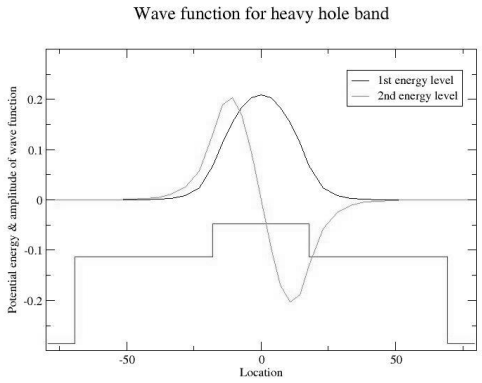

Fig. C.8.3. Wave envelop functions for heavy hole energy levels

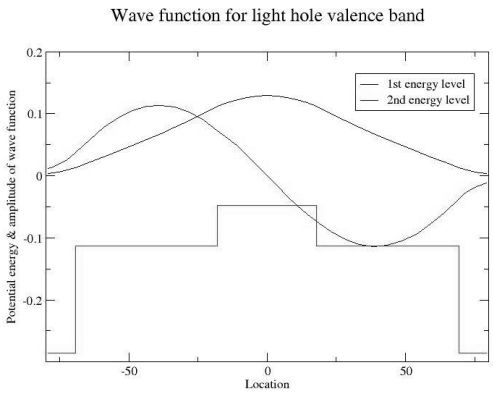

Fig. C.8.4. Wave envelop functions for light hole energy levels

C.8.3. Computation of Gain and Laser Characteristics

This is the last step of simulations using the GAIN program. With the previous calculated material composition, energy band edges, energy levels, and other parameters like material loss and Auger coefficient, the GAIN program can simulate the threshold current, threshold current density, slope efficiency, optical gain and mode gain as functions of wavelengths and photo energies, and L-I curve. The details are explained in Chapter 4 of the manual.

In this part of GAIN program, the input file needs to be constructed with the results of the previous steps and according to the laser design. In this example, single quantum well structure is used. For the three-quantum-well laser with a ridge length of 425 μm and ridge width of 3 μm, the input file is shown in Table C.8.6. The detailed steps of simulations are listed in Table C.8.7. The main output files: L-I curve, optical gain as a function of the wavelength, and mode gain vs. current density are plotted in Fig. C.8.5, Fig. C.8.6, and Fig. C.8.7.

a) The input file:

Table C.8.6. Input file for gain and threshold current calculation

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c    1. Input the compositions, width of well, effective index        c
c       and lasing wavelength.                                        c
c    Ex: xx,xz,qy,xy,lx,n,lam                                         c
c    for different materials the following are the forms of inputs.   c
c                                                                     c
c    w -- > well, b -- > barrier  cxz and cxy for cladding.            c
c                                                                     c
c    a.  AlxGa1-xAs : xx (Al w) xz (Al b) qy (0) xy (0)               c
c    b.  In1-xGaxAsyP1-y : xx (Ga w) xz (Ga b) qy (As w) xy (As b)    c
c    c.  In1-xGaxAs/InGaAsP : xx (Ga w) xz (Ga b) qy (0) xy (As b)    c
c    d.  AlxGayIn1-x-yAs/InP : xx (Ga w) xz (Ga b) qy (Al w) xy (Al b)c
c    e.                                                               c
c    f.  InxGa1-xAs/AlGaAs : xx (In w) xz (0) qy (0) xy (Al b)        c
```

```
c     g.                                                    c
c     h.  AlyInxGa1-x-yAs/AlGaAs : xx (Al w) xz (al b) qy (In w) xz (0)c
c     i.  In1-xGaxAs/AlGaInAs : xx (In w) xz (0) qy (Al b) xy (Ga b)   c
c     j.  In(y)Ga(1-y)As(x)N(1-x) :xx(As w),xz(As, b),qy(In w),xy(In b)c
c     k.  InGaAs/InGaAsP/GaAs: xx (In w), (0), xz(Ga w) xy (As b)
c     2. Input the energy gap,temperature, barrier band edges(both bands)
c     Ex: eg,temp,ec,ev                                     c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
0.22040026E+00 0.19999336E+00 0.1504008 0.0000  7.0 3.2567 0.8500d0
1.31957 298  0.2405987 0.1132229
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c     3. Input the ist level sub-band energy levels.              c
c     Ex: ec1,eh1,el1                                       c
c                                                           c
c     4. Input the material loss, reflectivities, number of quantum    c
c       wells and beta(for spontaneous emission).                c
c     Ex: alpha,r1,r2,mm,beta.                                c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
0.138709276765E+00     0.972318690802E-02     0.110796843027E+00     0.232901930540E+00
0.453040076948E-01  1
3.0d0                  0.996                  0.9994                  1                  5.D-
5ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c     5. Input the cavity length, ridge width, internal efficiency     c
c       Auger, strain(except AlGaAs,put 0) and confinement factor.    c
c     Ex: cl,cw,etha,ca,es,confine                            c
c                                                           c
c     6. Input the cladding composition and band edges.           c
c     Ex: cxz,cxy,ecc,evv                                   c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
425.D-4  3.0D-4  0.90  1.00d-29   0.016  0.977
0.61015643E+00  0.00  0.6084067 0.2863090
```

b) The steps for these calculations mentioned are listed in Table C.4.7

Table C.8.7. The steps for the gain and threshold current density calculations

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

5
  THE INPUT FILE NAME=
2schsqwalingaas85.tex
  SELECT MATERIAL=?
  1--AlGaAs
  2--InGaAsP
  3--In1-zGazAs/InGaAsP/InP
  4-- InGaAlAs
  5--GaInP/AlzGawIn1-z-wP/Al0.5In0.5P
  6-- InxGa1-xAs/AlxGa1-xAs/AlGaAs
  7--In1-xGaxAs/InGaAsP/GaxIn1-xP(X=0.51) MATCHED TO GaAs
  8--AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
```

```
 9--InzGa1-zAs/AlxGayIn1-x-yAs/InP
 10-- InGaAlAs/InGaAlAs/AlAsSb
 11--InzGa1-zAs/AlxGayIn1-x-yAs/AlAsSb
 12--In(y)Ga(1-y)As(x)N(1-x)/GaAs
 13--InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
 INPUT SELECTION
8
 INPUT MODE = ? FOR TE--> MODE =1, FOR TM--> MODE =2
 INPUT TE OR TM ?
1
 IF EL1 BELOW EH1 THEN SELECT 1, OTHERWISE SELECT 2
 SELECTION=?
1
 ************************************************
 CALCULATE THE EFFECTIVE MASS
 ************************************************
 FOR QUASI-FERMI LEVEL SELECT=1,
 FOR READ EXISTING QUASI-FERMI LEVEL SELECT=2
 SELECT=?
1

 J(LEAKAGE)=0.282088D-01 A/cm^2  N=0.239674D+19 1/cm^3
J(LEAKAGE)=0.288770D-01 A/cm^2  N=0.241654D+19 1/cm^3
J(LEAKAGE)=0.295579D-01 A/cm^2  N=0.243634D+19 1/cm^3
J(LEAKAGE)=0.302516D-01 A/cm^2  N=0.245614D+19 1/cm^3
J(LEAKAGE)=0.309583D-01 A/cm^2  N=0.247594D+19 1/cm^3
J(LEAKAGE)=0.316783D-01 A/cm^2  N=0.249574D+19 1/cm^3
J(LEAKAGE)=0.324116D-01 A/cm^2  N=0.251554D+19 1/cm^3
…….
J(LEAKAGE)=0.377958D+01 A/cm^2  N=0.786140D+19 1/cm^3
 J(LEAKAGE)=0.384091D+01 A/cm^2  N=0.788120D+19 1/cm^3
 J(LEAKAGE)=0.390322D+01 A/cm^2  N=0.790100D+19 1/cm^3
 J(LEAKAGE)=0.396654D+01 A/cm^2  N=0.792080D+19 1/cm^3
 J(LEAKAGE)=0.403088D+01 A/cm^2  N=0.794060D+19 1/cm^3
 J(LEAKAGE)=0.409626D+01 A/cm^2  N=0.796040D+19 1/cm^3
 J(LEAKAGE)=0.416269D+01 A/cm^2  N=0.798020D+19 1/cm^3
 J(LEAKAGE)=0.423019D+01 A/cm^2  N=0.800000D+19 1/cm^3
************************************************
 G(J) PARAMETERS FROM SINGLE WELL
 Go=0.195832D+04 1/cm  Jo=0.338688D+03 A/cm^2

 G(N) PARAMETERS FROM SINGLE WELL
 NGo=0.200442D+04 1/cm  XNo=0.162456D+19 1/cm^3

 Jtr=0.124596D+03 A/cm^2  NTR=0.597643D+18 1/cm^3


 THE OPTIMUM NUMBER OF QUANTUM WELL FOLLOWS THE ARTICLE
 BY McIlory et al. IEEE JQE-21 1985.

 THE OPTIMUM NUMBER OF QUANTUM WELL Nopt =           1
 INPUT Nopt(CAN BE DIFFERENT FROM ABOVE CALCULATION)=?
1
 NUMBER OF QUANTUM WELL(MAY OR MAY NOT BE Nopt)=?
1
```

```
**************************************************
 **************************************************
 1ST CHECK USE SINGLE WELL TIMES # OF WELLS
 **************************************************
 **************************************************
 2ND CHECK FOLLOWS FORMULA BY McIlory IN IEEE
 JOURNAL OF QUANTUM ELECTRONIC QE-21 1985.
 **************************************************
 Gth=   3.0542 1/cm Nth=0.456391D+18 1/cm^3 IY=   19
  1ST CHECK Jth=    93.18144132 A/cm^2
  2ND CHECK Jth=   376.31987 A/cm^2

  1ST CHECK Ith=0.118806D+01 mA NUMBER OF WELLS=  1
  2ND CHECK Ith=0.479808D+01 mA

 **************************************************
CALCULATE THE P-I RELATION

NDATA=        382
 **************************************************
 CALCULATE THE SLOPE: mW/mA Y=A+BX
 CONSTANT A=  -0.0238953   SLOPE B=   0.0201129

 **************************************************
  INPUT POWER PO FOR THE LINEWIDTH, PO=0 FOR STOP
  INPUT PO=    mW
0
 INPUT 1 FOR THE DYNAMIC CALCULATION. 2 FOR SKIP
 INPUT =
2
   K-FACTOR= 1.46476 nS  MAXIUM FREQ.=  6.0663 GHz

  **************************************************
  INPUT 1 FOR CALCULATE THE GAIN(E) RELATION.

  INPUT 2 FOR CALCULATE THE LINEWIDTH ENHENCEMENT
  FACTOR AND PHOTON ENERGY RELATION

  INPUT 3 FOR EXIT THE PROGRAM

 THE INPUT # IS
1
 INPUT FERMILEVELS IN C-BAND, V-BAND, AND CARRIER DENSITY
0.240516079684E+00 0.192582838033E-02 0.301052631579E+19
 CALCULATE THE CONVOLUTION GAIN(E) COEFFICIENT
  **************************************************
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(LAMBDA)
ol1.txt
  **************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(LAMBDA)
ml1.txt
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(E)
oe1.txt
  **************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(E)
me1.txt
```

```
 ************************************************
 INPUT 1 FOR REPEAT THE G(E) CALCULATION
 INPUT 2 FOR REPEAT THE ALPHA(E) CALCULATION
 INPUT 3 FOR EXIT
1
 ************************************************
  INPUT 1 FOR CALCULATE THE GAIN(E) RELATION.

  INPUT 2 FOR CALCULATE THE LINEWIDTH ENHENCEMENT
  FACTOR AND PHOTON ENERGY RELATION

  INPUT 3 FOR EXIT THE PROGRAM

 THE INPUT # IS
1
 INPUT FERMILEVELS IN C-BAND, V-BAND, AND CARRIER DENSITY
0.292773620684 -0.223794117473E-01 0.301052631579E+19
 CALCULATE THE CONVOLUTION GAIN(E) COEFFICIENT
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(LAMBDA)
ol2.txt
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(LAMBDA)
ml2.txt
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(E)
oe2.txt
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(E)
me2.txt
 ************************************************
 INPUT 1 FOR REPEAT THE G(E) CALCULATION
 INPUT 2 FOR REPEAT THE ALPHA(E) CALCULATION
 INPUT 3 FOR EXIT
3
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

7
```

c) The Output characteristics of designed laser from step 5 are summarized in Table C.8.7.

Table C.8.7 Characteristics of the designed laser

Optimized number of QWs (Nopt)	1
Number of QWs	1
Slope efficiency (%)	2.01
Jth (A/cm^2)	93.18- 1st check, for matching threshold conditions 376.32 – 2nd check, using McIlory method
Ith (mA)	1.188mA - 1st check, for matching threshold conditions 4.798 mA - 2nd check, using McIlory method

Peak λ at operating temperature (um)	0.84699um for carrier density of 1.0E18 /cm3 0.8512um for carrier density of 3.0E18 /cm3
Peak material gain (1/cm)	1481/cm for carrier density of 2.0E18 /cm3 3518/cm for carrier density of 3.0E18 /cm3

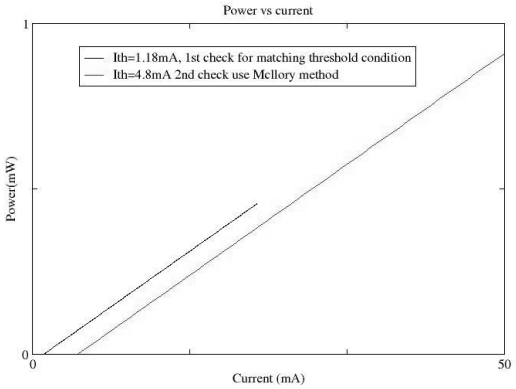

Fig. C.8.5. L-I curve of the laser

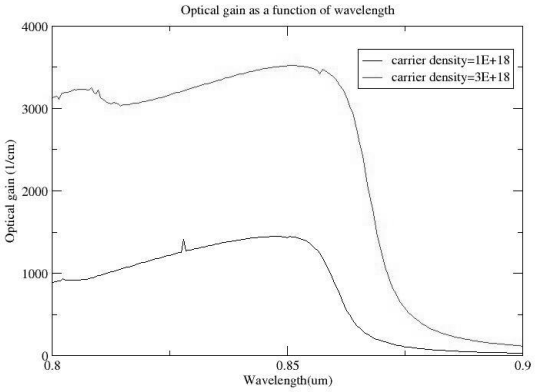

Fig. C.8.6. Optical gain-λ curve of the laser

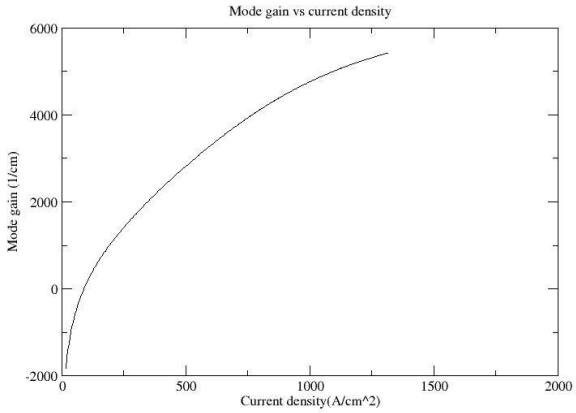

Fig. C.8.7. Mode gain as a function of current density (J)

C.9. Material system # 9: InGaAs/AlGaInAs/AlGaInAs (substrate InP)

This is a simulation of a five-layer laser structure that contains a single quantum well (QW), two separated confinement heterostructure (SCH) layers, and two cladding layers as shown in Fig. C.9.1.

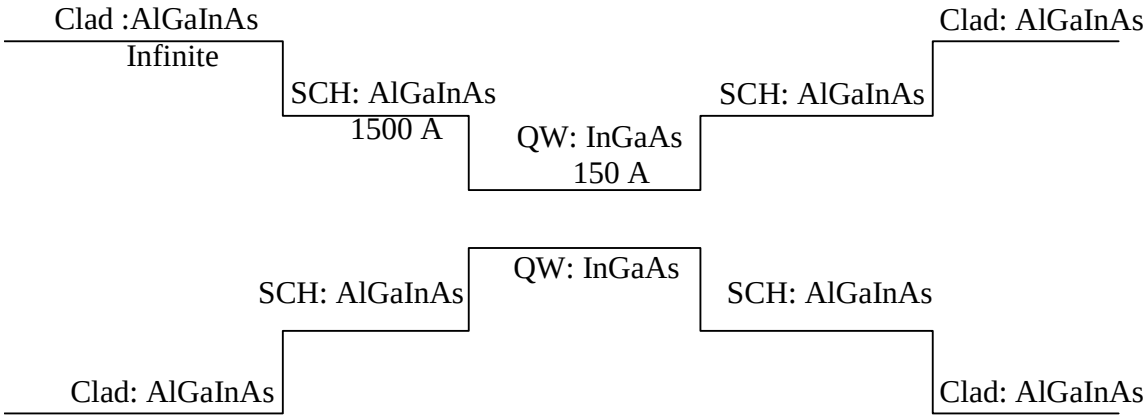

Figure C.9.8. Energy band diagram for the single quantum well structure

C.9.1. Calculation of material compositions and energy band edges.

The first step of the GAIN program is to calculate the material compositions and energy band edges of each layer. The user is asked to enter the photoluminescence wavelength, thickness, and strain of the QW, SCH, and cladding layers. After these parameters are input, the GAIN program generates two output files: cbandeg.dat and vbandeg.dat, containing the material compositions, and the conduction band edges and valence band edges respectively. The detailed explanation is provided in Chapter 2 of this manual.

a) The input parameters to the GAIN program in this step is listed in Table. C.9.1. The substrate is InP.

Table C.9.1. Input parameters to the GAIN program in this step.

Layer	λ (um)	Strain	Thickness (Å)
QW ($In_xGa_{1-x}As$)	1.51	5.1231E-003	150
SCH ($Al_xGa_yIn_{1-x-y}As$)	1.28	-	1500
Cladding ($Al_xGa_yIn_{1-x-y}As$)	0.83	-	380

b) The steps in using the GAIN program to calculate the material compositions and energy band edges are listed in Table C.9.2

Table C.9.2. steps to run the GAIN program for necessary parameters.

ENTER 1 **FOR THE NECESSARY PARAMETERS**
2 FOR THE ENERGY VALUES OF CONDUCTION BAND

```
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

1

 ENTER 1 FOR AlGaAs/AlGaAs
      2 FOR InGaAsP/InGaAsP/InP
      3 FOR InGaAs/InGaAsP/InP
      4 FOR InGaAlAs/InGaAlAs/InP
      5 FOR GaInP/(AlGa)0.5In0.5P/AlInP
      6 FOR InGaAs/AlGaAs/AlGaAs
      7 FOR InGaAs/InGaAsP/Ga0.51In0.49P(MATCHED GaAs)
      8 FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
      9 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/InP
     10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(matched InP)
     11 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/AlAsxSb1-x
     12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs (dilute N)
     13 FOR In(1-x)Ga(x)As(y)P(1-y)/GaAs
     14 FOR EXIT, BACK TO MAIN PAGE!
9
 INPUT THE LAYER # FOR GRIN STRUCTURE(STEP)
 STEP N=
2
  INPUT THE WELL WAVELENGTH (um)
1.51
  INPUT THE BARRIER WAVELENGTH (um)
1.28
  INPUT THE CLADDING WAVELENGTH (um)
0.83
BANDGAP ENERGY OF QUANTUM WELL=   0.821192052980132       eV
  INPUT CLADDING, BARRIER,QUANTUM WELL WIDTH (A)
380 1500 150
 THE In(z)Ga(1-z)As/Al(y)Ga(x)In(1-x-y)As/InP MATERIAL
 CALCULATE THE In(z)Ga(1-z)As QUANTUM WELL--Z

  FOR BARRIER IS LATTICE MATCHED SELECT ==>1
  FOR BARRIER IS STRAIN COMPENSATED SELECT ==> 2

  SELECTION IS ===> ?
1
  X is Ga=   0.293367442525692       Y is Al=   0.177652650765276
 CHECK STRAIN=  5.123144425669000E-003

  WRITE CONDUCTION BAND PARAMETERS INTO CBANDEG.DAT

  WRITE VALENCE BAND PARAMETERS INTO VBANDEG.DAT
  INPUT 1 FOR NEW CALCULATION
       2 FOR EXIT
  INPUT =?
2

 ENTER 1 FOR AlGaAs/AlGaAs
      2 FOR InGaAsP/InGaAsP/InP
```

```
      3 FOR InGaAs/InGaAsP/InP
      4 FOR InGaAlAs/InGaAlAs/InP
      5 FOR GaInP/(AlGa)0.5In0.5P/AlInP
      6 FOR InGaAs/AlGaAs/AlGaAs
      7 FOR InGaAs/InGaAsP/Ga0.51In0.49P(MATCHED GaAs)
      8 FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
      9 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/InP
     10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(matched InP)
     11 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/AlAsxSb1-x
     12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs (dilute N)
     13 FOR In(1-x)Ga(x)As(y)P(1-y)/GaAs
     14 FOR EXIT, BACK TO MAIN PAGE!
14
 THIS PROGRAM STOP HERE!, BACK TO MAIN PAGE
```

c) The output files, cbandeg.dat and vbandeg.dat are explained in Table C.9.3.

Table C.9.3. Material compositions and band offsets:

a) cbandeg.dat for conduction band

```
*************************************************************************
 QW strain   lattice constant
0.512314E-02  0.583873E-09
                        material compositions (see Table C.4.1 for x and y)
 layer thickness,          x              y        conduction band edges
  0.38000000E+03  0.00000000E+00  0.4806046   0.4844044     cladding layer
  0.15000000E+04  0.29336744E+00  0.1776527   0.1062417     SCH layer
  0.15000000E+03  0.45774735E+00  0.0000000  -0.0283436     quantum well
  0.15000000E+04  0.29336744E+00  0.1776527   0.1062417     SCH layer
  0.38000000E+03  0.00000000E+00  0.4806046   0.4844044     cladding layer
*************************************************************************
```

b) vbandeg.dat for valence band

```
*************************************************** ********************
 QW strain   lattice constant
 0.512314E-02  0.583873E-09
                        material compositions (see Table C.4.1 for x and y)
 layer thickness,          x              y        valence band edges
  0.38000000E+03  0.00000000E+00  0.4806046  -0.1883795     cladding layer
  0.15000000E+04  0.29336744E+00  0.1776527  -0.0413162     SCH layer
  0.15000000E+03  0.45774735E+00  0.0000000   0.0141718     quantum well
  0.15000000E+04  0.29336744E+00  0.1776527  -0.0413162     SCH layer
  0.38000000E+03  0.00000000E+00  0.4806046  -0.1883795     cladding layer
*************************************************************************
```

C.9.2. Energy level calculations

After the calculation of the material compositions and energy band edges, the GAIN program calculates energy levels in the conduction band and valence bands. The detailed explanations are discussed in Chapter 3 of this manual.

a) The steps of how to calculate the energy levels are shown in Table C.9.4.

Table C.9.4. Steps to calculate the energy levels

i) Steps to calculate the conduction band energy levels

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

2
 INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
 INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
 INPUT N=
5
 INPUT THE LOWEST POTENTIAL LAYER(1st Q-WELL) IC= ?
3
 INPUT THE SELECTED CENTER LAYER OF STRUCTURE ICR=
3
 ******************************************************
  INPUT I=1  FOR AlGaAs
       I=2  FOR InGaAsP
       I=3  FOR In1-xGaxAs/InGaAsP/InP
       I=4  FOR InGaAlAs/InGaAlAs
       I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
       I=6  FOR InGaAs/AlGaAs/AlGaAs
       I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
       I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
       I=9  FOR InzGa1-zAs/AlxGayIn1-x-yAs/InP
       I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
       I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
       I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
       I=13 FOR InGaAs/In(1-y)Ga(x)As(y)P(1-y)/GaAs
  INPUT I= ?
 ******************************************************
9
 ENERGY EIGENVALUE===> -0.992710047952E-02 ERROR= .3115362E-14
 ENERGY EIGENVALUE===>  0.441920512738E-01 ERROR= .2426294E-14
 ENERGY EIGENVALUE===>  0.106443501424E+00 ERROR= .4979896E-14
                        ……..

 FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
 SKIP INPUT I==> 2
 I=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
-0.992710047952E-02
 INPUT THE NAME OF OUTPUT FILE
cb1.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.92691705E-62
 CONFINEMENT FACTOR OF    2 th LAYER = 0.19816721E-01
 CONFINEMENT FACTOR OF    3 th LAYER = 0.96036656E+00
```

```
 CONFINEMENT FACTOR OF    4 th LAYER = 0.19816721E-01
 CONFINEMENT FACTOR OF    5 th LAYER = 0.92691705E-62
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
1
  INPUT THE EIGENVALUE
  EIGEN VALUE=
0.441920512738E-01
  INPUT THE NAME OF OUTPUT FILE
cb2.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.23632038E-45
 CONFINEMENT FACTOR OF    2 th LAYER = 0.86213358E-01
 CONFINEMENT FACTOR OF    3 th LAYER = 0.82757328E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.86213358E-01
 CONFINEMENT FACTOR OF    5 th LAYER = 0.23632038E-45
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
2
```

ii) Steps to calculate the heavy hole energy levels

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

3
  INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
  INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
  INPUT N=
5
  INPUT THE HIGHEST POTENTIAL(1st Q-WELL) LAYER IC= ?
3
  INPUT THE SELECTED CENTER OF THE STRUCTURE ICR=?
3
 *******************************************************
   INPUT I=1  FOR AlGaAs
        I=2  FOR InGaAsP
        I=3  FOR In(1-x)Ga(x)As/InGaAsP/InP
        I=4  FOR InGaAlAs/InGaAlAs
        I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
        I=6  FOR InGaAs/AlGaAs/AlGaAs
        I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
        I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
        I=9  FOR In(z)Ga(1-z)As/AlxGayIn1-x-yAs/InP
        I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
        I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
        I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
        I=13 FOR InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
   INPUT I= ?
 *******************************************************
9
 *******************************************************
```

```
 DOES THE STRUCTURE STRAIN OR STRAIN-COMPENSATED?
 IF STRAIN ONLY INPUT 1, STRAIN-COMPENSATED INPUT 2
 INPUT SELECT = ?

1
                                   ……….
 ENERGY EIGENVALUE===> -0.321196505162E-01 ERROR= .2209942E-14
 ENERGY EIGENVALUE===> -0.168788071783E-01 ERROR= .2462727E-14
 ENERGY EIGENVALUE===> -0.689461835889E-02 ERROR= .1860138E-14

 FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
 SKIP INPUT I==> 2
 I=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
-0.689461835889E-02
 INPUT THE NAME OF OUTPUT FILE
hh1.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.50739096E-73
 CONFINEMENT FACTOR OF    2 th LAYER = 0.91099066E-02
 CONFINEMENT FACTOR OF    3 th LAYER = 0.98178019E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.91099066E-02
 CONFINEMENT FACTOR OF    5 th LAYER = 0.50739096E-73
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
-0.168788071783E-01
 INPUT THE NAME OF OUTPUT FILE
hh2.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.19697388E-61
 CONFINEMENT FACTOR OF    2 th LAYER = 0.40620496E-01
 CONFINEMENT FACTOR OF    3 th LAYER = 0.91875901E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.40620496E-01
 CONFINEMENT FACTOR OF    5 th LAYER = 0.19697388E-61
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
2
```

iii) Steps to calculate the light hole energy levels

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

4
 INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
 INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
 INPUT N=
```

```
5
 INPUT THE HIGHEST POTENTIAL(1st Q-WELL) LAYER IC= ?
3
 INPUT THE SELECTED CENTER OF THE STRUCTURE ICR=?
3
 ********************************************************
  INPUT I=1  FOR AlGaAs
      I=2  FOR InGaAsP
      I=3  FOR In(1-x)Ga(x)As/InGaAsP/InP
      I=4  FOR InGaAlAs/InGaAlAs
      I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
      I=6  FOR InGaAs/AlGaAs/AlGaAs
      I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
      I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
      I=9  FOR In(z)Ga(1-z)As/AlxGayIn1-x-yAs/InP
      I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
      I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
      I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
      I=13 FOR InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
  INPUT I= ?
 ********************************************************
9
 ********************************************************

  DOES THE STRUCTURE STRAIN OR STRAIN-COMPENSATED?
  IF STRAIN ONLY INPUT 1, STRAIN-COMPENSATED INPUT 2
  INPUT SELECT = ?

1
                                ……..
  ENERGY EIGENVALUE===> -0.416760055833E-01 ERROR= .2632360E-14
  ENERGY EIGENVALUE===> -0.293879437609E-01 ERROR= .2884725E-14
  ENERGY EIGENVALUE===>  0.143716677955E-01 ERROR= .2231081E-14

  FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
  SKIP INPUT I==> 2
  I=?
1
  INPUT THE EIGENVALUE
  EIGEN VALUE=
0.143716677955E-01
  INPUT THE NAME OF OUTPUT FILE
lh1.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.12528826E-34
 CONFINEMENT FACTOR OF    2 th LAYER = 0.41196175E-01
 CONFINEMENT FACTOR OF    3 th LAYER = 0.91760765E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.41196175E-01
 CONFINEMENT FACTOR OF    5 th LAYER = 0.12528826E-34
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
1
  INPUT THE EIGENVALUE
  EIGEN VALUE=
-0.293879437609E-01
  INPUT THE NAME OF OUTPUT FILE
lh2.txt
```

```
 CONFINEMENT FACTOR OF    1 th LAYER = 0.65284158E-17
 CONFINEMENT FACTOR OF    2 th LAYER = 0.22295907E+00
 CONFINEMENT FACTOR OF    3 th LAYER = 0.55408185E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.22295907E+00
 CONFINEMENT FACTOR OF    5 th LAYER = 0.65284158E-17
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
2
```

b) The main output file from this part of GAIN program is energy.dat, containing all the energy levels as shown in Table C.9.5. After the energy eigen values are calculated, the GAIN program asks the users whether they would like to check the wave envelope function or not. We suggest that the user should check the wave envelope functions of the first and second energy levels for conduction and valence bands. The plots of the envelope functions are shown in Fig. C.9.2, Fig. C.9.3, Fig C.9.4.

Table C.9.5. Output file energy.dat

```
 CONDUCTION BAND ENERGY===> -0.992710047952E-02 ERROR= .3115362E-14
 CONDUCTION BAND ENERGY===>  0.441920512738E-01 ERROR= .2426294E-14
                                        ……
                                        ……
                                        ……
 HEAVY HOLE ENERGY===> -0.168788071783E-01 ERROR= .2462727E-14
 HEAVY HOLE ENERGY===> -0.689461835889E-02 ERROR= .1860138E-14
                                        ……
                                        ……
                                        ……
 LIGHT HOLE ENERGY===> -0.293879437609E-01 ERROR= .2884725E-14
 LIGHT HOLE ENERGY===>  0.143716677955E-01 ERROR= .2231081E-14
```

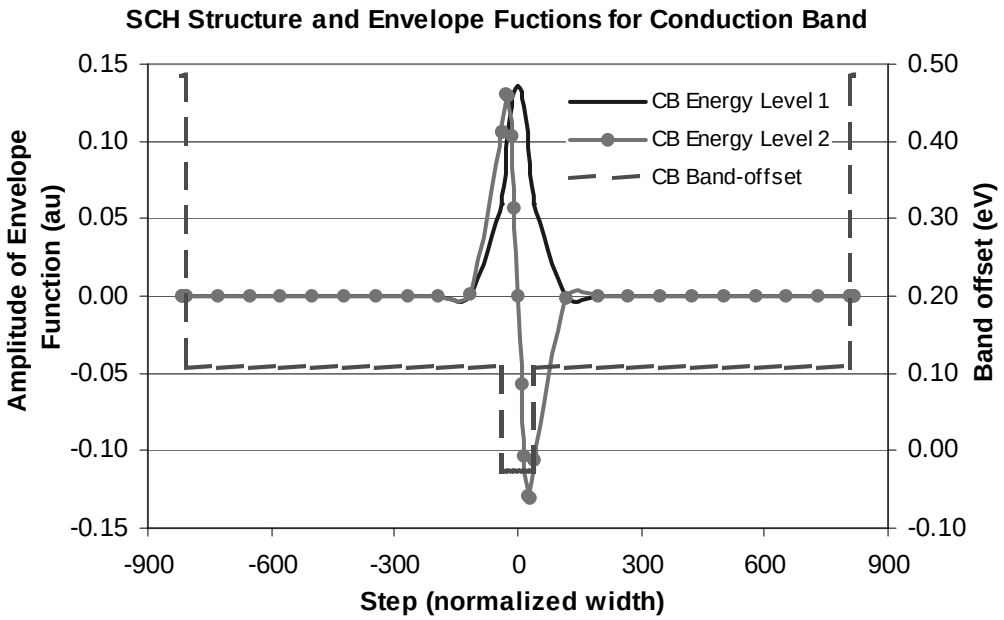

Fig. C.9.2. Wave envelope functions for energy levels in conduction band

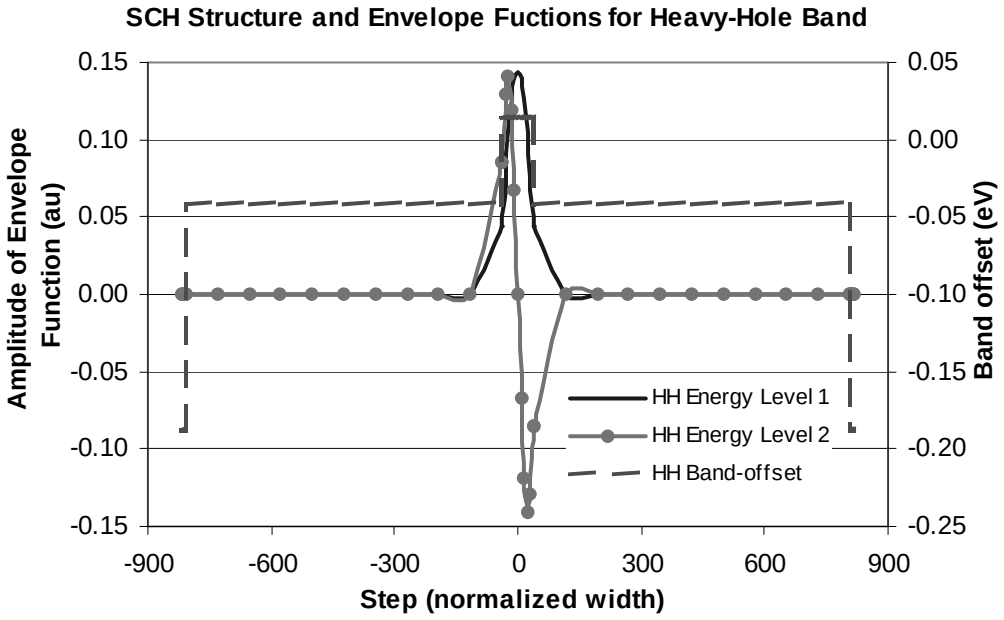

Fig. C.9.3. Wave envelope functions for heavy hole energy levels

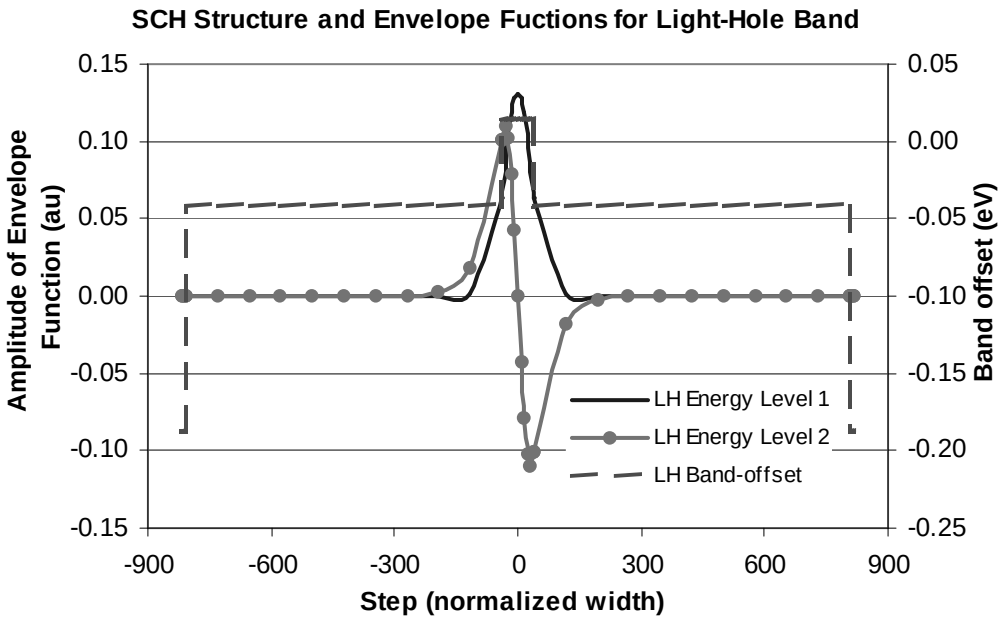

Fig. C.9.4. Wave envelope functions for light hole energy levels

C.9.3. Computation of Gain and Laser Characteristics

This is the last step of simulations using the GAIN program. With the previously calculated material composition, energy band edges, energy levels; and other parameters like material loss and Auger coefficient, the GAIN program can simulate the threshold current, threshold current density, slope efficiency, optical gain and modal gain as functions of wavelengths and photon energies, and also the L-I curve. The details are explained in Chapter 4 of the manual.

In this part of the GAIN program, the input file needs to be constructed with the results from the previous steps and according to the laser design. In this example, single quantum well structure is used to simulate a three-QW laser. For the three-quantum-well laser with a ridge length of 750 μm and ridge width of 5 μm, the input file is shown in Table C.9.6. The detailed steps of simulations are listed in Table C.9.7. The main output files: L-I curve, optical gain as a function of the wavelength, and mode gain vs. current density are plotted in Fig. C.9.5, Fig. C.9.6, and Fig. C.9.7.

a) The input file:

Table C.9.6. Input file for gain and threshold current calculation

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c     1. Input the compositions, width of well, effective index        c
c        and lasing wavelength.                                        c
c     Ex: xx,xz,qy,xy,lx,n,lam                                         c
c     for different materials the following are the forms of inputs.   c
c                                                                      c
c     w -- > well, b -- > barrier  cxz and cxy for cladding.            c
c                                                                      c
c     a.  AlxGa1-xAs : xx (Al w) xz (Al b) qy (0) xy (0)               c
c     b.  In1-xGaxAsyP1-y : xx (Ga w) xz (Ga b) qy (As w) xy (As b)    c
c     c.  In1-xGaxAs/InGaAsP : xx (Ga w) xz (Ga b) qy (0) xy (As b)    c
c     d.  AlxGayIn1-x-yAs/InP : xx (Ga w) xz (Ga b) qy (Al w) xy (Al b)c
c     e.                                                               c
c     f.  InxGa1-xAs/AlGaAs : xx (In w) xz (0) qy (0) xy (Al b)        c
c     g.                                                               c
c     h.  AlyInxGa1-x-yAs/AlGaAs : xx (Al w) xz (al b) qy (In w) xz (0)c
c     i.  InxGa1-xAs/AlGaInAs : xx (In w) xz (0) qy (Al b) xy (Ga b)   c
c     j.  In(y)Ga(1-y)As(x)N(1-x) :xx(As w),xz(As, b),qy(In w),xy(In b)c
c     k.  InGaAs/InGaAsP/GaAs: xx (In w), (0), xz(Ga w) xy (As b)
c        2.  Input  the  energy  gap,temperature,  barrier  band  edges(both
bands)
c     Ex: eg,temp,ec,ev                                                c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
0.45774735  0.0  0.1776527  0.29336744  15.0  3.273915  1.55
0.82119205  298  0.1062417  0.0413162
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c     3. Input the ist level sub-band energy levels.                   c
c     Ex: ec1,eh1,el1                                                  c
c                                                                      c
c     4. Input the material loss, reflectivities, number of quantum    c
c        wells and beta(for spontaneous emission).                     c
c     Ex: alpha,r1,r2,mm,beta.                                         c
```

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
-0.99271E-02   0.689462E-02   -0.143717E-01   0.44192E-01   0.168788E-01
0.29388E-01
3.0d0  0.30   0.30   1  5.D-5
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c     5. Input the cavity length, ridge width, internal efficiency     c
c        Auger, strain(except AlGaAs,put 0) and confinement factor.    c
c     Ex: cl,cw,etha,ca,es,confine                                     c
c                                                                      c
c     6. Input the cladding composition and band edges.                c
c     Ex: cxz,cxy,ecc,evv                                              c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
750.D-4    5D-4  0.96  1.00d-29   0.000  0.03050213
0.0  0.48  0.4844044   0.1883795
```

b) The steps for these calculations mentioned are listed in Table C.9.7

Table C.9.7. The steps for the gain and threshold current density calculations

```
ENTER 1 FOR THE NECESSARY PARAMETERS
     2 FOR THE ENERGY VALUES OF CONDUCTION BAND
     3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
     4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
     5 FOR THE LASER G-J AND G(LAMBDA)
     6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
     7 FOR EXIT
5
 THE INPUT FILE NAME=
ms9in
 SELECT MATERIAL=?
 1--AlGaAs
 2--InGaAsP
 3--In1-zGazAs/InGaAsP/InP
 4-- InGaAlAs
 5--GaInP/AlzGawIn1-z-wP/Al0.5In0.5P
 6-- InxGa1-xAs/AlxGa1-xAs/AlGaAs
 7--In1-xGaxAs/InGaAsP/GaxIn1-xP(X=0.51) MATCHED TO GaAs
 8--AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
 9--InzGa1-zAs/AlxGayIn1-x-yAs/InP
 10-- InGaAlAs/InGaAlAs/AlAsSb
 11--InzGa1-zAs/AlxGayIn1-x-yAs/AlAsSb
 12--In(y)Ga(1-y)As(x)N(1-x)/GaAs
 13--InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
 INPUT SELECTION
9
 INPUT MODE = ? FOR TE--> MODE =1, FOR TM--> MODE =2
 INPUT TE OR TM ?
2
 IF EL1 BELOW EH1 THEN SELECT 1, OTHERWISE SELECT 2
 SELECTION=?
2
 ************************************************
 CALCULATE THE EFFECTIVE MASS
 ************************************************
 FOR QUASI-FERMI LEVEL SELECT=1,
 FOR READ EXISTING QUASI-FERMI LEVEL SELECT=2
 SELECT=?
```

```
1
                    .................
 J(LEAKAGE)=0.421436D+04 A/cm^2  N=0.794060D+19 1/cm^3
 J(LEAKAGE)=0.428431D+04 A/cm^2  N=0.796040D+19 1/cm^3
 J(LEAKAGE)=0.435419D+04 A/cm^2  N=0.798020D+19 1/cm^3
 J(LEAKAGE)=0.442397D+04 A/cm^2  N=0.800000D+19 1/cm^3
 ************************************************
 G(J) PARAMETERS FROM SINGLE WELL
 Go=0.747571D+01 1/cm  Jo=0.117454D+03 A/cm^2

 G(N) PARAMETERS FROM SINGLE WELL
 NGo=0.245088D+03 1/cm  XNo=0.128797D+19 1/cm^3

 Jtr=0.432090D+02 A/cm^2  NTR=0.473818D+18 1/cm^3

 THE OPTIMUM NUMBER OF QUANTUM WELL FOLLOWS THE ARTICLE
 BY McIlory et al. IEEE JQE-21 1985.

 THE OPTIMUM NUMBER OF QUANTUM WELL Nopt =          3
 INPUT Nopt(CAN BE DIFFERENT FROM ABOVE CALCULATION)=?
3
 NUMBER OF QUANTUM WELL(MAY OR MAY NOT BE Nopt)=?
3

 ************************************************
 1ST CHECK USE SINGLE WELL TIMES # OF WELLS
 ************************************************
 2ND CHECK FOLLOWS FORMULA BY McIlory IN IEEE
 JOURNAL OF QUANTUM ELECTRONIC QE-21 1985.
 ************************************************
 Gth=  19.0530 1/cm Nth=0.396090D+19 1/cm^3 IY=  196
  1ST CHECK Jth=  1347.91345919 A/cm^2
  2ND CHECK Jth=   367.04422 A/cm^2

  1ST CHECK Ith=0.505468D+02 mA NUMBER OF WELLS=  3
  2ND CHECK Ith=0.137642D+02 mA

 ************************************************
 CALCULATE THE P-I RELATION

 NDATA=        205
 ************************************************
 CALCULATE THE SLOPE: mW/mA Y=A+BX
 CONSTANT A= -15.3972372   SLOPE B=   0.3046138

 ************************************************
 INPUT POWER PO FOR THE LINEWIDTH, PO=0 FOR STOP
 INPUT PO=    mW
0
 INPUT 1 FOR THE DYNAMIC CALCULATION. 2 FOR SKIP
 INPUT =
2
 K-FACTOR= 0.44360 nS  MAXIUM FREQ.= 20.0309 GHz

 ************************************************
 INPUT 1 FOR CALCULATE THE GAIN(E) RELATION.
```

```
 INPUT 2 FOR CALCULATE THE LINEWIDTH ENHENCEMENT
 FACTOR AND PHOTON ENERGY RELATION

 INPUT 3 FOR EXIT THE PROGRAM

 THE INPUT # IS
1
 INPUT FERMILEVELS IN C-BAND, V-BAND, AND CARRIER DENSITY
0.155952069365, 0.148892829364E-01, 2.0E+18
 CALCULATE THE CONVOLUTION GAIN(E) COEFFICIENT
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(LAMBDA)
ogl2.txt
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(LAMBDA)
mgl2.txt
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(E)
oge2.txt
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(E)
mge2.txt
 ************************************************
 INPUT 1 FOR REPEAT THE G(E) CALCULATION
 INPUT 2 FOR REPEAT THE ALPHA(E) CALCULATION
 INPUT 3 FOR EXIT
1
 ************************************************
 INPUT 1 FOR CALCULATE THE GAIN(E) RELATION.

 INPUT 2 FOR CALCULATE THE LINEWIDTH ENHENCEMENT
 FACTOR AND PHOTON ENERGY RELATION

 INPUT 3 FOR EXIT THE PROGRAM

 THE INPUT # IS
1
 INPUT FERMILEVELS IN C-BAND, V-BAND, AND CARRIER DENSITY
0.226279415596, 0.314766742996E-01, 3.0E+18
 CALCULATE THE CONVOLUTION GAIN(E) COEFFICIENT
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(LAMBDA)
ogl3.txt
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(LAMBDA)
mgl3.txt
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(E)
oge3.txt
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(E)
mge3.txt
 ************************************************
 INPUT 1 FOR REPEAT THE G(E) CALCULATION
 INPUT 2 FOR REPEAT THE ALPHA(E) CALCULATION
 INPUT 3 FOR EXIT
1
```

```
 ************************************************
 INPUT 1 FOR CALCULATE THE GAIN(E) RELATION.

 INPUT 2 FOR CALCULATE THE LINEWIDTH ENHENCEMENT
 FACTOR AND PHOTON ENERGY RELATION

 INPUT 3 FOR EXIT THE PROGRAM

 THE INPUT # IS
1
 INPUT FERMILEVELS IN C-BAND, V-BAND, AND CARRIER DENSITY
0.295069951213, 0.449714150578E-01, 4.0E+18
 CALCULATE THE CONVOLUTION GAIN(E) COEFFICIENT
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(LAMBDA)
ogl4.txt
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(LAMBDA)
mgl4.txt
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(E)
oge4.txt
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(E)
mge4.txt
 ************************************************
 INPUT 1 FOR REPEAT THE G(E) CALCULATION
 INPUT 2 FOR REPEAT THE ALPHA(E) CALCULATION
 INPUT 3 FOR EXIT
3

ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT
7
```

c) The Output characteristics of designed laser from step 5 are summarized in Table C.9.7.

Table C.9.7 Characteristics of the designed laser

Optimized number of QWs (Nopt)	3
Number of QWs	3
Slope efficiency (%)	30.46
Jth (A/cm^2)	1347.91 – 1^{st} check, for matching threshold conditions 367.04 – 2^{nd} check, using McIlory method
Ith (mA)	50.54 A - 1^{st} check, for matching threshold conditions 13.76 A - 2^{nd} check, using McIlory method
Peak λ at operating temperature (um)	1.5488 μm for carrier density of 2.0E18 $/cm^3$ 1.5538 μm for carrier density of 3.0E18 $/cm^3$ 1.5551 μm for carrier density of 4.0E18 $/cm^3$
Peak material gain (1/cm)	1074 /cm for carrier density of 2.0E18 $/cm^3$ 1501 /cm for carrier density of 3.0E18 $/cm^3$

	1824 /cm for carrier density of 4.0E18 /cm^3

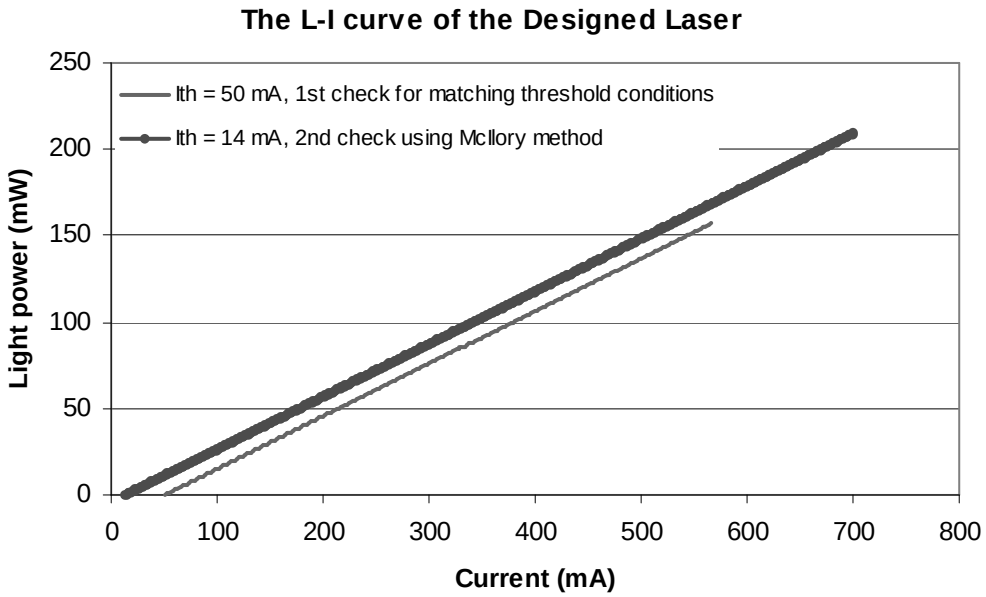

Fig. C.9.5. L-I curve of the laser

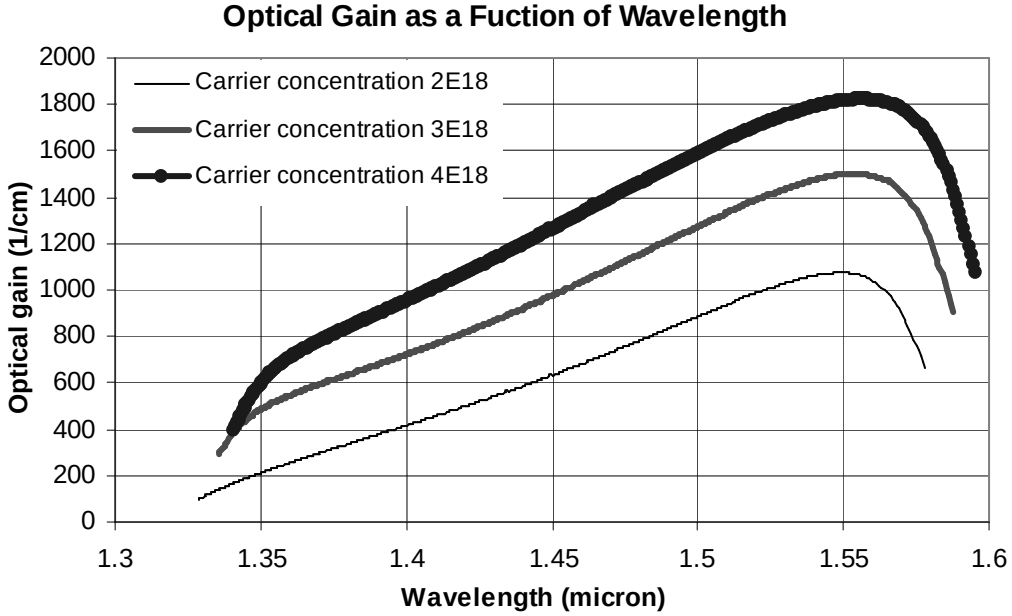

Fig. C.9.6. Optical gain-λ curve of the laser

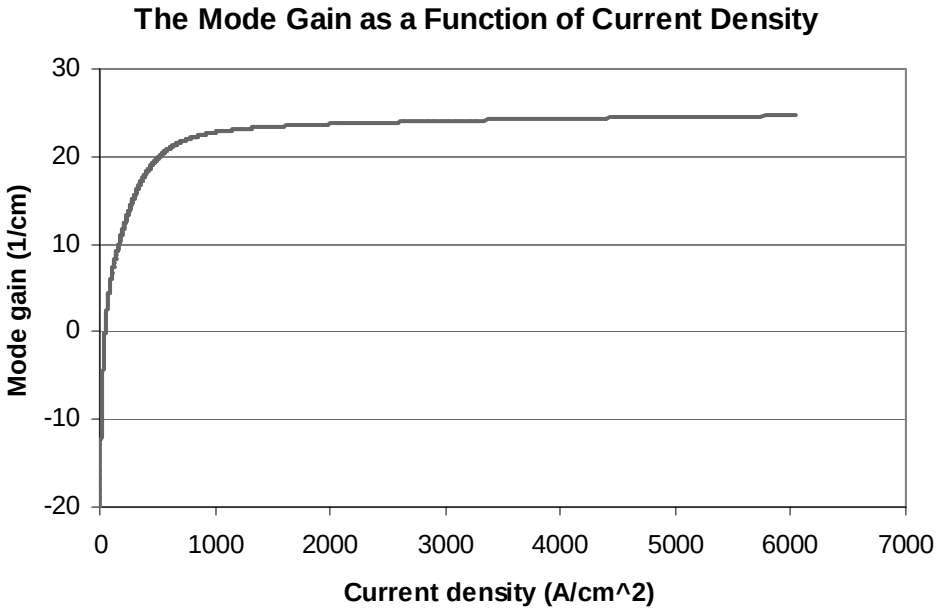

Fig. C.9.7. Mode gain as a function of current density (J)

C.12. Material system #12: In(y)Ga(1-y)As(x)N(1-x)/GaAs (dilute N)

This is a simulation of a five-layer laser structure that contains a single quantum well (QW), two separated confinement heterostructure (SCH) layers, and two cladding layers as shown in Fig. C.12.1. The structure is based on a published SQW structure [1]. From this example, the users will know how to simulate an existing structure using the GAIN program. The simulations results Jth and peak wavelength agree well with the published experimental data [1].

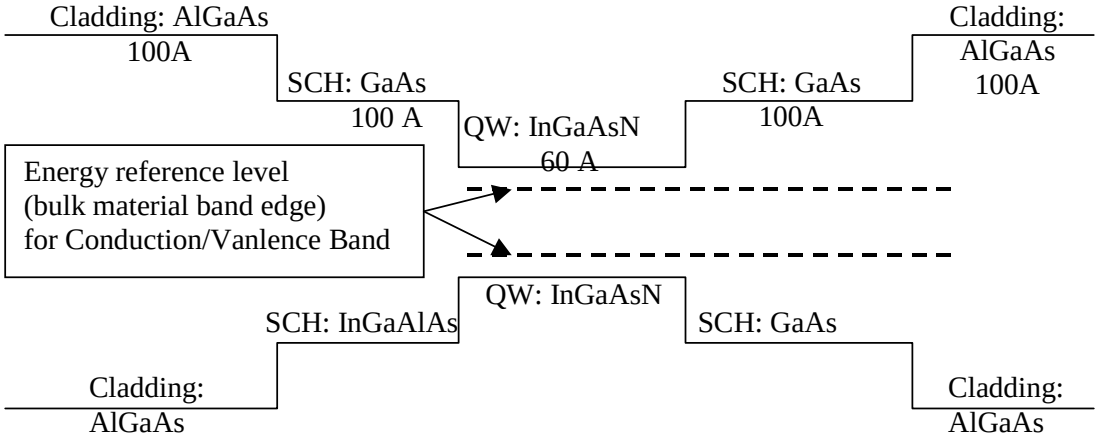

Figure C.12.9. Energy band diagram for the single quantum well structure

C.12.1. Calculation of material compositions and energy band edges.

The first step of the GAIN program is to calculate the material compositions and energy band edges of the each layer. The user is asked to enter the photoluminescence wavelength, thickness, and strain of the QW, SCH, and cladding layers. After these parameters are input, the GAIN program generates two output files: cbandeg.dat and vbandeg.dat, containing the material compositions, and the conduction band edges and valence band edges respectively. The detailed explanation is provided in Chapter 2 of this manual.

a) The input parameters to the GAIN program in this step are listed in Table. C.12.1.

Table C.12.1. Input parameters to the GAIN program in this step.

Layer	λ (um)	Strain	Thickness (Å)
QW (In(y)Ga(1-y)As(x)N(1-x))	1.333925998	-0.02	70
SCH (GaAs)	0.874283651		100
Cladding (AlGaAs)	0.644892865		100

b) The steps in using the GAIN program to calculate the material compositions and energy band edges are listed in Table C.12.2

Table C.12.2. steps to run the GAIN program for necessary parameters.

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

1

 ENTER 1 FOR AlGaAs/AlGaAs
      2 FOR InGaAsP/InGaAsP/InP
      3 FOR InGaAs/InGaAsP/InP
      4 FOR InGaAlAs/InGaAlAs/InP
      5 FOR GaInP/(AlGa)0.5In0.5P/AlInP
      6 FOR InGaAs/AlGaAs/AlGaAs
      7 FOR InGaAs/InGaAsP/Ga0.51In0.49P(MATCHED GaAs)
      8 FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
      9 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/InP
     10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(matched InP)
     11 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/AlAsxSb1-x
     12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs (dilute N)
     13 FOR In(1-x)Ga(x)As(y)P(1-y)/GaAs
     14 FOR EXIT, BACK TO MAIN PAGE!
12
 INPUT THE LAYER # FOR GRIN STRUCTURE(STEP)
 STEP N=
2
  INPUT THE WELL WAVELENGTH (um)
1.333925998
  INPUT THE BARRIER WAVELENGTH (um)
0.874283651
  INPUT THE CLADDING WAVELENGTH (um)
0.644892865
  BANDGAP ENERGY OF QUANTUM WELL=   0.929586800061753       eV
  INPUT CLADDING, BARRIER,QUANTUM WELL WIDTH (A)
100 100 70

  For dilute InGaAsN only (X>0.953, Y<0.289)

  In(y)Ga(1-y)As(x)N(1-x),output read In first then As

  IF ONE OF THE COMPONENTS IN ACTIVE REGION IS ZERO,
  YOU HAVE TO TRY ANOTHER INITIAL GUESS FOR
  BOTH WAVELENGTH AND STRAIN

  INPUT STRAIN=?
-0.02
 C[                                                  ]*
 C[  STARTING VECTOR:      0.100D+01 0.713D-03                    ]*
 C[                                                  ]*
```

```
 C[                                                  ]*
 C[  STARTING VECTOR:      0.995D+00 0.292D+00                ]*
 C[                                                  ]*
  STRAIN= -2.000000000000016E-002  AZ2=   5.65329980850220

  WRITE CONDUCTION BAND PARAMETERS INTO CBANDEG.DAT

  WRITE VALENCE BAND PARAMETERS INTO VBANDEG.DAT
  INPUT 1 FOR NEW CALCULATION
      2 FOR EXIT
  INPUT =?
2
```

c) The output files, cbandeg.dat and vbandeg.dat are explained in Table C.12.3.

Table C.12.3. Material compositions and band offsets:

a) cbandeg.dat for conduction band

```
QW strain    lattice constant
-.200000E-01  0.576637E-09
                          material compositions
 layer thickness,            Ga                Al       conduction band edges
  0.10000000E+03  0.40000000E+00   0.0000000   0.6952492      cladding layer
  0.10000000E+03  0.99974922E+00   0.0007133   0.3421020      SCH layer
  0.70000000E+02  0.99522355E+00   0.2924459   0.1076710      quantum well
  0.10000000E+03  0.99974922E+00   0.0007133   0.3421020      SCH layer
  0.10000000E+03  0.40000000E+00   0.0000000   0.6952492      cladding layer
*********************************************************************************
```

b) vbandeg.dat for valence band

```
 QW strain    lattice constant
 -.200000E-01  0.576637E-09
                          material compositions
 layer thickness,            Ga                Al       valence band edges
  0.10000000E+03  0.40000000E+00   0.0000000   -0.2979640     cladding layer
  0.10000000E+03  0.99974922E+00   0.0007133   -0.1466152     SCH layer
  0.70000000E+02  0.99522355E+00   0.2924459   -0.0538355     quantum well
  0.10000000E+03  0.99974922E+00   0.0007133   -0.1466152     SCH layer
  0.10000000E+03  0.40000000E+00   0.0000000   -0.2979640     cladding layer
*********************************************************************************
```

C.12.2. Energy level calculations

After the calculation of the material compositions and energy band edges, the GAIN program calculates energy levels in the conduction band and valence bands. The detailed explanations are discussed in Chapter 3 of this manual.

a) The steps of how to calculate the energy levels are shown in Table C.12.4.

Table C.12.4. Steps to calculate the energy levels

i) Steps to calculate the conduction band energy levels

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

2
 INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
 INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
 INPUT N=
5
 INPUT THE LOWEST POTENTIAL LAYER(1st Q-WELL) IC= ?
3
 INPUT THE SELECTED CENTER LAYER OF STRUCTURE ICR=
3
 ******************************************************
  INPUT I=1  FOR AlGaAs
       I=2  FOR InGaAsP
       I=3  FOR In1-xGaxAs/InGaAsP/InP
       I=4  FOR InGaAlAs/InGaAlAs
       I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
       I=6  FOR InGaAs/AlGaAs/AlGaAs
       I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
       I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
       I=9  FOR InzGa1-zAs/AlxGayIn1-x-yAs/InP
       I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
       I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
       I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
       I=13 FOR InGaAs/In(1-y)Ga(x)As(y)P(1-y)/GaAs
  INPUT I= ?
 ******************************************************
12
 ENERGY EIGENVALUE===>  0.166825507851E+00 ERROR= .524871
 ENERGY EIGENVALUE===>  0.316718310711E+00 ERROR= .428128
 ENERGY EIGENVALUE===>  0.379784585626E+00 ERROR= .237362
 ENERGY EIGENVALUE===>  0.399968049847E+00 ERROR= .224208
 ENERGY EIGENVALUE===>  0.481341035928E+00 ERROR= .238450
 ENERGY EIGENVALUE===>  0.531507743261E+00 ERROR= .299977
 ENERGY EIGENVALUE===>  0.626588219321E+00 ERROR= .248585

 FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
 SKIP INPUT I==> 2
 I=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
0.166825507851
 INPUT THE NAME OF OUTPUT FILE
cb1.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.29553906E-06
 CONFINEMENT FACTOR OF    2 th LAYER = 0.47656595E-01
 CONFINEMENT FACTOR OF    3 th LAYER = 0.90468622E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.47656595E-01
```

```
 CONFINEMENT FACTOR OF    5 th LAYER = 0.29553906E-06
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
1
  INPUT THE EIGENVALUE
  EIGEN VALUE=
0.316718310711
  INPUT THE NAME OF OUTPUT FILE
cb2.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.21750109E-03
 CONFINEMENT FACTOR OF    2 th LAYER = 0.25182782E+00
 CONFINEMENT FACTOR OF    3 th LAYER = 0.49590936E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.25182782E+00
 CONFINEMENT FACTOR OF    5 th LAYER = 0.21750109E-03
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
2
```

ii) Steps to calculate the heavy hole energy levels

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

3
  INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
  INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
  INPUT N=
5
  INPUT THE HIGHEST POTENTIAL(1st Q-WELL) LAYER IC= ?
3
  INPUT THE SELECTED CENTER OF THE STRUCTURE ICR=?
3
 ********************************************************
   INPUT I=1  FOR AlGaAs
        I=2  FOR InGaAsP
        I=3  FOR In(1-x)Ga(x)As/InGaAsP/InP
        I=4  FOR InGaAlAs/InGaAlAs
        I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
        I=6  FOR InGaAs/AlGaAs/AlGaAs
        I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
        I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
        I=9  FOR In(z)Ga(1-z)As/AlxGayIn1-x-yAs/InP
        I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
        I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
        I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
        I=13 FOR InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
   INPUT I= ?
 ********************************************************
12
 ********************************************************
```

```
 DOES THE STRUCTURE STRAIN OR STRAIN-COMPENSATED?
 IF STRAIN ONLY INPUT 1, STRAIN-COMPENSATED INPUT 2
 INPUT SELECT = ?

1
 ENERGY EIGENVALUE===> -0.280844081259E+00 ERROR= .4292362E-14
 ENERGY EIGENVALUE===> -0.261654918264E+00 ERROR= .5060880E-14
 ENERGY EIGENVALUE===> -0.230050446372E+00 ERROR= .4085794E-14
 ENERGY EIGENVALUE===> -0.215971305480E+00 ERROR= .3569352E-14
 ENERGY EIGENVALUE===> -0.191389154282E+00 ERROR= .1495427E-13
 ENERGY EIGENVALUE===> -0.179058584723E+00 ERROR= .2864169E-14
 ENERGY EIGENVALUE===> -0.166390752259E+00 ERROR= .3290070E-14
 ENERGY EIGENVALUE===> -0.155038585857E+00 ERROR= .2022241E-14
 ENERGY EIGENVALUE===> -0.151912036949E+00 ERROR= .1853312E-14
 ENERGY EIGENVALUE===> -0.949214838256E-01 ERROR= .3591541E-14
 ENERGY EIGENVALUE===> -0.294250467453E-01 ERROR= .1947900E-14
 ENERGY EIGENVALUE===>  0.126045078739E-01 ERROR= .1384266E-14

 FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
 SKIP INPUT I==> 2
 I=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
0.126045078739E-01
 INPUT THE NAME OF OUTPUT FILE
hh1.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.49924329E-13
 CONFINEMENT FACTOR OF    2 th LAYER = 0.80920305E-02
 CONFINEMENT FACTOR OF    3 th LAYER = 0.98381594E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.80920305E-02
 CONFINEMENT FACTOR OF    5 th LAYER = 0.49924329E-13
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
-0.294250467453E-01
 INPUT THE NAME OF OUTPUT FILE
hh2.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.65742276E-11
 CONFINEMENT FACTOR OF    2 th LAYER = 0.35421992E-01
 CONFINEMENT FACTOR OF    3 th LAYER = 0.92915602E+00
 CONFINEMENT FACTOR OF    4 th LAYER = 0.35421992E-01
 CONFINEMENT FACTOR OF    5 th LAYER = 0.65742276E-11
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
2
```

iii) Steps to calculate the light hole energy levels

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
```

```
      7 FOR EXIT

4
 INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
 INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
 INPUT N=
5
 INPUT THE HIGHEST POTENTIAL(1st Q-WELL) LAYER IC= ?
3
 INPUT THE SELECTED CENTER OF THE STRUCTURE ICR=?
3
 ******************************************************
  INPUT I=1  FOR AlGaAs
       I=2  FOR InGaAsP
       I=3  FOR In(1-x)Ga(x)As/InGaAsP/InP
       I=4  FOR InGaAlAs/InGaAlAs
       I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
       I=6  FOR InGaAs/AlGaAs/AlGaAs
       I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
       I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
       I=9  FOR In(z)Ga(1-z)As/AlxGayIn1-x-yAs/InP
       I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
       I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
       I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
       I=13 FOR InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
  INPUT I= ?
 ******************************************************
12
 ******************************************************

 DOES THE STRUCTURE STRAIN OR STRAIN-COMPENSATED?
 IF STRAIN ONLY INPUT 1, STRAIN-COMPENSATED INPUT 2
 INPUT SELECT = ?

1
 ENERGY EIGENVALUE===> -0.295278683327E+00 ERROR= .2131495E-14
 ENERGY EIGENVALUE===> -0.256122699275E+00 ERROR= .2338818E-14
 ENERGY EIGENVALUE===> -0.217375554875E+00 ERROR= .5742157E-14
 ENERGY EIGENVALUE===> -0.183928037223E+00 ERROR= .3316695E-14
 ENERGY EIGENVALUE===> -0.164785601442E+00 ERROR= .3822678E-14
 ENERGY EIGENVALUE===> -0.145241224988E+00 ERROR= .1407070E-14

 FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
 SKIP INPUT I==> 2
 I=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
0.145241224988
 INPUT THE NAME OF OUTPUT FILE
lh1.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.37276532E-07
 CONFINEMENT FACTOR OF    2 th LAYER = 0.99872870E+00
 CONFINEMENT FACTOR OF    3 th LAYER = 0.12712252E-02
 CONFINEMENT FACTOR OF    4 th LAYER = 0.35599162E-07
```

```
 CONFINEMENT FACTOR OF    5 th LAYER = 0.13287025E-14
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
1
  INPUT THE EIGENVALUE
  EIGEN VALUE=
-0.164785601442
  INPUT THE NAME OF OUTPUT FILE
lh2.txt
 CONFINEMENT FACTOR OF    1 th LAYER = 0.73199745E-02
 CONFINEMENT FACTOR OF    2 th LAYER = 0.45864444E+00
 CONFINEMENT FACTOR OF    3 th LAYER = 0.68071179E-01
 CONFINEMENT FACTOR OF    4 th LAYER = 0.45864444E+00
 CONFINEMENT FACTOR OF    5 th LAYER = 0.73199745E-02
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
2
```

b) The main output file from this part of GAIN program is energy.dat, containing all the energy levels as shown in Table C.12.5. After the energy eigen values are calculated, the GAIN program asks the user whether he would like to check the wave envelope function or not. We suggest that the user check the wave envelope functions of the first and second energy levels for conduction and valence bands. The plots of the envelope functions are shown in Fig. C.12.2, Fig. C.12.3, Fig C.12.4.

Table C.12.5. output file energy.dat

```
 CONDUCTION BAND ENERGY===>  0.166825507851E+00 ERROR= .5248710E-14

 CONDUCTION BAND ENERGY===>  0.316718310711E+00 ERROR= .4281281E-14

 CONDUCTION BAND ENERGY===>  0.379784585626E+00 ERROR= .2373624E-14

 CONDUCTION BAND ENERGY===>  0.399968049847E+00 ERROR= .2242087E-14

 CONDUCTION BAND ENERGY===>  0.481341035928E+00 ERROR= .2384506E-14

 CONDUCTION BAND ENERGY===>  0.531507743261E+00 ERROR= .2999773E-14

 CONDUCTION BAND ENERGY===>  0.626588219321E+00 ERROR= .2485859E-14

 HEAVY HOLE ENERGY===> -0.280844081259E+00 ERROR= .4292362E-14

 HEAVY HOLE ENERGY===> -0.261654918264E+00 ERROR= .5060880E-14

 HEAVY HOLE ENERGY===> -0.230050446372E+00 ERROR= .4085794E-14

 HEAVY HOLE ENERGY===> -0.215971305480E+00 ERROR= .3569352E-14

 HEAVY HOLE ENERGY===> -0.191389154282E+00 ERROR= .1495427E-13

 HEAVY HOLE ENERGY===> -0.179058584723E+00 ERROR= .2864169E-14

 HEAVY HOLE ENERGY===> -0.166390752259E+00 ERROR= .3290070E-14
```

HEAVY HOLE ENERGY===> -0.155038585857E+00 ERROR= .2022241E-14

HEAVY HOLE ENERGY===> -0.151912036949E+00 ERROR= .1853312E-14

HEAVY HOLE ENERGY===> -0.949214838256E-01 ERROR= .3591541E-14

HEAVY HOLE ENERGY===> -0.294250467453E-01 ERROR= .1947900E-14

HEAVY HOLE ENERGY===> 0.126045078739E-01 ERROR= .1384266E-14

LIGHT HOLE ENERGY===> -0.295278683327E+00 ERROR= .2131495E-14

LIGHT HOLE ENERGY===> -0.256122699275E+00 ERROR= .2338818E-14

LIGHT HOLE ENERGY===> -0.217375554875E+00 ERROR= .5742157E-14

LIGHT HOLE ENERGY===> -0.183928037223E+00 ERROR= .3316695E-14

LIGHT HOLE ENERGY===> -0.164785601442E+00 ERROR= .3822678E-14

LIGHT HOLE ENERGY===> -0.145241224988E+00 ERROR= .1407070E-14

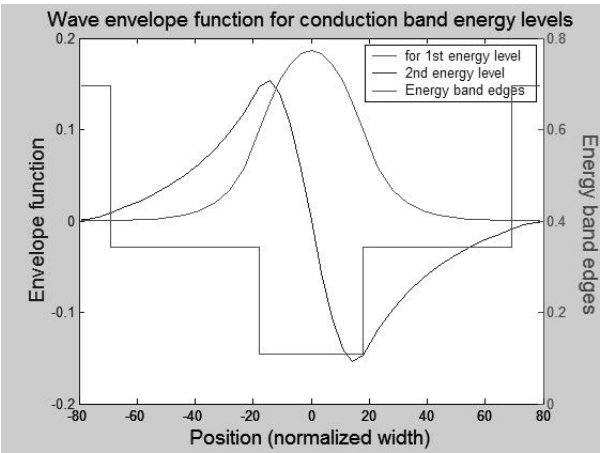

Fig. C.12.2. Wave envelope functions for energy levels in conduction band

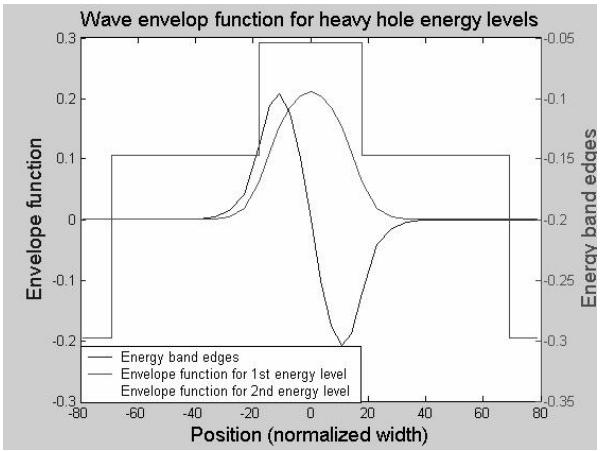

Fig. C.12.3. Wave envelope functions for heavy hole energy levels

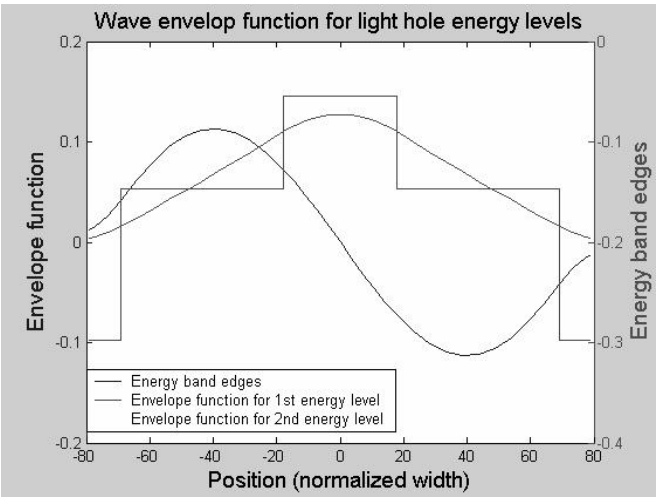

Fig. C.12.4. Wave envelope functions for light hole energy levels

C.12.3. Computation of Gain and Laser Characteristics

This is the last step of simulations using the GAIN program. With the previous calculated material composition, energy band edges, energy levels, and other parameters like material loss and Auger coefficient, the GAIN program can simulate the threshold current, threshold current density, slope efficiency, optical gain and mode gain as functions of wavelengths and photon energies, and L-I curve. The details are explained in Chapter 4 of the manual.

In this part of GAIN program, the input file needs to be constructed with the results of the previous steps and according to the laser design. In this example, single quantum well structure is used to simulate a three-QW laser. For the three-quantum-well laser with a ridge length of 750 μm and ridge width of 3 μm, the input file is shown in Table C.12.6. The detailed steps of simulations are listed in Table C.12.7. The main output files: L-I curve, optical gain as a function of the wavelength, and mode gain vs. current density are plotted in Fig. C.12.5, Fig. C.12.6, and Fig. C.12.7.

a) The input file:

Table C.12.6. Input file for gain and threshold current calculation

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c    1. Input the compositions, width of well, effective index        c
c       and lasing wavelength.                                        c
c    Ex: xx,xz,qy,xy,lx,n,lam                                         c
c    for different materials the following are the forms of inputs.   c
c                                                                     c
c    w -- > well, b -- > barrier  cxz and cxy for cladding.            c
c                                                                     c
c    a.  AlxGa1-xAs : xx (Al w) xz (Al b) qy (0) xy (0)               c
c    b.  In1-xGaxAsyP1-y : xx (Ga w) xz (Ga b) qy (As w) xy (As b)    c
c    c.  In1-xGaxAs/InGaAsP : xx (Ga w) xz (Ga b) qy (0) xy (As b)    c
```

```
c     d.  AlxGayIn1-x-yAs/InP : xx (Ga w) xz (Ga b) qy (Al w) xy (Al b)c
c     e.                                                                c
c     f.  InxGa1-xAs/AlGaAs : xx (In w) xz (0) qy (0) xy (Al b)        c
c     g.                                                                c
c     h.  AlyInxGa1-x-yAs/AlGaAs : xx (Al w) xz (al b) qy (In w) xz (0)c
c     i.  In1-xGaxAs/AlGaInAs : xx (In w) xz (0) qy (Al b) xy (Ga b)    c
c     12. In(y)Ga(1-y)As(x)N(1-x) :xx(As w),xz(As, b),qy(In w),xy(In b)c
c                                                                       c
c     2. Input the energy gap,temperature, barrier band edges(both bands)
c     Ex: eg,temp,ec,ev                                                 c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
0.996 1.0 0.3 0.0000  7.0 3.353749 1.31
0.93 298  0.3421020 0.1466152
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c     3. Input the ist level sub-band energy levels.                  c
c     Ex: ec1,eh1,el1                                                   c
c                                                                       c
c     4. Input the material loss, reflectivities, number of quantum     c
c       wells and beta(for spontaneous emission).                       c
c     Ex: alpha,r1,r2,mm,beta.                                          c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
0.166825507851   -0.126045078739E-01   0.145241224988  0.316718310711   0.294250467453E-01
0.164785601442
6.0d0  0.3000   0.300   1  5.D-5
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c     5. Input the cavity length, ridge width, internal efficiency      c
c       Auger, strain(except AlGaAs,put 0) and confinement factor.      c
c     Ex: cl,cw,etha,ca,es,confine                                      c
c                                                                       c
c     6. Input the cladding composition and band edges.                 c
c     Ex: cxz,cxy,ecc,evv                                               c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
1000.D-4  20D-4  0.96  1.00d-28   0.000  0.01
0.40000  0.00  0.6952492  0.2979640
```

b) The steps for these calculations mentioned are listed in Table C.12.7

Table C.12.7. The steps for the gain and threshold current density calculations

```
  ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

5
  THE INPUT FILE NAME=
in12.txt
  SELECT MATERIAL=?
  1--AlGaAs
  2--InGaAsP
  3--In1-zGazAs/InGaAsP/InP
  4-- InGaAlAs
  5--GaInP/AlzGawIn1-z-wP/Al0.5In0.5P
```

```
 6-- InxGa1-xAs/AlxGa1-xAs/AlGaAs
 7--In1-xGaxAs/InGaAsP/GaxIn1-xP(X=0.51) MATCHED TO GaAs
 8--AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
 9--InzGa1-zAs/AlxGayIn1-x-yAs/InP
 10-- InGaAlAs/InGaAlAs/AlAsSb
 11--InzGa1-zAs/AlxGayIn1-x-yAs/AlAsSb
 12--In(y)Ga(1-y)As(x)N(1-x)/GaAs
 13--InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
 INPUT SELECTION
12
 INPUT MODE = ? FOR TE--> MODE =1, FOR TM--> MODE =2
 INPUT TE OR TM ?
1
 IF EL1 BELOW EH1 THEN SELECT 1, OTHERWISE SELECT 2
 SELECTION=?
1
 **************************************************
 CALCULATE THE EFFECTIVE MASS
 **************************************************
 FOR QUASI-FERMI LEVEL SELECT=1,
 FOR READ EXISTING QUASI-FERMI LEVEL SELECT=2
 SELECT=?
1
 J(LEAKAGE)=0.124580D+02 A/cm^2  N=0.782180D+19 1/cm^3
 J(LEAKAGE)=0.124580D+02 A/cm^2  N=0.782180D+19 1/cm^3
 J(LEAKAGE)=0.127429D+02 A/cm^2  N=0.784160D+19 1/cm^3
……..

 J(LEAKAGE)=0.149281D+02 A/cm^2  N=0.798020D+19 1/cm^3
 J(LEAKAGE)=0.152694D+02 A/cm^2  N=0.800000D+19 1/cm^3
 **************************************************
 G(J) PARAMETERS FROM SINGLE WELL
 Go=0.888745D+01 1/cm  Jo=0.172961D+03 A/cm^2

 G(N) PARAMETERS FROM SINGLE WELL
 NGo=0.888745D+03 1/cm  XNo=0.128797D+19 1/cm^3

 Jtr=0.636289D+02 A/cm^2  NTR=0.473818D+18 1/cm^3


 THE OPTIMUM NUMBER OF QUANTUM WELL FOLLOWS THE ARTICLE
 BY McIlory et al. IEEE JQE-21 1985.

 THE OPTIMUM NUMBER OF QUANTUM WELL Nopt =          3
 INPUT Nopt(CAN BE DIFFERENT FROM ABOVE CALCULATION)=?
3
 NUMBER OF QUANTUM WELL(MAY OR MAY NOT BE Nopt)=?
1

 **************************************************
 **************************************************
 1ST CHECK USE SINGLE WELL TIMES # OF WELLS
 **************************************************
 **************************************************
 2ND CHECK FOLLOWS FORMULA BY McIlory IN IEEE
 JOURNAL OF QUANTUM ELECTRONIC QE-21 1985.
```

```
 ************************************************
 Gth=  18.0397 1/cm Nth=0.245614D+19 1/cm^3 IY=  120
  1ST CHECK Jth=  1410.15179344 A/cm^2
  2ND CHECK Jth=  1331.27210 A/cm^2

  1ST CHECK Ith=0.282030D+03 mA NUMBER OF WELLS=  3
  2ND CHECK Ith=0.266254D+03 mA

 ************************************************
 CALCULATE THE P-I RELATION

 NDATA=        281
 ************************************************
 CALCULATE THE SLOPE: mW/mA Y=A+BX
 CONSTANT A= -95.8802667   SLOPE B=   0.3399643

 ************************************************
 INPUT POWER PO FOR THE LINEWIDTH, PO=0 FOR STOP
 INPUT PO=    mW
0
 INPUT 1 FOR THE DYNAMIC CALCULATION. 2 FOR SKIP
 INPUT =
2
 K-FACTOR= 0.24875 nS  MAXIUM FREQ.= 35.7219 GHz

 ************************************************
 INPUT 1 FOR CALCULATE THE GAIN(E) RELATION.

 INPUT 2 FOR CALCULATE THE LINEWIDTH ENHENCEMENT
 FACTOR AND PHOTON ENERGY RELATION

 INPUT 3 FOR EXIT THE PROGRAM

 THE INPUT # IS
1
INPUT FERMILEVELS IN C-BAND, V-BAND, AND CARRIER DENSITY
0.277843825747 -0.188854176754E-01 0.200075187970E+19
CALCULATE THE CONVOLUTION GAIN(E) COEFFICIENT
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(LAMBDA)
ol1.txt
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(LAMBDA)
ml1.txt
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(E)
oe1.txt
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(E)
me1.txt
 ************************************************
 INPUT 1 FOR REPEAT THE G(E) CALCULATION
 INPUT 2 FOR REPEAT THE ALPHA(E) CALCULATION
 INPUT 3 FOR EXIT
1
 ************************************************
 INPUT 1 FOR CALCULATE THE GAIN(E) RELATION.
```

```
 INPUT 2 FOR CALCULATE THE LINEWIDTH ENHENCEMENT
 FACTOR AND PHOTON ENERGY RELATION

 INPUT 3 FOR EXIT THE PROGRAM

 THE INPUT # IS
0.321632806946 -0.503649146984E-02 0.301052631579E+19
 CALCULATE THE CONVOLUTION GAIN(E) COEFFICIENT
 ************************************************
INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(LAMBDA)
ol2.txt
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(LAMBDA)
ml2.txt
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(E)
oe2.txt
 ************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(E)
me2.txt
 ************************************************
 INPUT 1 FOR REPEAT THE G(E) CALCULATION
 INPUT 2 FOR REPEAT THE ALPHA(E) CALCULATION
 INPUT 3 FOR EXIT
3
```

c) The Output characteristics of designed laser from step 5 are summarized in Table C.12.7.

Table C.12.7 Characteristics of the designed laser

Optimized number of QWs (Nopt)	3
Number of QWs	1
Slope efficiency (%)	33.99643
Jth (A/cm^2)	1410.15 - 1st check, for matching threshold conditions 1331.27– 2nd check, using McIlory method
Ith (mA)	282.03 - 1st check, for matching threshold conditions 266.25 - 2nd check, using McIlory method
Peak λ at operating temperature (um)	1.126um for carrier density of 2.0E18 /cm3 1.145 um for carrier density of 3.0E18 /cm3
Peak material gain (1/cm)	2042.7/cm for carrier density of 2.0E18 /cm3 2843.4/cm for carrier density of 2.0E18 /cm3

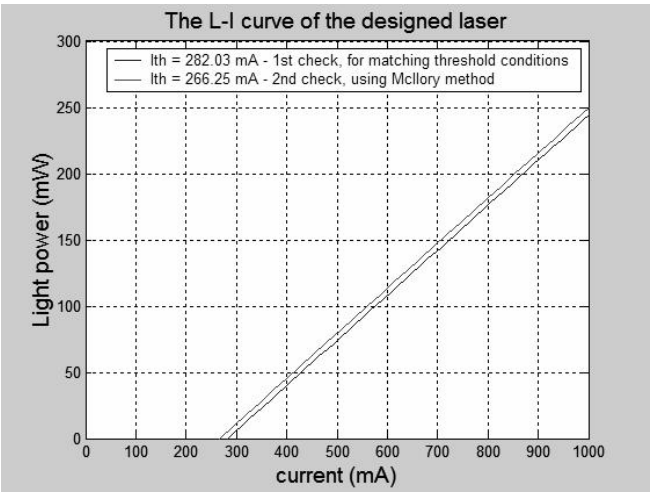

Fig. C.12.5. L-I curve of the laser

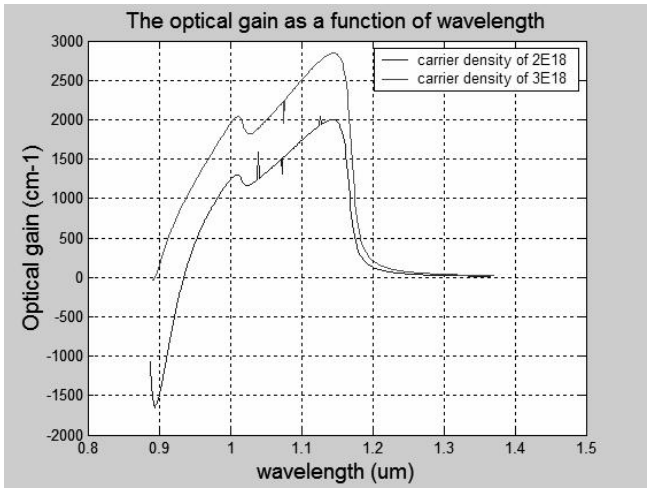

Fig. C.12.6. Optical gain-λ curve of the laser

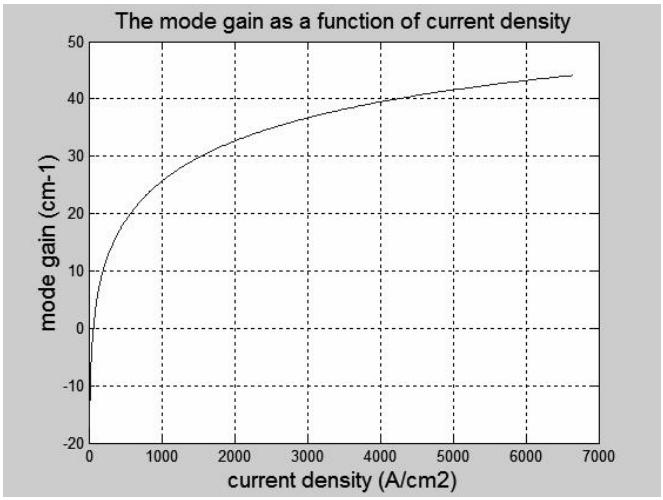

Fig. C.12.7. Mode gain as a function of current density (J)

[1] Masahiko Kondow, Takeshi Kitatani, Shi'ichi Nakatsuka, "GaInNAs: A Novel Material for Long-Wavelength Semiconductor Lasers", IEEE J. Quantum Electronics, vol. 3, no. 3, 1997.

C.13. Material system #13: In(1-x)Ga(x)As(y)P(1-y)/GaAs

This is a simulation of a five-layer laser structure that contains a single compressively strained quantum well (QW), two separated confinement heterostructure (SCH) layers, and two cladding layers as shown in Fig. C.13.1.

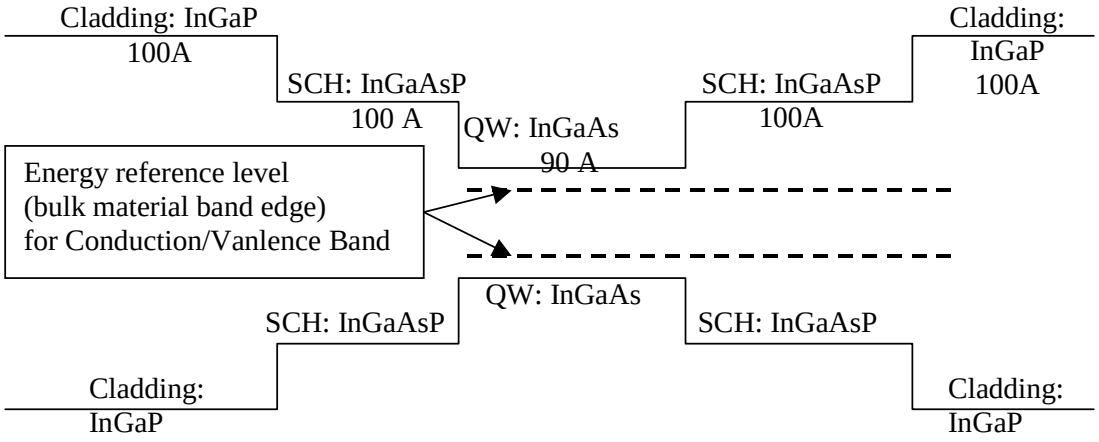

Figure C.13.10. Energy band diagram for the simple quantum well structure

C.13.1. Calculation of material compositions and energy band edges.

The first step of the GAIN program is to calculate the material compositions and energy band edges of the each layer. The user is asked to enter the photoluminescence wavelength, thickness, and strain of the QW, SCH, and cladding layers. After these parameters are input, the GAIN program generates two output files: cbandeg.dat and vbandeg.dat, containing the material compositions, and the conduction band edges and valence band edges respectively. The detailed explanation is provided in Chapter 2 of this manual.

a) The input parameters to the GAIN program in this step are listed in Table. C.13.1.

Table C.13.1. Input parameters to the GAIN program in this step.

Layer	λ (um)	Strain	Thickness (Å)
QW ($In_xGa_{1-x}As$)	1.05	-.113737E-01	90
SCH ($In_{1-x}Ga_xAs_yP_{1-y}$)	0.775		100
Cladding ($In_{1-x}Ga_xP$)	0.65		100

b) The steps in using the GAIN program to calculate the material compositions and energy band edges are listed in Table C.13.2

Table C.13.2. steps to run the GAIN program for necessary parameters.

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

1

 ENTER 1 FOR AlGaAs/AlGaAs
      2 FOR InGaAsP/InGaAsP/InP
      3 FOR InGaAs/InGaAsP/InP
      4 FOR InGaAlAs/InGaAlAs/InP
      5 FOR GaInP/(AlGa)0.5In0.5P/AlInP
      6 FOR InGaAs/AlGaAs/AlGaAs
      7 FOR InGaAs/InGaAsP/Ga0.51In0.49P(MATCHED GaAs)
      8 FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
      9 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/InP
     10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(matched InP)
     11 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/AlAsxSb1-x
     12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs (dilute N)
     13 FOR In(1-x)Ga(x)As(y)P(1-y)/GaAs
     14 FOR EXIT, BACK TO MAIN PAGE!
13
 INPUT THE LAYER # FOR GRIN STRUCTURE(STEP)
 STEP N=
2
  INPUT THE WELL WAVELENGTH (um)
1.05
  INPUT THE BARRIER WAVELENGTH (um)
0.775
  INPUT THE CLADDING WAVELENGTH (um)
0.65
  BANDGAP ENERGY OF QUANTUM WELL=   0.683804000019804
  INPUT CLADDING, BARRIER, QUANTUM WELL WIDTH (A)
100 100 90
  FOR LATTICE MATCHED BARRIER SELLECT --> 1
  FOR STRAIN COMPENSATED SELECT -->2

  INPUT SELECTION ===> ?
1
 C[                                          ]*
 C[      34 ITERATIONS                               ]*
  ROOT (Y)=  0.457504996552668      ROOT (X)=  0.713274608740734
  ROOT(  2)IS COMPLEX!Real=      0.3293112 Imag=      -0.5242450
  ROOT(  3)IS COMPLEX!Real=      0.3293112 Imag=       0.5242450
  ROOT(  4) WITH REAL PART > 1 Real=       1.3495216
  Ga=  0.713274608740734       As=  0.457504996552668
 C[                                          ]*
 C[      31 ITERATIONS                               ]*
  ROOT (Y)=  1.607682884018472E-003  ROOT (X)=  0.481571950395300
  ROOT(  2)IS COMPLEX!Real=      0.4871066 Imag=      -0.7058294
  ROOT(  3)IS COMPLEX!Real=      0.4871066 Imag=       0.7058294
  ROOT(  4) WITH REAL PART > 1 Real=       1.4898280
  CLADDING Ga=  0.481571950395300      CLADDING As=  1.607682884018472E-003
```

```
 STRAIN FOR InGaAs/InGaAsP/GaAs IS  -1.137372501690129E-002

 WRITE CONDUCTION BAND PARAMETERS INTO CBANDEG.DAT

 WRITE VALENCE BAND PARAMETERS INTO VBANDEG.DAT
 INPUT 1 FOR NEW CALCULATION, 2 FOR EXIT
 I= ?
2

 ENTER 1 FOR AlGaAs/AlGaAs
      2 FOR InGaAsP/InGaAsP/InP
      3 FOR InGaAs/InGaAsP/InP
      4 FOR InGaAlAs/InGaAlAs/InP
      5 FOR GaInP/(AlGa)0.5In0.5P/AlInP
      6 FOR InGaAs/AlGaAs/AlGaAs
      7 FOR InGaAs/InGaAsP/Ga0.51In0.49P(MATCHED GaAs)
      8 FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
      9 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/InP
     10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(matched InP)
     11 FOR InzGa1-zAs/AlyGaxIn1-x-yAs/AlAsxSb1-x
     12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs (dilute N)
     13 FOR In(1-x)Ga(x)As(y)P(1-y)/GaAs
     14 FOR EXIT, BACK TO MAIN PAGE!
14
 THIS PROGRAM STOP HERE!, BACK TO MAIN PAGE
```

c) The output files, cbandeg.dat and vbandeg.dat are explained in Table C.13.3.

Table C.13.3. Material compositions and band offsets:

a) cbandeg.dat for conduction band

```
**************************************************************************
 QW strain   lattice constant
-.113737E-01  0.571760E-09
                        material compositions(see Table C.13.1 for x and y)
 layer thickness,            x              y       conduction band edges
  0.10000000E+03  0.48157195E+00   0.0016077    0.2978522      cladding layer
  0.10000000E+03  0.71327461E+00   0.4575050    0.2304440      SCH layer
  0.90000000E+02  0.15876268E+00   0.0000000    0.0746203      quantum well
  0.10000000E+03  0.71327461E+00   0.4575050    0.2304440      SCH layer
  0.10000000E+03  0.48157195E+00   0.0016077    0.2978522      cladding layer
**************************************************************************
```

b) vbandeg.dat for valence band

```
**************************************************** ********************
 QW strain   lattice constant
 -.113737E-01  0.571760E-09
                        material compositions(see Table C.13.1 for x and y)
 layer thickness,            x              y       valence band edges
  0.10000000E+03  0.48157195E+00   0.0016077   -0.4467784     cladding layer
  0.10000000E+03  0.71327461E+00   0.4575050   -0.3456660      SCH layer
  0.90000000E+02  0.15876268E+00   0.0000000   -0.0373101      quantum well
  0.10000000E+03  0.71327461E+00   0.4575050   -0.3456660      SCH layer
  0.10000000E+03  0.48157195E+00   0.0016077   -0.4467784      cladding layer
**************************************************************************
```

C.13.2. Energy level calculations

After the calculation of the material compositions and energy band edges, the GAIN program calculates energy levels in the conduction band and valence bands. The detailed explanations are discussed in Chapter 3 of this manual.

a) The steps of how to calculate the energy levels are shown in Table C.13.4.

Table C.13.4. Steps to calculate the energy levels

i) Steps to calculate the conduction band energy levels

```
ENTER 1 FOR THE NECESSARY PARAMETERS

      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
     3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
     4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
     5 FOR THE LASER G-J AND G(LAMBDA)
     6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
     7 FOR EXIT

2
 INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
 INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
 INPUT N=
5
 INPUT THE LOWEST POTENTIAL LAYER(1st Q-WELL) IC= ?
3
 INPUT THE SELECTED CENTER LAYER OF STRUCTURE ICR=
3
 ******************************************************
  INPUT I=1  FOR AlGaAs
      I=2  FOR InGaAsP
      I=3  FOR In1-xGaxAs/InGaAsP/InP
      I=4  FOR InGaAlAs/InGaAlAs
      I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
      I=6  FOR InGaAs/AlGaAs/AlGaAs
      I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
      I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
      I=9  FOR InzGa1-zAs/AlxGayIn1-x-yAs/InP
      I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
      I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
      I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs

      I=13 FOR InGaAs/In(1-y)Ga(x)As(y)P(1-y)/GaAs
  INPUT I= ?
 ******************************************************
13
ENERGY EIGENVALUE===>  0.969908633581E-01 ERROR= .4024812E-1
ENERGY EIGENVALUE===>  0.159263664462E+00 ERROR= .3355458E-1
ENERGY EIGENVALUE===>  0.233016713571E+00 ERROR= .2446655E-1
```

```
ENERGY EIGENVALUE===>  0.251588768045E+00 ERROR= .2853046E-1
ENERGY EIGENVALUE===>  0.266059578219E+00 ERROR= .2658063E-1
ENERGY EIGENVALUE===>  0.297760175518E+00 ERROR= .1439724E-1
 FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
 SKIP INPUT I==> 2
 I=?
1
 INPUT THE EIGENVALUE
0.969908633581E-01
 INPUT THE NAME OF OUTPUT FILE
cb1.txt
CONFINEMENT FACTOR OF    1 th LAYER = 0.63852474E-07
CONFINEMENT FACTOR OF    2 th LAYER = 0.17340584E-01
CONFINEMENT FACTOR OF    3 th LAYER = 0.96531870E+00
CONFINEMENT FACTOR OF    4 th LAYER = 0.17340584E-01
CONFINEMENT FACTOR OF    5 th LAYER = 0.63852474E-07
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
0.159263664462E+00
 INPUT THE NAME OF OUTPUT FILE
cb2.txt
CONFINEMENT FACTOR OF    1 th LAYER = 0.63347186E-05
CONFINEMENT FACTOR OF    2 th LAYER = 0.86169326E-01
CONFINEMENT FACTOR OF    3 th LAYER = 0.82764868E+00
CONFINEMENT FACTOR OF    4 th LAYER = 0.86169326E-01
CONFINEMENT FACTOR OF    5 th LAYER = 0.63347186E-05
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
2
```

ii) Steps to calculate the heavy hole energy levels

```
 ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT
3
 INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
 INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
 INPUT N=
5
 INPUT THE HIGHEST POTENTIAL(1st Q-WELL) LAYER IC= ?
3
 INPUT THE SELECTED CENTER OF THE STRUCTURE ICR=?
3
 *******************************************************
  INPUT I=1  FOR AlGaAs
       I=2  FOR InGaAsP
       I=3  FOR In(1-x)Ga(x)As/InGaAsP/InP
       I=4  FOR InGaAlAs/InGaAlAs
```

```
       I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
       I=6  FOR InGaAs/AlGaAs/AlGaAs
       I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
       I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
       I=9  FOR In(z)Ga(1-z)As/AlxGayIn1-x-yAs/InP
       I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
       I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
       I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
```

I=13 FOR InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs

```
  INPUT I= ?
 *********************************************************
13
 *********************************************************

  DOES THE STRUCTURE STRAIN OR STRAIN-COMPENSATED?
  IF STRAIN ONLY INPUT 1, STRAIN-COMPENSATED INPUT 2
  INPUT SELECT = ?

1
ENERGY EIGENVALUE===> -0.431144978171E+00 ERROR= .3048383E-14
ENERGY EIGENVALUE===> -0.416154706432E+00 ERROR= .4027410E-14

                                                ……..

ENERGY EIGENVALUE===> -0.360098024766E-01 ERROR= .1582591E-14
ENERGY EIGENVALUE===> -0.880918208839E-02 ERROR= .2485319E-14
  FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
  SKIP INPUT I==> 2
  I=?
1
  INPUT THE EIGENVALUE
  EIGEN VALUE=
-0.880918208839E-02
  INPUT THE NAME OF OUTPUT FILE
hh1.txt
CONFINEMENT FACTOR OF    1 th LAYER = 0.13106920E-18
CONFINEMENT FACTOR OF    2 th LAYER = 0.13394211E-02
CONFINEMENT FACTOR OF    3 th LAYER = 0.99734154E+00
CONFINEMENT FACTOR OF    4 th LAYER = 0.13190393E-02
CONFINEMENT FACTOR OF    5 th LAYER = 0.13146527E-18
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
  SELECT=?
1
  INPUT THE EIGENVALUE
  EIGEN VALUE=
-0.360098024766E-01
  INPUT THE NAME OF OUTPUT FILE
hh2.txt
CONFINEMENT FACTOR OF    1 th LAYER = 0.24159076E-17
CONFINEMENT FACTOR OF    2 th LAYER = 0.54971662E-02
CONFINEMENT FACTOR OF    3 th LAYER = 0.98900594E+00
CONFINEMENT FACTOR OF    4 th LAYER = 0.54968902E-02
CONFINEMENT FACTOR OF    5 th LAYER = 0.24238529E-17
  INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
```

```
 SELECT=?
2
```

iii) Steps to calculate the light hole energy levels

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

4
 INPUT THE NUMBER OF QUANTUM WELLS NUM=?
1
 INPUT TOTAL LAYERS FOR STRUCTURE--N ODD
 INPUT N=
5
 INPUT THE HIGHEST POTENTIAL(1st Q-WELL) LAYER IC= ?
3
 INPUT THE SELECTED CENTER OF THE STRUCTURE ICR=?
3
 ********************************************************
  INPUT I=1  FOR AlGaAs
       I=2  FOR InGaAsP
       I=3  FOR In(1-x)Ga(x)As/InGaAsP/InP
       I=4  FOR InGaAlAs/InGaAlAs
       I=5  FOR GaInP/(AlGa)0.5In0.5P/AlInP
       I=6  FOR InGaAs/AlGaAs/AlGaAs
       I=7  FOR InGaAs/InGaAsP/Ga0.51In0.49P(GaAs)
       I=8  FOR AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
       I=9  FOR In(z)Ga(1-z)As/AlxGayIn1-x-yAs/InP
       I=10 FOR InGaAlAs/InGaAlAs/AlAsxSb1-x(InP)
       I=11 FOR InzGa1-zAs/AlxGayIn1-x-yAs/AlAsxSb1-x
       I=12 FOR In(y)Ga(1-y)As(x)N(1-x)/GaAs
       I=13 FOR InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
  INPUT I= ?
 ********************************************************
13
 ********************************************************

  DOES THE STRUCTURE STRAIN OR STRAIN-COMPENSATED?
  IF STRAIN ONLY INPUT 1, STRAIN-COMPENSATED INPUT 2
  INPUT SELECT = ?

1
ENERGY EIGENVALUE===> -0.437001414290E+00 ERROR= .3575176E-14
ENERGY EIGENVALUE===> -0.417816439139E+00 ERROR= .9797945E-14

                                          …….

ENERGY EIGENVALUE===> -0.155259330638E+00 ERROR= .3235995E-14
ENERGY EIGENVALUE===> -0.953949376087E-01 ERROR= .2429016E-14
```

```
 FOR CHECKING THE Schrodinger WAVE FUNCTION INPUT I==> 1
 SKIP INPUT I==> 2
 I=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
-0.953949376087E-01
 INPUT THE NAME OF OUTPUT FILE
lh1.txt
CONFINEMENT FACTOR OF    1 th LAYER = 0.45515149E-10
CONFINEMENT FACTOR OF    2 th LAYER = 0.62110303E-02
CONFINEMENT FACTOR OF    3 th LAYER = 0.98757794E+00
CONFINEMENT FACTOR OF    4 th LAYER = 0.62110309E-02
CONFINEMENT FACTOR OF    5 th LAYER = 0.48346799E-10
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
1
 INPUT THE EIGENVALUE
 EIGEN VALUE=
-0.155259330638E+00
 INPUT THE NAME OF OUTPUT FILE
lh2.txt
CONFINEMENT FACTOR OF    1 th LAYER = 0.19585995E-08
CONFINEMENT FACTOR OF    2 th LAYER = 0.28328869E-01
CONFINEMENT FACTOR OF    3 th LAYER = 0.94334223E+00
CONFINEMENT FACTOR OF    4 th LAYER = 0.28328892E-01
CONFINEMENT FACTOR OF    5 th LAYER = 0.20998482E-08
 INPUT NEW EIGENVALUE--> 1, BACK TO MAIN PAGE--> 2
 SELECT=?
2
```

b) The main output file from this part of GAIN program is energy.dat, containing all the energy levels as shown in Table C.13.5. After the energy eigen values are calculated, the GAIN program asks the user whether he would like to check the wave envelope function or not. We suggest that the user check the wave envelope functions of the first and second energy levels for conduction, heavy-hole and light hole bands. The plots of the envelope functions are shown in Fig. C.13.2, Fig. C.13.3, Fig C.13.4.

Table C.13.5. output file energy.dat

```
 CONDUCTION BAND ENERGY===>  0.969908633581E-01 ERROR= .4024812E-14

 CONDUCTION BAND ENERGY===>  0.159263664462E+00 ERROR= .3355458E-14

                                        ……

 HEAVY HOLE ENERGY===> -0.360098024766E-01 ERROR= .1582591E-14

 HEAVY HOLE ENERGY===> -0.880918208839E-02 ERROR= .2485319E-14

                                        …….

 LIGHT HOLE ENERGY===> -0.155259330638E+00 ERROR= .3235995E-14
```

LIGHT HOLE ENERGY===> -0.953949376087E-01 ERROR= .2429016E-14

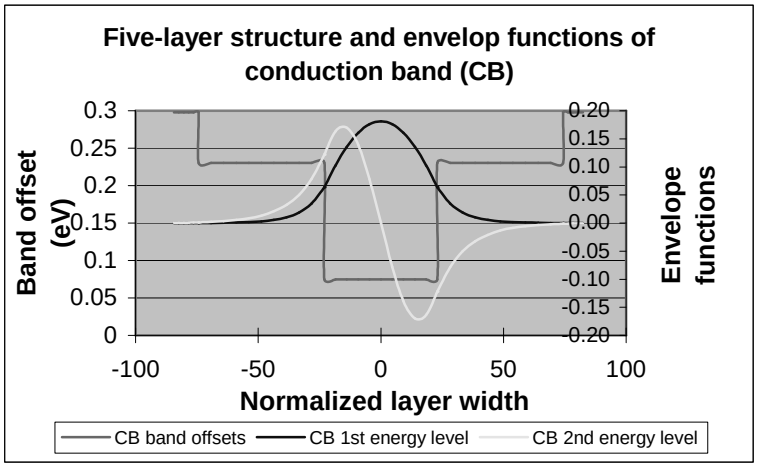

Fig. C.13.2. Wave envelope functions for energy levels in conduction band

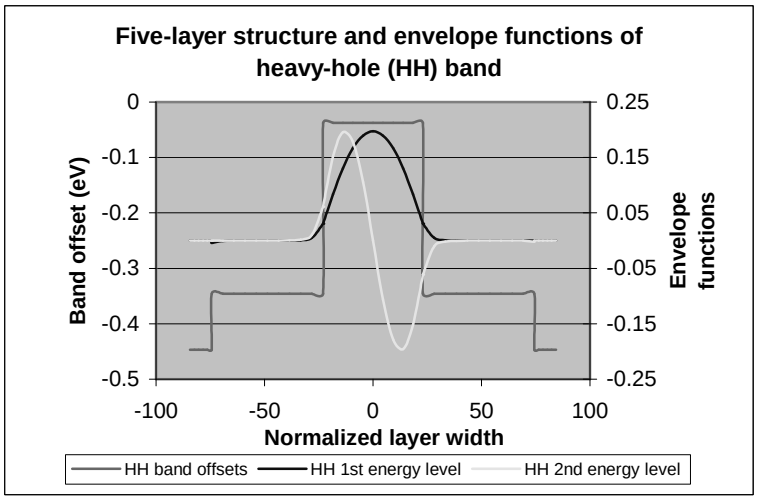

Fig. C.13.3. Wave envelope functions for heavy hole energy levels

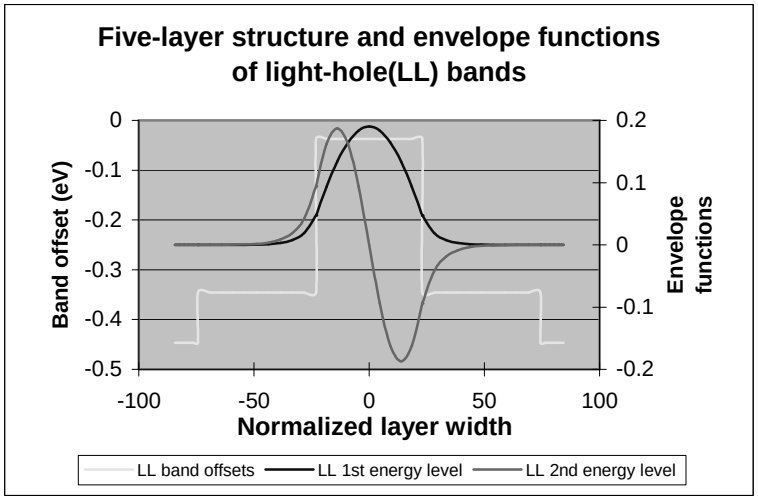

Fig. C.13.4. Wave envelope functions for light hole energy levels

C.13.3. Computation of Gain and Laser Characteristics

This is the last step of simulations using the GAIN program. With the previous calculated material composition, energy band edges, energy levels, and other parameters like material loss and Auger coefficient, the GAIN program can simulate the threshold current, threshold current density, slope efficiency, optical gain and mode gain as functions of wavelengths and photon energies, and L-I curve. The details are explained in Chapter 4 of the manual.

In this part of GAIN program, the input file needs to be constructed with the results of the previous steps and according to the laser design. The input file of material system #13 is shown in Table C.13.6. The detailed steps of simulations are listed in Table C.13.7. The main output files: L-I curve, optical gain as a function of the wavelength, and mode gain vs. current density are plotted in Fig. C.13.5, Fig. C.13.6, and Fig. C.13.7.

a) The input file:

Table C.13.6. Input file (mat_13.txt) for gain and threshold current calculation

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c    1. Input the compositions, width of well, effective index                 c
c       and lasing wavelength.                                                 c
c    Ex: xx,xz,qy,xy,lx,n,lam                                                  c
c    for different materials the following are the forms of inputs.            c
c                                                                              c
c    w -- > well, b -- > barrier  cxz and cxy for cladding.                     c
c                                                                              c
c    a.  AlxGa1-xAs : xx (Al w) xz (Al b) qy (0) xy (0)                        c
c    b.  In1-xGaxAsyP1-y : xx (Ga w) xz (Ga b) qy (As w) xy (As b)             c
c    c.  In1-xGaxAs/InGaAsP : xx (Ga w) xz (Ga b) qy (0) xy (As b)             c
c    d.  AlxGayIn1-x-yAs/InP : xx (Ga w) xz (Ga b) qy (Al w) xy (Al b)         c
c    e.                                                                        c
c    f.  InxGa1-xAs/AlGaAs : xx (In w) xz (0) qy (0) xy (Al b)                 c
c    g.                                                                        c
c    h.  AlyInxGa1-x-yAs/AlGaAs : xx (Al w) xz (al b) qy (In w) xz (0)         c
c    i.  In1-xGaxAs/AlGaInAs : xx (In w) xz (0) qy (Al b) xy (Ga b)            c
c    j.  In(y)Ga(1-y)As(x)N(1-x) :xx(As w),xz(As, b),qy(In w),xy(In b)         c
c    k.  InGaAs/InGaAsP/GaAs: xx (In w), (0), xz(Ga w) xy (As b)
c    2. Input the energy gap,temperature, barrier band edges(both bands)
c    Ex: eg,temp,ec,ev                                                         c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
0.15876268E+00  0.0  0.71327461E+00  0.4575050  9.0  3.33  0.975
1.181  298  0.2304440  0.3456660
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c    3. Input the ist level sub-band energy levels.                            c
c    Ex: ec1,eh1,el1                                                           c
c                                                                              c
c    4. Input the material loss, reflectivities, number of quantum             c
c       wells and beta(for spontaneous emission).                              c
c    Ex: alpha,r1,r2,mm,beta.                                                  c
```

```
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
0.09699086  0.00880918  0.0953949  0.15926366  0.0360098  0.1552593
2.0d0  0.3000  0.300  1  5.D-5
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
c   5. Input the cavity length, ridge width, internal efficiency                c
c     Auger, strain(except AlGaAs,put 0) and confinement factor.                c
c   Ex: cl,cw,etha,ca,es,confine                                                c
c                                                                               c
c   6. Input the cladding composition and band edges.                           c
c   Ex: cxz,cxy,ecc,evv                                                         c
ccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccccc
1000.D-4  100.0D-4  0.86  1.00d-29  0.000  0.018
0.48  157195E+00  0.0016077  0.2978522  0.4467784
```

b) The steps for these calculations mentioned are listed in Table C.13.7

Table C.13.7. The steps for the gain and threshold current density calculations

```
ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

5
 THE INPUT FILE NAME=
mat_13.tex
 SELECT MATERIAL=?
 1--AlGaAs
 2--InGaAsP
 3--In1-zGazAs/InGaAsP/InP
 4-- InGaAlAs
 5--GaInP/AlzGawIn1-z-wP/Al0.5In0.5P
 6-- InxGa1-xAs/AlxGa1-xAs/AlGaAs
 7--In1-xGaxAs/InGaAsP/GaxIn1-xP(X=0.51) MATCHED TO GaAs
 8--AlyInxGa1-x-yAs/AlzGa1-zAs/GaAs
 9--InzGa1-zAs/AlxGayIn1-x-yAs/InP
 10-- InGaAlAs/InGaAlAs/AlAsSb
 11--InzGa1-zAs/AlxGayIn1-x-yAs/AlAsSb
 12--In(y)Ga(1-y)As(x)N(1-x)/GaAs
 13--InGaAs/In(1-x)Ga(x)As(y)P(1-y)/GaAs
 INPUT SELECTION
13
 INPUT MODE = ? FOR TE--> MODE =1, FOR TM--> MODE =2
 INPUT TE OR TM ?
1
 IF EL1 BELOW EH1 THEN SELECT 1, OTHERWISE SELECT 2
 SELECTION=?
1
 ************************************************
 CALCULATE THE EFFECTIVE MASS
 ************************************************
 FOR QUASI-FERMI LEVEL SELECT=1,
 FOR READ EXISTING QUASI-FERMI LEVEL SELECT=2
```

```
 SELECT=?
1


                                                  …….
J(LEAKAGE)=0.737102D+05 A/cm^2  N=0.788120D+19 1/cm^3
 J(LEAKAGE)=0.745813D+05 A/cm^2  N=0.790100D+19 1/cm^3
 J(LEAKAGE)=0.754584D+05 A/cm^2  N=0.792080D+19 1/cm^3
 J(LEAKAGE)=0.763412D+05 A/cm^2  N=0.794060D+19 1/cm^3
 J(LEAKAGE)=0.772298D+05 A/cm^2  N=0.796040D+19 1/cm^3
 J(LEAKAGE)=0.781241D+05 A/cm^2  N=0.798020D+19 1/cm^3
 J(LEAKAGE)=0.790240D+05 A/cm^2  N=0.800000D+19 1/cm^3
 ************************************************
 G(J) PARAMETERS FROM SINGLE WELL
 Go=0.223602D+02 1/cm  Jo=0.330614D+03 A/cm^2

 G(N) PARAMETERS FROM SINGLE WELL
 NGo=0.124223D+04 1/cm  XNo=0.116917D+19 1/cm^3

 Jtr=0.121626D+03 A/cm^2  NTR=0.430115D+18 1/cm^3


 THE OPTIMUM NUMBER OF QUANTUM WELL FOLLOWS THE ARTICLE
 BY McIlory et al. IEEE JQE-21 1985.

 THE OPTIMUM NUMBER OF QUANTUM WELL Nopt =          1
 INPUT Nopt(CAN BE DIFFERENT FROM ABOVE CALCULATION)=?
1
  NUMBER OF QUANTUM WELL(MAY OR MAY NOT BE Nopt)=?
1

 ************************************************
 ************************************************
 1ST CHECK USE SINGLE WELL TIMES # OF WELLS
 ************************************************
 ************************************************
 2ND CHECK FOLLOWS FORMULA BY McIlory IN IEEE
 JOURNAL OF QUANTUM ELECTRONIC QE-21 1985.
 ************************************************
   Gth=  14.0397 1/cm Nth=0.872180D+18 1/cm^3 IY=   40
   1ST CHECK Jth=   234.12059582 A/cm^2
   2ND CHECK Jth=   384.43491 A/cm^2

   1ST CHECK Ith=0.234121D+03 mA NUMBER OF WELLS=  1
   2ND CHECK Ith=0.384435D+03 mA

 ************************************************
 CALCULATE THE P-I RELATION

 NDATA=        361
************************************************
CALCULATE THE SLOPE: mW/mA Y=A+BX
 CONSTANT A=-108.9198070   SLOPE B=   0.4652295
 ************************************************
 INPUT POWER PO FOR THE LINEWIDTH, PO=0 FOR STOP
 INPUT PO=    mW
0
```

```
 INPUT 1 FOR THE DYNAMIC CALCULATION. 2 FOR SKIP
 INPUT =
2
  K-FACTOR= 0.32466 nS  MAXIUM FREQ.= 27.3693 GHz
  **************************************************
  INPUT 1 FOR CALCULATE THE GAIN(E) RELATION.

  INPUT 2 FOR CALCULATE THE LINEWIDTH ENHENCEMENT
  FACTOR AND PHOTON ENERGY RELATION

  INPUT 3 FOR EXIT THE PROGRAM

 THE INPUT # IS
1
INPUT FERMILEVELS IN C-BAND, V-BAND, AND CARRIER DENSITY
0.210195297051E+00  0.516850978058E-02 0.200075187970E+19
 CALCULATE THE CONVOLUTION GAIN(E) COEFFICIENT
  **************************************************
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(LAMBDA)
ol1_mat_13
  **************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(LAMBDA)
ml1_mat_13
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(E)
oe1_mat_13
  **************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(E)
me1_mat_13
  **************************************************
 INPUT 1 FOR REPEAT THE G(E) CALCULATION
 INPUT 2 FOR REPEAT THE ALPHA(E) CALCULATION
 INPUT 3 FOR EXIT
1
  **************************************************
  INPUT 1 FOR CALCULATE THE GAIN(E) RELATION.

  INPUT 2 FOR CALCULATE THE LINEWIDTH ENHENCEMENT
  FACTOR AND PHOTON ENERGY RELATION

  INPUT 3 FOR EXIT THE PROGRAM

 THE INPUT # IS
1
INPUT FERMILEVELS IN C-BAND, V-BAND, AND CARRIER DENSITY
0.210195297051E+00 0.189627393147E-01 0.299072681704E+19
 CALCULATE THE CONVOLUTION GAIN(E) COEFFICIENT
  **************************************************
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(LAMBDA)
ol2_mat_13
  **************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(LAMBDA)
ml2_mat_13
 INPUT THE NAME FOR THE CONVOLUTION OPTICAL GAIN(E)
oe2_mat_13
  **************************************************
 INPUT THE NAME FOR THE CONVOLUTION MODE GAIN(E)
```

```
me2_mat_13
 ************************************************
 INPUT 1 FOR REPEAT THE G(E) CALCULATION
 INPUT 2 FOR REPEAT THE ALPHA(E) CALCULATION
 INPUT 3 FOR EXIT
3

ENTER 1 FOR THE NECESSARY PARAMETERS
      2 FOR THE ENERGY VALUES OF CONDUCTION BAND
      3 FOR THE ENERGY VALUES OF HEAVY HOLE BAND
      4 FOR THE ENERGY VALUES OF LIGHT HOLE BAND
      5 FOR THE LASER G-J AND G(LAMBDA)
      6 FOR RATE EQUATIONS(TWO SECTION MODEL INCLUDED)
      7 FOR EXIT

7
```

c) The Output characteristics of designed laser from step 5 are summarized in Table C.13.7.

Table C.13.7 Characteristics of the designed laser

Optimized number of QWs (Nopt)	1
Number of QWs	1
Slope efficiency (%)	47.43
Jth (A/cm^2)	234.12 - 1st check, for matching threshold conditions 384.43– 2nd check, using McIlory method
Peak λ at operating temperature (um)	0.970 um for carrier density of 2.0E18 /cm3 0.973 um for carrier density of 3.0E18 /cm3
Peak material gain (1/cm)	2723/cm for carrier density of 2.0E18 /cm3 3451 /cm for carrier density of 3.0E18 /cm3

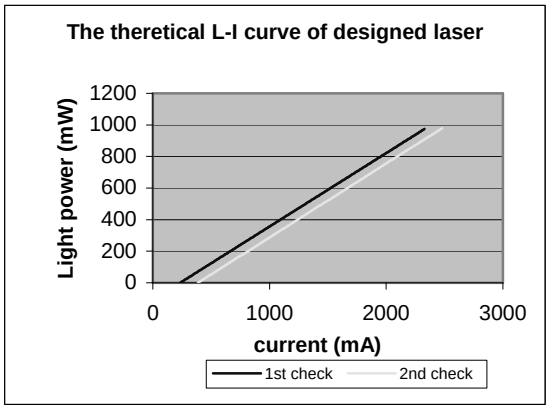

Fig. C.13.5. L-I curve of the laser

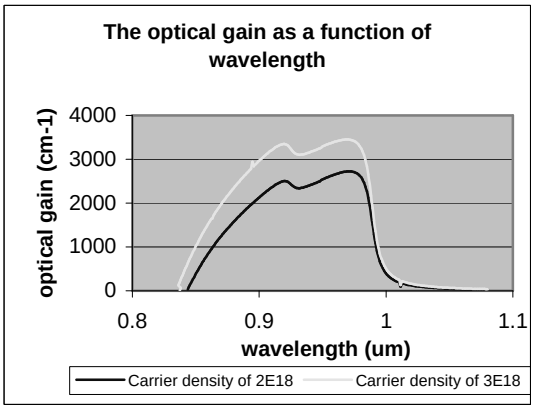

Fig. C.13.6. Optical gain-λ curve of the laser

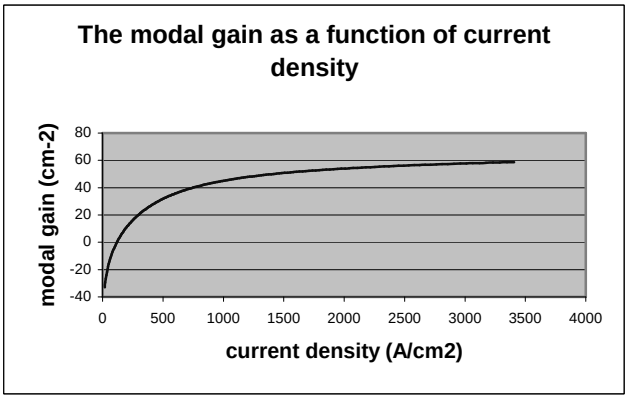

Fig. C.13.7. Mode gain as a function of current density (J)